Graph Neural Networks: hands-on session

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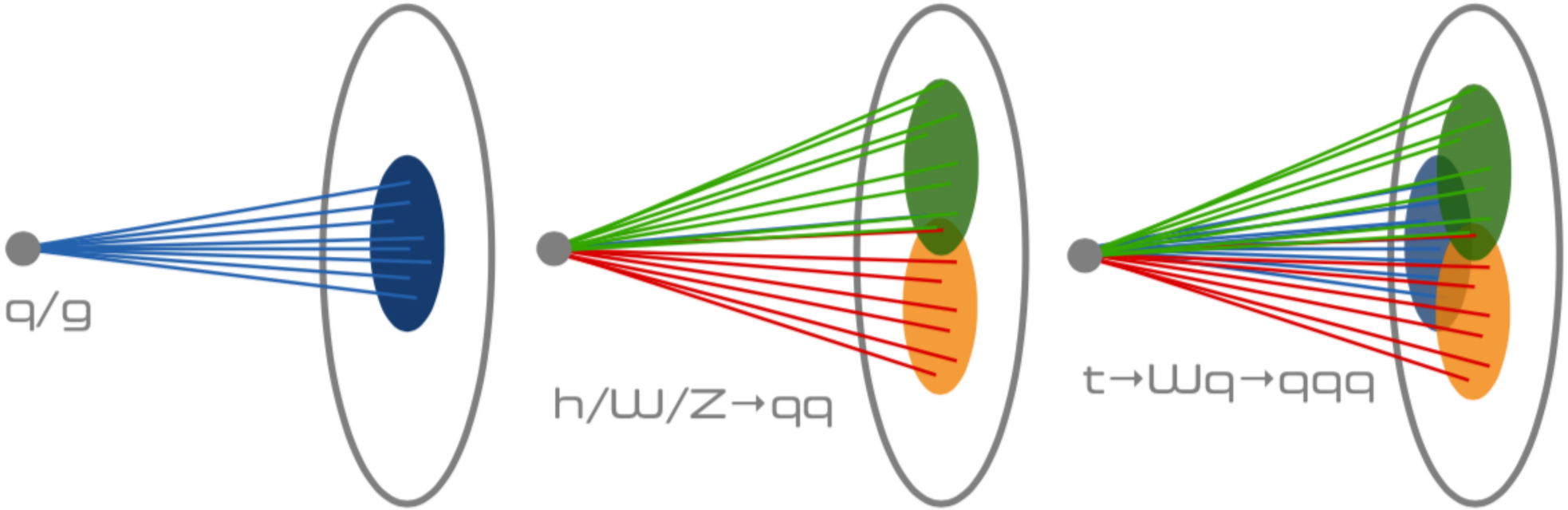
The problem: jet tagging

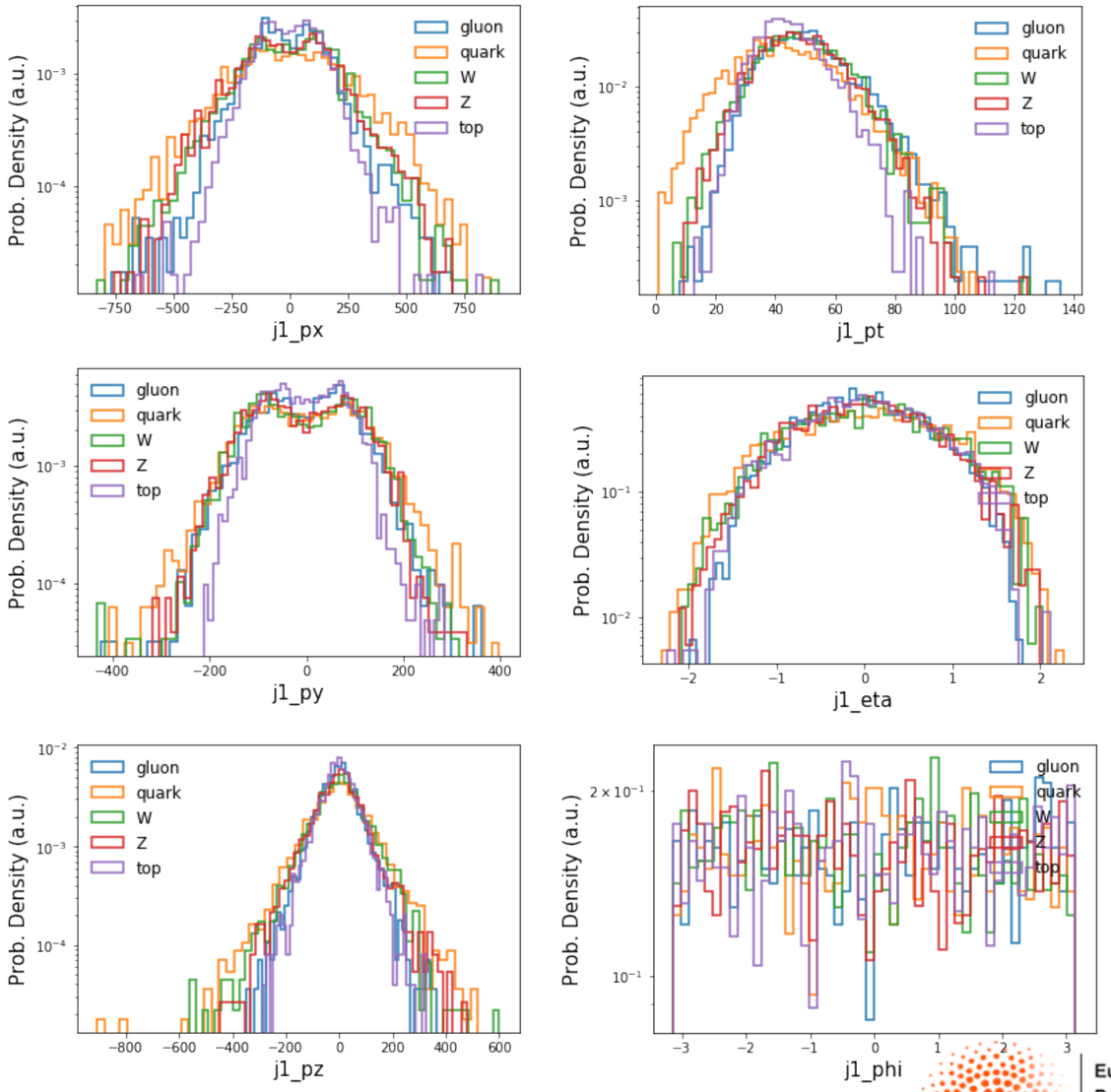
- *At the LHC, a jet is a spray of hadrons coming from a "shower" initiated by a quark or a gluon*

- *When heavy particles (W, Z, top quark) decaying to quarks are produced at large momentum, multiple jets overlap in a single jet*



The data representation

- Each jet is represented as a list of up to 100 particles, ordered by decreasing transverse momentum
  - We will cut the list at 30, to make the training faster
- Each particle is represented as a list of 16 features
  - We will use only 3 coordinates: (px, py, pz) as a default, but you can switch to (p_T, η, φ) if you want to
- See ***this notebook*** for more info



Step1: we read the data

- *Nothing particularly enlightening. Just push Shift+Enter*

Import needed libraries

```
import os
import h5py
import glob
import numpy as np
import matplotlib.pyplot as plt
```

```
import torch
import torch.nn as nn
from torch.autograd.variable import *
import torch.optim as optim
```

```
%matplotlib inline
```

Download dataset

```
! git clone https://github.com/pierinim/tutorials.git
! ls tutorials/Data/JetDataset/
```

Step1: we read the data

- *Nothing particularly enlightening. Just push Shift+Enter*

Append ground-truth and jet data in 2 numpy arrays

```
target = np.array([])
jetList = np.array([])
# we cannot load all data on Colab. So we just take a few files
datafiles = ['tutorials/Data/JetDataset/jetImage_7_100p_30000_40000.h5',
            'tutorials/Data/JetDataset/jetImage_7_100p_60000_70000.h5',
             'tutorials/Data/JetDataset/jetImage_7_100p_50000_60000.h5',
             'tutorials/Data/JetDataset/jetImage_7_100p_10000_20000.h5',
             'tutorials/Data/JetDataset/jetImage_7_100p_0_10000.h5']
# if you are running locallt, you can use the full dataset doing
# for fileIN in glob.glob("tutorials/HiggsSchool/data/*h5"):
for fileIN in datafiles:
    print("Appending %s" %fileIN)
    f = h5py.File(fileIN)
    # for pT, eta, phi
    myJetList = np.array(f.get("jetConstituentList")[:,:,[5,8,11]])
    # for px, py, pz
    #myJetList = np.array(f.get("jetConstituentList")[:,:,[0,1,2]])
    mytarget = np.array(f.get('jets')[0:,-6:-1])
    jetList = np.concatenate([jetList, myJetList], axis=0) if jetList.size else myJetList
    target = np.concatenate([target, mytarget], axis=0) if target.size else mytarget
    del myJetList, mytarget
    f.close()
print(target.shape, jetList.shape)
```

Step1: we read the data

- *Nothing particularly enlightening. Just push Shift+Enter*

Data preparation: transpose, encoding, train/val/test split

```
# pytorch Cross Entropy doesn't support one-hot encoding
target = np.argmax(target, axis=1)
# the dataset is N_jets x N_particles x N_features
# the IN wants N_jets x N_features x N_particles
jetList = np.swapaxes(jetList, 1, 2)
```

```
nParticle = 30
jetList = jetList[:,:,:nParticle]
print(jetList.shape)
```

```
from sklearn.model_selection import train_test_split
X_train, X_val, y_train, y_val = train_test_split(jetList, target, test_size=0.33)
print(X_train.shape, X_val.shape, y_train.shape, y_val.shape)
del jetList, target
```

```
# check if a GPU is available. Otherwise run on CPU
device = 'cpu'
args_cuda = torch.cuda.is_available()
if args_cuda: device = "cuda"
```

```
# Convert dataset to pytorch
X_train = Variable(torch.FloatTensor(X_train)).to(device)
X_val = Variable(torch.FloatTensor(X_val)).to(device)
y_train = Variable(torch.LongTensor(y_train).long()).to(device)
y_val = Variable(torch.LongTensor(y_val).long()).to(device)
```

Step2: setup the device

- *Nothing particularly enlightening. Just push Shift+Enter*

If GPU available (it should) we move data there

```
# check if a GPU is available. Otherwise run on CPU
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```

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```


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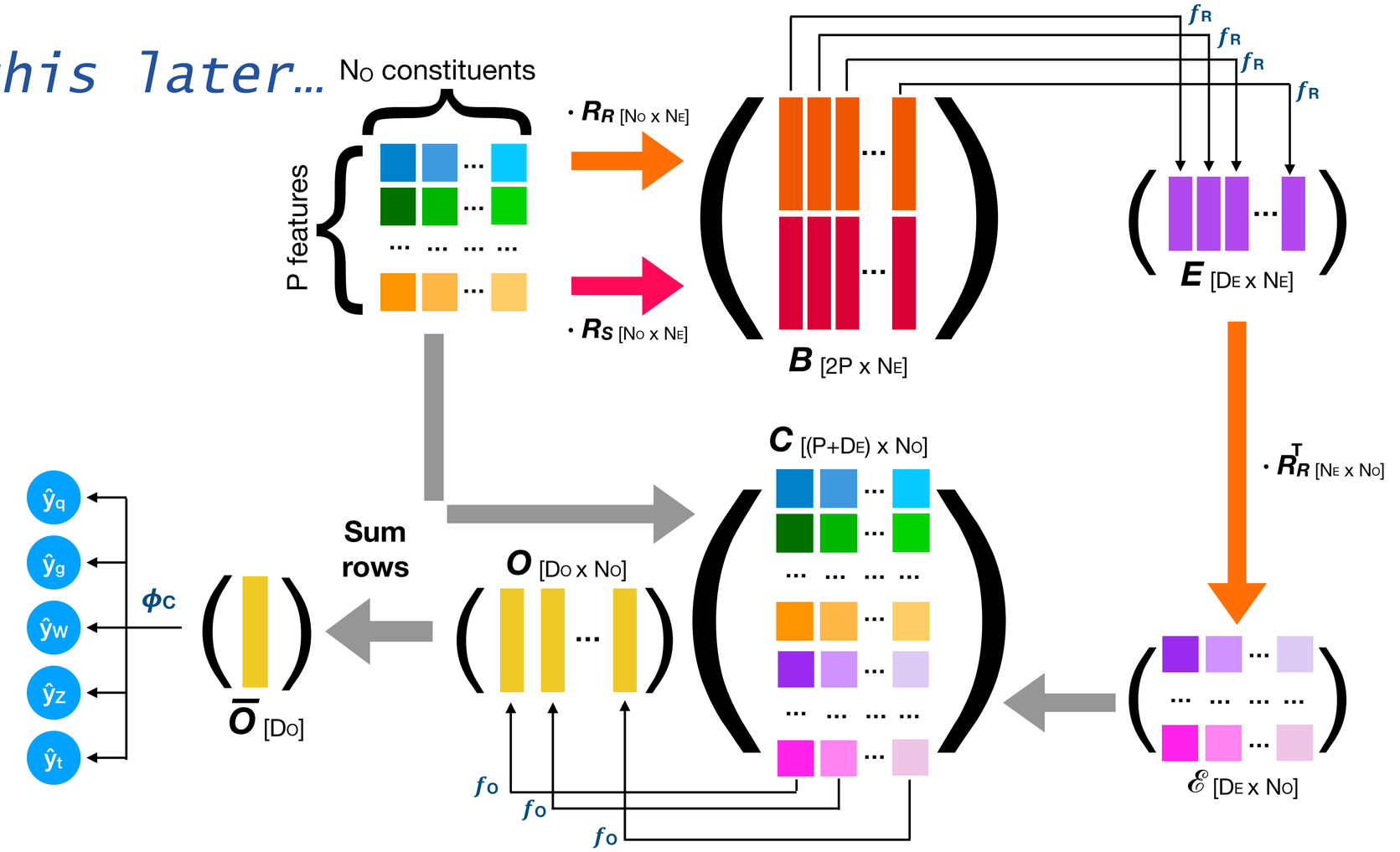
Step3: we build the model

- *More on this later…*



No: # of constituents
P: # of features
$N_E = N_O(N_O-1)$: # of edges
D_E: size of internal representations
D_O: size of post-interaction internal representation

ϕ_C, f_O, f_R parameterized as neural networks

Step4: we train

- *Nothing particularly enlightening. Just push Shift+Enter*

```
n_epochs = 300
batch_size = 100
patience =  10
```

```
#import util
# instantiate the model & setup training
# relu
gnn = GraphNet()
gnn.to(device)
loss = nn.CrossEntropyLoss()
optimizer = optim.Adam(gnn.parameters(), lr = 0.0001)

loss_train = np.zeros(n_epochs)
acc_train = np.zeros(n_epochs)
loss_val = np.zeros(n_epochs)
acc_val = np.zeros(n_epochs)
for i in range(n_epochs):
    print("Epoch %s" % i)
    for j in range(0, X_train.size()[0], batch_size):
        optimizer.zero_grad()
        out = gnn(X_train[j:j + batch_size,:,:])
        target = y_train[j:j + batch_size]
        l = loss(out, target)
        l.backward()
        optimizer.step()
        loss_train[i] += l.cpu().data.numpy()*batch_size
    loss_train[i] = loss_train[i]/X_train.shape[0]
```

Step4: we train

- *Nothing particularly enlightening. Just push Shift+Enter*

```
    #### val loss & accuracy
    for j in range(0, X_val.size()[0], batch_size):
        out_val = gnn(X_val[j:j + batch_size])
        target_val =  y_val[j:j + batch_size]

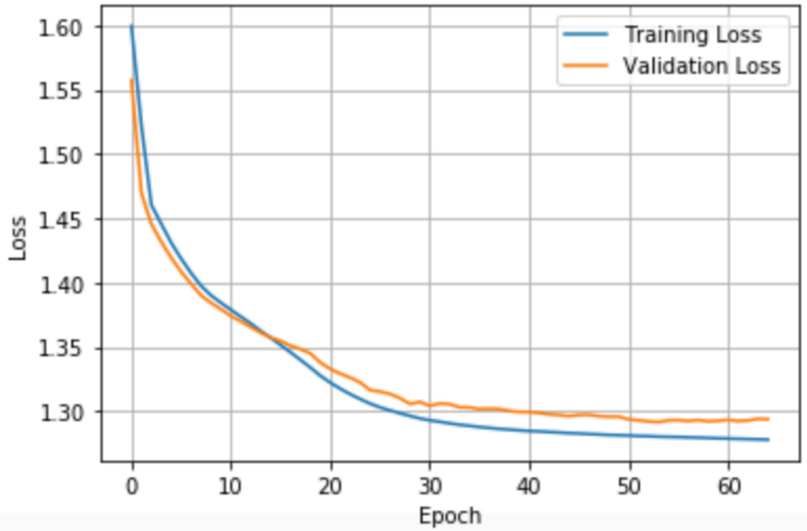
        l_val = loss(out_val,target_val)
        loss_val[i] += l_val.cpu().data.numpy()*batch_size
    loss_val[i] = loss_val[i]/X_val.shape[0]
    print("Training   Loss: %f" %l.cpu().data.numpy())
    print("Validation Loss: %f" %l_val.cpu().data.numpy())
    if all(loss_val[max(0, i - patience):i] > min(np.append(loss_val[0:max(0, i - patience)], 200))) and i > patienc
        print("Early Stopping")
        break
    print
```

Step5: we validate

- *Nothing particularly enlightening. Just push Shift+Enter*

Training history

```
epoch_number = list(range((loss_train > 0.).sum()))
plt.figure()
plt.plot(epoch_number, loss_train[loss_train>0.],label='Training Loss')
plt.plot(epoch_number, loss_val[loss_train>0.],label='Validation Loss')
plt.ylabel("Loss")
plt.xlabel("Epoch")
plt.grid(True)
plt.legend(loc='upper right')
#plt.savefig('%s/ROC.pdf'%(options.outputDir))
plt.show()
```



Step5: we validate

- *Nothing particularly enlightening. Just push Shift+Enter*

Compute TPR and FPR for each class

```
labels = ['gluon', 'quark', 'W', 'Z', 'top']
```

```
lst = []
n_batches_val = int(X_val.size()[0]/batch_size)
if args_cuda:
    for j in torch.split(X_val, n_batches_val).cuda():
        a = gnn(j).cpu().data.numpy()
        lst.append(a)
else:
    for j in torch.split(X_val, n_batches_val):
        a = gnn(j).cpu().data.numpy()
        lst.append(a)
predicted = Variable(torch.FloatTensor(np.concatenate(lst)))
```

```
# there is no softmax in the output layer. We have to put it by
predicted = torch.nn.functional.softmax(predicted, dim=1)
```

Pytorch puts the softmax in activation function
- **Not at the output layer**
- **- We need to include it when we run the model**

```
predict_val = predicted.data.numpy()
true_val = y_val.data.numpy()
```

Step5: we validate

- *Nothing particularly enlightening. Just push Shift+Enter*

Build the ROC curve

```
:
from sklearn.metrics import roc_curve, auc
#### get the ROC curves
fpr = {}
tpr = {}
auc1 = {}
plt.figure()
for i, label in enumerate(labels):
        fpr[label], tpr[label], threshold = roc_curve((true_val== i), predict_val[:,i])
        auc1[label] = auc(fpr[label], tpr[label])
        plt.plot(tpr[label],fpr[label],label='%s tagger, auc = %.1f%%'%(label,auc1[label]*100.))
plt.semilogy()
plt.xlabel("sig. efficiency")
plt.ylabel("bkg. mistag rate")
plt.ylim(0.001,1)
plt.grid(True)
plt.legend(loc='lower right')
#plt.savefig('%s/ROC.pdf'%(options.outputDir))
plt.show()
```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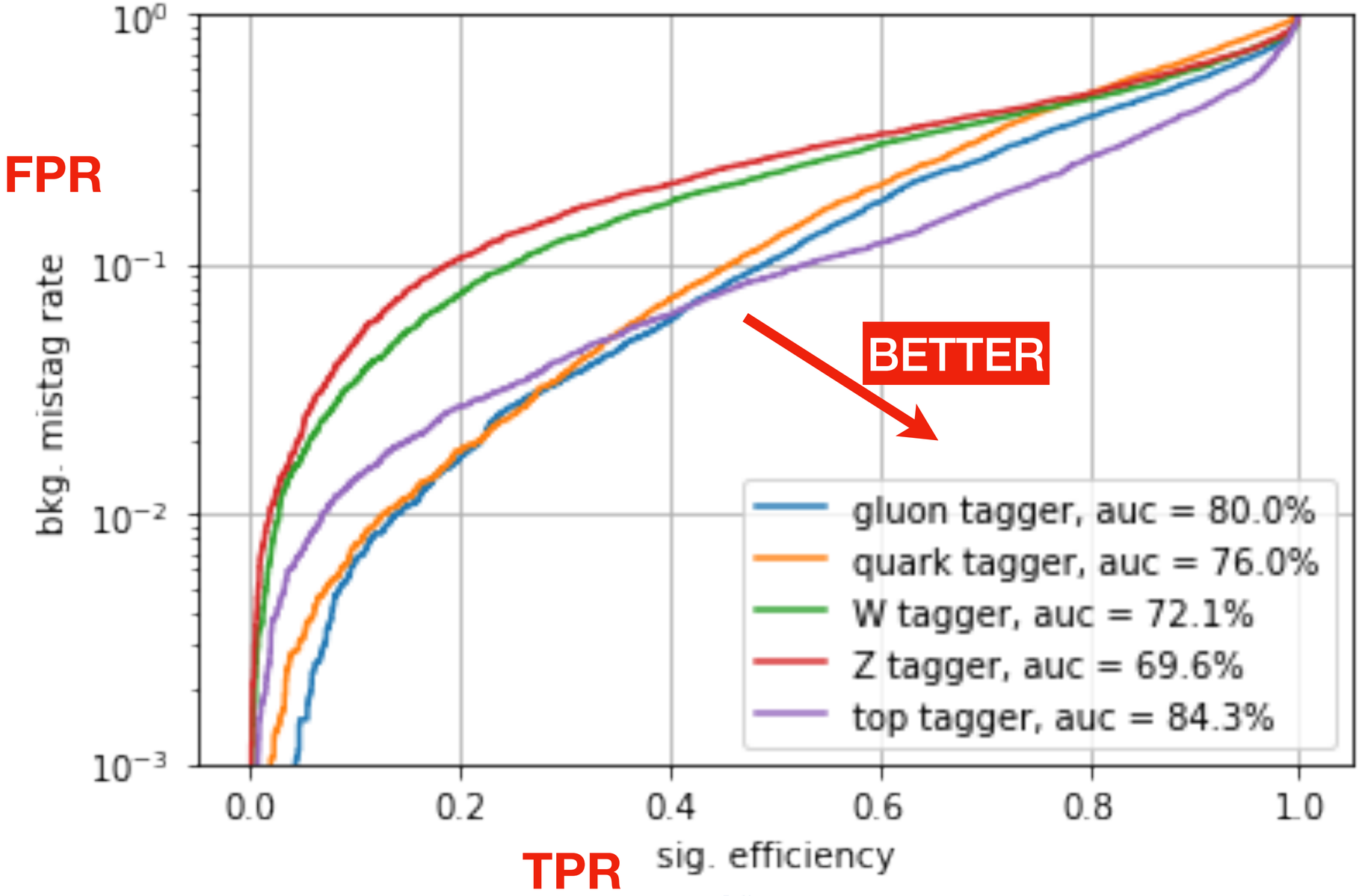
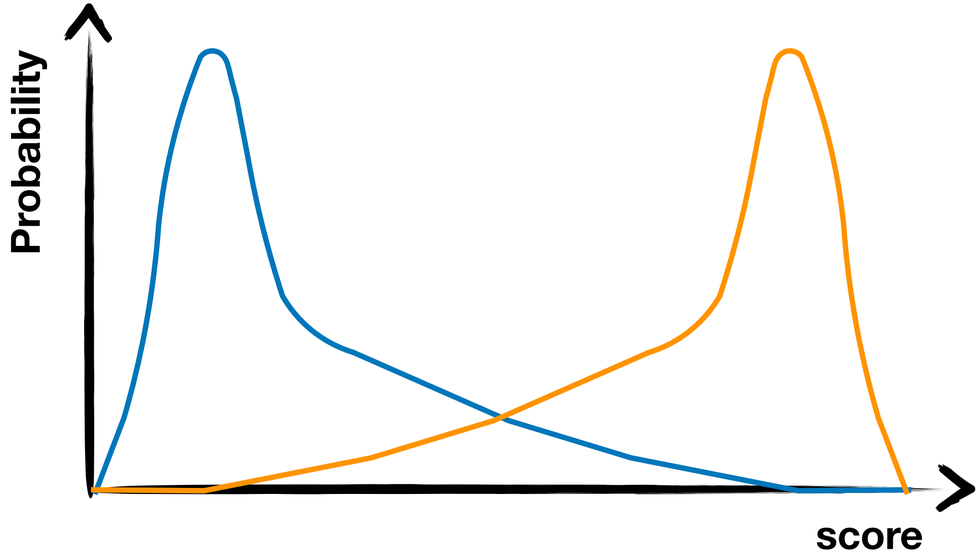
Jet tagging ROC curve

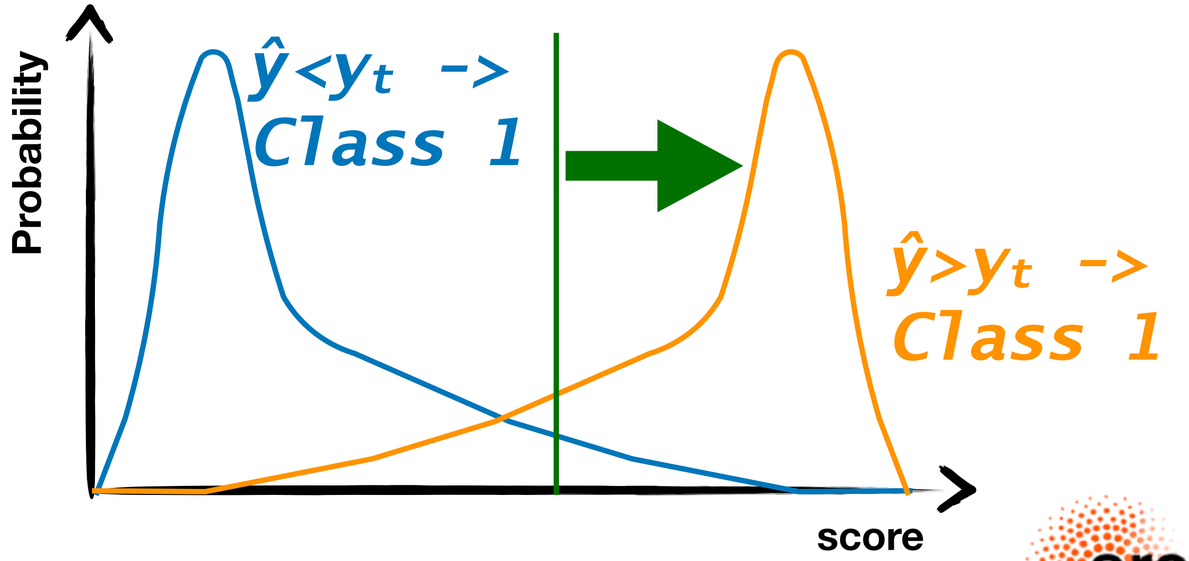


Backup

What is a ROC curve?

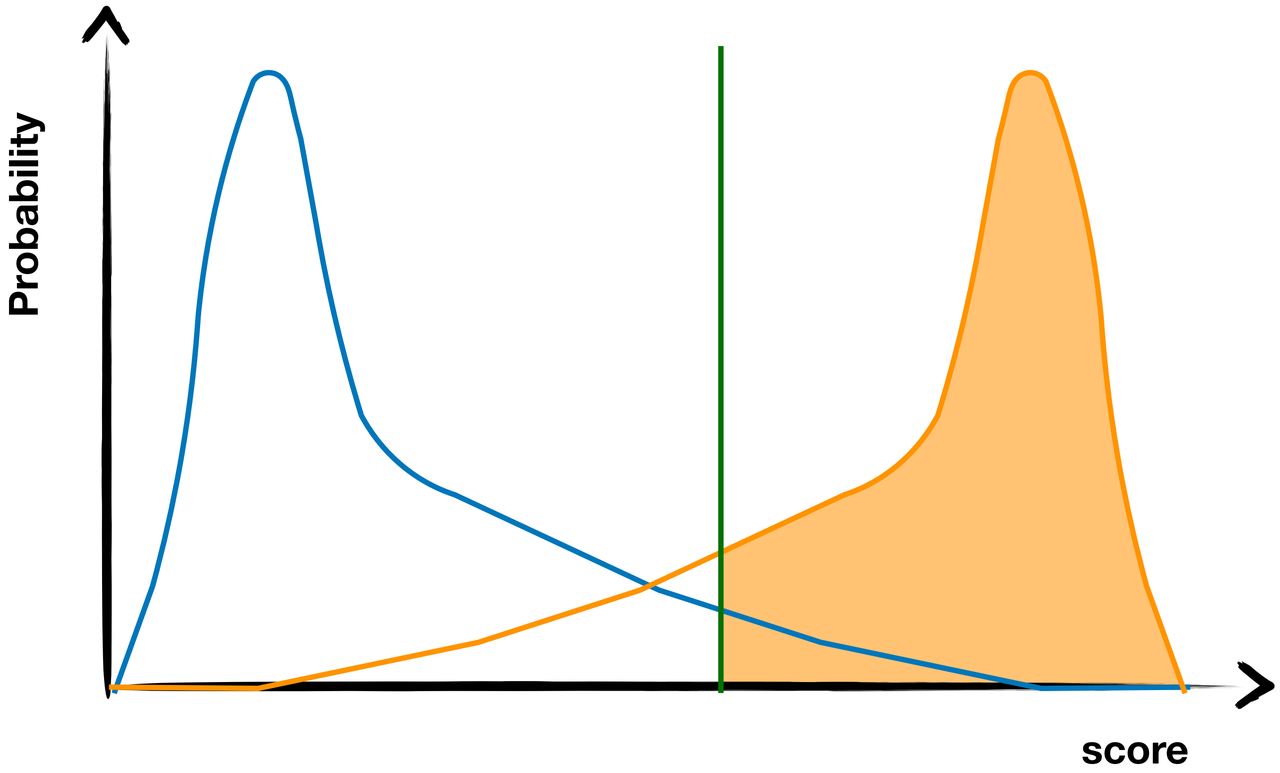
- Consider a binary classifier
- Its output $\hat{y}$ is a number in [0,1]
- If well trained, value should be close to 0 (1) for class-0 (class-1) examples
- One usually defines a threshold y_t such that:
  - $\hat{y} > y_t$ -> Class 1
  - $\hat{y} < y_t$ -> Class 0





What is a ROC curve?

- *A given threefold defines the following qualities*
  - *True-positives: Class-1 events above the threshold*
  - *True-negatives: Class-0 events below the threshold*
  - *False-positives: Class-0 events above the threshold*
  - *False-negatives: Class-1 events below the threshold*



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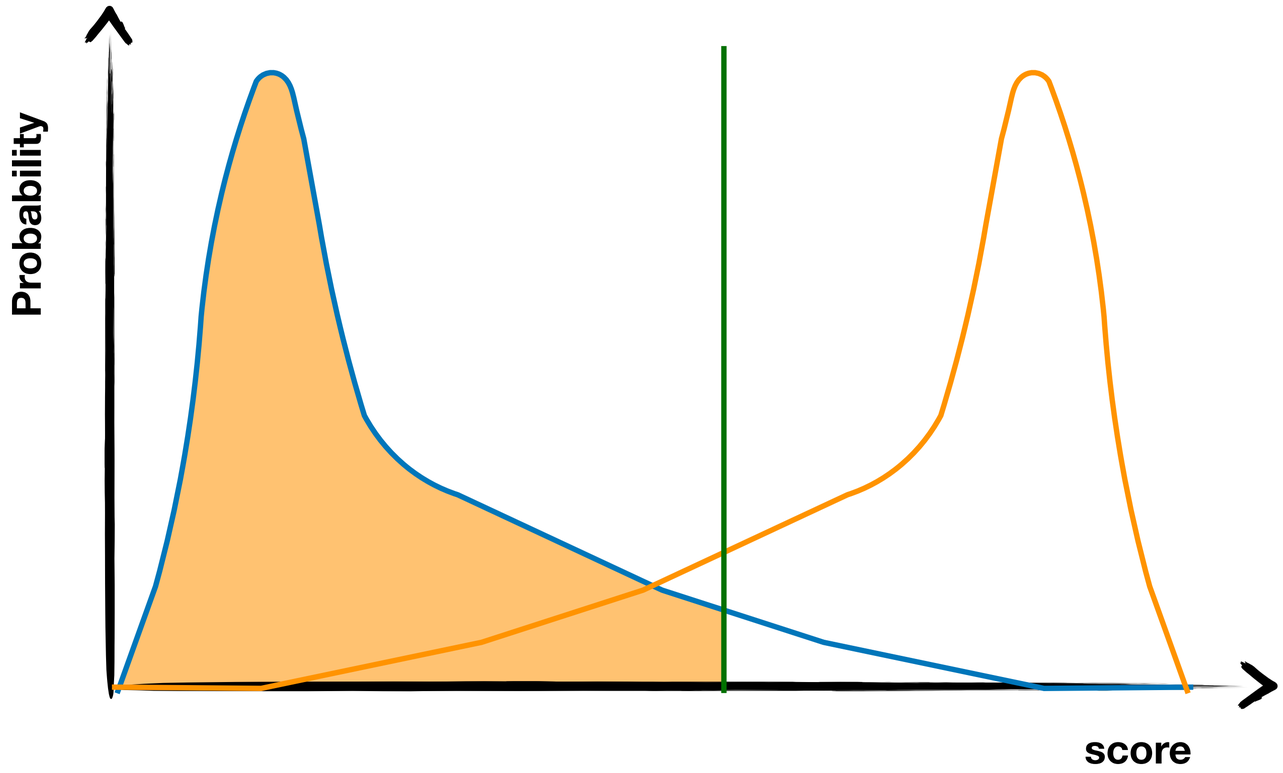

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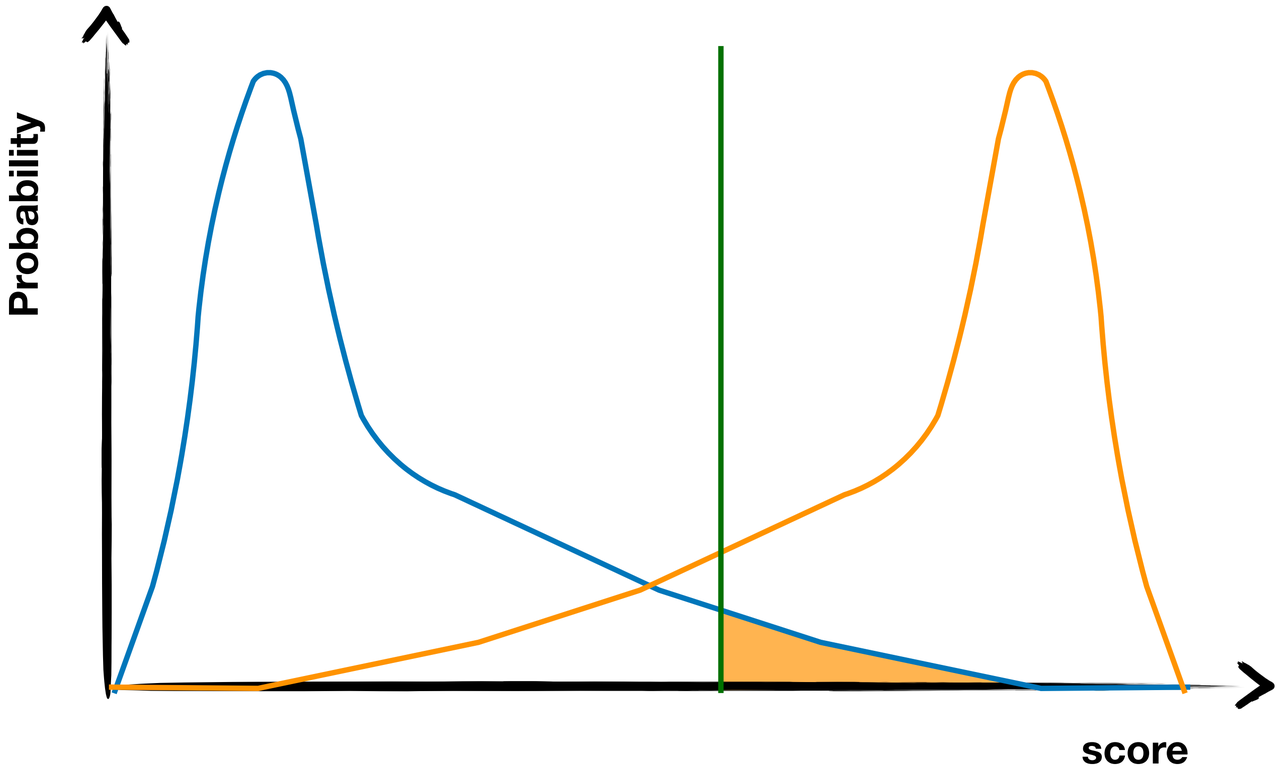

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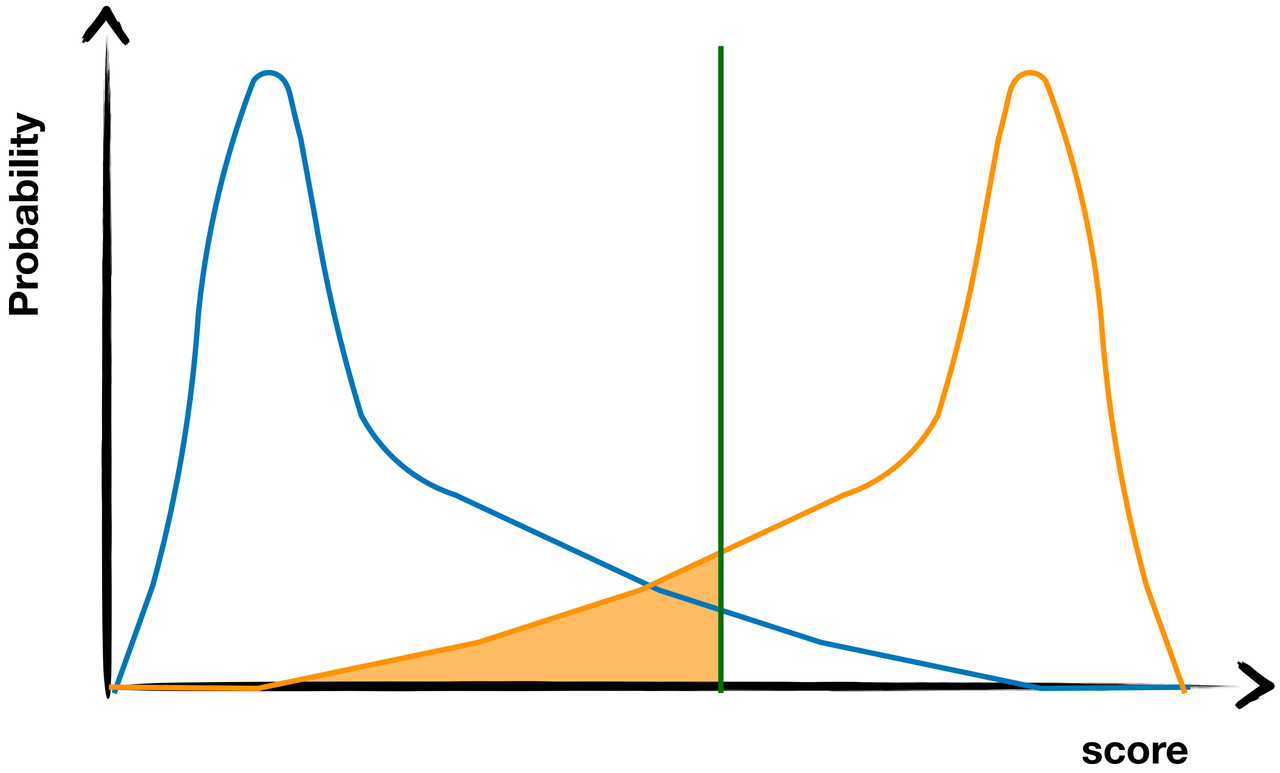
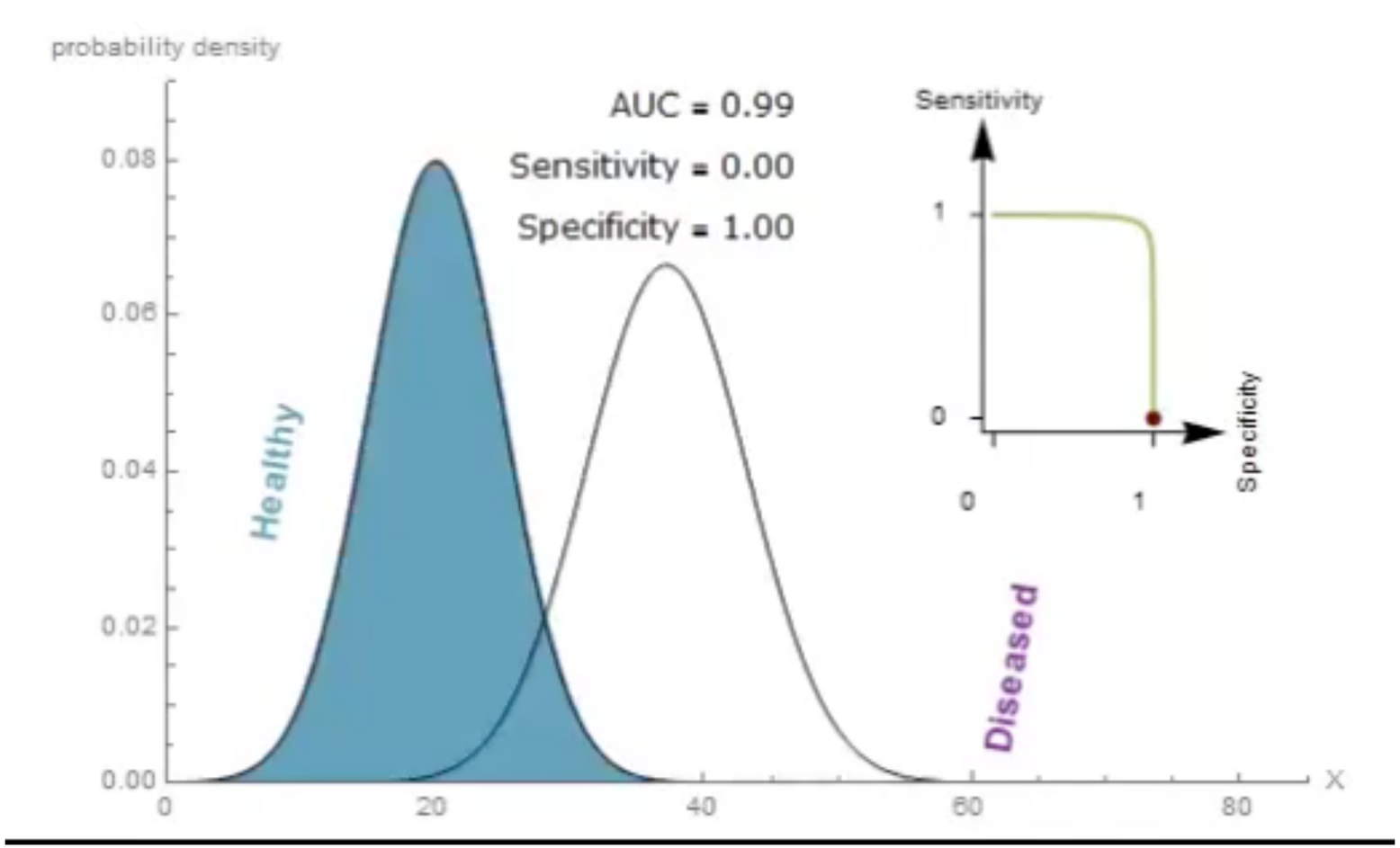


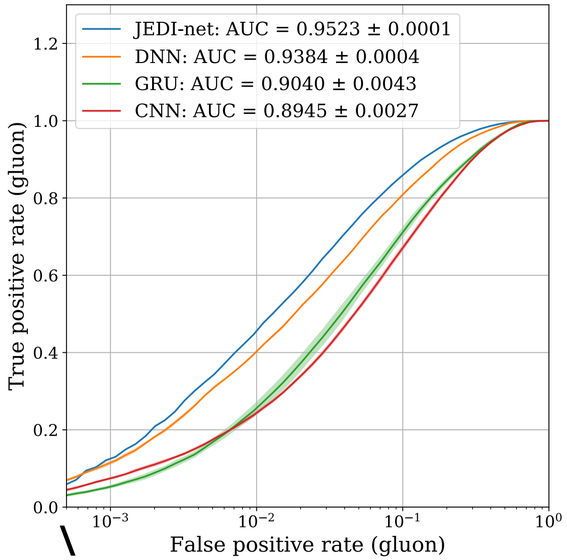
Classifier metrics

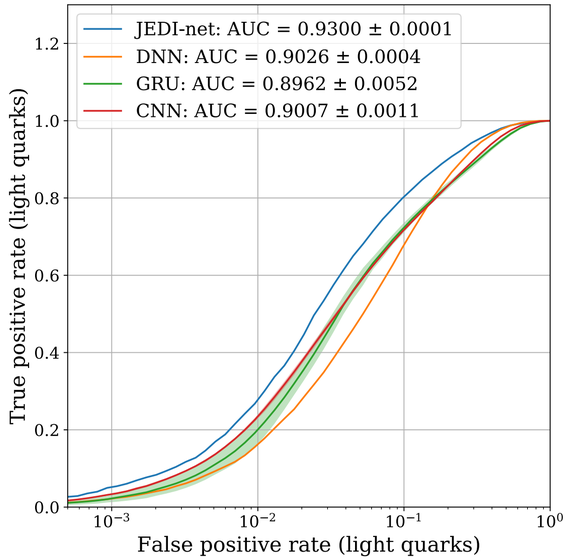
- *Accuracy: (TP+TN)/Total*
  - *The fraction of events correctly classified*
- *Sensitivity: TP/(Total positive)*
  - *We call it signal efficiency*
- *Specificity: TN/(Total negative)*
  - *We call it 1-mistag*
- *These metrics depend o the chosen threshold*
- *To build a threshold-independent metric, we need a ROC curve*

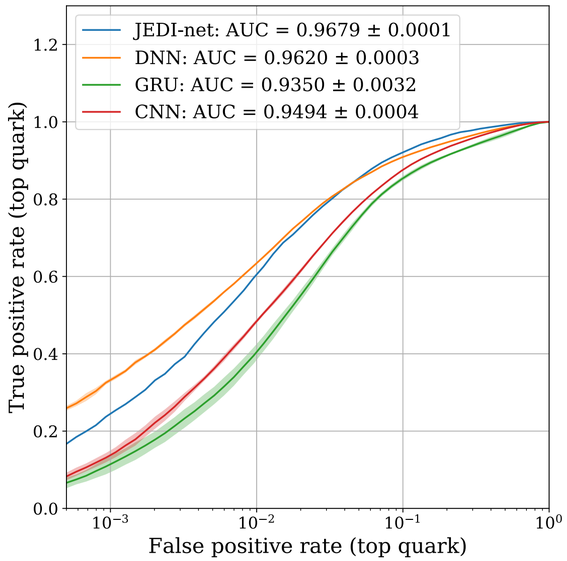
What is a ROC curve?

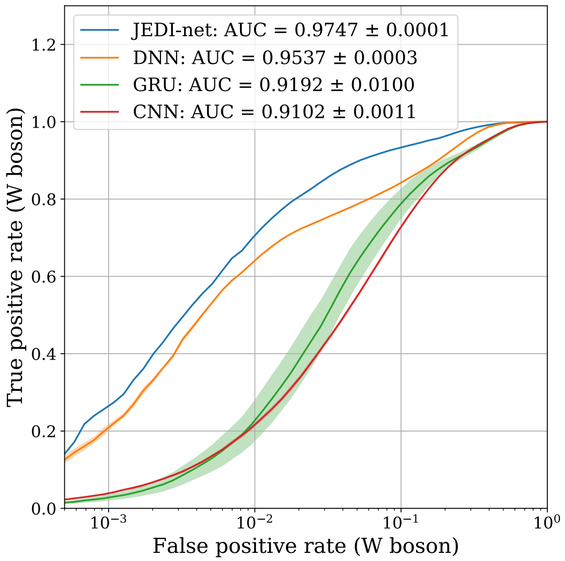


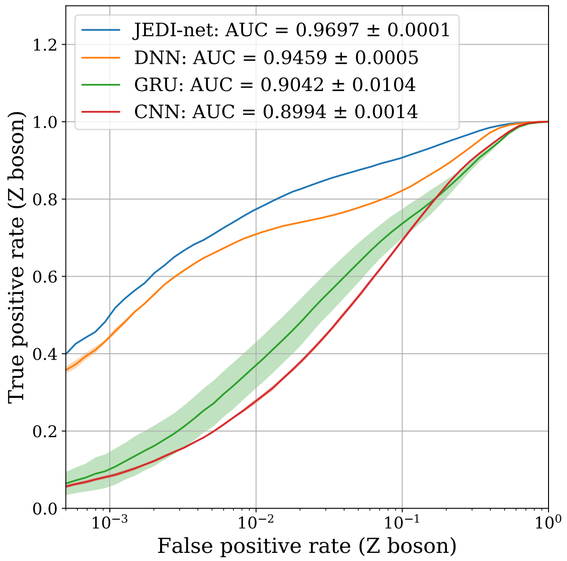
A comparison











http://arxiv.org/abs/1908.05318