Importing modules and dependences

```
import numpy as np
import matplotlib
import matplotlib.pyplot as plt
import torch
from torch import nn
import torch.nn.functional as F
import torchvision
import torch.optim as optim
import random
from tqdm import tqdm
from sklearn.model_selection import train_test_split
from sklearn.metrics import confusion_matrix
from sklearn.model_selection import train_test_split, GridSearchCV, ShuffleSplit
```

```
Loading VDFs and augmenting them with the particle
       abundances and power spectrum
featurevector_allvdfs_all_4040 = np.load('allsimulations.mldata_vdfs_4040.npy')
featurevector_allvdfs_all_6060 = np.load('allsimulations.mldata_vdfs_6060.npy')
print(featurevector_allvdfs_all_4040.shape)
print(featurevector_allvdfs_all_6060.shape)
\rightarrow \overline{\phantom{a}} (1596, 2, 40, 40)
           (1596, 2, 60, 60)
featurevector_allmoments = np.load('allsimulations.featurevector_allmoments_allps.npy')
print(featurevector_allmoments.shape)
extra_features = featurevector_allmoments[:,18:]
<del>→•</del> (1596, 30)
ncases = featurevector_allvdfs_all_4040.shape[0]
featurevector_allvdfs_all_4040_norm = np.copy(np.log10(featurevector_allvdfs_all_4040 + 1))
for ncase in range (0, ncases, 1):
    if (np.amax(featurevector_allvdfs_all_4040_norm[ncase,1,:,:]) != 0):
        featurevector_allvdfs_all_4040_norm[ncase,1,:,:] /= np.amax(featurevector_allvdfs_all_4040_norm[ncase,1,:,:]
ncases = featurevector_allvdfs_all_6060.shape[0]
featurevector_allvdfs_all_6060_norm = np.copy(np.log10(featurevector_allvdfs_all_6060 + 1))
for ncase in range (0, ncases, 1):
    featurevector_allvdfs_all_6060_norm[ncase,0,:,:] /= np.amax(featurevector_allvdfs_all_6060_norm[ncase
    if (np.amax(featurevector_allvdfs_all_6060_norm[ncase,1,:,:]) != 0):
        featurevector_allvdfs_all_6060_norm[ncase,1,:,:] /= np.amax(featurevector_allvdfs_all_6060_norm[ncase,1,:,:] /= np.amax(featurevector_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_allvdfs_
```

```
ncases = featurevector_allvdfs_all_4040_norm.shape[0]
featurevector_allvdfs_all_4040_aug = np.zeros([ncases,2*40*40+12], dtype=float)
featurevector_allvdfs_all_4040_aug[:,:-12] = np.log10(featurevector_allvdfs_all_4040_norm.reshape(feat
featurevector_allvdfs_all_4040_aug[:,-12:] = extra_features
ncases = featurevector_allvdfs_all_6060_norm.shape[0]
featurevector_allvdfs_all_6060_aug = np.zeros([ncases,2*60*60+12], dtype=float)
featurevector_allvdfs_all_6060_aug[:,:-12] = np.log10(featurevector_allvdfs_all_6060_norm.reshape(feat
featurevector_allvdfs_all_6060_aug[:,-12:] = extra_features
print(featurevector_allvdfs_all_4040_aug.shape)
print(featurevector_allvdfs_all_6060_aug.shape)
print(np.amin(featurevector_allvdfs_all_6060_aug[:,-10:]))
print(np.amax(featurevector_allvdfs_all_6060_aug[:,-10:]))
\rightarrow \overline{\phantom{a}} (1596, 3212)
     (1596, 7212)
     0.00020191832627305094
     1.0
featurevector_allmoments = np.load('allsimulations.featurevector_allmoments_all.npy')
times_allmoments = np.load('allsimulations.timep_array_all.npy')
labels_an = np.load('allsimulations.labels_allmoments_an_01_all.npy')
labels_me = np.load('allsimulations.labels_allmoments_me_01_all.npy')
# merging both labels
labels_allmoments = np.copy(labels_me)
labels_allmoments[np.where(labels_an == 1)] = 1
print('The total number of data points is: ' + str(len(labels_allmoments)))
print('Among them unstable (positive) samples: ' + str(len(np.where(labels_allmoments == 1)[0])))
print(labels allmoments.shape)
\rightarrow The total number of data points is: 1596
     Among them unstable (positive) samples: 418
     (1596,)
simnames = np.load('allsimulations.simnames_all.npy')
data_split = ShuffleSplit(n_splits=10, test_size=0.33, random_state=0)
data_split.split(labels_allmoments)
```

Best architecture for 40x40 VDFs (5-fold CV for faster assessment)

```
class VDFCNN_4040_CNN3_CONN2(nn.Module):
   def __init__(self):
```

```
super(VDFCNN_4040_CNN3_CONN2, self).__init__()
    self.cnncell = nn.Sequential(
        nn.Conv2d(2, 4, kernel_size=3, padding=1),
        nn.ReLU(True),
        nn.MaxPool2d(kernel_size=2, stride=2),
        nn.Conv2d(4, 8, kernel_size=3, padding=1),
        nn.ReLU(True),
        nn.MaxPool2d(kernel_size=2, stride=2),
        nn.Conv2d(8, 16, kernel_size=3, padding=1),
        nn.ReLU(True),
        nn.MaxPool2d(kernel_size=2, stride=2),
    self.linearcell = nn.Sequential(
        nn.Linear(16*5*5+12, 50),
        nn.ReLU(True),
        nn.Linear(50, 10),
        nn.ReLU(True),
       nn.Linear(10,2),
        nn.Sigmoid()
  def forward(self, x):
   x_{cnn} = x[:, :-12]
   x_p = x[:, -12:]
   x_{cnn} = x_{cnn.reshape}(-1, 2, 40, 40)
   x_cnn = self.cnncell(x_cnn)
   x_{cnn} = x_{cnn.view}(-1, 16 * 5 * 5)
   x = torch.cat((x_cnn, x_p), dim=1)
   x = self.linearcell(x)
    return x
class VDFCNN_4040_CNN3_CONN1(nn.Module):
 def __init__(self):
    super(VDFCNN_4040_CNN3_CONN1, self).__init__()
    self.cnncell = nn.Sequential(
        nn.Conv2d(2, 4, kernel_size=3, padding=1),
        nn.ReLU(True),
        nn.MaxPool2d(kernel_size=2, stride=2),
        nn.Conv2d(4, 8, kernel_size=3, padding=1),
        nn.ReLU(True),
        nn.MaxPool2d(kernel_size=2, stride=2),
        nn.Conv2d(8, 16, kernel_size=3, padding=1),
        nn.ReLU(True),
        nn.MaxPool2d(kernel_size=2, stride=2),
    self.linearcell = nn.Sequential(
        nn.Linear(16*5*5+12, 10),
        nn.ReLU(True),
        nn.Linear(10,2),
       nn.Sigmoid()
  def forward(self, x):
   x_{cnn} = x[:, :-12]
   x_p = x[:, -12:]
    x_{cnn} = x_{cnn.reshape}(-1, 2, 40, 40)
```

```
x_cnn = self.cnncell(x_cnn)
    x_{cnn} = x_{cnn.view}(-1, 16 * 5 * 5)
    x = torch.cat((x_cnn, x_p), dim=1)
   x = self.linearcell(x)
    return x
class VDFCNN_4040_CNN2_CONN2(nn.Module):
  def __init__(self):
    super(VDFCNN_4040_CNN2_CONN2, self).__init__()
    self.cnncell = nn.Sequential(
        nn.Conv2d(2, 4, kernel_size=3, padding=1),
        nn.ReLU(True),
        nn.MaxPool2d(kernel_size=2, stride=2),
        nn.Conv2d(4, 8, kernel_size=3, padding=1),
        nn.ReLU(True),
        nn.MaxPool2d(kernel_size=2, stride=2),
    self.linearcell = nn.Sequential(
        nn.Linear(8*10*10+12, 50),
        nn.ReLU(True),
        nn.Linear(50, 10),
        nn.ReLU(True),
        nn.Linear(10,2),
        nn.Sigmoid()
 def forward(self, x):
   x_{cnn} = x[:, :-12]
   x_p = x[:, -12:]
   x_{cnn} = x_{cnn.reshape}(-1, 2, 40, 40)
   x_cnn = self.cnncell(x_cnn)
   x_{cnn} = x_{cnn.view}(-1, 8 * 10 * 10)
   x = torch.cat((x_cnn, x_p), dim=1)
   x = self.linearcell(x)
    return x
class VDFCNN_4040_CNN2_CONN1(nn.Module):
  def __init__(self):
    super(VDFCNN_4040_CNN2_CONN1, self).__init__()
    self.cnncell = nn.Sequential(
        nn.Conv2d(2, 4, kernel_size=3, padding=1),
        nn.ReLU(True),
        nn.MaxPool2d(kernel_size=2, stride=2),
        nn.Conv2d(4, 8, kernel_size=3, padding=1),
        nn.ReLU(True),
        nn.MaxPool2d(kernel_size=2, stride=2),
    self.linearcell = nn.Sequential(
        nn.Linear(8*10*10+12, 10),
        nn.ReLU(True),
        nn.Linear(10,2),
        nn.Sigmoid()
 def forward(self, x):
```

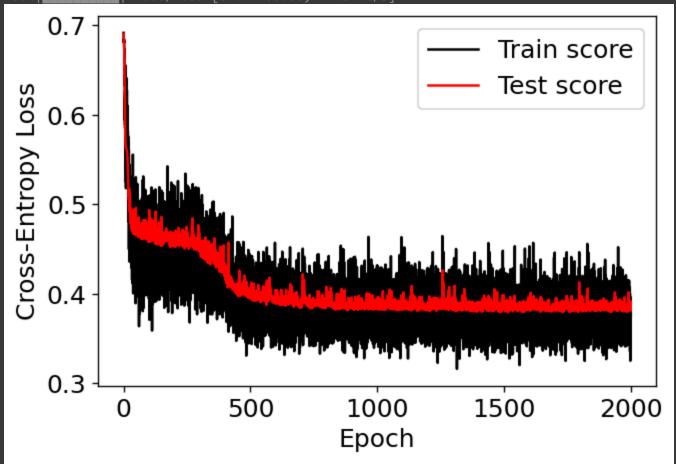
```
x_{cnn} = x[:, :-12]
    x_p = x[:, -12:]
    x_{cnn} = x_{cnn.reshape}(-1, 2, 40, 40)
   x_cnn = self.cnncell(x_cnn)
   x_{cnn} = x_{cnn.view}(-1, 8 * 10 * 10)
    x = torch.cat((x_cnn, x_p), dim=1)
   x = self.linearcell(x)
    return x
class VDFCNN_4040_CNN1_CONN2(nn.Module):
  def __init__(self):
    super(VDFCNN_4040_CNN1_CONN2, self).__init__()
    self.cnncell = nn.Sequential(
        nn.Conv2d(2, 4, kernel_size=3, padding=1),
        nn.ReLU(True),
        nn.MaxPool2d(kernel_size=2, stride=2),
    self.linearcell = nn.Sequential(
        nn.Linear(4*20*20+12, 50),
        nn.ReLU(True),
        nn.Linear(50, 10),
        nn.ReLU(True),
        nn.Linear(10,2),
        nn.Sigmoid()
 def forward(self, x):
   x_{cnn} = x[:, :-12]
   x_p = x[:, -12:]
   x_{cnn} = x_{cnn.reshape}(-1, 2, 40, 40)
   x_cnn = self.cnncell(x_cnn)
   x_{cnn} = x_{cnn.view}(-1, 4 * 20 * 20)
   x = torch.cat((x_cnn, x_p), dim=1)
   x = self.linearcell(x)
    return x
class VDFCNN_4040_CNN1_CONN1(nn.Module):
  def __init__(self):
    super(VDFCNN_4040_CNN1_CONN1, self).__init__()
    self.cnncell = nn.Sequential(
        nn.Conv2d(2, 4, kernel_size=3, padding=1),
        nn.ReLU(True),
        nn.MaxPool2d(kernel_size=2, stride=2),
    self.linearcell = nn.Sequential(
        nn.Linear(4*20*20+12, 10),
        nn.ReLU(True),
        nn.Linear(10,2),
        nn.Sigmoid()
 def forward(self, x):
   x_{cnn} = x[:, :-12]
   x_p = x[:, -12:]
    x_{cnn} = x_{cnn.reshape}(-1, 2, 40, 40)
```

```
x_{cnn} = self.cnncell(x_{cnn})
   x_{cnn} = x_{cnn.view}(-1, 4 * 20 * 20)
    x = torch.cat((x_cnn, x_p), dim=1)
   x = self.linearcell(x)
    return x
def outputclass_analysis_scorereturn(test_labels, predicted_labels):
    tn, fp, fn, tp = confusion_matrix(test_labels, predicted_labels).ravel()
    precision = tp/(tp+fp)
   recall = tp/(tp+fn)
   acc = (tp+tn)/(tp+fn+fp+tn)
   tss = tp/(tp+fn) - fp/(fp+tn)
   hss = 2*(tp*tn - fp*fn)/((tp+fn)*(fn+tn) + (tp+fp)*(fp+tn))
    return tp, tn, fp, fn, acc, tss
# NETWORK: VDFCNN_4040_CNN3_CONN2
ARCH = 'VDFCNN_4040_CNN3_CONN2'
tp = np.zeros([7,5], dtype=int)
tn = np.zeros([7,5], dtype=int)
fp = np.zeros([7,5], dtype=int)
fn = np.zeros([7,5], dtype=int)
acc = np.zeros([7,5], dtype=float)
tss = np.zeros([7,5], dtype=float)
for n_e, split_indexes in enumerate(data_split.split(labels_allmoments)):
 if (n_e >= 5): continue
 train_index, test_index = split_indexes
 X_train, X_test = featurevector_allvdfs_all_4040_aug[train_index], featurevector_allvdfs_all_4040_au
 f_train, f_test = labels_allmoments[train_index], labels_allmoments[test_index]
 while(True):
    # training the network
    device = torch.device("cuda:0")
    net = VDFCNN_4040_CNN3_CONN2().to(device)
    optimizer = optim.Adam(net.parameters(), lr=0.001, weight_decay=0.001)
    loss_history_train = []
    loss_history_test = []
    outputs_history_train = []
    outputs_labels_train = []
    outputs_history_test = []
    outputs_labels_test = []
    n_{epochs} = 2000
    n_iterations = 7 # based on the total size / batch size, approximately
    # test data tensors
    testdata_tensor = torch.tensor(X_test).float().to(device=device)
    testlabels_tensor = torch.tensor(f_test).long().to(device=device)
```

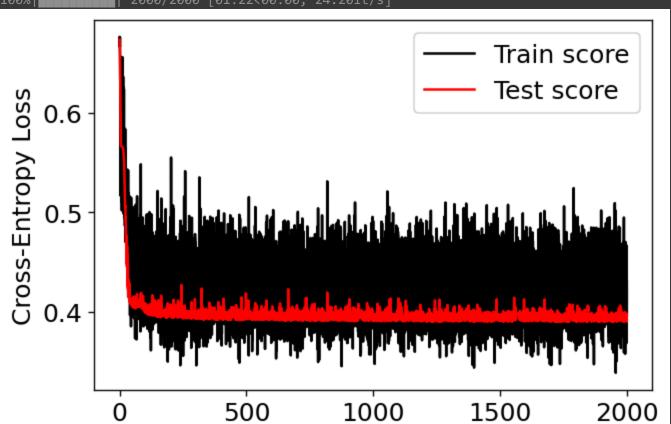
```
for ep in tqdm(range(n_epochs)):
     for n_iter in range (n_iterations):
       train_indexes = np.random.choice(X_train.shape[0], size=128, replace=False)
       traindata_tensor = torch.tensor(X_train[train_indexes]).float().to(device=device)
       trainlabels_tensor = torch.tensor(f_train[train_indexes]).long().to(device=device)
       outputs = net(traindata_tensor)
       criteria = nn.CrossEntropyLoss()
       loss = criteria(outputs, trainlabels_tensor)
       optimizer.zero_grad()
       loss.backward()
       optimizer.step()
       loss_history_train.append(loss.item())
       outputs_history_train.append(outputs.detach())
       outputs_labels_train.append(f_train[train_indexes])
       outputs = net(testdata_tensor)
       criteria = nn.CrossEntropyLoss()
       loss = criteria(outputs, testlabels_tensor)
       loss_history_test.append(loss.item())
       outputs_history_test.append(outputs.detach())
       outputs_labels_test.append(f_test)
   # visualizing the result
   matplotlib.rcParams.update({'font.size': 15})
   im, ax = plt.subplots(1, 1, figsize=(6,4), dpi=120)
   ax.plot(np.arange(n_epochs*n_iterations)/n_iterations, loss_history_train, color='black', label='
   ax.plot(np.arange(n_epochs*n_iterations)/n_iterations, loss_history_test, color='red', label='Test
   ax.set(xlabel='Epoch', ylabel='Cross-Entropy Loss')
   ax.legend()
   plt.show()
   # finding the optimum
   optim_indexes = np.arange(250,2000,250)*n_iterations
   oi = 6
   optim_index = optim_indexes[oi]
   outputs_optim = outputs_history_test[optim_index]
   labels_optim = np.argmax(outputs_optim.cpu(), axis=1)
    _tp, _tn, _fp, _fn, _acc, _tss = outputclass_analysis_scorereturn(f_test, labels_optim)
   if (_acc < 0.88):
     print("RERUNNING THE SAMPLE...")
     continue
   break
 for oi in range (0, 7, 1):
   optim_index = optim_indexes[oi]
   outputs_optim = outputs_history_test[optim_index]
   labels_optim = np.argmax(outputs_optim.cpu(), axis=1)
   tp[oi,n_e], tn[oi,n_e], fp[oi,n_e], fn[oi,n_e], acc[oi,n_e], tss[oi,n_e] = outputclass_analysis_s(
   print(oi*250+250,acc[oi,n_e], tss[oi,n_e])
 print('-----
# final results
print("ARCH = " + str(ARCH))
```

```
for oi in range (0, 7, 1):
    print("=>=>=> NUMBER OF EPOCHS:", oi*250+250)
    print("TP = " + str(np.mean(tp[oi,:])) + "+/-" + str(np.std(tp[oi,:])))
    print("TN = " + str(np.mean(tn[oi,:])) + "+/-" + str(np.std(tn[oi,:])))
    print("FP = " + str(np.mean(fp[oi,:])) + "+/-" + str(np.std(fp[oi,:])))
    print("FN = " + str(np.mean(fn[oi,:])) + "+/-" + str(np.std(fn[oi,:])))
    print("Acc = " + str(np.mean(acc[oi,:])) + "+/-" + str(np.std(acc[oi,:])))
    print("TSS = " + str(np.mean(tss[oi,:])) + "+/-" + str(np.std(tss[oi,:])))
```

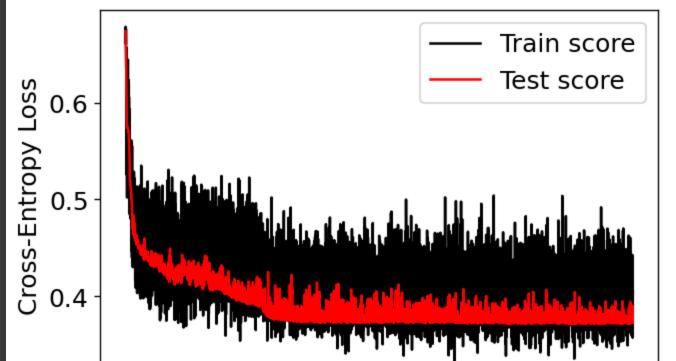
[01:27<00:00, 22.87it/s]

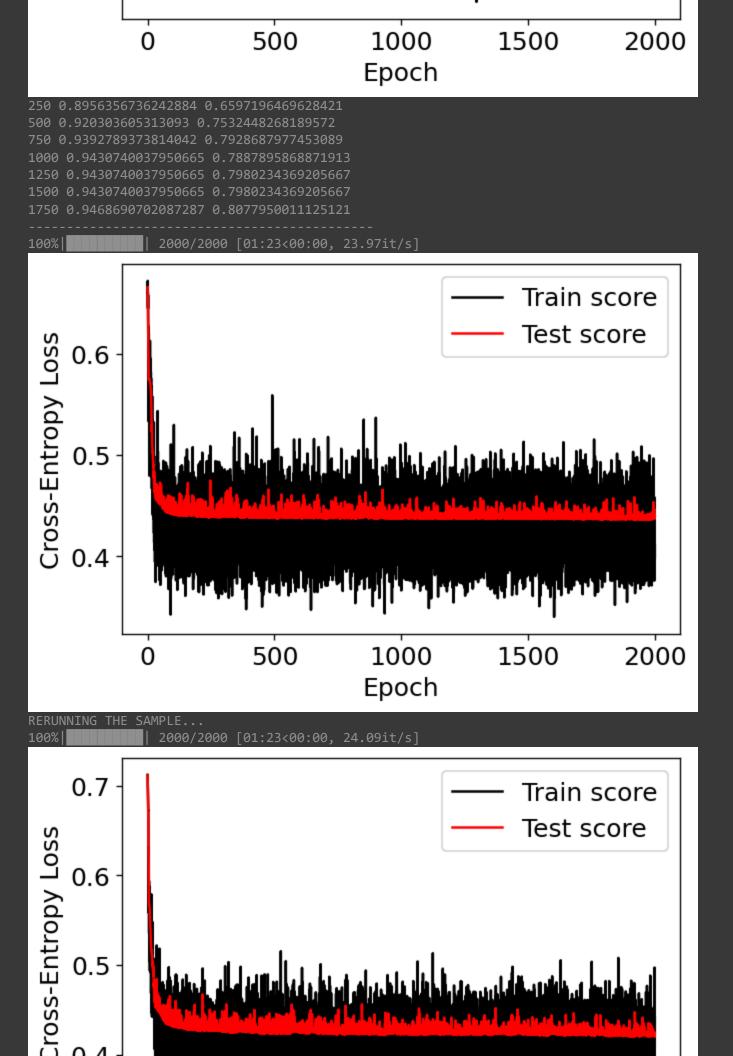


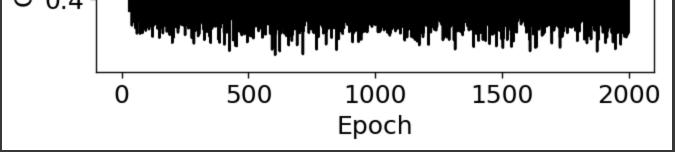
250 0.8519924098671727 0.5330712568222588
500 0.9146110056925996 0.7662493797946643
750 0.9297912713472486 0.7915346742490744
1000 0.9240986717267552 0.7938819129040876
1250 0.9316888045540797 0.8040341971680469
1500 0.9278937381404174 0.7989580550360673
1750 0.9316888045540797 0.7990534712415557



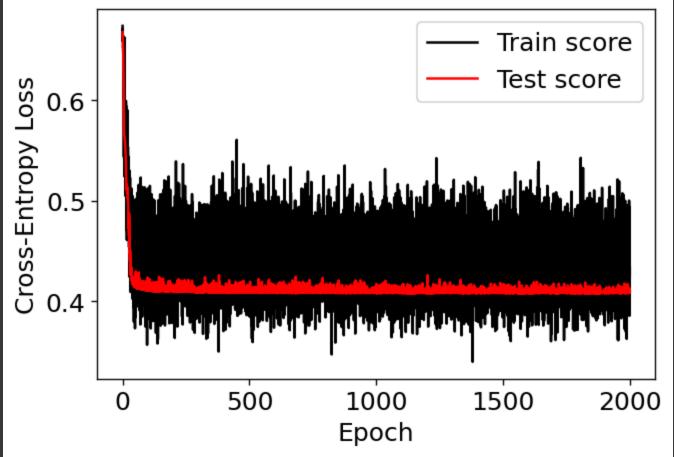
Epoch 500 0.9127134724857685 0.6890004198313041 750 0.9222011385199241 0.6917293233082706 1000 0.9184060721062619 0.6866531811762909 1250 0.9222011385199241 0.6967100492347621 0.7 Train score Test score **Cross-Entropy Loss** 0.6 0.5 0.4 500 1000 1500 2000 0 **Epoch** 2000/2000 [01:23<00:00, 23.94it/s] Train score Test score 0.6







250 0.8918406072106262 0.6293281653746771 500 0.889943074003795 0.62218530823182 750 0.8804554079696395 0.5682355112587671 1000 0.889943074003795 0.6176264304171281 1250 0.8918406072106262 0.6293281653746771 1500 0.8766603415559773 0.608656330749354 1750 0.8937381404174574 0.6273532668881506



250 0.8937381404174574 0.6755345410352815 500 0.8994307400379506 0.6831681288215411 750 0.9070208728652751 0.6884280885648095 1000 0.8975332068311196 0.6806235995594546 1250 0.9070208728652751 0.6933462458698871 1500 0.9013282732447818 0.6857126580836277 1750 0.9032258064516129 0.6882571873457142

ARCH = VDFCNN_4040_CNN3_CONN2

=>=> NUMBER OF EPOCHS: 250

TP = 91.6 + / -6.621178142898739

TN = 377.2 + / -5.706137047074842

FN = 44.2 + / -6.49307323229917

Acc = 0.8895635673624287+/-0.020486329527538153

TSS = 0.6388345654037689+/-0.057248306413644104

=>=> NUMBER OF EPOCHS: 500

```
TP = 99.8+/-7.833262411026456
TN = 378.4 + / -4.715930449020639
FP = 12.8+/-5.192301994298868
Acc = 0.9074003795066414+/-0.011090428232411739
TSS = 0.7027696126996574+/-0.05223995987720622
=>=> NUMBER OF EPOCHS: 750
TP = 98.2+/-11.565465835840769
TN = 384.4 + / -4.923413450036469
FP = 6.8+/-5.035871324805669
FN = 37.6 + / -12.611106216347556
Acc = 0.9157495256166983+/-0.020563517547087774
=>=> NUMBER OF EPOCHS: 1000
TP = 100.0 + / -9.359487165438072
TN = 382.0 + / -6.54217089351845
FP = 9.2+/-7.493997598078078
Acc = 0.9146110056925997+/-0.019051082198119382
TSS = 0.7135149421888305+/-0.06800459312555461
=>=> NUMBER OF EPOCHS: 1250
TP = 101.0+/-9.186947262284681
TN = 383.4 + / -5.276362383309167
FP = 7.8+/-5.2687759489277965
FN = 34.8 + / -9.846826900072937
Acc = 0.9191650853889943+/-0.018065472843130034
TSS = 0.724288418913588+/-0.06712924300017296
=>=> NUMBER OF EPOCHS: 1500
TP = 101.4+/-8.867919710958146
TN = 379.8 + / -6.046486583132389
FP = 11.4+/-5.748043145279966
```

Acc = 0.9130929791271347+/-0.022783045191352755 TSS = 0.7180815537358781+/-0.07254689610459417

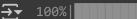
Acc = 0.9206831119544592+/-0.019440225388790422 TSS = 0.7273489281747294+/-0.06828038690843315

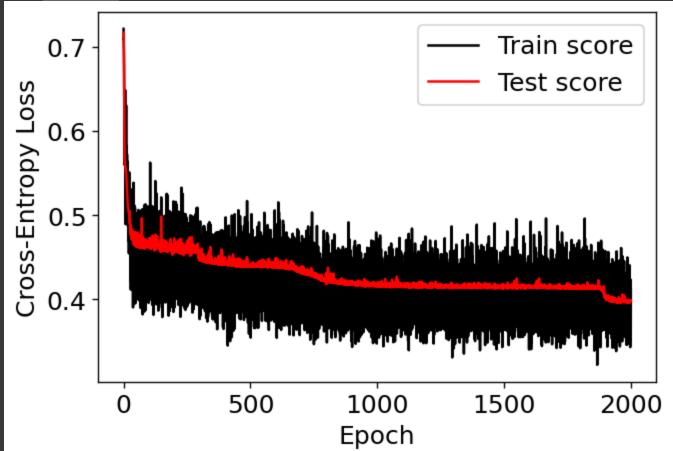
=>=>=> NUMBER OF EPOCHS: 1750 TP = 101.2+/-9.130169768410662 TN = 384.0+/-5.549774770204643 FP = 7.2+/-5.878775382679628 FN = 34.6+/-9.871170143402454

```
# NETWORK: VDFCNN_4040_CNN3_CONN1
ARCH = 'VDFCNN_4040_CNN3_CONN1'
tp = np.zeros([7,5], dtype=int)
tn = np.zeros([7,5], dtype=int)
fp = np.zeros([7,5], dtype=int)
fn = np.zeros([7,5], dtype=int)
acc = np.zeros([7,5], dtype=float)
tss = np.zeros([7,5], dtype=float)
for n_e, split_indexes in enumerate(data_split.split(labels_allmoments)):
 if (n_e >= 5): continue
 train_index, test_index = split_indexes
 X_train, X_test = featurevector_allvdfs_all_4040_aug[train_index], featurevector_allvdfs_all_4040_au
 f_train, f_test = labels_allmoments[train_index], labels_allmoments[test_index]
 while(True):
    # training the network
    device = torch.device("cuda:0")
    net = VDFCNN_4040_CNN3_CONN1().to(device)
    optimizer = optim.Adam(net.parameters(), lr=0.001, weight_decay=0.001)
    loss_history_train = []
    loss_history_test = []
    outputs_history_train = []
    outputs_labels_train = []
    outputs_history_test = []
    outputs_labels_test = []
    n_{epochs} = 2000
    n_iterations = 7 # based on the total size / batch size, approximately
    # test data tensors
    testdata_tensor = torch.tensor(X_test).float().to(device=device)
    testlabels_tensor = torch.tensor(f_test).long().to(device=device)
    for ep in tqdm(range(n_epochs)):
      for n_iter in range (n_iterations):
        train_indexes = np.random.choice(X_train.shape[0], size=128, replace=False)
        traindata_tensor = torch.tensor(X_train[train_indexes]).float().to(device=device)
        trainlabels_tensor = torch.tensor(f_train[train_indexes]).long().to(device=device)
        outputs = net(traindata_tensor)
        criteria = nn.CrossEntropyLoss()
        loss = criteria(outputs, trainlabels_tensor)
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
        loss_history_train.append(loss.item())
        outputs_history_train.append(outputs.detach())
        outputs_labels_train.append(f_train[train_indexes])
        outputs = net(testdata_tensor)
```

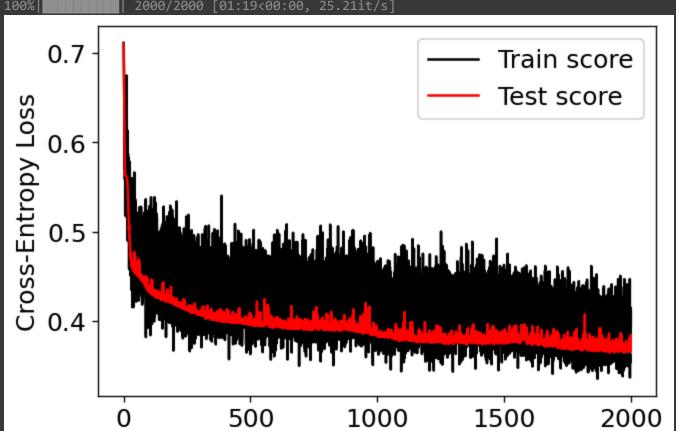
```
criteria = nn.CrossEntropyLoss()
       loss = criteria(outputs, testlabels_tensor)
       loss_history_test.append(loss.item())
       outputs_history_test.append(outputs.detach())
       outputs_labels_test.append(f_test)
   # visualizing the result
   matplotlib.rcParams.update({'font.size': 15})
   im, ax = plt.subplots(1, 1, figsize=(6,4), dpi=120)
   ax.plot(np.arange(n_epochs*n_iterations)/n_iterations, loss_history_train, color='black', label='
   ax.plot(np.arange(n_epochs*n_iterations)/n_iterations, loss_history_test, color='red', label='Test
   ax.set(xlabel='Epoch', ylabel='Cross-Entropy Loss')
   ax.legend()
   plt.show()
   # finding the optimum
   optim_indexes = np.arange(250,2000,250)*n_iterations
   oi = 6
   optim_index = optim_indexes[oi]
   outputs_optim = outputs_history_test[optim_index]
   labels_optim = np.argmax(outputs_optim.cpu(), axis=1)
   _tp, _tn, _fp, _fn, _acc, _tss = outputclass_analysis_scorereturn(f_test, labels_optim)
   if (_acc < 0.88):
     print("RERUNNING THE SAMPLE...")
     continue
   break
 for oi in range (0, 7, 1):
   optim_index = optim_indexes[oi]
   outputs_optim = outputs_history_test[optim_index]
   labels_optim = np.argmax(outputs_optim.cpu(), axis=1)
   tp[oi,n_e], tn[oi,n_e], fp[oi,n_e], fn[oi,n_e], acc[oi,n_e], tss[oi,n_e] = outputclass_analysis_s(
   print(oi*250+250,acc[oi,n_e], tss[oi,n_e])
 print('----')
# final results
print("ARCH = " + str(ARCH))
for oi in range (0, 7, 1):
 print("=>=>=> NUMBER OF EPOCHS:", oi*250+250)
 print("TP = " + str(np.mean(tp[oi,:])) + "+/-" + str(np.std(tp[oi,:])))
 print("TN = " + str(np.mean(tn[oi,:])) + "+/-" + str(np.std(tn[oi,:])))
 print("FP = " + str(np.mean(fp[oi,:])) + "+/-" + str(np.std(fp[oi,:])))
 print("FN = " + str(np.mean(fn[oi,:])) + "+/-" + str(np.std(fn[oi,:])))
 print("Acc = " + str(np.mean(acc[oi,:])) + "+/-" + str(np.std(acc[oi,:])))
```

print("TSS = " + str(np.mean(tss[oi,:])) + "+/-" + str(np.std(tss[oi,:])))





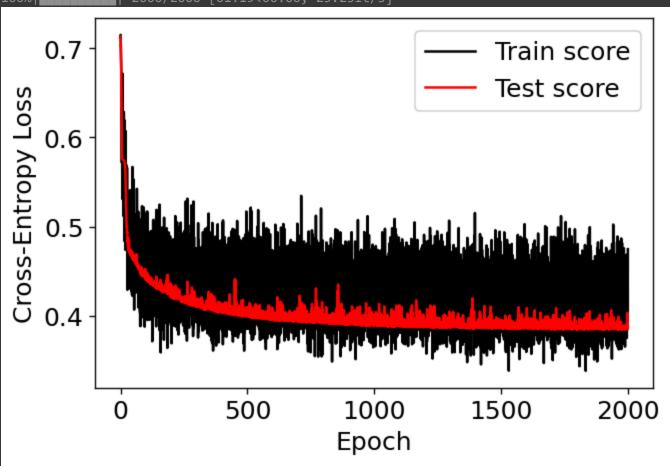
500 0.8766603415559773 0.6308156177245143 1000 0.8994307400379506 0.7210411816342888 1250 0.9013282732447818 0.72855997862677 1500 0.8994307400379506 0.7260219075607801



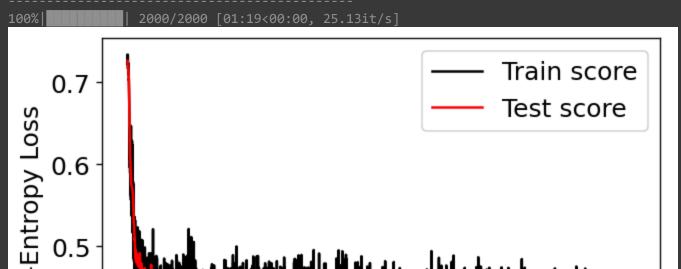
Epoch

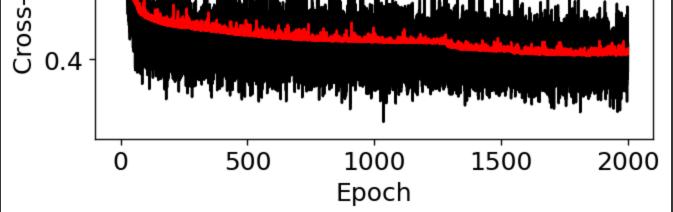
250 0.9013282732447818 0.6787527193618564 500 0.920303605313093 0.7539406892866685 750 0.905123339658444 0.6888095874203274 1000 0.9278937381404174 0.7740544254036106 1250 0.9335863377609108 0.8065722682340368 1500 0.9430740037950665 0.819262623563986 1750 0.937381404174573 0.8216098622189992

100%|**| | 100%| | 100%**| 2000/2000 [01:19<00:00, 25.23it/s]

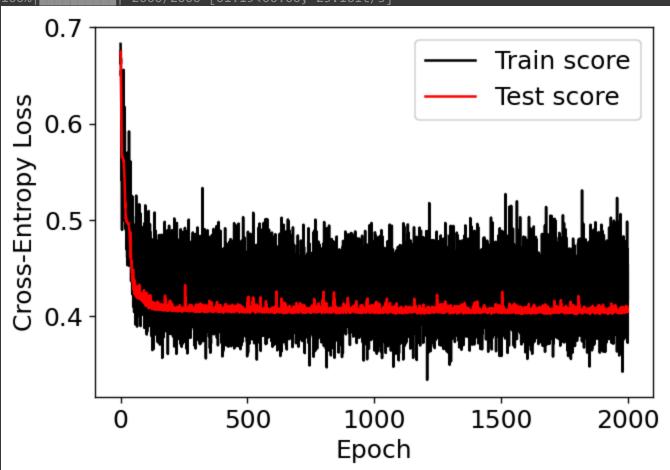


250 0.889943074003795 0.7397092635170214 500 0.9165085388994307 0.7665578877104502 750 0.9316888045540797 0.8241118445449827 1000 0.9316888045540797 0.8333456945783579 1250 0.9278937381404174 0.8281910554031002 1500 0.9259962049335864 0.816379885782096 1750 0.9259962049335864 0.8025291107320329





250 0.8633776091081594 0.5723329641934293 500 0.8671726755218216 0.5866186784791435 750 0.8937381404174574 0.6957364341085271 1000 0.8937381404174574 0.6866186784791436 1250 0.8956356736242884 0.6983204134366925 1500 0.8956356736242884 0.7211148025101514 1750 0.905123339658444 0.7522702104097453



=>=>=> NUMBER OF EPOCHS: 250 TP = 94.6+/-11.056219968868202 TN = 371.0+/-10.507140429250958

```
FP = 20.2+/-8.704022058795578
FN = 41.2 + / -10.225458424931373
Acc = 0.8834914611005692+/-0.019484626418206363
TSS = 0.6445064816371981+/-0.06810733696767045
=>=> NUMBER OF EPOCHS: 500
TP = 98.4+/-9.112628599915615
TN = 374.4 + / -6.374950980203691
FN = 37.4 + / -9.264987857520376
Acc = 0.8971537001897533+/-0.02141439996913226
=>=> NUMBER OF EPOCHS: 750
TP = 102.0+/-10.807404868885037
TN = 374.0 + / -8.508818954473059
FP = 17.2+/-7.413501197140255
FN = 33.8+/-8.795453370918407
Acc = 0.903225806451613+/-0.01636725514447651
TSS = 0.7061729414773706+/-0.06112246716757385
=>=> NUMBER OF EPOCHS: 1000
TP = 106.6 + / -8.957678270623477
TN = 374.2 + / -6.823488843692792
FN = 29.2+/-8.034923770640267
Acc = 0.9123339658444023+/-0.015104173618316782
TSS = 0.7412065195844594+/-0.05563907012564536
=>=> NUMBER OF EPOCHS: 1250
TP = 107.6+/-9.830564581955606
TN = 374.0 + / -8.17312669668102
FP = 17.2+/-6.523802572120037
FN = 28.2+/-9.064215354899728
Acc = 0.9138519924098671+/-0.01472759613808899
TSS = 0.7480812781748698+/-0.05916259940743479
=>=> NUMBER OF EPOCHS: 1500
TP = 108.0 + / -9.528903399657276
TN = 373.6 + / -9.58331884056875
FP = 17.6+/-7.578918128598566
FN = 27.8 + / -8.35224520712844
Acc = 0.9138519924098671+/-0.017985572085119996
TSS = 0.7497980298998852+/-0.0593857021319266
=>=> NUMBER OF EPOCHS: 1750
TP = 109.2+/-8.541662601625049
```

TN = 372.8 + / -8.840814442120138

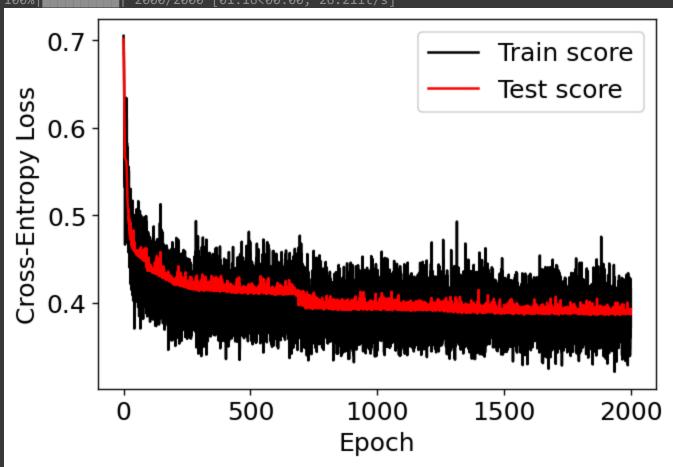
FN = 26.6 + / -7.337574531137657

Acc = 0.9146110056925997+/-0.01541563264636803 TSS = 0.7566956872257814+/-0.05054637616070908

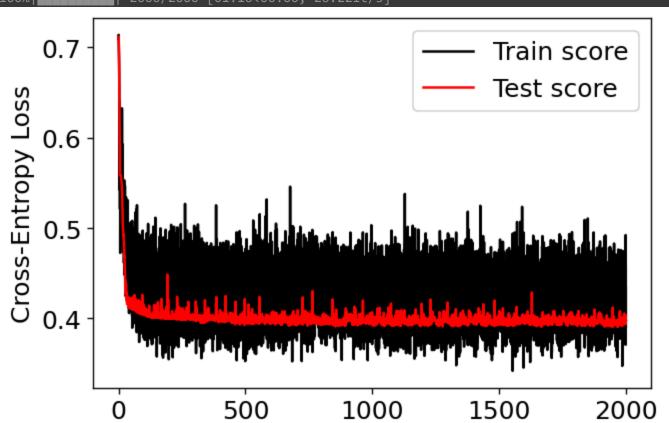
```
# NETWORK: VDFCNN_4040_CNN2_CONN2
ARCH = 'VDFCNN_4040_CNN2_CONN2'
tp = np.zeros([7,5], dtype=int)
tn = np.zeros([7,5], dtype=int)
fp = np.zeros([7,5], dtype=int)
fn = np.zeros([7,5], dtype=int)
acc = np.zeros([7,5], dtype=float)
tss = np.zeros([7,5], dtype=float)
for n_e, split_indexes in enumerate(data_split.split(labels_allmoments)):
 if (n_e >= 5): continue
 train_index, test_index = split_indexes
 X_train, X_test = featurevector_allvdfs_all_4040_aug[train_index], featurevector_allvdfs_all_4040_au
 f_train, f_test = labels_allmoments[train_index], labels_allmoments[test_index]
 while(True):
    # training the network
    device = torch.device("cuda:0")
    net = VDFCNN_4040_CNN2_CONN2().to(device)
    optimizer = optim.Adam(net.parameters(), lr=0.001, weight_decay=0.001)
    loss_history_train = []
    loss_history_test = []
    outputs_history_train = []
    outputs_labels_train = []
    outputs_history_test = []
    outputs_labels_test = []
    n_{epochs} = 2000
    n_iterations = 7 # based on the total size / batch size, approximately
    # test data tensors
    testdata_tensor = torch.tensor(X_test).float().to(device=device)
    testlabels_tensor = torch.tensor(f_test).long().to(device=device)
    for ep in tqdm(range(n_epochs)):
      for n_iter in range (n_iterations):
        train_indexes = np.random.choice(X_train.shape[0], size=128, replace=False)
        traindata_tensor = torch.tensor(X_train[train_indexes]).float().to(device=device)
        trainlabels_tensor = torch.tensor(f_train[train_indexes]).long().to(device=device)
        outputs = net(traindata_tensor)
        criteria = nn.CrossEntropyLoss()
        loss = criteria(outputs, trainlabels_tensor)
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
        loss_history_train.append(loss.item())
        outputs_history_train.append(outputs.detach())
        outputs_labels_train.append(f_train[train_indexes])
        outputs = net(testdata_tensor)
```

```
criteria = nn.CrossEntropyLoss()
       loss = criteria(outputs, testlabels_tensor)
       loss_history_test.append(loss.item())
       outputs_history_test.append(outputs.detach())
       outputs_labels_test.append(f_test)
   # visualizing the result
   matplotlib.rcParams.update({'font.size': 15})
   im, ax = plt.subplots(1, 1, figsize=(6,4), dpi=120)
   ax.plot(np.arange(n_epochs*n_iterations)/n_iterations, loss_history_train, color='black', label='
   ax.plot(np.arange(n_epochs*n_iterations)/n_iterations, loss_history_test, color='red', label='Test
   ax.set(xlabel='Epoch', ylabel='Cross-Entropy Loss')
   ax.legend()
   plt.show()
   # finding the optimum
   optim_indexes = np.arange(250,2000,250)*n_iterations
   oi = 6
   optim_index = optim_indexes[oi]
   outputs_optim = outputs_history_test[optim_index]
   labels_optim = np.argmax(outputs_optim.cpu(), axis=1)
   _tp, _tn, _fp, _fn, _acc, _tss = outputclass_analysis_scorereturn(f_test, labels_optim)
   if (_acc < 0.88):
     print("RERUNNING THE SAMPLE...")
     continue
   break
 for oi in range (0, 7, 1):
   optim_index = optim_indexes[oi]
   outputs_optim = outputs_history_test[optim_index]
   labels_optim = np.argmax(outputs_optim.cpu(), axis=1)
   tp[oi,n_e], tn[oi,n_e], fp[oi,n_e], fn[oi,n_e], acc[oi,n_e], tss[oi,n_e] = outputclass_analysis_s(
   print(oi*250+250,acc[oi,n_e], tss[oi,n_e])
 print('----')
# final results
print("ARCH = " + str(ARCH))
for oi in range (0, 7, 1):
 print("=>=>=> NUMBER OF EPOCHS:", oi*250+250)
 print("TP = " + str(np.mean(tp[oi,:])) + "+/-" + str(np.std(tp[oi,:])))
 print("TN = " + str(np.mean(tn[oi,:])) + "+/-" + str(np.std(tn[oi,:])))
 print("FP = " + str(np.mean(fp[oi,:])) + "+/-" + str(np.std(fp[oi,:])))
 print("FN = " + str(np.mean(fn[oi,:])) + "+/-" + str(np.std(fn[oi,:])))
 print("Acc = " + str(np.mean(acc[oi,:])) + "+/-" + str(np.std(acc[oi,:])))
```

print("TSS = " + str(np.mean(tss[oi,:])) + "+/-" + str(np.std(tss[oi,:])))

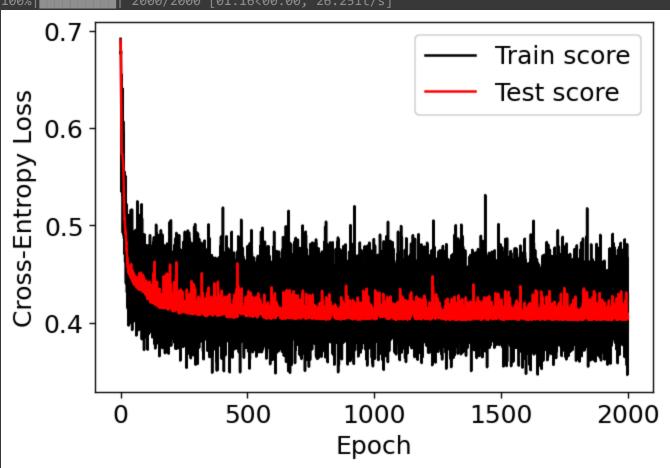


250 0.8956356736242884 0.7458493950612571
500 0.8994307400379506 0.7459448112667455
750 0.9127134724857685 0.743788405022709
1000 0.920303605313093 0.7838250448456165
1250 0.9222011385199241 0.7863631159116065
1500 0.9184060721062619 0.7763062478531353
1750 0.9278937381404174 0.793977329109576



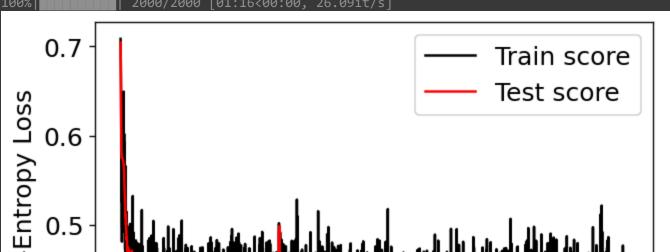
Epoch

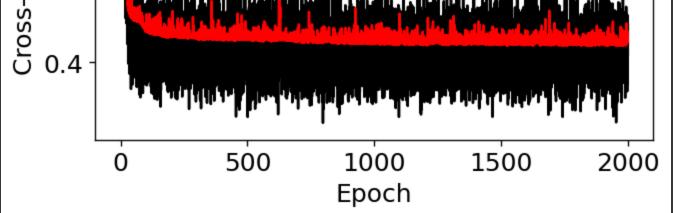
250 0.9108159392789373 0.6765008969123315 500 0.9146110056925996 0.6965192168237854 750 0.9127134724857685 0.6790389679783214 1000 0.9089184060721063 0.6938857295523071 1250 0.9184060721062619 0.6966146330292736 1500 0.9127134724857685 0.6890004198313041 1750 0.9184060721062619 0.6966146330292736



250 0.905123339658444 0.6679893198842988 500 0.9013282732447818 0.676685455759104 750 0.9070208728652751 0.6751835644886153 1000 0.905123339658444 0.6679893198842988 1250 0.9013282732447818 0.6536008306756655 1500 0.9127134724857685 0.6782985982348142 1750 0.8804554079696395 0.6483349402951865

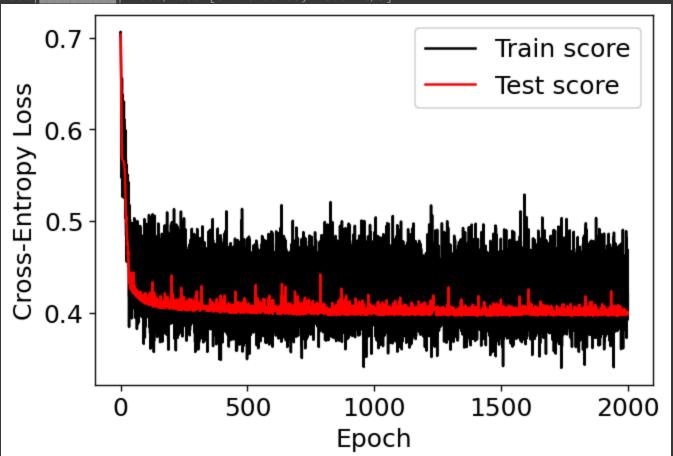
. | 180%| **| | 1808| | 1808**| | 2009/2000 | 101:16<00:00. 26.09it/s





250 0.8804554079696395 0.5864710225175341 500 0.889943074003795 0.62218530823182 750 0.8918406072106262 0.6293281653746771 1000 0.8823529411764706 0.6164082687338501 1250 0.8709677419354839 0.6009043927648579 1500 0.8918406072106262 0.6293281653746771 1750 0.8937381404174574 0.6319121447028424

100%|**| | 1000|| 1000||**| 2000/2000 [01:16<00:00, 26.07it/s



250 0.9013282732447818 0.6857126580836277 500 0.9108159392789373 0.6738445178686719 750 0.9127134724857685 0.6763890471307584 1000 0.9070208728652751 0.6736736166495766 1250 0.9070208728652751 0.6835099312597319 1500 0.9089184060721063 0.6860544605218184 1750 0.9146110056925996 0.6986062056131556

ARCH = VDFCNN_4040_CNN2_CONN2

=>=> NUMBER OF EPOCHS: 250

TP = 95.8+/-8.182909018191513

TN = 377.8 + / -8.634813257969162

FP = 13.4+/-9.871170143402454

```
FN = 40.0 + / -10.392304845413264
TSS = 0.6725046584918097+/-0.050974594375762135
=>=> NUMBER OF EPOCHS: 500
TP = 96.8 + / -6.675327707311453
TN = 379.2+/-8.304215796810679
FP = 12.0+/-8.717797887081348
Acc = 0.903225806451613 + (-0.008736899000547497)
TSS = 0.6830358619900254+/-0.03991725219853976
=>=> NUMBER OF EPOCHS: 750
TP = 95.2+/-5.192301994298868
FP = 8.2+/-5.075431016179809
FN = 40.6+/-6.887670143089026
=>=> NUMBER OF EPOCHS: 1000
TP = 97.2+/-7.11055553385247
TN = 379.6 + / -4.673328578219169
FP = 11.6+/-4.841487374764082
FN = 38.6+/-9.178235124467012
Acc = 0.9047438330170777+/-0.012379132015408044
=>=> NUMBER OF EPOCHS: 1250
TP = 96.8 + / -7.222188034107115
FP = 11.6+/-6.343500610861482
Acc = 0.9039848197343454+/-0.01814502176528566
TSS = 0.684198580728227+/-0.06077231096284698
=>=> NUMBER OF EPOCHS: 1500
TP = 97.0 + / -6.663332499583072
TN = 382.0 + / -4.857983120596447
FP = 9.2+/-5.912698199637792
FN = 38.8+/-8.726969691708572
Acc = 0.9089184060721063+/-0.009060596877657178
TSS = 0.6917975783631498+/-0.04747035441407377
=>=> NUMBER OF EPOCHS: 1750
TP = 98.0 + / -6.899275324264136
TN = 380.0 + / -8.19756061276768
```

FP = 11.2+/-6.734983296193095 FN = 37.8+/-8.795453370918409

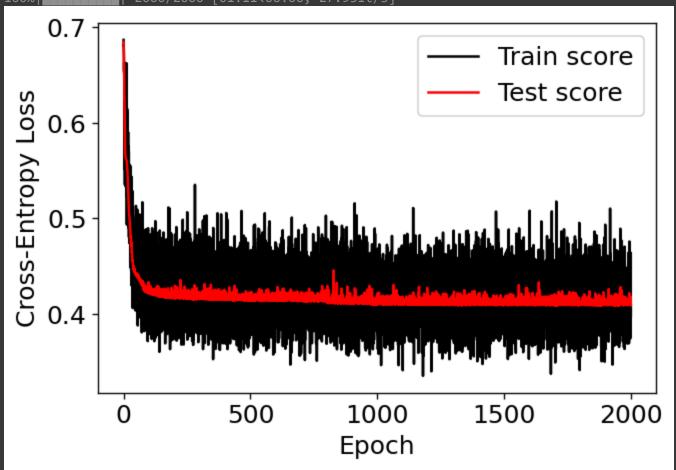
Acc = 0.9070208728652751+/-0.0173497221262428 TSS = 0.6938890505500068+/-0.056504261213213995

```
# NETWORK: VDFCNN_4040_CNN2_CONN1
ARCH = 'VDFCNN_4040_CNN2_CONN1'
tp = np.zeros([7,5], dtype=int)
tn = np.zeros([7,5], dtype=int)
fp = np.zeros([7,5], dtype=int)
fn = np.zeros([7,5], dtype=int)
acc = np.zeros([7,5], dtype=float)
tss = np.zeros([7,5], dtype=float)
for n_e, split_indexes in enumerate(data_split.split(labels_allmoments)):
 if (n_e >= 5): continue
 train_index, test_index = split_indexes
 X_train, X_test = featurevector_allvdfs_all_4040_aug[train_index], featurevector_allvdfs_all_4040_au
 f_train, f_test = labels_allmoments[train_index], labels_allmoments[test_index]
 while(True):
    # training the network
    device = torch.device("cuda:0")
    net = VDFCNN_4040_CNN2_CONN1().to(device)
    optimizer = optim.Adam(net.parameters(), lr=0.001, weight_decay=0.001)
    loss_history_train = []
    loss_history_test = []
    outputs_history_train = []
    outputs_labels_train = []
    outputs_history_test = []
    outputs_labels_test = []
    n_{epochs} = 2000
    n_iterations = 7 # based on the total size / batch size, approximately
    # test data tensors
    testdata_tensor = torch.tensor(X_test).float().to(device=device)
    testlabels_tensor = torch.tensor(f_test).long().to(device=device)
    for ep in tqdm(range(n_epochs)):
      for n_iter in range (n_iterations):
        train_indexes = np.random.choice(X_train.shape[0], size=128, replace=False)
        traindata_tensor = torch.tensor(X_train[train_indexes]).float().to(device=device)
        trainlabels_tensor = torch.tensor(f_train[train_indexes]).long().to(device=device)
        outputs = net(traindata_tensor)
        criteria = nn.CrossEntropyLoss()
        loss = criteria(outputs, trainlabels_tensor)
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
        loss_history_train.append(loss.item())
        outputs_history_train.append(outputs.detach())
        outputs_labels_train.append(f_train[train_indexes])
        outputs = net(testdata_tensor)
```

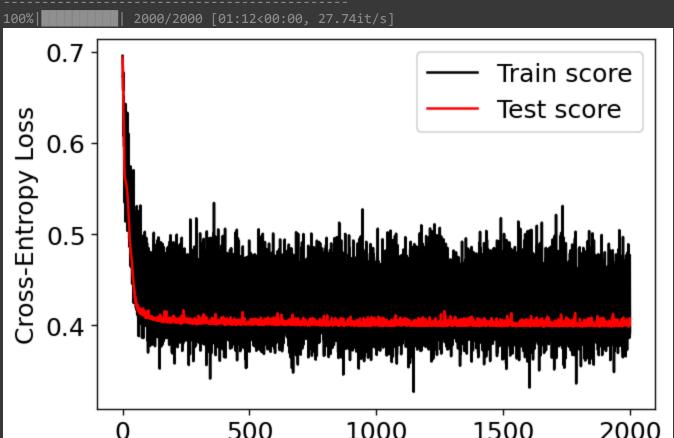
```
criteria = nn.CrossEntropyLoss()
       loss = criteria(outputs, testlabels_tensor)
       loss_history_test.append(loss.item())
       outputs_history_test.append(outputs.detach())
       outputs_labels_test.append(f_test)
   # visualizing the result
   matplotlib.rcParams.update({'font.size': 15})
   im, ax = plt.subplots(1, 1, figsize=(6,4), dpi=120)
   ax.plot(np.arange(n_epochs*n_iterations)/n_iterations, loss_history_train, color='black', label='
   ax.plot(np.arange(n_epochs*n_iterations)/n_iterations, loss_history_test, color='red', label='Test
   ax.set(xlabel='Epoch', ylabel='Cross-Entropy Loss')
   ax.legend()
   plt.show()
   # finding the optimum
   optim_indexes = np.arange(250,2000,250)*n_iterations
   oi = 6
   optim_index = optim_indexes[oi]
   outputs_optim = outputs_history_test[optim_index]
   labels_optim = np.argmax(outputs_optim.cpu(), axis=1)
   _tp, _tn, _fp, _fn, _acc, _tss = outputclass_analysis_scorereturn(f_test, labels_optim)
   if (_acc < 0.88):
     print("RERUNNING THE SAMPLE...")
     continue
   break
 for oi in range (0, 7, 1):
   optim_index = optim_indexes[oi]
   outputs_optim = outputs_history_test[optim_index]
   labels_optim = np.argmax(outputs_optim.cpu(), axis=1)
   tp[oi,n_e], tn[oi,n_e], fp[oi,n_e], fn[oi,n_e], acc[oi,n_e], tss[oi,n_e] = outputclass_analysis_s(
   print(oi*250+250,acc[oi,n_e], tss[oi,n_e])
 print('----')
# final results
print("ARCH = " + str(ARCH))
for oi in range (0, 7, 1):
 print("=>=>=> NUMBER OF EPOCHS:", oi*250+250)
 print("TP = " + str(np.mean(tp[oi,:])) + "+/-" + str(np.std(tp[oi,:])))
 print("TN = " + str(np.mean(tn[oi,:])) + "+/-" + str(np.std(tn[oi,:])))
 print("FP = " + str(np.mean(fp[oi,:])) + "+/-" + str(np.std(fp[oi,:])))
 print("FN = " + str(np.mean(fn[oi,:])) + "+/-" + str(np.std(fn[oi,:])))
 print("Acc = " + str(np.mean(acc[oi,:])) + "+/-" + str(np.std(acc[oi,:])))
```

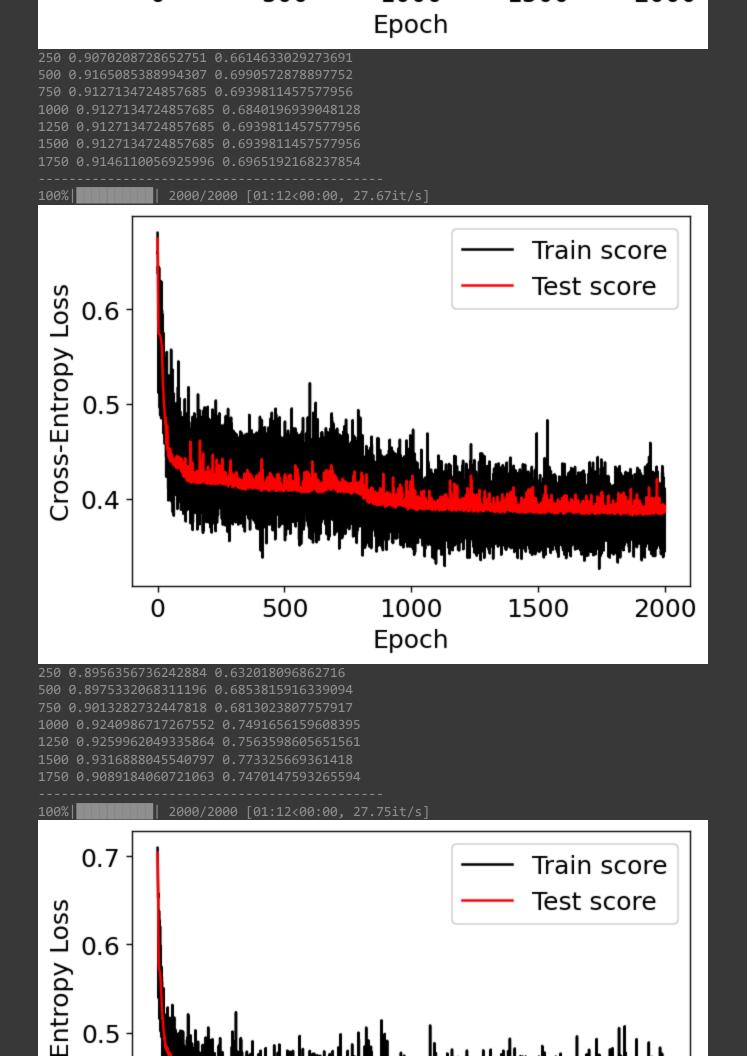
print("TSS = " + str(np.mean(tss[oi,:])) + "+/-" + str(np.std(tss[oi,:])))

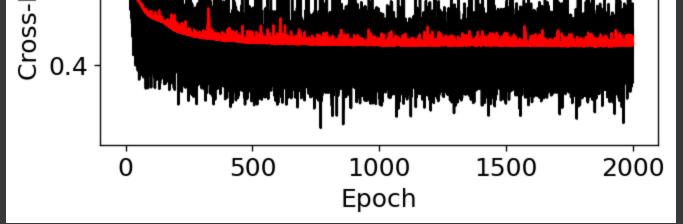




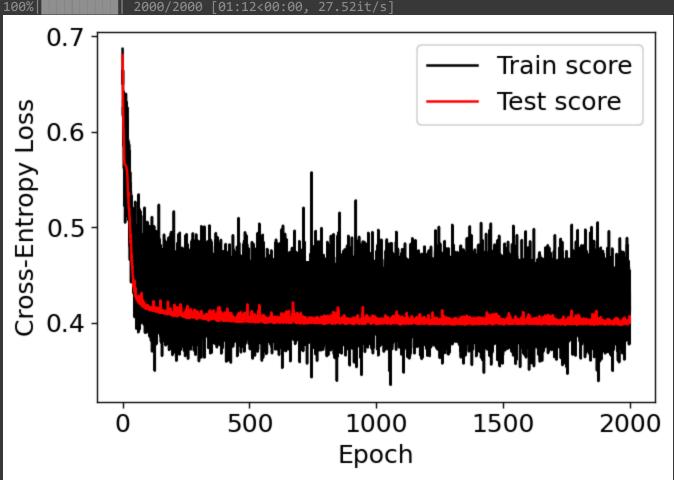
500 0.8956356736242884 0.6412541506049387 750 0.905123339658444 0.653944505934888 1000 0.8937381404174574 0.6486775313919316 1250 0.9070208728652751 0.6664440288538606 1500 0.905123339658444 0.6489637800083966







250 0.8861480075901328 0.6033407161314138 500 0.889943074003795 0.6267441860465116 750 0.8918406072106262 0.6293281653746771 1000 0.889943074003795 0.6267441860465116 1250 0.889943074003795 0.6176264304171281 1500 0.8937381404174574 0.6319121447028424 1750 0.889943074003795 0.6176264304171281



250 0.9032258064516129 0.6685845581254035 500 0.9146110056925996 0.6986062056131556 750 0.9165085388994307 0.6962325775701645 1000 0.9184060721062619 0.7086134214424062 1250 0.9108159392789373 0.6935171470889825 1500 0.9146110056925996 0.6838517336979226 1750 0.9108159392789373 0.6787626751737496

ARCH = VDFCNN_4040_CNN2_CONN1 =>=>=> NUMBER OF EPOCHS: 250 TP = 89.6+/-2.0591260281974

```
FP = 7.2+/-1.469693845669907
FN = 46.2 + / -4.308131845707603
Acc = 0.8986717267552182+/-0.007260389552071728
TSS = 0.6418588623846638+/-0.023165496276400854
=>=> NUMBER OF EPOCHS: 500
TP = 94.4+/-4.17612260356422
TN = 381.4 + / -5.782732917920384
FP = 9.8+/-3.54400902933387
FN = 41.4+/-4.454211490264018
Acc = 0.9028462998102466+/-0.010693740268391169
TSS = 0.6702086843576581+/-0.03031965003986837
=>=> NUMBER OF EPOCHS: 750
TP = 93.8 + / -3.4871191548325386
TN = 383.4 + / -4.963869458396343
FN = 42.0+/-4.049691346263317
Acc = 0.9055028462998103+/-0.008687304092796652
TSS = 0.6709577550826633+/-0.025684150118331542
=>=> NUMBER OF EPOCHS: 1000
TP = 95.8+/-6.013318551349163
TN = 382.6 + / -4.079215610874228
FP = 8.6+/-2.939387691339814
FN = 40.0+/-5.621387729022079
Acc = 0.9077798861480076+/-0.013556410701701521
TSS = 0.6834440897493004+/-0.04330528430923252
=>=> NUMBER OF EPOCHS: 1250
TP = 95.8+/-6.615134163416491
FP = 7.8+/-0.7483314773547882
FN = 40.0 + / -6.54217089351845
Acc = 0.9092979127134726+/-0.011598259423101448
TSS = 0.6855857225365846+/-0.04500497541961731
=>=> NUMBER OF EPOCHS: 1500
TN = 385.0 + / -3.847076812334269
FP = 6.2+/-1.469693845669907
Acc = 0.91157495256167+/-0.012448743428354215
TSS = 0.6864068947056751+/-0.04897026879758102
=>=> NUMBER OF EPOCHS: 1750
TP = 95.2+/-8.304215796810679
```

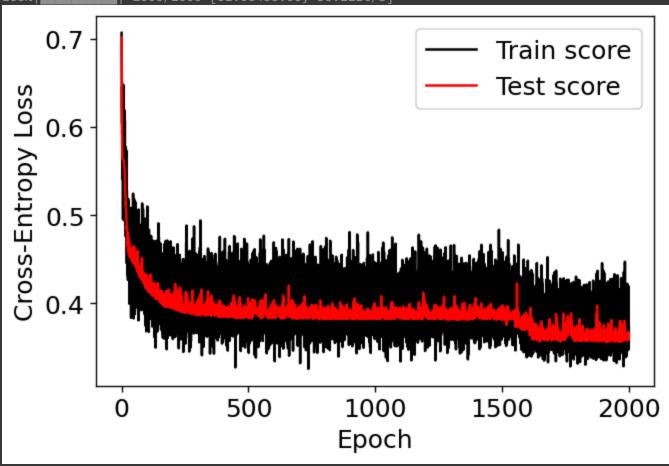
TN = 382.2+/-7.730459236035076 FP = 9.0+/-5.549774770204643 FN = 40.6+/-7.657675887630659

TSS = 0.6777773723499239+/-0.043805027634543775

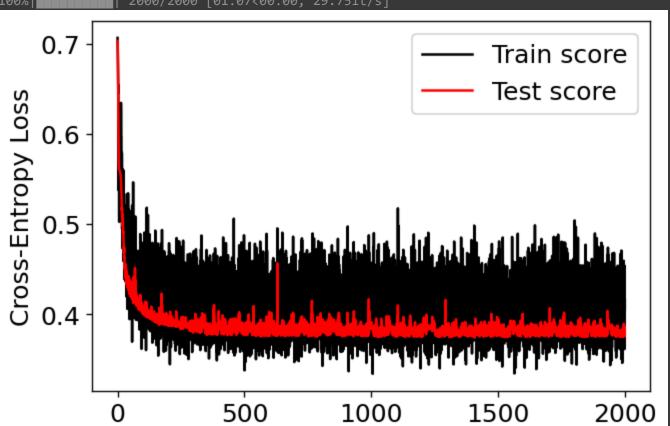
```
# NETWORK: VDFCNN_4040_CNN1_CONN2
ARCH = 'VDFCNN_4040_CNN1_CONN2'
tp = np.zeros([7,5], dtype=int)
tn = np.zeros([7,5], dtype=int)
fp = np.zeros([7,5], dtype=int)
fn = np.zeros([7,5], dtype=int)
acc = np.zeros([7,5], dtype=float)
tss = np.zeros([7,5], dtype=float)
for n_e, split_indexes in enumerate(data_split.split(labels_allmoments)):
 if (n_e >= 5): continue
 train_index, test_index = split_indexes
 X_train, X_test = featurevector_allvdfs_all_4040_aug[train_index], featurevector_allvdfs_all_4040_au
 f_train, f_test = labels_allmoments[train_index], labels_allmoments[test_index]
 while(True):
    # training the network
    device = torch.device("cuda:0")
    net = VDFCNN_4040_CNN1_CONN2().to(device)
    optimizer = optim.Adam(net.parameters(), lr=0.001, weight_decay=0.001)
    loss_history_train = []
    loss_history_test = []
    outputs_history_train = []
    outputs_labels_train = []
    outputs_history_test = []
    outputs_labels_test = []
    n_{epochs} = 2000
    n_iterations = 7 # based on the total size / batch size, approximately
    # test data tensors
    testdata_tensor = torch.tensor(X_test).float().to(device=device)
    testlabels_tensor = torch.tensor(f_test).long().to(device=device)
    for ep in tqdm(range(n_epochs)):
      for n_iter in range (n_iterations):
        train_indexes = np.random.choice(X_train.shape[0], size=128, replace=False)
        traindata_tensor = torch.tensor(X_train[train_indexes]).float().to(device=device)
        trainlabels_tensor = torch.tensor(f_train[train_indexes]).long().to(device=device)
        outputs = net(traindata_tensor)
        criteria = nn.CrossEntropyLoss()
        loss = criteria(outputs, trainlabels_tensor)
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
        loss_history_train.append(loss.item())
        outputs_history_train.append(outputs.detach())
        outputs_labels_train.append(f_train[train_indexes])
        outputs = net(testdata_tensor)
```

```
criteria = nn.CrossEntropyLoss()
       loss = criteria(outputs, testlabels_tensor)
       loss_history_test.append(loss.item())
       outputs_history_test.append(outputs.detach())
       outputs_labels_test.append(f_test)
   # visualizing the result
   matplotlib.rcParams.update({'font.size': 15})
   im, ax = plt.subplots(1, 1, figsize=(6,4), dpi=120)
   ax.plot(np.arange(n_epochs*n_iterations)/n_iterations, loss_history_train, color='black', label='
   ax.plot(np.arange(n_epochs*n_iterations)/n_iterations, loss_history_test, color='red', label='Test
   ax.set(xlabel='Epoch', ylabel='Cross-Entropy Loss')
   ax.legend()
   plt.show()
   # finding the optimum
   optim_indexes = np.arange(250,2000,250)*n_iterations
   oi = 6
   optim_index = optim_indexes[oi]
   outputs_optim = outputs_history_test[optim_index]
   labels_optim = np.argmax(outputs_optim.cpu(), axis=1)
   _tp, _tn, _fp, _fn, _acc, _tss = outputclass_analysis_scorereturn(f_test, labels_optim)
   if (_acc < 0.88):
     print("RERUNNING THE SAMPLE...")
     continue
   break
 for oi in range (0, 7, 1):
   optim_index = optim_indexes[oi]
   outputs_optim = outputs_history_test[optim_index]
   labels_optim = np.argmax(outputs_optim.cpu(), axis=1)
   tp[oi,n_e], tn[oi,n_e], fp[oi,n_e], fn[oi,n_e], acc[oi,n_e], tss[oi,n_e] = outputclass_analysis_s(
   print(oi*250+250,acc[oi,n_e], tss[oi,n_e])
 print('----')
# final results
print("ARCH = " + str(ARCH))
for oi in range (0, 7, 1):
 print("=>=>=> NUMBER OF EPOCHS:", oi*250+250)
 print("TP = " + str(np.mean(tp[oi,:])) + "+/-" + str(np.std(tp[oi,:])))
 print("TN = " + str(np.mean(tn[oi,:])) + "+/-" + str(np.std(tn[oi,:])))
 print("FP = " + str(np.mean(fp[oi,:])) + "+/-" + str(np.std(fp[oi,:])))
 print("FN = " + str(np.mean(fn[oi,:])) + "+/-" + str(np.std(fn[oi,:])))
 print("Acc = " + str(np.mean(acc[oi,:])) + "+/-" + str(np.std(acc[oi,:])))
```

print("TSS = " + str(np.mean(tss[oi,:])) + "+/-" + str(np.std(tss[oi,:])))

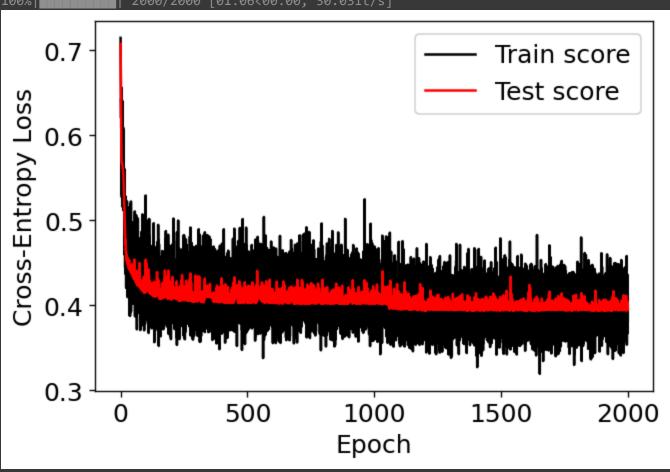


250 0.9259962049335864 0.7366512728521811
500 0.9316888045540797 0.7492462119766421
750 0.920303605313093 0.748959963360177
1000 0.920303605313093 0.7539406892866685
1250 0.9278937381404174 0.7541315216976452
1500 0.9240986717267552 0.7590168314186482
1750 0.9506641366223909 0.8343956337544368



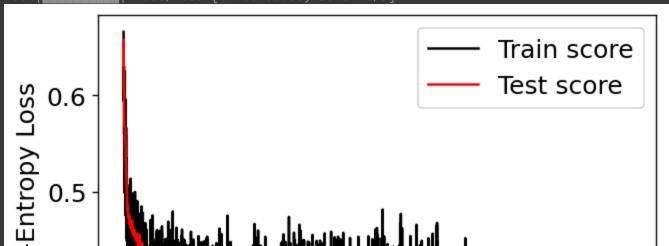
Epoch

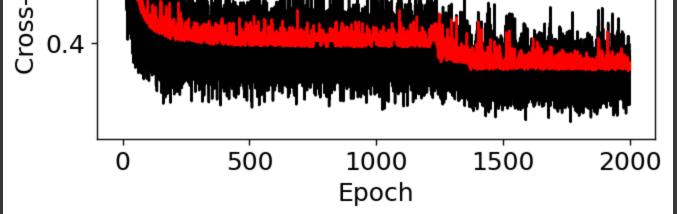
250 0.9278937381404174 0.7690736994771191 500 0.9316888045540797 0.7691691156826076 750 0.937381404174573 0.7668218770275944 1000 0.9278937381404174 0.7541315216976452 1250 0.9297912713472486 0.7765924964696004 1500 0.9335863377609108 0.7766879126750887 1750 0.9335863377609108 0.7766879126750887



250 0.9032258064516129 0.6654120002966698 500 0.9108159392789373 0.6803382036638731 750 0.9108159392789373 0.6711043536304977 1000 0.9127134724857685 0.696766298301565 1250 0.920303605313093 0.7116925016687681 1500 0.9127134724857685 0.7013832233182525 1750 0.9222011385199241 0.7235036712897723

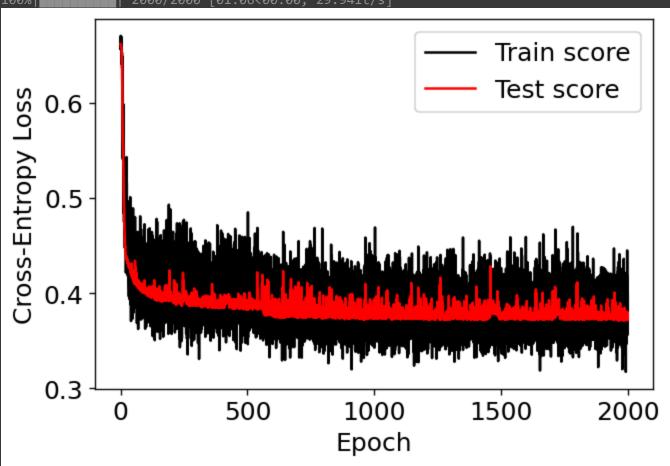






250 0.8956356736242884 0.7119970468807678 500 0.9184060721062619 0.7247692875599853 750 0.9184060721062619 0.7247692875599853 1250 0.9013282732447818 0.6513658176448874 1500 0.9392789373814042 0.8124584717607973 1750 0.9240986717267552 0.7917866371354744

29.94it/s]



250 0.9165085388994307 0.730659678705708 500 0.9278937381404174 0.7557631688883826 750 0.9222011385199241 0.718620637271657 1000 0.937381404174573 0.7930766017242035 1250 0.9392789373814042 0.79562113098629 1500 0.9392789373814042 0.7857848163761346

ARCH = VDFCNN_4040_CNN1_CONN2

=>=> NUMBER OF EPOCHS: 250

TP = 102.2+/-4.578209256903839

TN = 379.4 + / -8.114185110040317

FP = 11.8+/-6.046486583132389

```
FN = 33.6 + / -5.607138307550474
Acc = 0.9138519924098671+/-0.012621092332687586
TSS = 0.7227587396424893 + (-0.03407334843023653)
=>=> NUMBER OF EPOCHS: 500
TN = 385.0 + / -3.22490309931942
FP = 6.2+/-1.8330302779823362
Acc = 0.9240986717267552+/-0.008227507927392323
TSS = 0.7358571975542981+/-0.031274583041151334
=>=> NUMBER OF EPOCHS: 750
TP = 100.6+/-3.97994974842648
TN = 385.2 + / -4.166533331199931
FP = 6.0+/-3.8987177379235853
FN = 35.2 + / -5.706137047074842
Acc = 0.9218216318785579 + (-0.008687304092796666)
TSS = 0.7260552237699823+/-0.03244401932851345
=>=> NUMBER OF EPOCHS: 1000
TN = 381.4 + / -4.2708313008125245
FP = 9.8+/-3.1240998703626617
Acc = 0.9218216318785577+/-0.009852565454077552
=>=> NUMBER OF EPOCHS: 1250
TN = 384.4 + / -1.624807680927192
FP = 6.8+/-2.7129319932501077
FN = 33.4 + / -8.404760555780276
Acc = 0.9237191650853889+/-0.012723381111377769
TSS = 0.7378806936934382+/-0.05151173917271604
=>=> NUMBER OF EPOCHS: 1500
TP = 107.0 + / -5.549774770204643
TN = 383.0 + / -3.5777087639996634
FP = 8.2+/-2.315167380558045
FN = 28.8+/-5.3814496188294845
Acc = 0.9297912713472487+/-0.010183231776090143
TSS = 0.7670662511097843+/-0.03710112680166281
=>=> NUMBER OF EPOCHS: 1750
TP = 110.0+/-5.329165037789691
```

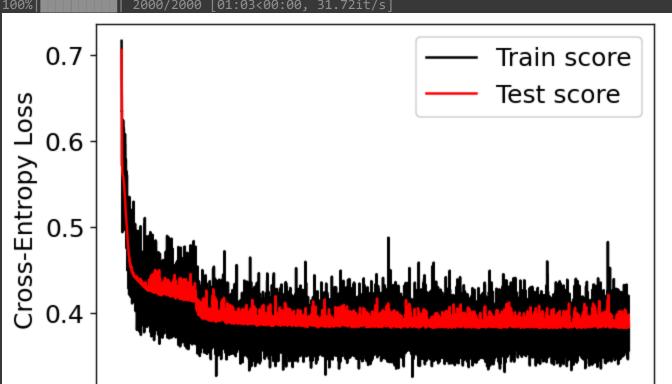
FP = 9.0+/-4.47213595499958 FN = 25.8+/-6.046486583132389

Acc = 0.933965844402277+/-0.010420895800945722 TSS = 0.787349891551259+/-0.03729125256476849

```
# NETWORK: VDFCNN_4040_CNN1_CONN1
ARCH = 'VDFCNN_4040_CNN1_CONN1'
tp = np.zeros([7,5], dtype=int)
tn = np.zeros([7,5], dtype=int)
fp = np.zeros([7,5], dtype=int)
fn = np.zeros([7,5], dtype=int)
acc = np.zeros([7,5], dtype=float)
tss = np.zeros([7,5], dtype=float)
for n_e, split_indexes in enumerate(data_split.split(labels_allmoments)):
 if (n_e >= 5): continue
 train_index, test_index = split_indexes
 X_train, X_test = featurevector_allvdfs_all_4040_aug[train_index], featurevector_allvdfs_all_4040_au
 f_train, f_test = labels_allmoments[train_index], labels_allmoments[test_index]
 while(True):
    # training the network
    device = torch.device("cuda:0")
    net = VDFCNN_4040_CNN1_CONN1().to(device)
    optimizer = optim.Adam(net.parameters(), lr=0.001, weight_decay=0.001)
    loss_history_train = []
    loss_history_test = []
    outputs_history_train = []
    outputs_labels_train = []
    outputs_history_test = []
    outputs_labels_test = []
    n_{epochs} = 2000
    n_iterations = 7 # based on the total size / batch size, approximately
    # test data tensors
    testdata_tensor = torch.tensor(X_test).float().to(device=device)
    testlabels_tensor = torch.tensor(f_test).long().to(device=device)
    for ep in tqdm(range(n_epochs)):
      for n_iter in range (n_iterations):
        train_indexes = np.random.choice(X_train.shape[0], size=128, replace=False)
        traindata_tensor = torch.tensor(X_train[train_indexes]).float().to(device=device)
        trainlabels_tensor = torch.tensor(f_train[train_indexes]).long().to(device=device)
        outputs = net(traindata_tensor)
        criteria = nn.CrossEntropyLoss()
        loss = criteria(outputs, trainlabels_tensor)
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
        loss_history_train.append(loss.item())
        outputs_history_train.append(outputs.detach())
        outputs_labels_train.append(f_train[train_indexes])
        outputs = net(testdata_tensor)
```

```
criteria = nn.CrossEntropyLoss()
       loss = criteria(outputs, testlabels_tensor)
       loss_history_test.append(loss.item())
       outputs_history_test.append(outputs.detach())
       outputs_labels_test.append(f_test)
   # visualizing the result
   matplotlib.rcParams.update({'font.size': 15})
   im, ax = plt.subplots(1, 1, figsize=(6,4), dpi=120)
   ax.plot(np.arange(n_epochs*n_iterations)/n_iterations, loss_history_train, color='black', label='
   ax.plot(np.arange(n_epochs*n_iterations)/n_iterations, loss_history_test, color='red', label='Test
   ax.set(xlabel='Epoch', ylabel='Cross-Entropy Loss')
   ax.legend()
   plt.show()
   # finding the optimum
   optim_indexes = np.arange(250,2000,250)*n_iterations
   oi = 6
   optim_index = optim_indexes[oi]
   outputs_optim = outputs_history_test[optim_index]
   labels_optim = np.argmax(outputs_optim.cpu(), axis=1)
   _tp, _tn, _fp, _fn, _acc, _tss = outputclass_analysis_scorereturn(f_test, labels_optim)
   if (_acc < 0.88):
     print("RERUNNING THE SAMPLE...")
     continue
   break
 for oi in range (0, 7, 1):
   optim_index = optim_indexes[oi]
   outputs_optim = outputs_history_test[optim_index]
   labels_optim = np.argmax(outputs_optim.cpu(), axis=1)
   tp[oi,n_e], tn[oi,n_e], fp[oi,n_e], fn[oi,n_e], acc[oi,n_e], tss[oi,n_e] = outputclass_analysis_s(
   print(oi*250+250,acc[oi,n_e], tss[oi,n_e])
 print('----')
# final results
print("ARCH = " + str(ARCH))
for oi in range (0, 7, 1):
 print("=>=>=> NUMBER OF EPOCHS:", oi*250+250)
 print("TP = " + str(np.mean(tp[oi,:])) + "+/-" + str(np.std(tp[oi,:])))
 print("TN = " + str(np.mean(tn[oi,:])) + "+/-" + str(np.std(tn[oi,:])))
 print("FP = " + str(np.mean(fp[oi,:])) + "+/-" + str(np.std(fp[oi,:])))
 print("FN = " + str(np.mean(fn[oi,:])) + "+/-" + str(np.std(fn[oi,:])))
 print("Acc = " + str(np.mean(acc[oi,:])) + "+/-" + str(np.std(acc[oi,:])))
```

print("TSS = " + str(np.mean(tss[oi,:])) + "+/-" + str(np.std(tss[oi,:])))



1000

Epoch

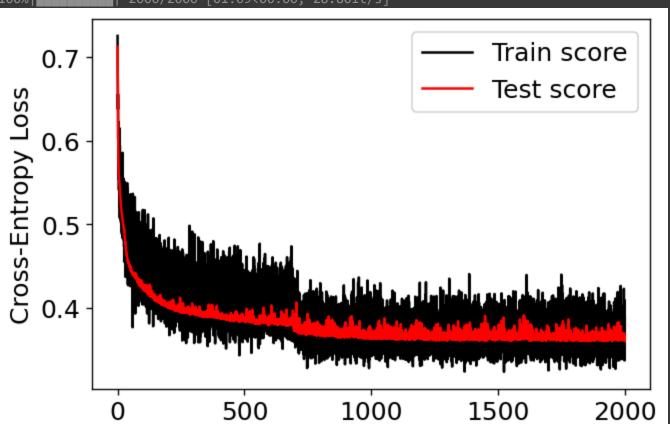
1500

2000

500 0.9297912713472486 0.756669592763635 750 0.9316888045540797 0.7592076638296248 1000 0.9278937381404174 0.7342086179916797 1250 0.9146110056925996 0.7513072020151902 1500 0.9165085388994307 0.7389030953017061

0

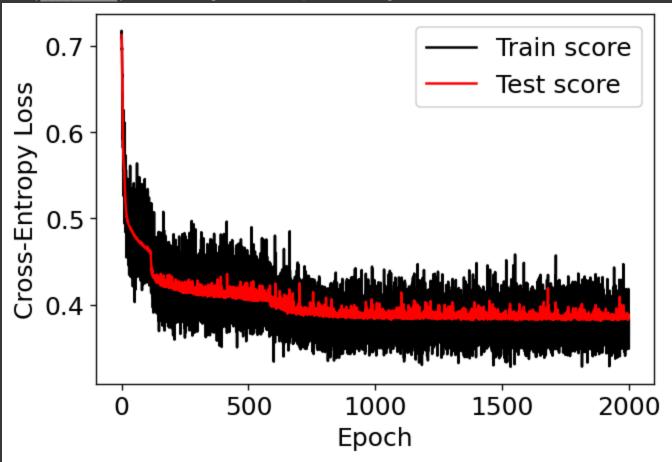
500



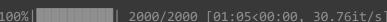
Epoch

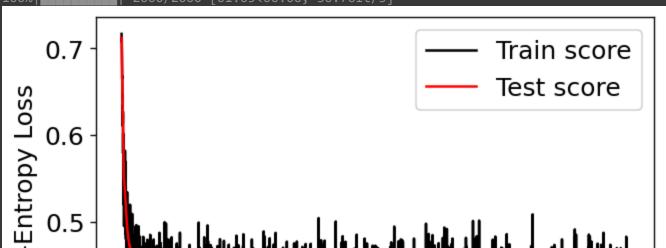
250 0.9184060721062619 0.7165375367352391 500 0.9335863377609108 0.7766879126750887 750 0.9449715370018975 0.7968970649975192 1000 0.9430740037950665 0.8541277050494256 1250 0.9506641366223909 0.8742414411663677 1500 0.9544592030360531 0.8643754055188733 1750 0.9487666034155597 0.8617419182473951

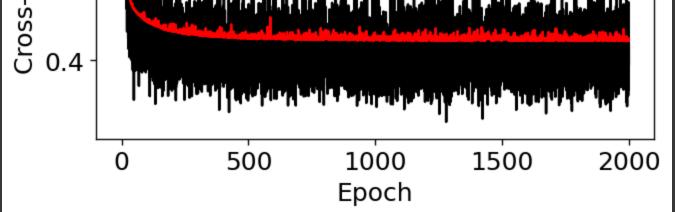
100%|**| | 100%| | 100%**| 2000/2000 [01:05<00:00, 30.46it/s]



250 0.8994307400379506 0.6787250611881629 500 0.9070208728652751 0.707502039605429 750 0.937381404174573 0.7810576281243047 1000 0.9259962049335864 0.7609767855818438 1250 0.9316888045540797 0.773325669361418 1500 0.9354838709677419 0.7877141585700511 1750 0.9354838709677419 0.7969480086034265

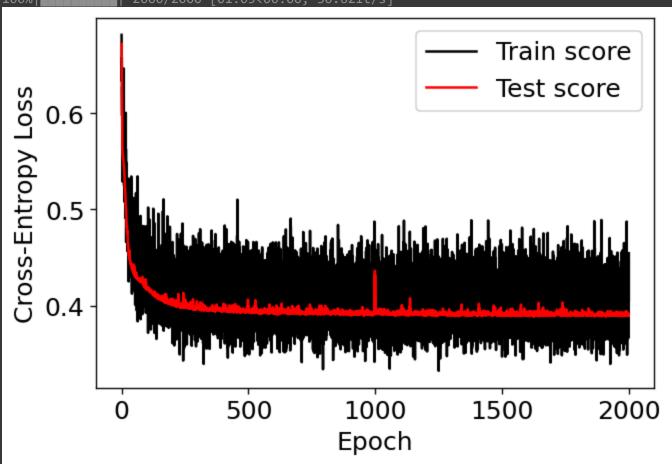






250 0.889943074003795 0.62218530823182 500 0.888045540796964 0.628719084533038 750 0.8918406072106262 0.6384459210040605 1000 0.889943074003795 0.6176264304171281 1250 0.9013282732447818 0.6468069398301957 1500 0.9013282732447818 0.6513658176448874 1750 0.8937381404174574 0.6364710225175342

100%|**| | 100%|| 100%**| 2000/2000 [01:05<00:00, 30.62it/s



250 0.9070208728652751 0.6589191447343437 500 0.920303605313093 0.7259124226197259 750 0.9184060721062619 0.7233678933576393 1000 0.9184060721062619 0.7577949944931829 1250 0.9259962049335864 0.7483004823212184 1500 0.9297912713472486 0.7484713835403137 1750 0.9297912713472486 0.7484713835403137

ARCH = VDFCNN_4040_CNN1_CONN1

=>=> NUMBER OF EPOCHS: 250

TP = 94.4+/-3.826225293941798

TN = 379.2 + / -7.30479294709987

FP = 12.0+/-7.4565407529228995

```
Acc = 0.8986717267552182 + (-0.013714847058514366)
TSS = 0.6649325834919088+/-0.031602452366995874
=>=> NUMBER OF EPOCHS: 500
TP = 100.8+/-4.791659420284375
TN = 381.8+/-5.192301994298868
FP = 9.4+/-2.244994432064365
Acc = 0.9157495256166983+/-0.016611816795627548
TSS = 0.7190982104393834+/-0.05114190774422929
=>=> NUMBER OF EPOCHS: 750
TP = 102.6+/-5.885575587824865
FP = 6.4 + / -2.727636339397171
FN = 33.2 + / -7.359347797189639
Acc = 0.9248576850094878+/-0.01865382273615863
TSS = 0.7397952342626297+/-0.05635882800299856
=>=> NUMBER OF EPOCHS: 1000
TN = 380.8 + / -4.707440918375927
FP = 10.4+/-4.841487374764082
FN = 31.2+/-11.9565881421081
Acc = 0.9210626185958255+/-0.017498507602882
TSS = 0.7449469067066521+/-0.07572092396478855
=>=> NUMBER OF EPOCHS: 1250
FP = 10.2+/-5.075431016179809
FN = 29.4 + / -11.46472851837321
Acc = 0.9248576850094876+/-0.01656840983145584
TSS = 0.7587963469388781+/-0.0724521204128168
=>=> NUMBER OF EPOCHS: 1500
TP = 105.6 + / -8.63944442658207
TN = 383.2 + / -2.9257477676655586
FP = 8.0+/-3.3466401061363023
FN = 30.2 + / -10.264501936285072
Acc = 0.9275142314990512 + (-0.017897269256245293)
=>=> NUMBER OF EPOCHS: 1750
```

TP = 106.2+/-9.47417542586161 TN = 382.8+/-3.919183588453085 FP = 8.4+/-2.65329983228432 FN = 29.6+/-11.038115781237304

Acc = 0.9278937381404175+/-0.018318813489407434 TSS = 0.7615641445329572+/-0.07363993537735601

Best Network Architecture

CONCLUSION:

Best network configuration: VDFCNN_4040_CNN1_CONN2 with 1750 epochs

Running for the best configuration now...

```
# NETWORK: VDFCNN_4040_CNN1_CONN2
ARCH = 'VDFCNN 4040 CNN1 CONN2'
tp = np.zeros([10], dtype=int)
tn = np.zeros([10], dtype=int)
fp = np.zeros([10], dtype=int)
fn = np.zeros([10], dtype=int)
acc = np.zeros([10], dtype=float)
tss = np.zeros([10], dtype=float)
for n_e, split_indexes in enumerate(data_split.split(labels_allmoments)):
 train_index, test_index = split_indexes
 X train, X test = featurevector allvdfs all 4040 aug[train index], featurevector allvdfs all 4040 au
 f_train, f_test = labels_allmoments[train_index], labels_allmoments[test_index]
 while(True):
    # training the network
    device = torch.device("cuda:0")
    net = VDFCNN_4040_CNN1_CONN2().to(device)
    optimizer = optim.Adam(net.parameters(), lr=0.001, weight_decay=0.001)
    loss_history_train = []
    loss_history_test = []
    outputs_history_train = []
    outputs_labels_train = []
    outputs_history_test = []
    outputs_labels_test = []
    n = 1750
    n_iterations = 7 # based on the total size / batch size, approximately
    # test data tensors
    testdata_tensor = torch.tensor(X_test).float().to(device=device)
    testlabels_tensor = torch.tensor(f_test).long().to(device=device)
    for ep in tqdm(range(n_epochs)):
      for n_iter in range (n_iterations):
        train_indexes = np.random.choice(X_train.shape[0], size=128, replace=False)
        traindata_tensor = torch.tensor(X_train[train_indexes]).float().to(device=device)
        trainlabels_tensor = torch.tensor(f_train[train_indexes]).long().to(device=device)
        outputs = net(traindata_tensor)
```

```
criteria = nn.CrossEntropyLoss()
       loss = criteria(outputs, trainlabels_tensor)
       optimizer.zero_grad()
       loss.backward()
       optimizer.step()
       loss_history_train.append(loss.item())
       outputs_history_train.append(outputs.detach())
       outputs_labels_train.append(f_train[train_indexes])
       outputs = net(testdata_tensor)
       criteria = nn.CrossEntropyLoss()
       loss = criteria(outputs, testlabels_tensor)
       loss_history_test.append(loss.item())
       outputs_history_test.append(outputs.detach())
       outputs_labels_test.append(f_test)
   # visualizing the result
   matplotlib.rcParams.update({'font.size': 15})
   im, ax = plt.subplots(1, 1, figsize=(6,4), dpi=120)
   ax.plot(np.arange(n_epochs*n_iterations)/n_iterations, loss_history_train, color='black', label='
   ax.plot(np.arange(n_epochs*n_iterations)/n_iterations, loss_history_test, color='red', label='Test
   ax.set(xlabel='Epoch', ylabel='Cross-Entropy Loss')
   ax.legend()
   plt.show()
   # finding the optimum
   optim_index = -1
   outputs_optim = outputs_history_test[optim_index]
   labels_optim = np.argmax(outputs_optim.cpu(), axis=1)
   _tp, _tn, _fp, _fn, _acc, _tss = outputclass_analysis_scorereturn(f_test, labels_optim)
   print(_acc, optim_index)
   if (_acc < 0.88):
     print("RERUNNING THE SAMPLE...")
     continue
   break
 tp[n_e], tn[n_e], fp[n_e], fn[n_e], acc[n_e], tss[n_e] = outputclass_analysis_scorereturn(f_test, 1
 print(acc[n_e], tss[n_e])
 print('----')
# final results
print("ARCH = " + str(ARCH))
print("TP = " + str(np.mean(tp)) + "+/-" + str(np.std(tp)))
print("TN = " + str(np.mean(tn)) + "+/-" + str(np.std(tn)))
print("FP = " + str(np.mean(fp)) + "+/-" + str(np.std(fp)))
print("FN = " + str(np.mean(fn)) + "+/-" + str(np.std(fn)))
print("Acc = " + str(np.mean(acc)) + "+/-" + str(np.std(acc)))
print("TSS = " + str(np.mean(tss)) + "+/-" + str(np.std(tss)))
```