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SDA PH4515 Week 8 Discussion Notes

From 2016 Exam Q5, averaging measurements

$$y_i \sim \text{Gauss}(\lambda, \sigma_i) \qquad i = 1, 2$$

↳ indep. { param to be measured.

a) Likelihood function

$$L(\lambda) = \prod_{i=1}^{2} \frac{1}{\sqrt{2\pi}\,\sigma_i} e^{-(y_i - \lambda)^2 / 2\sigma_i^2}$$

$$\Rightarrow \ln L(\lambda) = -\frac{1}{2} \sum_{i=1}^{2} \frac{(y_i - \lambda)^2}{\sigma_i^2} + C$$

$$\Rightarrow \text{minimize} \quad \chi^2(\lambda) = \sum_{i=1}^{2} \frac{(y_i - \lambda)^2}{\sigma_i^2}$$

b) $$\frac{\partial \chi^2}{\partial \lambda} = -\frac{2(y_1 - \lambda)}{\sigma_1^2} - \frac{2(y_2 - \lambda)}{\sigma_2^2} \overset{\text{set}}{=} 0$$

$$\Rightarrow \hat{\lambda} = \frac{y_1/\sigma_1^2 + y_2/\sigma_2^2}{\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}}$$

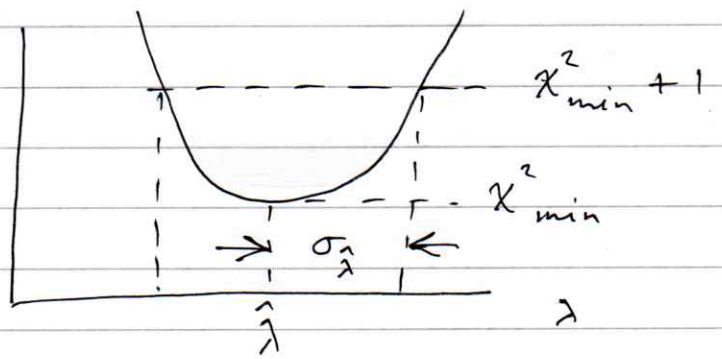
$$= \underbrace{\frac{\sigma_2^2}{\sigma_1^2 + \sigma_2^2}}_{w} y_1 + \underbrace{\frac{\sigma_1^2}{\sigma_1^2 + \sigma_2^2}}_{1 - w} y_2$$

c) $$E[\hat{\lambda}] = \frac{\frac{E[y_1]}{\sigma_1^2} + \frac{E[y_2]}{\sigma_2^2}}{\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}}$$, use $E[y_i] = \lambda$ $i = 1, 2$

$= \lambda \Rightarrow \hat{\lambda}$ is unbiased.

$$V[\hat{\lambda}] = \frac{1}{\left(\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}\right)^2}\left(\frac{V[y_1]}{\sigma_1^4} + \frac{V[y_2]}{\sigma_2^4}\right) = \frac{1}{\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}}$$ ($V[y_1] \to \sigma_1^2$, $V[y_2] \to \sigma_2^2$)

d)



$$p = \int_{\chi^2_{min}}^{\infty} f_{\chi^2}(t; n_d = 1)\, dt$$

↑ 2 measurements − 1 fitted param.

e) Suppose $\hat{\lambda} = w y_1 + (1-w) y_2$ for some w

= most general linear unbiased λ

$$E[\hat{\lambda}] = w E[y_1] + (1-w) E[y_2] = \lambda \Rightarrow \text{unbiased}$$ ✓

($E[y_1] \to \lambda$, $E[y_2] \to \lambda$)

$V[\hat{\lambda}] = w^2 \sigma_1^2 + (1-w)^2 \sigma_2^2$ ← adjust w to minimize

$$\frac{\partial V[\hat{\lambda}]}{\partial w} = 2w\sigma_1^2 - 2(1-w)\sigma_2^2 \overset{\text{set}}{=} 0$$

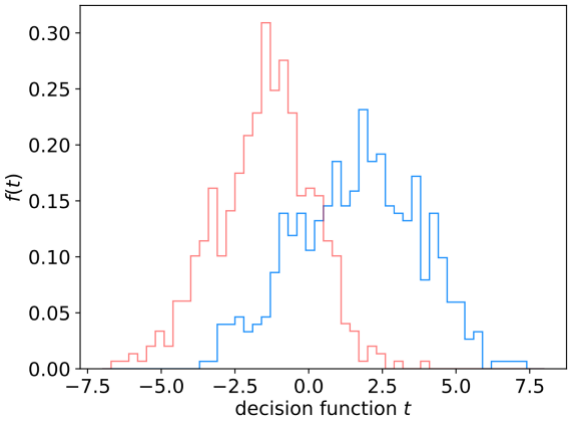
$$\Rightarrow w = \frac{\sigma_2^2}{\sigma_1^2 + \sigma_2^2} \Rightarrow \text{same as LS!}$$

$\hat{\lambda}$ = "BLUE" (Best Linear Unbiased Estimator)

G. Cowan / RHUL Physics
PH4515 Problem Sheet 5 (2023)

The complete code listings are given after the exercises.

Question 1, python version: For the linear discriminant, the program as given already produced the following distribution for the decision function (not necessary to submit):



1(a) [5 marks] To calculate the background efficiency (size of the test), add

```
size = 1. - metrics.accuracy_score(y_bkg_test, y_bkg_pred)
print('size of test of background = ', size)
```

1(b) [3 marks] To calculate the purity, use

$$\text{signal purity} = P(s|t > t_c) = \frac{P(t > t_c|s)\pi_s}{P(t > t_c|s)\pi_s + P(t > t_c|b)\pi_b}$$

with prior probabilities $\pi_s = \pi_b = 0.5$. To get this, add

```
purity = effSig*piSig / (effSig*piSig + effBkg*piBkg)
```

where

$$\texttt{effSig} = \varepsilon_s = P(t > t_c|s),$$
$$\texttt{effBkg} = \varepsilon_s = P(t > t_c|b).$$

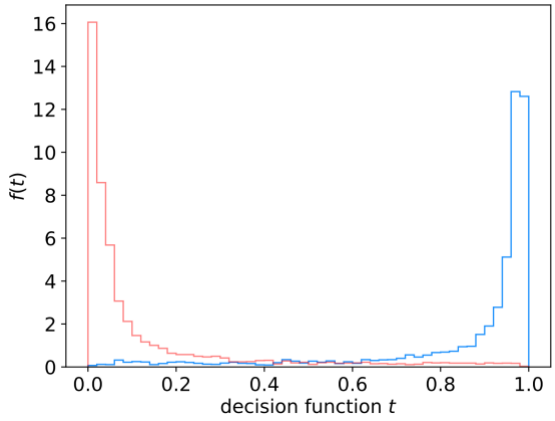
Combined with the existing code to find the test's power, the output for the LDA was:

```
power of test with respect to signal    = 0.7916666666666666
size of test of background              = 0.2338709677419355
purity of signal sample                 = 0.7719528178243775
```

1(c) [8 marks] To include a multilayer perceptron with 3 hidden layers in a single node, the classifier was created using

```
clf = MLPClassifier(hidden_layer_sizes=(3,), activation='tanh',
                    max_iter=2000, random_state=0)
```

The histogram of the MLP output (as given by predict_proba) is shown below:



1(d) [4 marks] To select events with the MLP, the function predict_proba is used instead of the decision function. As in (b), to find the purity, use the efficiencies in Bayes' theorem:

Signal efficiency = $\varepsilon_s = P(t>t_c|s)$
Background efficiency = $\varepsilon_b = P(t>t_c|b)$
Signal purity = $P(s|t>t_c) = \varepsilon_s\pi_s/(\varepsilon_s\pi_s + \varepsilon_b\pi_b)$

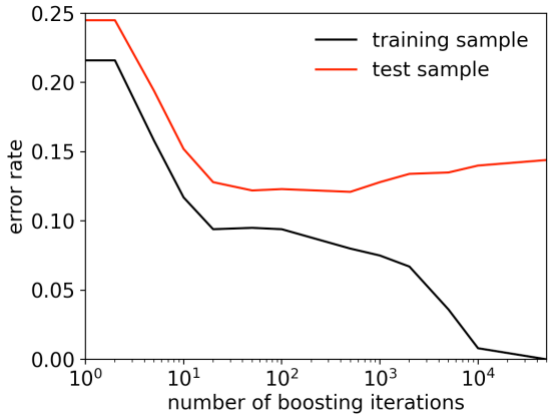
By defining the critical region with a minimum threshold on its value of 0.5, the program produced the following output:

power of test with respect to signal = 0.876984126984127

size of test of background = 0.11290322580645162

purity of signal sample = 0.8859433596275701

Exercise 2 [bonus]: The total error rate of a BDT (using AdaBoost) as a function of the number of boosting iterations is shown below. As can be seen in the figure, the error rate from the training sample goes to zero after around 10^4 iterations. For the test sample, a minimum error rate of 12.1% is found at 500 iterations, with a shallow minimum around 12% from 10^2 to 10^3 iterations. For more than 10^3 iterations the error rate increases slowly.



Appendix – Python code listing

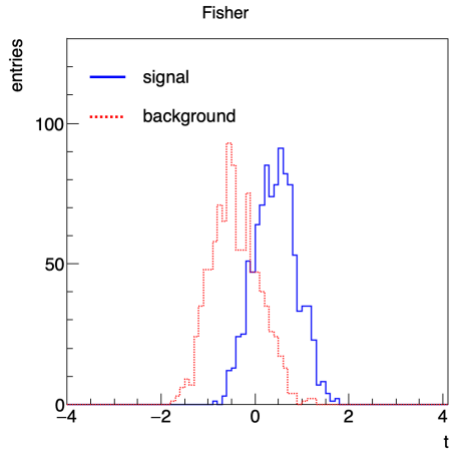
```
#  simpleClassifier_solution.py
#  G. Cowan / RHUL Physics / November 2021
#  Simple program to illustrate classification with scikit-learn

import scipy as sp
import numpy as np
import matplotlib
import matplotlib.pyplot as plt
import matplotlib.ticker as ticker

from sklearn.discriminant_analysis import LinearDiscriminantAnalysis as LDA
from sklearn.neural_network import MLPClassifier
from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import AdaBoostClassifier
from sklearn.model_selection import train_test_split
from sklearn import metrics

#  read the data in from files,
#  assign target values 1 for signal, 0 for background
sigData = np.loadtxt('signal.txt')
nSig = sigData.shape[0]
sigTargets = np.ones(nSig)

bkgData = np.loadtxt('background.txt')
nBkg = bkgData.shape[0]
bkgTargets = np.zeros(nBkg)

# concatenate arrays into data X and targets y
X = np.concatenate((sigData,bkgData),0)
```

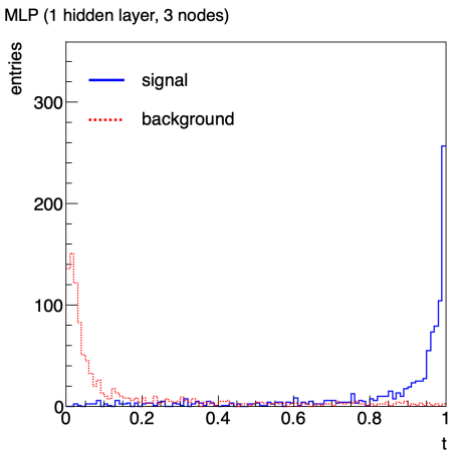
```
y = np.concatenate((sigTargets, bkgTargets))
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.5, random_state=1)

# make histograms of input components
for comp in [1,2,3]:
    plt.figure(figsize=(5,5))
    plt.gcf().subplots_adjust(bottom=0.2)
    plt.gcf().subplots_adjust(left=0.2)
    matplotlib.rcParams.update({'font.size':20})    # set all font sizes
    nBins = 50
    xMin = min( np.floor(np.min(sigData[:,comp-1])), np.floor(np.min(bkgData[:,comp-1])))
    xMax = max( np.ceil(np.max(sigData[:,comp-1])), np.ceil(np.max(bkgData[:,comp-1])))
    xSig = sigData[:,comp-1]
    xBkg = bkgData[:,comp-1]
    bins = np.linspace(xMin, xMax, nBins+1)
    xLabel = '$x_{' + str(comp) + '}$'
    yLabel = '$f_{' + str(comp) + '}(x_{' + str(comp) + '})$'
    plt.xlabel(xLabel, labelpad=2)
    plt.ylabel(yLabel, labelpad=2)
    n, bins, patches = plt.hist(xSig, bins=bins, density=True, histtype='step', fill=False,        color='dodgerblue')
    n, bins, patches = plt.hist(xBkg, bins=bins, density=True, histtype='step', fill=False,        color='red', alpha=0.5)
    fileName = "inputs_" + str(comp) + ".pdf"
    plt.savefig(fileName, format='pdf')
    plt.show()

# Create classifier object and train
# Add code here to include other claassifiers (MLP, BDT,...)
# Select classifier
classifier = "MLP"
if classifier == "LDA":
    clf = LDA()
elif classifier == "MLP":
    clf = MLPClassifier(hidden_layer_sizes=(3,), activation='tanh',
                max_iter=2000, random_state=0)
elif classifier == "BDT":
    clf = AdaBoostClassifier(DecisionTreeClassifier(max_depth=1), algorithm="SAMME",      n_estimators=100)
clf.fit(X_train, y_train)



# Evaluate accuracy using the test data.
# If available, use the decision function, else (e.g. for MLP) use predict_proba
# Adjust threshold value tCut or pMin as appropriate
```

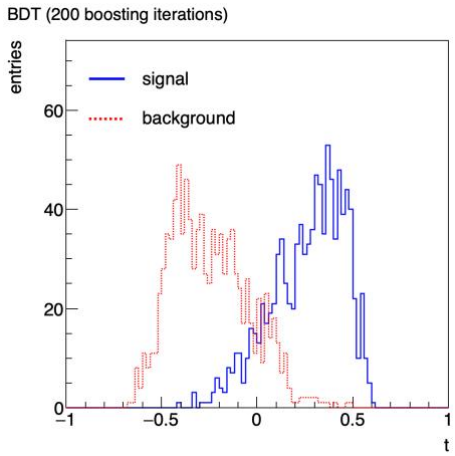
```
X_bkg_test = X_test[y_test==0]
X_sig_test = X_test[y_test==1]
y_bkg_test = y_test[y_test==0]
y_sig_test = y_test[y_test==1]
if hasattr(clf, "decision_function"):
    tCut = 0.
    y_bkg_pred = (clf.decision_function(X_bkg_test) >= tCut).astype(bool)
    y_sig_pred = (clf.decision_function(X_sig_test) >= tCut).astype(bool)
else:
    pCut = 0.5
    y_bkg_pred = (clf.predict_proba(X_bkg_test)[:,1]  >= pCut).astype(bool)
    y_sig_pred = (clf.predict_proba(X_sig_test)[:,1]  >= pCut).astype(bool)

power = metrics.accuracy_score(y_sig_test, y_sig_pred)           # = Prob(t >= tCut|sig)
print('power of test with respect to signal = ', power)

#  Ex. 1(a) Add code here to obtain the background efficiency
# = size of test alpha = Prob(t >= tCut|bkg)
size = 1. - metrics.accuracy_score(y_bkg_test, y_bkg_pred)       # = Prob(t >= tCut|bkg)
print('size of test of background = ', size)

#  Ex. 1(b) Purity of signal sample selected with t >= tCut
piSig = 0.5      # prior probability to be signal
piBkg = 0.5      # prior probability to be background
effSig = power
effBkg = size
purity = effSig*piSig / (effSig*piSig + effBkg*piBkg)
print('purity of signal sample = ', purity)

# Ex. 1(c) make histogram of decision function
plt.figure()                              # new window
matplotlib.rcParams.update({'font.size':14})    # set all font sizes
tTest = clf.predict_proba(X_test)[:,1]
if hasattr(clf, "decision_function"):
    tTest = clf.decision_function(X_test)       # if available use decision_function
else:
    tTest = clf.predict_proba(X_test)[:,1]      # for e.g. MLP need to use predict_proba
tBkg = tTest[y_test==0]
tSig = tTest[y_test==1]
nBins = 50
tMin = np.floor(np.min(tTest))
tMax = np.ceil(np.max(tTest))
bins = np.linspace(tMin, tMax, nBins+1)
plt.xlabel('decision function $t$', labelpad=3)
plt.ylabel('$f(t)$', labelpad=3)
```

```
n, bins, patches = plt.hist(tSig, bins=bins, density=True, histtype='step', fill=False, color='dodgerblue')
n, bins, patches = plt.hist(tBkg, bins=bins, density=True, histtype='step', fill=False, color='red', alpha=0.5)
plt.savefig("decision_function_hist.pdf", format='pdf')

#  2 -- total error rate for BDT as function of boosting iterations
boostingIterations = [1, 2, 5, 10, 20, 50, 100, 500, 1000, 2000, 5000, 10000, 50000]
trainErrorRate = []
testErrorRate = []
for i in range(len(boostingIterations)):
    clf = AdaBoostClassifier(DecisionTreeClassifier(max_depth=1), algorithm="SAMME",      n_estimators=boostingIterations[i])
    clf.fit(X_train, y_train)
    y_pred_train = clf.predict(X_train)
    y_pred_test = clf.predict(X_test)
    trainErrorRate.append(1. - metrics.accuracy_score(y_train, y_pred_train))
    testErrorRate.append(1. - metrics.accuracy_score(y_test, y_pred_test))
    print(boostingIterations[i], trainErrorRate[i], testErrorRate[i])

# make plot
fig, ax = plt.subplots(1,1)
plt.xlabel(r'number of boosting iterations', labelpad=3)
plt.ylabel(r'error rate', labelpad=3)
plt.xscale('log')
xMin=1.
xMax=5.e4
yMin=0.
yMax=0.25
plt.xlim(xMin, xMax)
plt.ylim(yMin, yMax)
plt.plot(boostingIterations, trainErrorRate, color='black', label=r'training sample')
plt.plot(boostingIterations, testErrorRate, color='red', label=r'test sample')
plt.subplots_adjust(left=0.2, right=0.9, top=0.9, bottom=0.2)
handles, labels = ax.get_legend_handles_labels()
plt.legend(handles, labels, loc='upper right', frameon=False)
plt.savefig("BDTErrorRate.pdf", format='pdf')
plt.show()
```

Exercise 1, C++ version. Using C++/Root, the following distributions were obtained for the Fisher discriminant, MLP (3 nodes in 1 hidden layer) and BDT with 200 boosting iterations:







the following efficiencies and purities were obtained:

signal efficiency (power) Fisher = 0.824

background efficiency (size) Fisher = 0.215

signal purity (Fisher) = 0.79307

signal efficiency (power) MLP3 = 0.904

background efficiency (size) MLP3 = 0.112

signal purity (MLP3) = 0.889764

The routine tmvaTrain.cc was modified to include a multilayer perceptron using

factory->BookMethod(dataLoader, TMVA::Types::kMLP, "MLP3",

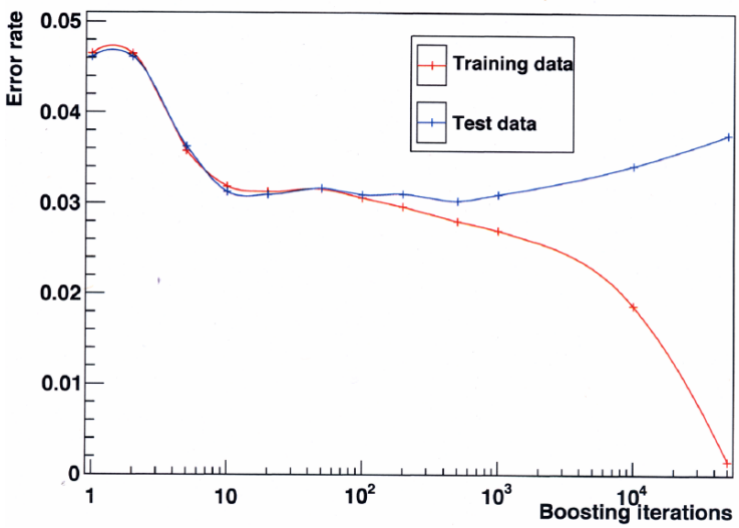
"H:!V:NeuronType=tanh:HiddenLayers=3");

And a boosted decision tree with 200 iterations was created with

factory->BookMethod(dataLoader, TMVA::Types::kBDT, "BDT200",

"NTrees=200:BoostType=AdaBoost");

Ex. 2 (bonus) The total error rate versus number of boosting iterations of BDT (using 1000 training events):



C++ code: The routine analyzeData.cc was modified to calculate the signal and background efficiencies and signal purity using the code below:

```
#include <iostream>
#include <fstream>
#include <vector>
#include <TFile.h>
#include <TTree.h>
#include <TH1D.h>
#include <TCanvas.h>
#include <TApplication.h>
#include <TROOT.h>
#include <TStyle.h>
#include <TPad.h>
#include <TAxis.h>
#include <TH2F.h>
#include <TF2.h>
#include <TLine.h>
#include "Event.h"
#include "OutFunc.h"
#include <TMVA/Reader.h>
```

```
using namespace std;

OutFunc* testFisher;      // need global for contour later
OutFunc* testMLP3;      // need global for contour later
OutFunc* testBDT200;      // need global for contour later

int main() {

// Set up an output file and book some histograms

  TFile* histFile = new TFile("analysis.root", "RECREATE");
  TH1D* hSigFisher = new TH1D("hSigFisher", "Fisher, sig", 100, -5.0, 5.0);
  TH1D* hBkgFisher = new TH1D("hBkgFisher", "Fisher, bkg", 100, -5.0, 5.0);
  TList* hList = new TList();      // list of histograms to store
  hList->Add(hSigFisher);
  hList->Add(hBkgFisher);

  TH1D* hSigMLP3 = new TH1D("hSigMLP3", "MLP3, sig", 100, -5.0, 5.0);
  TH1D* hBkgMLP3 = new TH1D("hBkgMLP3", "MLP3, bkg", 100, -5.0, 5.0);
  hList->Add(hSigMLP3);
  hList->Add(hBkgMLP3);

  TH1D* hSigBDT200 = new TH1D("hSigBDT200", "BDT200, sig", 100, -5.0, 5.0);
  TH1D* hBkgBDT200 = new TH1D("hBkgBDT200", "BDT200, bkg", 100, -5.0, 5.0);
  hList->Add(hSigBDT200);
  hList->Add(hBkgBDT200);

// Set up the OutFunc object.  First argument must be one of the classifiers.
// 4th argument is offset for making contour; otherwise should be zero.
// 5th argument is bool array indicating which variables were used in training

  std::string dir    = "../train/dataset/weights/";
  std::string prefix = "tmvaTest";
  const double tCutFisher = 0.;
  const double tCutMLP3 = 0.5;
  const double tCutBDT200 = 0.;
  std::vector<bool> useVar(3);
  useVar[0] = true;      // x
  useVar[1] = true;      // y
  useVar[2] = true;      // z
  testFisher = new OutFunc("Fisher", dir, prefix, 0., useVar);
  testMLP3 = new OutFunc("MLP3", dir, prefix, 0., useVar);
  testBDT200 = new OutFunc("BDT200", dir, prefix, 0., useVar);

// Open input file, get the TTrees, put into a vector
```

```
  TFile* inputFile = new TFile("../generate/testData.root");
  inputFile->ls();
  TTree* sig = dynamic_cast<TTree*>(inputFile->Get("sig"));
  TTree* bkg = dynamic_cast<TTree*>(inputFile->Get("bkg"));
  std::vector<TTree*> treeVec;
  treeVec.push_back(sig);
  treeVec.push_back(bkg);

// Loop over TTrees, i=0 is signal, i=1 is background

  int nSig, nBkg;
  int nSigAccFisher = 0;
  int nSigAccMLP3 = 0;
  int nSigAccBDT200 = 0;
  int nBkgAccFisher = 0;
  int nBkgAccMLP3 = 0;
  int nBkgAccBDT200 = 0;
  for (int i=0; i<treeVec.size(); i++){

    treeVec[i]->Print();
    Event evt;
    treeVec[i]->SetBranchAddress("evt", &evt);
    int numEntries = treeVec[i]->GetEntries();
    if ( i == 0 ) { nSig = numEntries; }
    if ( i == 1 ) { nBkg = numEntries; }
    std::cout << "number of entries = " << numEntries << std::endl;

// Loop over events.

    for (int j=0; j<numEntries; j++){

      treeVec[i]->GetEntry(j);                  // sets evt
      double tFisher = testFisher->val(&evt);    // evaluate test statistic
      double tMLP3 = testMLP3->val(&evt);
      double tBDT200 = testBDT200->val(&evt);

      if ( i == 0 ){                     // signal
        hSigFisher->Fill(tFisher);
        hSigMLP3->Fill(tMLP3);
            hSigBDT200->Fill(tBDT200);
            if ( tFisher >= tCutFisher ) { nSigAccFisher++; }
            if ( tMLP3 >= tCutMLP3 ) { nSigAccMLP3++; }
            if ( tBDT200 >= tCutBDT200 ) { nSigAccBDT200++; }
      }
```

```
    else if ( i == 1 ){                 // background
      hBkgFisher->Fill(tFisher);
          hBkgMLP3->Fill(tMLP3);
      hBkgBDT200->Fill(tBDT200);
          if ( tFisher >= tCutFisher ) { nBkgAccFisher++; }
          if ( tMLP3 >= tCutMLP3 ) { nBkgAccMLP3++; }
          if ( tBDT200 >= tCutBDT200 ) { nBkgAccBDT200++; }
    }

  }

 }

//  Compute efficiencies (power, size) etc.

 double epsSigFisher = static_cast<double>(nSigAccFisher)
  / static_cast<double>(nSig);
 std::cout << "signal efficiency (power) Fisher = " << epsSigFisher
           << std::endl;
 double epsBkgFisher = static_cast<double>(nBkgAccFisher)
  / static_cast<double>(nBkg);
 std::cout << "background efficiency (size) Fisher = " << epsBkgFisher
           << std::endl;

 double epsSigMLP3 = static_cast<double>(nSigAccMLP3)
  / static_cast<double>(nSig);
 std::cout << "signal efficiency (power) MLP3 = " << epsSigMLP3
           << std::endl;
 double epsBkgMLP3 = static_cast<double>(nBkgAccMLP3)
  / static_cast<double>(nBkg);
 std::cout << "background efficiency (size) MLP3 = " << epsBkgMLP3
           << std::endl;

 double epsSigBDT200 = static_cast<double>(nSigAccBDT200)
  / static_cast<double>(nSig);
 std::cout << "signal efficiency (power) BDT200 = " << epsSigBDT200
           << std::endl;
 double epsBkgBDT200 = static_cast<double>(nBkgAccBDT200)
  / static_cast<double>(nBkg);
 std::cout << "background efficiency (size) BDT200 = " << epsBkgBDT200
           << std::endl;

 // Compute signal purity assuming equal prior probabilities
 double piSig = 0.5;
 double piBkg = 0.5;
```

```
  double purityFisher = epsSigFisher*piSig /
    (epsSigFisher*piSig + epsBkgFisher*piBkg);
  std::cout << "signal purity (Fisher) = " << purityFisher << std::endl;

  double purityMLP3 = epsSigMLP3*piSig/(epsSigMLP3*piSig + epsBkgMLP3*piBkg);
  std::cout << "signal purity (MLP3) = " << purityMLP3 << std::endl;

  double purityBDT200 = epsSigBDT200*piSig /
    (epsSigBDT200*piSig + epsBkgBDT200*piBkg);
  std::cout << "signal purity (BDT200) = " << purityBDT200 << std::endl;

// Close up

  inputFile->Close();
  histFile->Write();
  histFile->Close();

  return 0;
}
```