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In [1]: # simpleClassifier.py
        # G. Cowan / RHUL Physics / November 2020
        # 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.model_selection import train_test_split
        from sklearn import metrics
In [2]: # 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)
In [6]: # concatenate arrays into data X and targets y
        X = np.concatenate((sigData,bkgData),0)
        X = X[:, 0:2]
                                          # at first, only use x1 and x2
        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)
        # Create classifier object and train
        # Add code here to include other classifiers (MLP, BDT,...)
        clf = LDA()
        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:
            pMin = 0.9
            y bkg pred = (clf.predict proba(X bkg test)[:,1] >= pMin).astype(bool)
            y_sig_pred = (clf.predict_proba(X_sig_test)[:,1] >= pMin).astype(bool)
                                                                     \# = = Prob(t \ge tCut \mid sig)
        power = metrics.accuracy_score(y_sig_test, y_sig_pred)
        print('power of test with respect to signal = ', power)
        power of test with respect to signal = 0.7832195905258932
In [8]: # 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)
        print('size of test with respect to bkg = ', size)
        size of test with respect to bkg = 0.1606217616580311
# Using Bayes Theorem P(s|t>tc) = P(t>tc|s) pi(s)/(P(t>tc|s) pi(s) + P(t>tc|b)pi(b)
        # Since prior probabilities are the same, they cancel out.
        purity = power/(power + size)
        print("purity: ", purity)
        purity: 0.8298212286563059
In [4]: # make a scatter plot
        fig, ax = plt.subplots(1,1)
        plt.gcf().subplots_adjust(bottom=0.15)
        plt.gcf().subplots_adjust(left=0.15)
        ax.set_xlim((-2.5, 3.5))
        ax.set_ylim((-2,4))
        x0,x1 = ax.get xlim()
        y0,y1 = ax.get_ylim()
        ax.set_aspect(abs(x1-x0)/abs(y1-y0)) # make square plot
        xtick_spacing = 0.5
        ytick_spacing = 2.0
        ax.yaxis.set_major_locator(ticker.MultipleLocator(xtick_spacing))
        ax.yaxis.set_major_locator(ticker.MultipleLocator(ytick_spacing))
        plt.scatter(sigData[:,0], sigData[:,1], s=3, color='dodgerblue', marker='o')
        plt.scatter(bkgData[:,0], bkgData[:,1], s=3, color='red', marker='o')
        # add decision boundary to scatter plot
        x_{min}, x_{max} = X[:, 0].min() - .5, X[:, 0].max() + .5
        y_{min}, y_{max} = X[:, 1].min() - .5, X[:, 1].max() + .5
        h = .01 # step size in the mesh
        xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max, h))
        # depending on classifier call predict_proba or decision_function
        Z = clf.predict_proba(np.c_[xx.ravel(), yy.ravel()])[:, 1]
        Z = Z.reshape(xx.shape)
        plt.contour(xx, yy, Z, 1, colors='k')
        plt.xlabel(r'$x_{1}$', labelpad=0)
        plt.ylabel(r'$x {2}$', labelpad=15)
        plt.savefig("scatterplot.pdf", format='pdf')
In [5]: # 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:
                                                        # for e.g. MLP need to use predict proba
            tTest = clf.predict_proba(X_test)[:,1]
        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')
        plt.show()
           0.25
           0.20
         £ 0.15
           0.10
           0.05
           0.00
                                   0
                           decision function t
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In []: