Theoretical Questions

Q1:
To evaluate how well our model performs at T1D classification, we need to have evaluation metrics that measures of its performances/accuracy. Which evaluation metric is more important to us: model accuracy or model performance? Give a simple example that illustrates your claim

A1:
The model performance would be a better evaluation metric in this case. Model accuracy is just the number of correct predictions made by the model devided by the total number of predictions - which would not be a good model in this case because we have a relatively small number of people in the population with the T1D. For example, if we use a classifier that classifies all patients as being healthy, we would get an accuracy of at least 99.67% (according to the assignment that states that up to 0.33% suffer from T1D), which is a very high accuracy, but this is a terrible classifier.

Q2:
T1D is often associated with other comorbidities such as a heart attack. You are asked to design a ML algorithm to predict which patients are going to suffer a heart attack. Relevant patient features for the algorithm may include blood pressure (BP), body-mass index (BMI), age (A), level of physical activity (P), and income (I). You should choose between two classifiers: the first uses only BP and BMI features and the other one uses all of the features available to you. Explain the pros and cons of each choice.

A2:

Classifier1
Pros - Easy to visualize data, less weights to train.
Cons - Selected feature may not be the best features (we need prior information in order to choose the best ones), the less features we have - the more missing information in one of the features might increase errors in the classification.

Classifier2
Pros - Contains a wider selection of features which might help get a better classification.
Cons - Longer training time, may contain redundant features.

Q3:
A histologist wants to use machine learning to tell the difference between pancreas biopsies that show signs of T1D and those that do not. She has already come up with dozens of measurements to take, such as color, size, uniformity and cell-count, but she isn't sure which model to use. The biopsies are really similar, and it is difficult to distinguish them from the human eye, or by just looking at the features. Which of the following is better: logistic regression, linear SVM or nonlinear SVM? Explain your answer.

A3:

Since the data is difficult to distinguish by just looking at the features, logistic regression would not be useful for classification, nor would linear SVM, since the data is non-seperable, and therefore we cannot seperate the data using a linear line. In this case, nonlinear SVM would be the most useful method, since it would transform our non-seperable data into a higher dimensional space, where the data might prove to be seperable.

Q4:
What are the differences between LR and linear SVM and what is the difference in the effect/concept of their hyper-parameters tuning?

A4: The main difference between LR and Linear SVM is that linear SVM find the "best" margin that seperates the classes, while LR does not, and can have different boundaries with different weights (the boundary is not "optimized"). Another difference is that LR uses a probobilistic approach, while SVM is deterministic. The differnce in the concept of their hyper-parameters tuning is that LR uses a regularization (penalty) - for example, l1 or l2, and the lambda parameter which gives us the penalty strength. For linear SVM - we use the "kernel trick" in order to find the best hyper-parameters.

Coding Assignment

In [1]:
```
# imports
import pandas as pd
import numpy as np
%matplotlib inline
import matplotlib
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split,  GridSearchCV,  StratifiedKFold
from sklearn.preprocessing import StandardScaler
from sklearn.metrics import plot_confusion_matrix, confusion_matrix, log_loss, hinge_loss, roc_auc_score
from sklearn.linear_model import LogisticRegression
from sklearn.pipeline import Pipeline
from sklearn.svm import SVC
from sklearn.ensemble import RandomForestClassifier
from sklearn.decomposition import PCA
import csv
```

Functions:

In [2]:
```
def metrics (best_estimator,x_test,y_test,y_pred_test, y_pred_proba_test,loss_type):
    plot_confusion_matrix(best_estimator,x_test,y_test, cmap=plt.cm.Blues)
    plt.grid(False)
    TN = calc_TN(y_test, y_pred_test)
    FP = calc_FP(y_test, y_pred_test)
    FN = calc_FN(y_test, y_pred_test)
    TP = calc_TP(y_test, y_pred_test)
```

```
    Se = TP/(TP+FN)
    Sp = TN/(TN+FP)
    PPV = TP/(TP+FP)
    NPV = TN/(TN+FN)
    Acc = (TP+TN)/(TP+FP+TN+FN)
    F1 = 2*(PPV*Se)/(PPV+Se)
    print('Sensitivity is {:.2f}'.format(Se))
    print('Specificity is {:.2f}'.format(Sp))
    print('PPV is {:.2f}'.format(PPV))
    print('NPV is {:.2f}'.format(NPV))
    print('Accuracy is {:.2f}'.format(Acc))
    print('F1 is {:.2f}'.format(F1))
    print('AUROC is {:.2f}'.format(roc_auc_score(y_test, y_pred_proba_test[:,1])))
    if (loss_type=='log'):
        print('Log Loss is {:.2f}'.format(log_loss(y_test,y_pred_test)))
    elif (loss_type=='hinge'):
        print('Hinge Loss is {:.2f}'.format(hinge_loss(np.where(y_test==0, -1, y_test),np.where(y_pred_test==0, -1, y
        # We replaced all 0 with -1 since that how hinge loss is calculated
```

In [3]:
```
def plt_2d_pca(X_pca,y,title):
    fig = plt.figure(figsize=(8, 8))
    ax = fig.add_subplot(111, aspect='equal')
    ax.scatter(X_pca[y==0, 0], X_pca[y==0, 1], color='b')
    ax.scatter(X_pca[y==1, 0], X_pca[y==1, 1], color='r')
    ax.legend(('Negative','Positive'))
    ax.plot([0], [0], "ko")
    ax.arrow(0, 0, 0, 1, head_width=0.05, length_includes_head=True, head_length=0.1, fc='k', ec='k')
    ax.arrow(0, 0, 1, 0, head_width=0.05, length_includes_head=True, head_length=0.1, fc='k', ec='k')
    ax.set_xlabel('$U_1$')
    ax.set_ylabel('$U_2$')
    ax.set_title(title)
```

Load Data

In [4]:
```
#T1D data
df_raw = pd.read_csv("HW2_data.csv")
df = df_raw.copy()

#preprocessing
#converting family history to Yes/No
df['Family History'] = df['Family History'].map({1: 'Yes', 0 : 'No'})
#since only around 7% of data has missing values, we dropped these rows
df = df.dropna()
print(df.shape)
```

```
(523, 18)
```

The reason we dropped the rows and not entered NaN values is so when we convert the data into One hot vector, we won't have

extra categories due to the NaN values. We also didn't want to add random value to the dataset since the values are binary, and by adding random values instead of the missing values we can corrupt our data.

Train Test Split

In [5]:
```
# train test split
# feature columns
features = [0,1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,17]
X = df.iloc[:,features]
# T1D prediction
y = df.iloc[:,16]
X_train, x_test, Y_train, y_test = train_test_split(X, y, test_size = 0.20, random_state = 10, stratify=y)
```

Data visualization and exploration

The features in our data are devided into 3 sets of representation:

1. Age
2. Gender
3. Binary

In order to represent the distribution of the features we summary each feature representation in a different table

In [6]:
```
#Distribution in train and test set

fig1, ax1 =plt.subplots(1,1)
st1 = X_train.iloc[:,0].describe()
st2 = x_test.iloc[:,0].describe()
data = [['mean',st1['mean'],st2['mean']],['median',st1['50%'],st2['50%']],['std',st1['std'],st2['std']]]

column_labels=["Distribution Parameters", "Age in train set", "Age in test set"]
ax1.axis('tight')
ax1.axis('off')
ax1.table(cellText=data,colLabels=column_labels,loc="center")
plt.show()

fig2, ax2 =plt.subplots(1,1)
st1 = X_train.iloc[:,1].describe()
st2 = x_test.iloc[:,1].describe()
data = [['freq gender',st1['top'],st2['top']],['freq gender %',st1['freq']/st1['count'],st2['freq']/st2['count']],['l
column_labels=["Parameters", "Gender in train set", "Gender in test set"]
ax2.axis('tight')
ax2.axis('off')
ax2.table(cellText=data,colLabels=column_labels,loc="center")
plt.show()
```

Distribution Parameters	Age in train set	Age in test set
mean	48.49760765550239	46.161904761904765
median	48.0	45.0
std	12.178577095306338	11.85742530225406

Parameters	Gender in train set	Gender in test set
freq gender	Male	Male
freq gender %	0.6148325358851675	0.6952380952380952
less freq gender %	0.3851674641148325	0.3047619047619048

In [7]:
```
#computing positive feature distribution for train and test sets  in dictionaries
dict_stat_train={}
dict_stat_test={}
for f in X_train.columns:
    if f == 'Age' or f == 'Gender':
        continue
    count = X_train[f].describe(exclude=[np.number])['count']
    top = X_train[f].describe(exclude=[np.number])['top']
    freq = X_train[f].describe(exclude=[np.number])['freq']
    if top == 'Yes':
        dict_stat_train['%  Yes in ' + str(f)]=100*freq/count
    else:
        dict_stat_train['%  Yes in ' + str(f)]=100*(1-freq/count)

    count = x_test[f].describe(exclude=[np.number])['count']
    top = x_test[f].describe(exclude=[np.number])['top']
    freq = x_test[f].describe(exclude=[np.number])['freq']
    if top == 'Yes':
```

```
        dict_stat_test['%  Yes in ' + str(f)]=100*freq/count
    else:
        dict_stat_test['%  Yes in ' + str(f)]=100*(1-freq/count)
```

In [8]:
```
#creating csv file for positive feature distribution
with open('Positive_feature_dist.csv', 'w') as output:
    writer = csv.DictWriter(output, fieldnames = ["Positive feature", "Train %", "Test %","Delta %"])
    writer.writeheader()
    cw = csv.writer(output)
    for k in dict_stat_train.keys():
      cw.writerow([k, dict_stat_train[k], dict_stat_test[k],np.abs(dict_stat_train[k]-dict_stat_test[k])])

df_feature_Positive = pd.read_csv("Positive_feature_dist.csv")
print(df_feature_Positive)
```

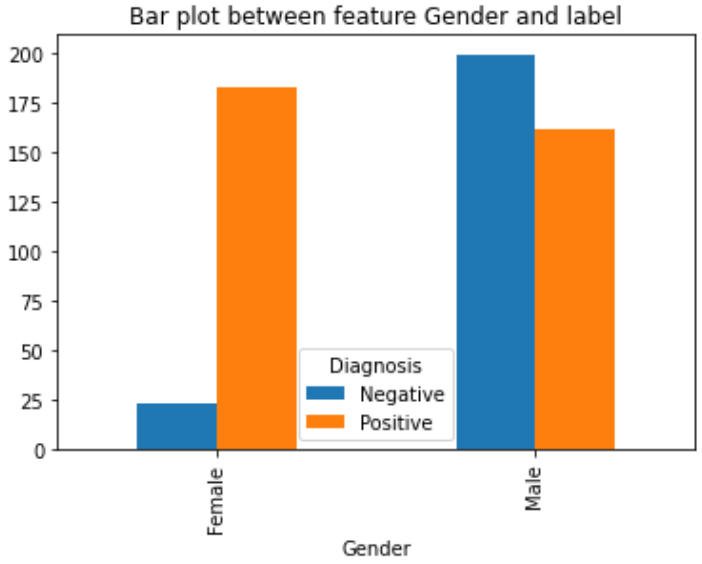
```
                 Positive feature    Train %     Test %   Delta %
0    %  Yes in Increased Urination  50.478469  45.714286  4.764183
1       %  Yes in Increased Thirst  46.172249  38.095238  8.077011
2     %  Yes in Sudden Weight Loss  41.626794  40.952381  0.674413
3               %  Yes in Weakness  58.133971  60.000000  1.866029
4       %  Yes in Increased Hunger  46.650718  40.952381  5.698337
5         %  Yes in Genital Thrush  20.334928  29.523810  9.188881
6        %  Yes in Visual Blurring  45.933014  39.047619  6.885395
7               %  Yes in Itching  49.521531  44.761905  4.759626
8          %  Yes in Irritability  24.641148  22.857143  1.784005
9        %  Yes in Delayed Healing  47.846890  38.095238  9.751652
10       %  Yes in Partial Paresis  43.779904  39.047619  4.732285
11      %  Yes in Muscle Stiffness  37.559809  36.190476  1.369332
12            %  Yes in Hair Loss  34.928230  33.333333  1.594896
13              %  Yes in Obesity  17.224880  15.238095  1.986785
14       %  Yes in Family History  49.760766  55.238095  5.477330
```

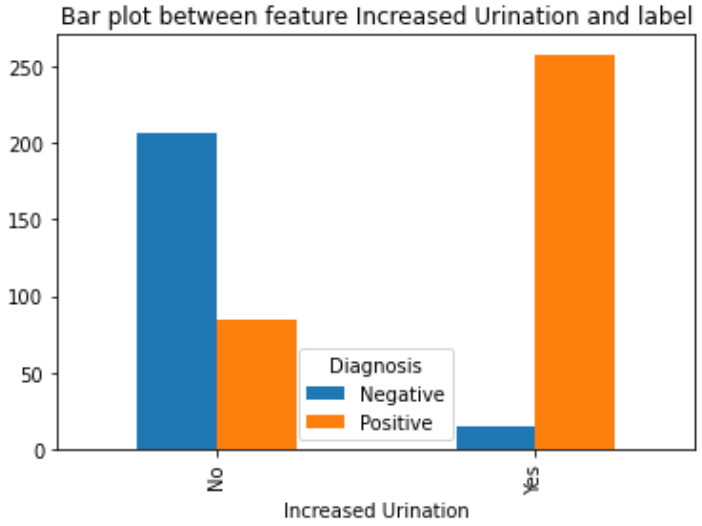
If training and test datasets are not sampled from the same distribution, there is an imbalance between them then training cannot be used to predict anything about the test dataset in a usable manner.
This problem is known as DataShift
We can treat DataShift by:

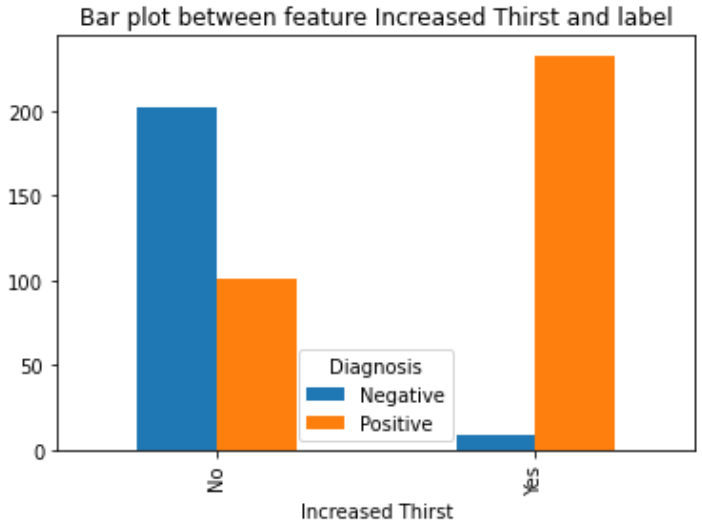
1. Dropping of drifting features
2. Importance weight using Density Ratio Estimation We can also use stratification when splitting the data in order to avoid this issue.

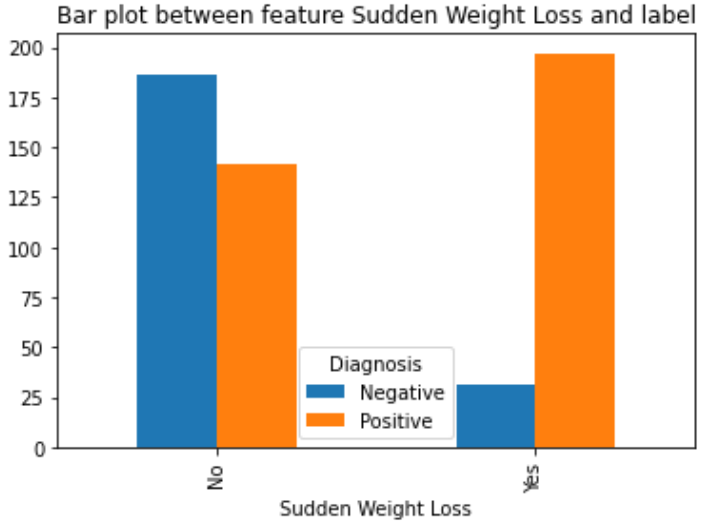
In [9]:
```
# relationship between feature and label
diagnosis_column = df_raw["Diagnosis"]
for f in df_raw.columns:
    if f == "Diagnosis" or f == "Age":
        continue
    series = df_raw.groupby([f,diagnosis_column]).size().unstack(level=1).plot(kind='bar')
```

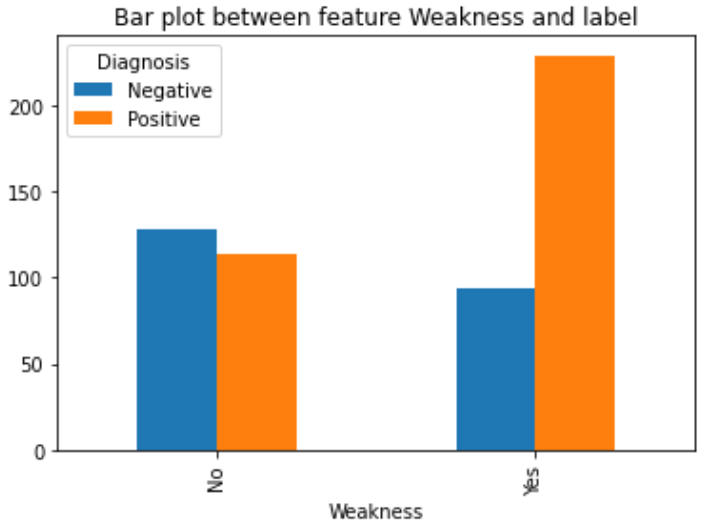
```
    plt.show
    plt.title('Bar plot between feature ' + str(f) + ' and label')
```

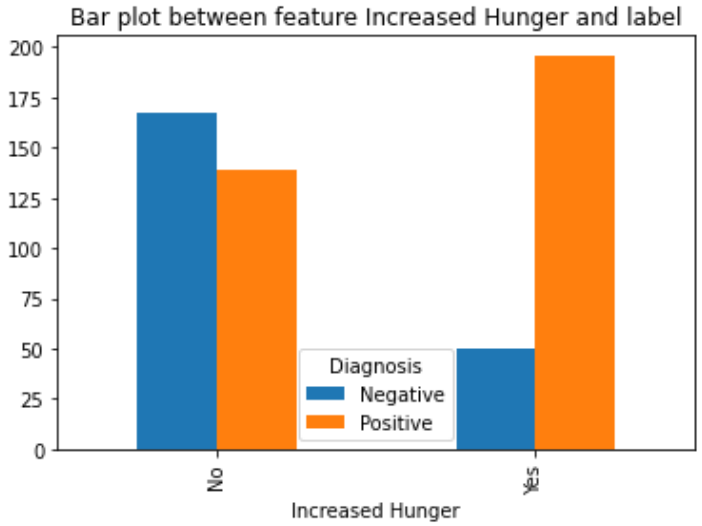


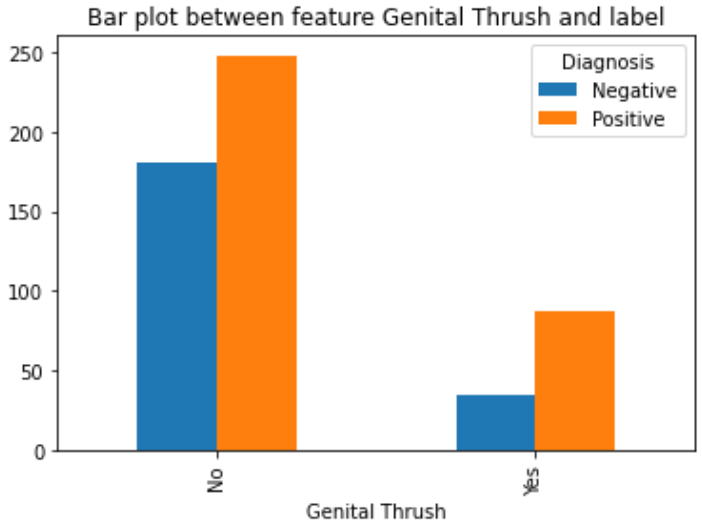


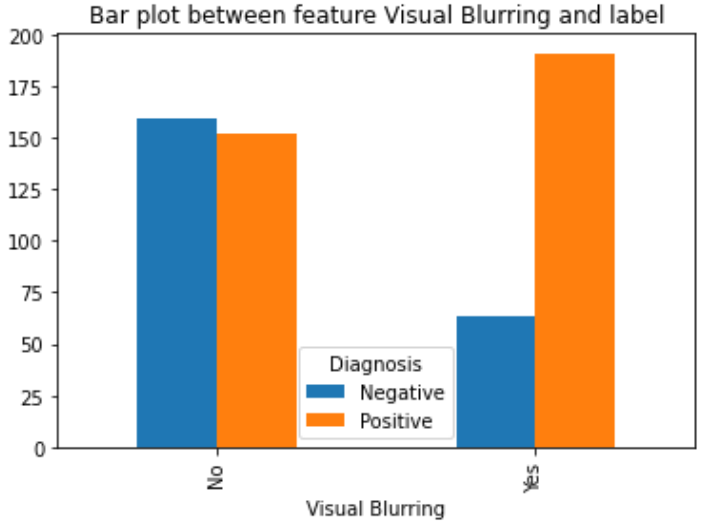

Bar plot between feature Increased Thirst and label
200
150
100
50
0
Diagnosis
Negative
Positive
No
Yes
Increased Thirst

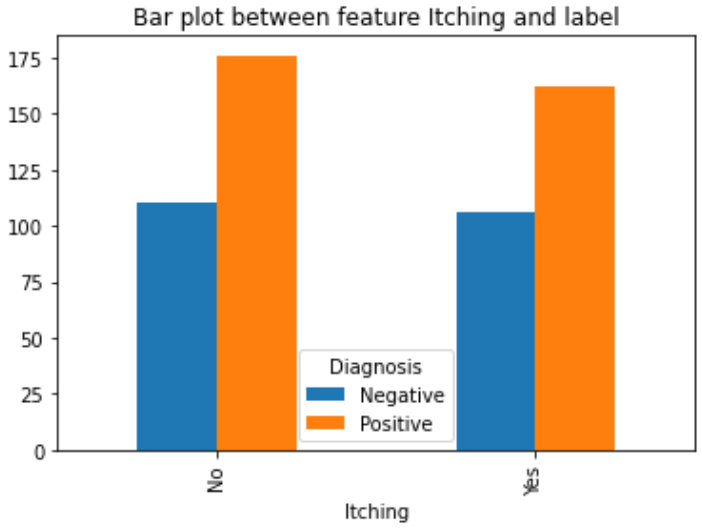

Bar plot between feature Sudden Weight Loss and label
200
175
150
125
100
75
50
25
0
Diagnosis
Negative
Positive
No
Yes
Sudden Weight Loss

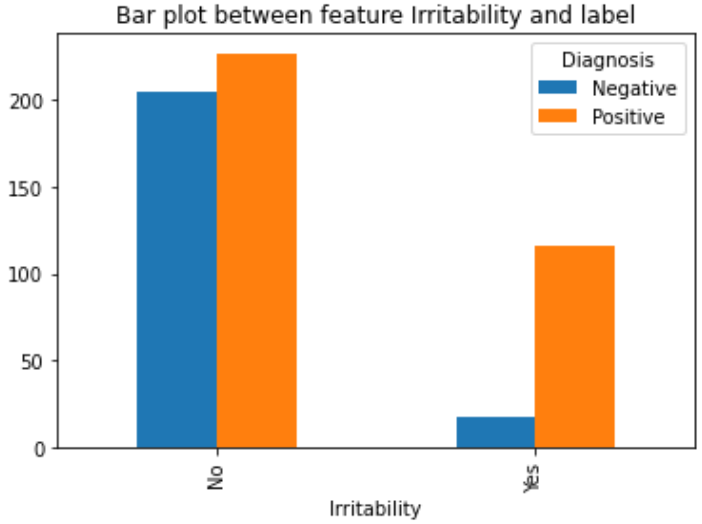

Bar plot between feature Weakness and label
Diagnosis
Negative
Positive
200
150
100
50
0
No
Yes
Weakness

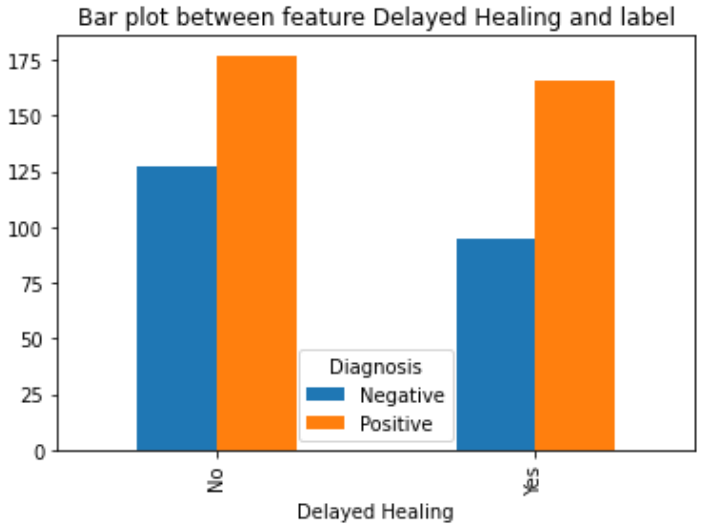

Bar plot between feature Increased Hunger and label
200
175
150
125
100
75
50
25
0
Diagnosis
Negative
Positive
No
Yes
Increased Hunger

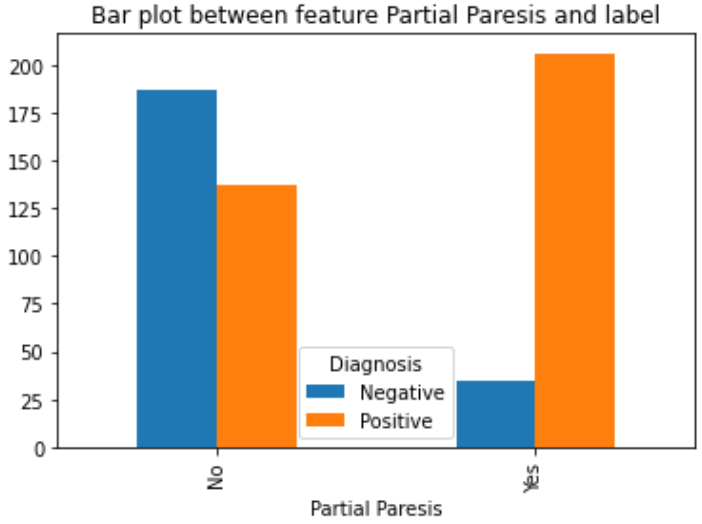

Bar plot between feature Genital Thrush and label
Diagnosis
Negative
Positive
250
200
150
100
50
0
No
Yes
Genital Thrush

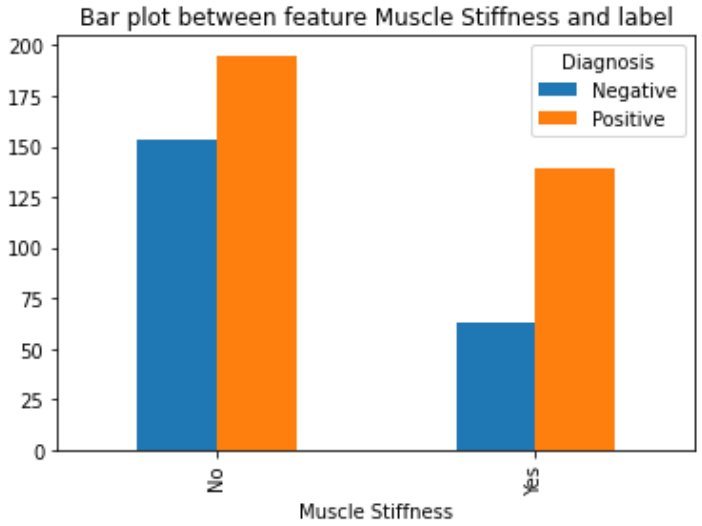

Bar plot between feature Visual Blurring and label
200
175
150
125
100
75
50
25
0
Diagnosis
Negative
Positive
No
Yes
Visual Blurring

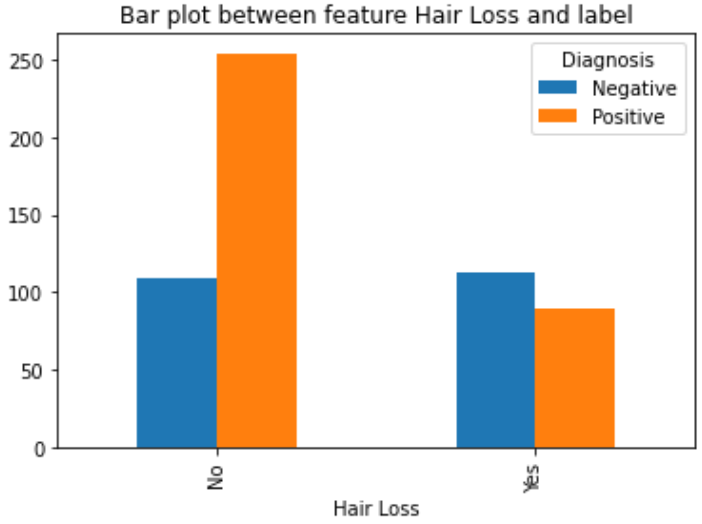

Bar plot between feature Itching and label
175
150
125
100
75
50
25
0
Diagnosis
Negative
Positive
No
Yes
Itching

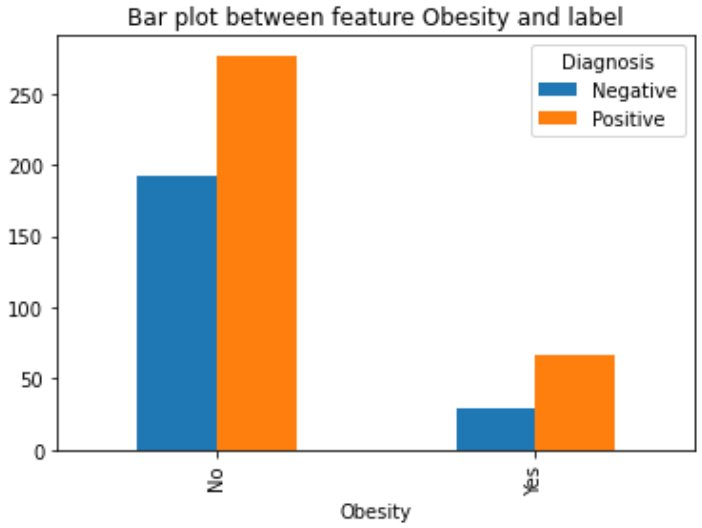

Bar plot between feature Irritability and label
200
150
100
50
0
Diagnosis
Negative
Positive
No
Yes
Irritability

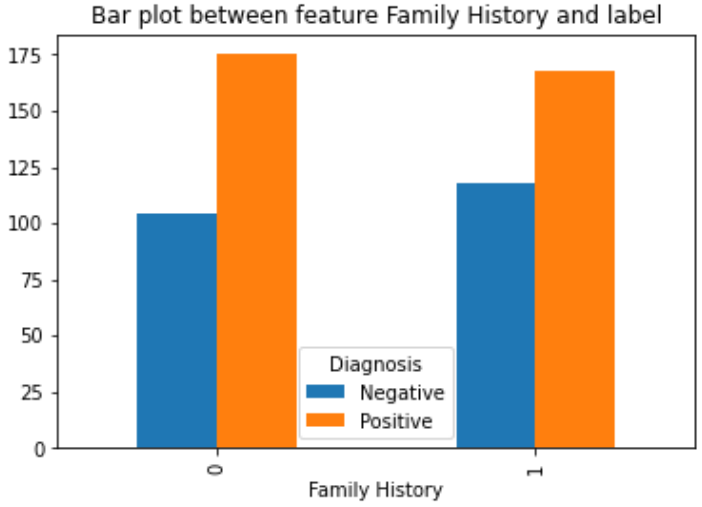

Bar plot between feature Delayed Healing and label
175
150
125
100
75
50
25
0
Diagnosis
Negative
Positive
No
Yes
Delayed Healing


Bar plot between feature Partial Paresis and label
200
175
150
125
100
75
50
25
0
Diagnosis
Negative
Positive
No
Yes
Partial Paresis


Bar plot between feature Muscle Stiffness and label
Diagnosis
Negative
Positive
200
175
150
125
100
75
50
25
0
No
Yes
Muscle Stiffness

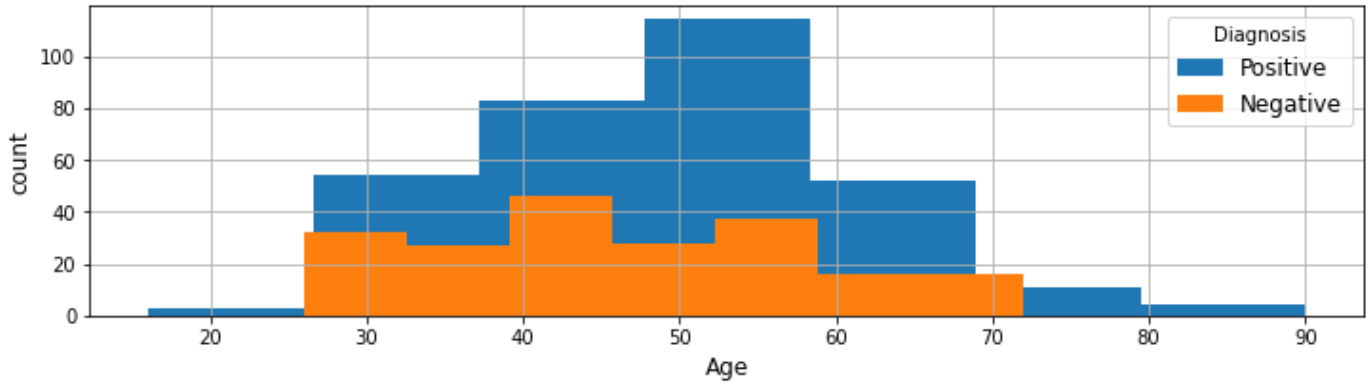

Bar plot between feature Hair Loss and label
Diagnosis
Negative
Positive
250
200
150
100
50
0
No
Yes
Hair Loss





In [25]:
```
idx_N=np.where(y=='Negative')
idx_P=np.where(y=='Positive')

fig, ax = plt.subplots(figsize=(12, 3))
age_P_hist=df_raw['Age'].iloc[idx_P].hist(label='Positive',bins=7,ax=ax)
age_N_hist=df_raw['Age'].iloc[idx_N].hist(label='Negative',bins=7,ax=ax)

ax.legend(title = 'Diagnosis', fontsize = 'large')
ax.set_xlabel('Age', fontsize = 'large')
ax.set_ylabel('count', fontsize = 'large')
```

Out[25]:
```
Text(0, 0.5, 'count')
```



We plotted the age histogram according to the diagnosis aswell in order to show that our data has a large variance in age - both for positive and negative patients, thus taking the factor of age into account as a feature.

Feature label bar plot revealed that women are more likely to have T1D. This is unexpected becasue according to the following paper males are more likley to have T1D. We were also surprised to see that there was not a significant sign of family history in T1D positives, whereas it is known that T1D is genetically linked (reference). We were also surprised by the link between age and diagnosis - we can see that after the age of 30, each age group has a higher percentage of positive diagnosis, until it reaches the age of 60, and then it starts going down.

We think that the following features - Increase Urination, Increased thirst, Sudden weight loss, Increased hunger, Visual Blurring, Irritability, Partial Paresis, are more important becasue their bar plot indicates that a person which is T1D positive is very likley to have these features/phyiscal phenotypes. This also fits the knowledge we have regarding the disease.

Encoding data as one hot vector:

In [11]:
```
for col in df:
    vector = pd.get_dummies(df[[col]].astype(str), drop_first=True) # convertion to string allows us to work with the
    df = pd.concat([df,vector],axis=1)
    df = df.drop(columns=[col])
df.head()
```

Out[11]:

	Age_25	Age_26	Age_27	Age_28	Age_29	Age_30	Age_31	Age_32	Age_33	Age_34	...	Visual Blurring_Yes	Itching_Yes	Irritability_Yes	He
0	0	0	0	0	0	0	0	0	0	0	...	0	1	0	
1	0	0	0	0	0	0	0	0	0	0	...	0	0	0	
2	0	0	0	0	0	0	0	0	0	0	...	0	0	0	
3	0	0	0	0	0	0	0	0	0	0	...	0	0	0	

	Age_25	Age_26	Age_27	Age_28	Age_29	Age_30	Age_31	Age_32	Age_33	Age_34	...	Visual Blurring_Yes	Itching_Yes	Irritability_Yes	He
4	0	0	0	0	0	0	0	0	0	0	...	1	1	0	

5 rows × 67 columns

Machine Learning Models:

In [12]:
```
y_1H = df["Diagnosis_Positive"]
X_1H = df.drop(['Diagnosis_Positive'],axis=1)

# splitting one hot vector data into train and test set
X_train, x_test, Y_train, y_test = train_test_split(X_1H, y_1H, test_size = 0.20, random_state = 10, stratify=y_1H)

# We define the functions for calculating our performances
calc_TN = lambda y_true, y_pred: confusion_matrix(y_true, y_pred)[0, 0]
calc_FP = lambda y_true, y_pred: confusion_matrix(y_true, y_pred)[0, 1]
calc_FN = lambda y_true, y_pred: confusion_matrix(y_true, y_pred)[1, 0]
calc_TP = lambda y_true, y_pred: confusion_matrix(y_true, y_pred)[1, 1]
```

We Start with our linear model - the logistic regression:

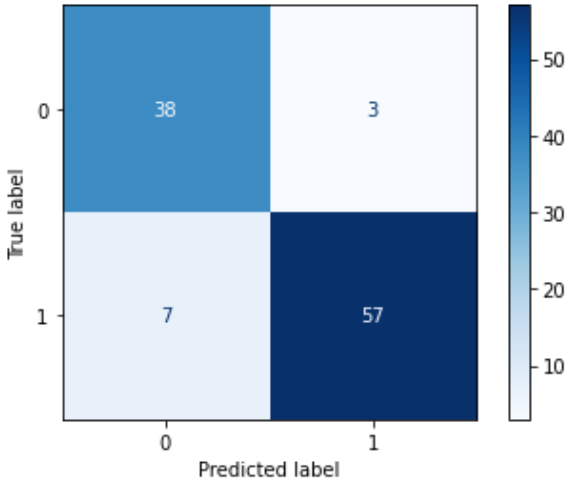
In [13]:
```
n_splits = 5
max_iter = 2000
solver = 'liblinear'

skf = StratifiedKFold(n_splits=n_splits, random_state=10, shuffle=True)

log_reg = LogisticRegression(random_state=5, max_iter=max_iter, solver=solver)
lmbda = np.array([0.001, 0.01, 1, 10, 100, 1000])
pipe = Pipeline(steps=[('logistic', log_reg)])
clf = GridSearchCV(estimator=pipe, param_grid={'logistic__C': 1/lmbda, 'logistic__penalty': ['l2']},
        scoring=['accuracy','f1','precision','recall','roc_auc'], cv=skf,
        refit='roc_auc', verbose=0, return_train_score=True)
clf.fit(X_train, Y_train)
log_reg_opt = clf.best_estimator_
y_pred_test = log_reg_opt.predict(x_test)
y_pred_proba_test = log_reg_opt.predict_proba(x_test)
```

Now we check the Logistic regression performance:

In [14]:
```
metrics (log_reg_opt,x_test,y_test,y_pred_test, y_pred_proba_test,'log')
```

```
Sensitivity is 0.89
Specificity is 0.93
```

```
PPV is 0.95
NPV is 0.84
Accuracy is 0.90
F1 is 0.92
AUROC is 0.95
Log Loss is 3.29
```



We continue with another linear model, this time - the linear SVM:

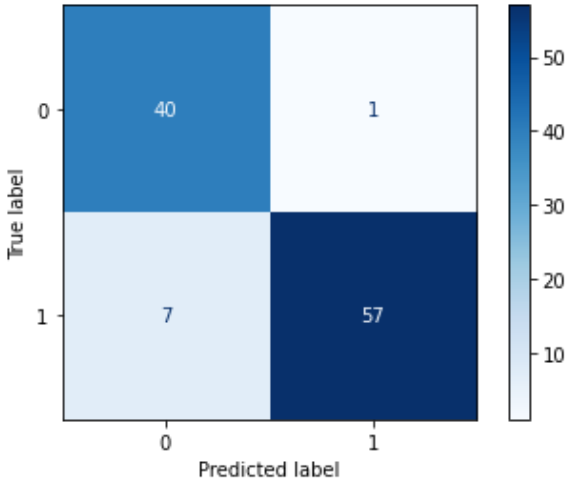
In [15]:
```
svc = SVC(probability=True)
C = np.array([0.001, 0.01, 1, 10, 100, 1000])
pipe = Pipeline(steps=[('svm', svc)])
svm_lin = GridSearchCV(estimator=pipe,
             param_grid={'svm__kernel':['linear'], 'svm__C':C},
             scoring=['accuracy','f1','precision','recall','roc_auc'],
             cv=skf, refit='roc_auc', verbose=0, return_train_score=True)
svm_lin.fit(X_train, Y_train)
best_svm_lin = svm_lin.best_estimator_
y_pred_test = best_svm_lin.predict(x_test)
y_pred_proba_test = best_svm_lin.predict_proba(x_test)
```

Now we check the linear SVM performance:

In [16]:
```
print('linear SVM has the best results with: {}'.format(svm_lin.best_params_))
metrics (best_svm_lin,x_test,y_test,y_pred_test, y_pred_proba_test,'hinge')
```

```
linear SVM has the best results with: {'svm__C': 100.0, 'svm__kernel': 'linear'}
Sensitivity is 0.89
Specificity is 0.98
PPV is 0.98
NPV is 0.85
Accuracy is 0.92
F1 is 0.93
```

```
AUROC is 0.95
Hinge Loss is 0.15
```



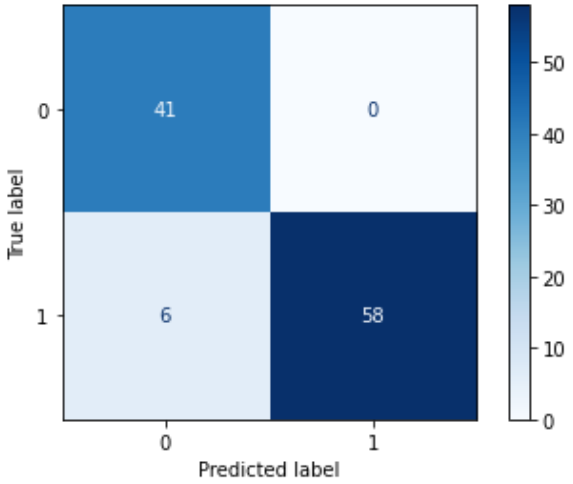
Now we want to train on a non-lionear model:

In [17]:
```
svc1 = SVC(degree=3, gamma='scale',probability=True)
C = np.array([0.001,0.1,1, 100, 1000])
param = [{'svm__C': C, 'svm__kernel': ['rbf','poly'], 'svm__gamma':['auto','scale']}]
pipe = Pipeline(steps=[('svm', svc1)])
# finding the best parameters
svm_nonlin = GridSearchCV(estimator=pipe, param_grid=param,scoring=['accuracy','f1','precision','recall','roc_auc'],
svm_nonlin.fit(X_train, Y_train)
svm_nonlin.best_params_

best_svm_nonlin = svm_nonlin.best_estimator_
y_pred_test = best_svm_nonlin.predict(x_test)
y_pred_proba_test = best_svm_nonlin.predict_proba(x_test)
```

Now we check the non-linear SVM performance:

In [18]:
```
print('non-linear SVM has the best results with: {}'.format(svm_nonlin.best_params_))
metrics (best_svm_nonlin,x_test,y_test,y_pred_test, y_pred_proba_test,'hinge')
```

```
non-linear SVM has the best results with: {'svm__C': 100.0, 'svm__gamma': 'scale', 'svm__kernel': 'rbf'}
Sensitivity is 0.91
Specificity is 1.00
PPV is 1.00
NPV is 0.87
Accuracy is 0.94
F1 is 0.95
AUROC is 0.98
Hinge Loss is 0.11
```

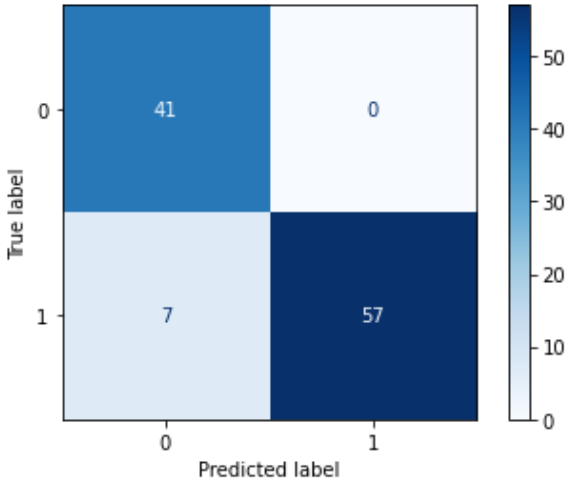


Q5: What performs best on this dataset? Linear or non-linear models?

We can see that using logistic regression produced the worst results in all aspects - Accuracy, F1, AUROC & loss. However, results were still good. Using SVM (both linear & nonlinear) produced very good results. We notice there is no big differnce in most metrics but in all of them we see a slight increase in the nonlinear model, for example the AUROC - where we in the linear model we get a value of 0.95 (which is great!) and for the nonlinear model we get a value of 0.98 (which is almost perfect). Due to this we will state that non-linear models performs slightly better on our dataset, even though the differnces are very slight. It is important to note - our dataset is not very big, and we get very good performance statstics, which might suggest that our model is a bit overfitted.

In [19]:
```
rfc = RandomForestClassifier(n_estimators=100,criterion='gini',max_depth=None,max_features='auto')
model=rfc.fit(X_train,Y_train)
y_pred_rfc = model.predict(x_test)

metrics (model,x_test,y_test,y_pred_test, y_pred_proba_test,'forest')
```

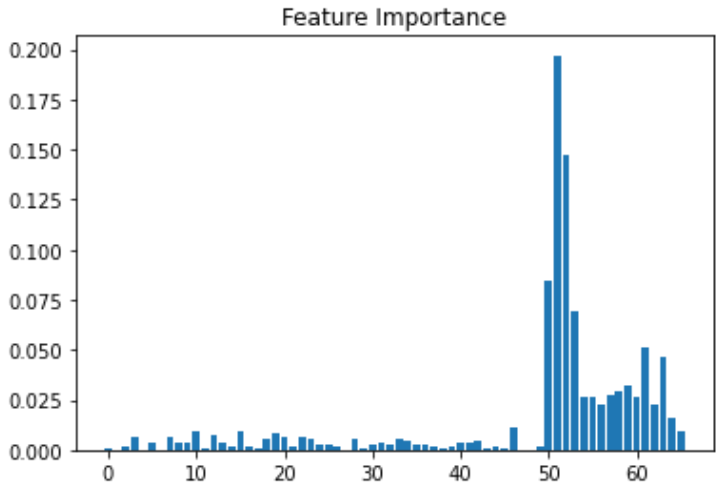
```
Sensitivity is 0.91
Specificity is 1.00
PPV is 1.00
NPV is 0.87
Accuracy is 0.94
F1 is 0.95
AUROC is 0.98
```



In [20]:
```
# finding 2 best features by RFC

m1=max(model.feature_importances_)
l=list(model.feature_importances_)
new_l=set(l)
new_l.remove(m1)
m2=max(new_l)

best_feature=np.where(model.feature_importances_==m1)
second_best_feature=(np.where(model.feature_importances_==m2))
best_feature=best_feature[0]
second_best_feature=second_best_feature[0]

l=X_1H.columns
name1=l[best_feature]
name2=l[second_best_feature]
print(name1,name2)
```

```
Index(['Increased Urination_Yes'], dtype='object') Index(['Increased Thirst_Yes'], dtype='object')
```

In [21]:
```
plt.figure()
plt.title('Feature Importance')
plt.bar(range(X_1H.shape[1]),model.feature_importances_)
plt.show()
```



Accroding to feature importance bar plot, we can see that features from index 50 in X_1H have higher significance:

In [22]:
```
print(l[50:-1])
```

```
Index(['Gender_Male', 'Increased Urination_Yes', 'Increased Thirst_Yes',
       'Sudden Weight Loss_Yes', 'Weakness_Yes', 'Increased Hunger_Yes',
       'Genital Thrush_Yes', 'Visual Blurring_Yes', 'Itching_Yes',
       'Irritability_Yes', 'Delayed Healing_Yes', 'Partial Paresis_Yes',
       'Muscle Stiffness_Yes', 'Hair Loss_Yes', 'Obesity_Yes'],
      dtype='object')
```

Q6,a: What are the 2 most improtant features according to the random forest?

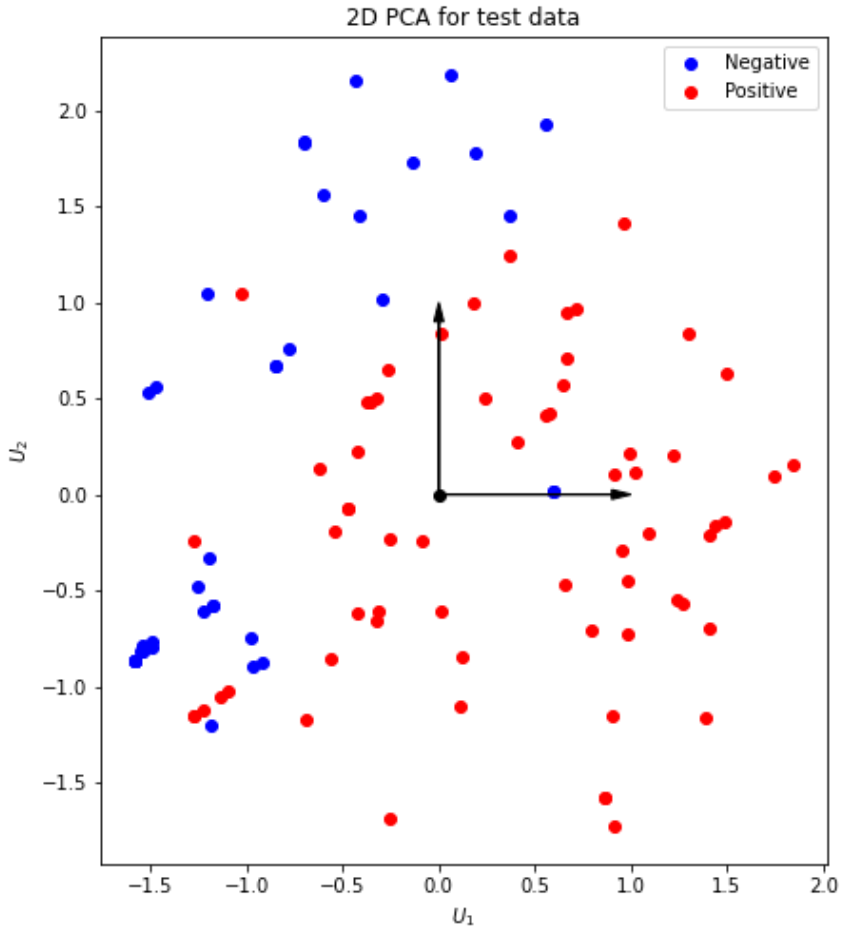
Increased urination & Increased thrist.

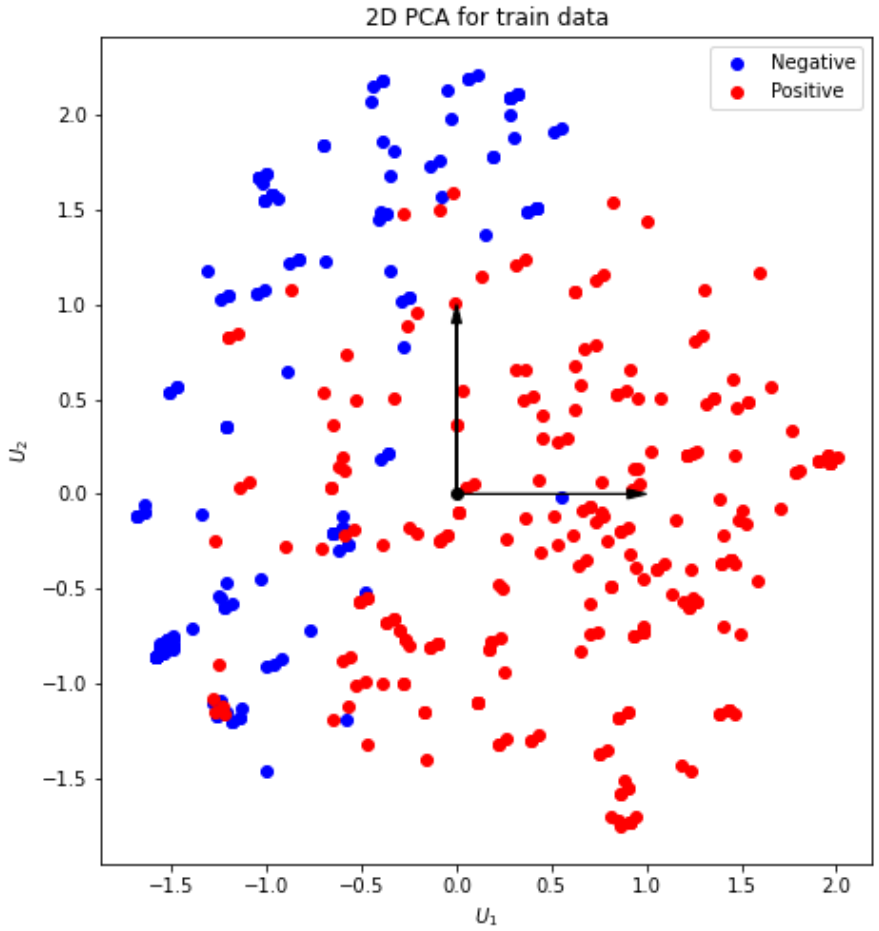
Q6,b: Does this match up exactly with the feature exploration you did?

Yes! We can notice in the plots we disaplyed in Q3 that for both our most important features - almost all positive patients experience these symptoms. This is also known to us from the literature (credit) - patients with T1D experience in very high concentration of glucose in their systems - making their bodies try to balance this concentration by either thirst or urination.

Data Separabillity Visualization

In [27]:
```
pca = PCA(n_components=2, whiten=True)
X_train_pca = pca.fit_transform(X_train)
x_test_pca = pca.transform(x_test)
plt_2d_pca(x_test_pca,y_test, '2D PCA for test data')
plt_2d_pca(X_train_pca,Y_train, '2D PCA for train data')
```


2D PCA for test data
Negative
Positive
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
U_2
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
U_1



By looking at the plots, we can see that other than some outliers (which will always be in the data), the data looks seperable (2nd or 3rd degree polynomial should do the job very well). We can also notice the similarities in both the plots, indicating that the same margin can be used for both test and train data in order to seperate between negative and positive patients.

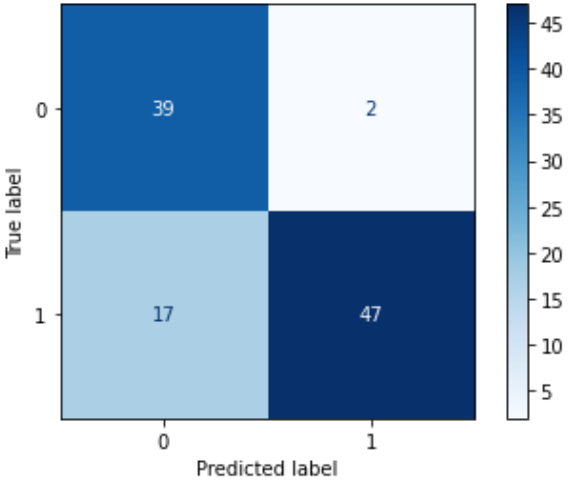
We will start by training on our dimensionality reduced training set:

Logistic regression:

In [28]:
```
skf = StratifiedKFold(n_splits=n_splits, random_state=10, shuffle=True)

log_reg = LogisticRegression(random_state=5, max_iter=max_iter, solver=solver)
lmbda = np.array([0.001, 0.01, 1, 10, 100, 1000])
pipe = Pipeline(steps=[('logistic', log_reg)])
clf = GridSearchCV(estimator=pipe, param_grid={'logistic__C': 1/lmbda, 'logistic__penalty': ['l2']},
        scoring=['accuracy','f1','precision','recall','roc_auc'], cv=skf,
        refit='roc_auc', verbose=0, return_train_score=True)
```

```
clf.fit(X_train_pca, Y_train)
log_reg_opt_pca = clf.best_estimator_
y_pred_test = log_reg_opt_pca.predict(x_test_pca)
y_pred_proba_test = log_reg_opt_pca.predict_proba(x_test_pca)
metrics (log_reg_opt_pca,x_test_pca,y_test,y_pred_test, y_pred_proba_test, 'log')
```

```
Sensitivity is 0.73
Specificity is 0.95
PPV is 0.96
NPV is 0.70
Accuracy is 0.82
F1 is 0.83
AUROC is 0.92
Log Loss is 6.25
```



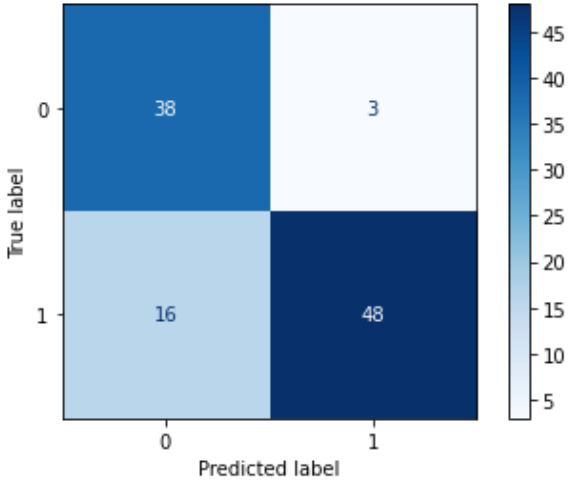
Linear SVM:

In [29]:

```
svc = SVC(probability=True)
C = np.array([0.001, 0.01, 1, 10, 100, 1000])
pipe = Pipeline(steps=[('svm', svc)])
svm_lin = GridSearchCV(estimator=pipe,
             param_grid={'svm__kernel':['linear'], 'svm__C':C},
             scoring=['accuracy','f1','precision','recall','roc_auc'],
             cv=skf, refit='roc_auc', verbose=0, return_train_score=True)
svm_lin.fit(X_train_pca, Y_train)
best_svm_lin_pca = svm_lin.best_estimator_
y_pred_test = best_svm_lin_pca.predict(x_test_pca)
y_pred_proba_test = best_svm_lin_pca.predict_proba(x_test_pca)
metrics (best_svm_lin_pca,x_test_pca,y_test,y_pred_test, y_pred_proba_test, 'hinge')
```

```
Sensitivity is 0.75
Specificity is 0.93
PPV is 0.94
```

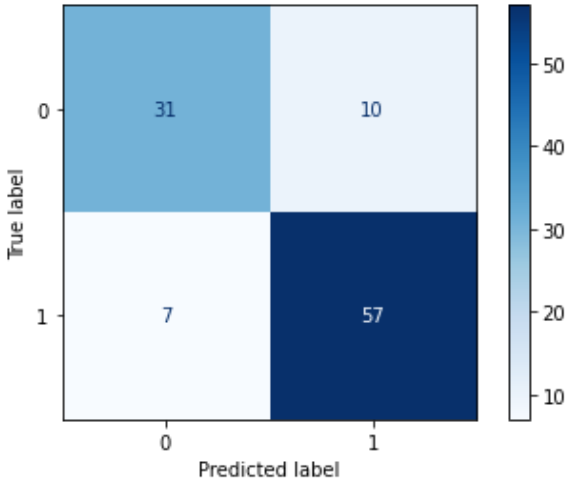
```
NPV is 0.70
Accuracy is 0.82
F1 is 0.83
AUROC is 0.92
Hinge Loss is 0.36
```



Non-linear SVM:

In [30]:
```
svc1 = SVC(degree=3, gamma='scale',probability=True)
C = np.array([0.001,0.1,1, 100, 1000])
param = [{'svm__C': C, 'svm__kernel': ['rbf','poly'], 'svm__gamma':['auto','scale']}]
pipe = Pipeline(steps=[('svm', svc1)])
# finding the best parameters
svm_nonlin = GridSearchCV(estimator=pipe, param_grid=param,scoring=['accuracy','f1','precision','recall','roc_auc'],
svm_nonlin.fit(X_train_pca, Y_train)
svm_nonlin.best_params_

best_svm_nonlin_pca = svm_nonlin.best_estimator_
y_pred_test = best_svm_nonlin_pca.predict(x_test_pca)
y_pred_proba_test = best_svm_nonlin_pca.predict_proba(x_test_pca)
metrics (best_svm_nonlin_pca,x_test_pca,y_test,y_pred_test, y_pred_proba_test,'hinge')
```

```
Sensitivity is 0.89
Specificity is 0.76
PPV is 0.85
NPV is 0.82
Accuracy is 0.84
F1 is 0.87
AUROC is 0.94
Hinge Loss is 0.32
```



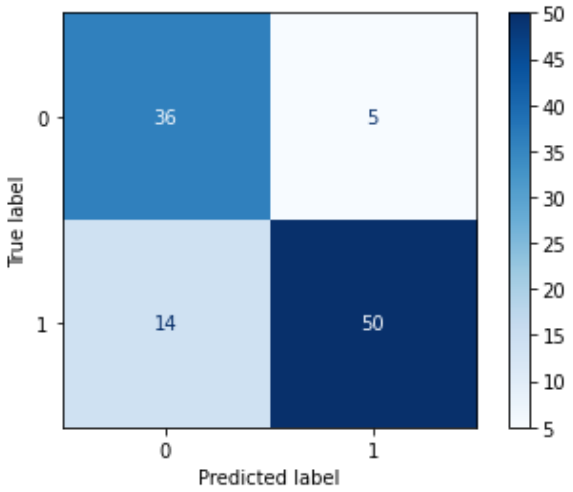
Now we will reduce the data to the 2 best features we found in section 6 and repeat the process:

In [31]:
```
X_train_2f = X_train.iloc[:,[51,52]]
x_test_2f = x_test.iloc[:,[51,52]]
```

Logistic Regression:

In [32]:
```
skf = StratifiedKFold(n_splits=n_splits, random_state=10, shuffle=True)

log_reg = LogisticRegression(random_state=5, max_iter=max_iter, solver=solver)
lmbda = np.array([0.001, 0.01, 1, 10, 100, 1000])
pipe = Pipeline(steps=[('logistic', log_reg)])
clf = GridSearchCV(estimator=pipe, param_grid={'logistic__C': 1/lmbda, 'logistic__penalty': ['l2']},
        scoring=['accuracy','f1','precision','recall','roc_auc'], cv=skf,
        refit='roc_auc', verbose=0, return_train_score=True)
clf.fit(X_train_2f, Y_train)
log_reg_opt_2f = clf.best_estimator_
y_pred_test = log_reg_opt_2f.predict(x_test_2f)
y_pred_proba_test = log_reg_opt_2f.predict_proba(x_test_2f)
metrics (log_reg_opt_2f,x_test_2f,y_test,y_pred_test, y_pred_proba_test,'log')
```

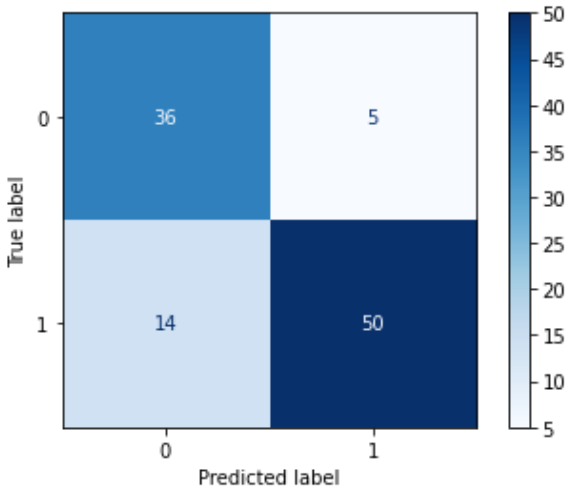
```
Sensitivity is 0.78
Specificity is 0.88
PPV is 0.91
NPV is 0.72
Accuracy is 0.82
F1 is 0.84
AUROC is 0.86
Log Loss is 6.25
```



Linear SVM:

In [33]:
```
svc = SVC(probability=True)
C = np.array([0.001, 0.01, 1, 10, 100, 1000])
pipe = Pipeline(steps=[('svm', svc)])
svm_lin = GridSearchCV(estimator=pipe,
             param_grid={'svm__kernel':['linear'], 'svm__C':C},
             scoring=['accuracy','f1','precision','recall','roc_auc'],
             cv=skf, refit='roc_auc', verbose=0, return_train_score=True)
svm_lin.fit(X_train_2f, Y_train)
best_svm_lin_2f = svm_lin.best_estimator_
y_pred_test = best_svm_lin_2f.predict(x_test_2f)
y_pred_proba_test = best_svm_lin_2f.predict_proba(x_test_2f)
metrics (best_svm_lin_2f,x_test_2f,y_test,y_pred_test, y_pred_proba_test,'hinge')
```

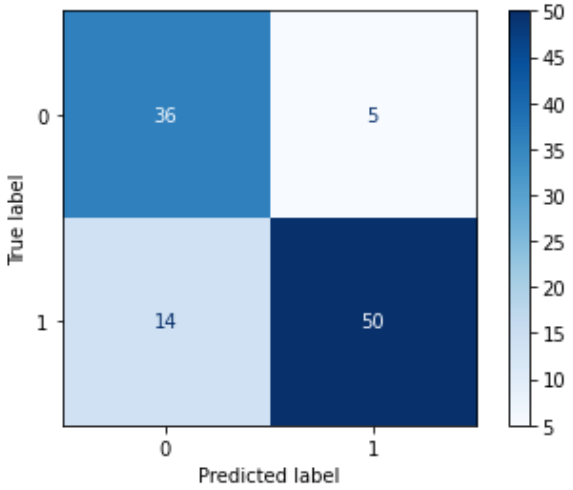
```
Sensitivity is 0.78
Specificity is 0.88
PPV is 0.91
NPV is 0.72
Accuracy is 0.82
F1 is 0.84
AUROC is 0.86
Hinge Loss is 0.36
```



Non-Linear SVM:

In [34]:
```
svc1 = SVC(degree=3, gamma='scale',probability=True)
C = np.array([0.001,0.1,1, 100, 1000])
param = [{'svm__C': C, 'svm__kernel': ['rbf','poly'], 'svm__gamma':['auto','scale']}]
pipe = Pipeline(steps=[('svm', svc1)])
# finding the best parameters
svm_nonlin = GridSearchCV(estimator=pipe, param_grid=param,scoring=['accuracy','f1','precision','recall','roc_auc'],
svm_nonlin.fit(X_train_2f, Y_train)
svm_nonlin.best_params_
best_svm_nonlin_2f = svm_nonlin.best_estimator_
y_pred_test = best_svm_nonlin_2f.predict(x_test_2f)
y_pred_proba_test = best_svm_nonlin_2f.predict_proba(x_test_2f)
metrics (best_svm_nonlin_2f,x_test_2f,y_test,y_pred_test, y_pred_proba_test,'hinge')
```

```
Sensitivity is 0.78
Specificity is 0.88
PPV is 0.91
NPV is 0.72
Accuracy is 0.82
F1 is 0.84
AUROC is 0.86
Hinge Loss is 0.36
```



Q7: What performs better? 2 features or reduced dimensionality?

In order to answer this question, we summarized the most important metrics in the table below:

	Accuracy	F1	AUROC	Loss
Log Regression PCA	0.82	0.83	0.92	6.25
Linear SVM PCA	0.82	0.83	0.92	0.36
Non-linear SVM PCA	0.84	0.87	0.94	0.32
Log Regression 2Features	0.82	0.84	0.86	6.25
Linear SVM 2Features	0.82	0.84	0.86	0.36
Non-linear SVM 2Features	0.82	0.84	0.86	0.36

First of all, we can notice that for the 2features data, all models perform exactly the same. This is expected because we have only 2 features with binary results, making even the simplest model very effective. When comparing between the different models for PCA, we can see that non-linear SVM improved all the evaluation metrics when compared to the linear models. When comparing between the 2 training sets, we can see that in general the PCA set shows better metrics, especially for AUROC. When using a non-linear model with the PCA data we see the highest increase in all of the metrics. We will conclude that the PCA data performs better. We might say we expected PCA to perform better, because the 2 axis contain not only the 2 most important features, but a linear combination of all the features, thus taking into account other important features which might affect our diagnosis. However, the 2feature data provides an advantage by being simple and quick, and still being a reliable estimator.