CS 534: Machine Learning Homework 4

Problem 1: Kernel Methods

(a) According to the given conditions, the kernel can be expressed as:

$$k_\beta(\mathbf{x},\mathbf{z}) = (1+\beta\mathbf{x}\cdot\mathbf{z})^2 - 1 = 2\beta\mathbf{x}\cdot\mathbf{z} + (\beta\mathbf{x}\cdot\mathbf{z})^2$$
$$= 2\beta(\mathrm{x}_1\mathrm{z}_1 + \mathrm{x}_2\mathrm{z}_2) + \beta^2(\mathrm{x}_1\mathrm{z}_1 + \mathrm{x}_2\mathrm{z}_2)^2$$
$$= 2\beta(\mathrm{x}_1\mathrm{z}_1 + \mathrm{x}_2\mathrm{z}_2) + \beta^2[(\mathrm{x}_1\mathrm{z}_1)^2 + 2\mathrm{x}_1\mathrm{z}_1\mathrm{x}_2\mathrm{z}_2 + (\mathrm{x}_2\mathrm{z}_2)^2]$$
$$= 2\beta\mathrm{x}_1\mathrm{z}_1 + 2\beta\mathrm{x}_2\mathrm{z}_2 + 2\beta^2\mathrm{x}_1\mathrm{z}_1\mathrm{x}_2\mathrm{z}_2 + \beta^2{\mathrm{x}_1}^2{\mathrm{z}_1}^2 + \beta^2{\mathrm{x}_2}^2{\mathrm{z}_2}^2$$

Let $\phi(\mathbf{x}) = \big(\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \phi_3(\mathbf{x}), \phi_4(\mathbf{x}), \phi_5(\mathbf{x})\big)$, then if we choose

$$\phi_1(\mathbf{x}) = \sqrt{2\beta}\mathrm{x}_1$$

$$\phi_2(\mathbf{x}) = \sqrt{2\beta}\mathrm{x}_2$$

$$\phi_3(\mathbf{x}) = \sqrt{2}\beta\mathrm{x}_1\mathrm{x}_2$$

$$\phi_4(\mathbf{x}) = \beta(\mathrm{x}_1)^2$$
$$\phi_5(\mathbf{x}) = \beta(\mathrm{x}_2)^2$$

then $k_\beta(\mathbf{x},\mathbf{z}) = \phi(\mathbf{x})\cdot\phi(\mathbf{z})$, where

$$\phi(\mathbf{x}) = \big(\sqrt{2\beta}\mathrm{x}_1, \sqrt{2\beta}\mathrm{x}_2, \sqrt{2}\beta\mathrm{x}_1\mathrm{x}_2, \beta(\mathrm{x}_1)^2, \beta(\mathrm{x}_2)^2\big)$$

(b) Because $k(\mathrm{x},\mathrm{z}) = \mathrm{x}^{\mathrm{T}}\mathrm{z}$, we can obtain some transformations according to the rules. Given the rule (i), let $k_0(\mathrm{x},\mathrm{z}) = \mathrm{x}^{\mathrm{T}}\mathrm{z}$ and $f(\mathbf{x}) = 1/\|\mathbf{x}\|_2$, then

$$k_1(\mathrm{x},\mathrm{z}) = f(\mathbf{x})f(\mathbf{z})k_0(\mathrm{x},\mathrm{z}) = \left(\frac{\mathbf{x}}{\|\mathbf{x}\|_2}\right)^{\mathrm{T}}\left(\frac{\mathbf{z}}{\|\mathbf{z}\|_2}\right)$$

Given the rule (iii) and the $k_1(\mathrm{x},\mathrm{z})$, we have

$$k_2(\mathrm{x},\mathrm{z}) = k_1(\mathrm{x},\mathrm{z})k_0(\mathrm{x},\mathrm{z}) = 1$$

Given the rule (ii) and the $k_2(\mathrm{x},\mathrm{z})$ and $k_1(\mathrm{x},\mathrm{z})$,

$$k_3(\mathrm{x},\mathrm{z}) = k_2(\mathrm{x},\mathrm{z}) + k_1(\mathrm{x},\mathrm{z}) = \left[1 + \left(\frac{\mathbf{x}}{\|\mathbf{x}\|_2}\right)^{\mathrm{T}}\left(\frac{\mathbf{z}}{\|\mathbf{z}\|_2}\right)\right]$$

Finally, given the rule (iii),

$$k_4(\mathrm{x},\mathrm{z}) = [k_3(\mathrm{x},\mathrm{z})]^3 = \left[1 + \left(\frac{\mathbf{x}}{\|\mathbf{x}\|_2}\right)^{\mathrm{T}}\left(\frac{\mathbf{z}}{\|\mathbf{z}\|_2}\right)\right]^3$$

Then, the required kernel is obtained by the rules and $k(\mathrm{x},\mathrm{z}) = \mathrm{x}^{\mathrm{T}}\mathrm{z}$.

In [1]:
```
import numpy as np
import pandas as pd
from sklearn import tree,svm
from sklearn import model_selection
from sklearn import preprocessing
import matplotlib.pyplot as plt
from sklearn.externals.six import StringIO
#import pydot
from IPython.display import Image
from sklearn import metrics
from mpl_toolkits.mplot3d import Axes3D
from sklearn.utils import shuffle,resample
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import KFold,cross_val_score
import seaborn as sns
%matplotlib inline
```

Problem 2

In [415]:
```
data = pd.read_csv('allhyper.data')
data['class'] = data['class'].str.rsplit('.',expand=True)[0]
data.dropna(axis=1, how='all', inplace=True)
label_types = data.dtypes.values
labels = data.columns
```

Preprocessing

In [296]:
```
print 'percentage of class = "hyperthyroid" in the data:\t',
(data[data['class']=='hyperthyroid'].shape[0]*1.0/data.shape[0])*100,'%'
```

```
percentage of class = "hyperthyroid" in the data:       2.21428571429 %
```

Because the value of the class is highly imbalanced such that the class only has 2.21 % of the key value 'hyperthyroid', the misclassification cannot exactly show the performance of models. So F1 score with 'recall' is more suitable for validate the performance of models. Particularly, F2 score may be more expected than F1 score **because it weights recall higher than precision by placing more emphasis on false negatives**.

In [416]:
```
miss = pd.DataFrame(data.isnull().sum())/data.shape[0]*100
miss = pd.concat([miss,data.dtypes],axis=1)
miss.columns = ['percentage of missing values','data type']
miss[miss['percentage of missing values']>0]
```

Out[416]:

	percentage of missing values	data type
age	0.035714	float64
sex	3.928571	object
TSH	10.142857	float64
T3	20.892857	float64
TT4	6.571429	float64
T4U	10.607143	float64
FTI	10.535714	float64

As you can see from the table above,

1.There are missing values in data set. We handle the missing values according to their typye:

(1)using the mean to fill 'float' missing values; (2)the missing 'object' value would not be handled because of the advantage of tree.

2.Because original data are object values, we transform the **object vaues to binary values or multinomial values for the use of sklearn package**.

In [417]:
```
for i in range(len(label_types)-1):
    if label_types[i] == 'float':
        data[labels[i]].fillna(data[labels[i]].mean(), inplace=True)
    else:
        data[labels[i]].fillna('None', inplace=True)
object_names = data.dtypes[data.dtypes=='object'].index.values
objects = {}
for key in object_names[:-1]: # not include 'class' column
    objects[key] = data.groupby(key).sum().index.values
objects
```

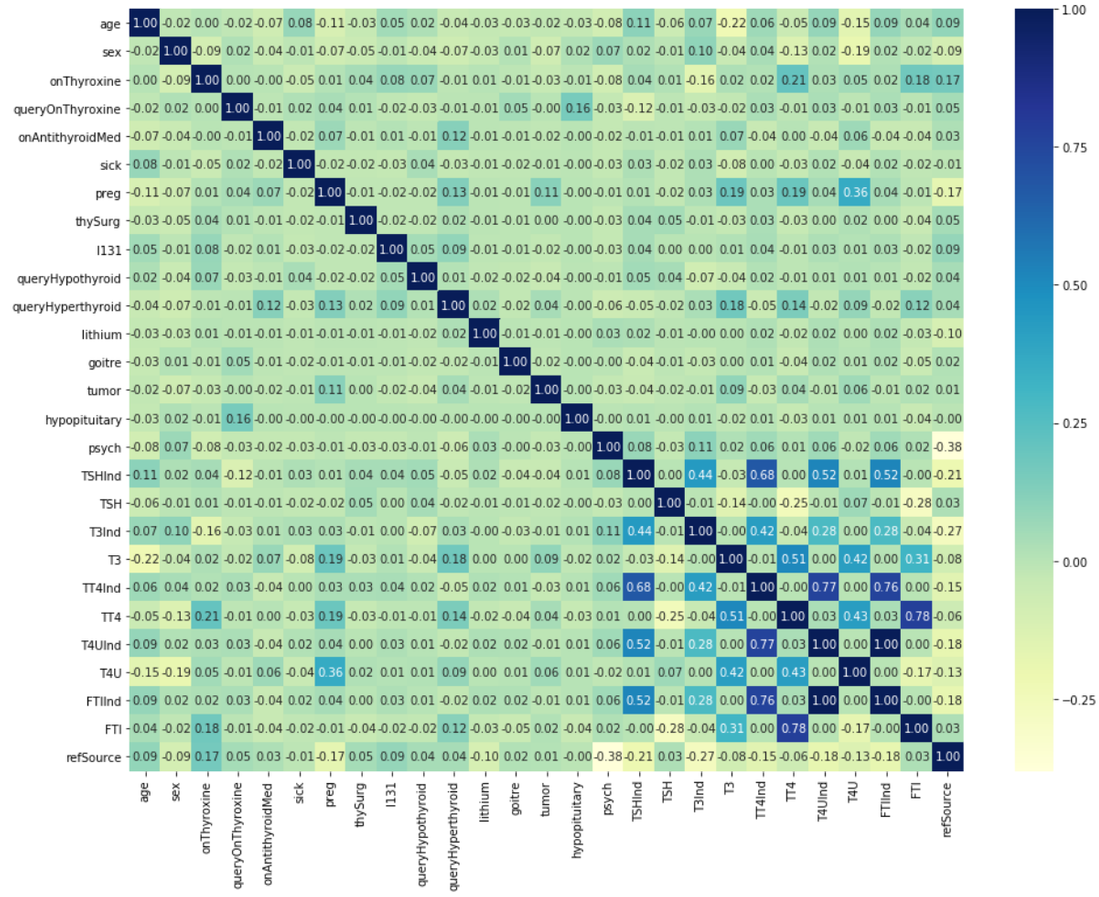
Out[417]:
```
{'FTIInd': array(['f', 't'], dtype=object),
 'I131': array(['f', 't'], dtype=object),
 'T3Ind': array(['f', 't'], dtype=object),
 'T4UInd': array(['f', 't'], dtype=object),
 'TBGInd': array(['f'], dtype=object),
 'TSHInd': array(['f', 't'], dtype=object),
 'TT4Ind': array(['f', 't'], dtype=object),
 'goitre': array(['f', 't'], dtype=object),
 'hypopituitary': array(['f', 't'], dtype=object),
 'lithium': array(['f', 't'], dtype=object),
 'onAntithyroidMed': array(['f', 't'], dtype=object),
 'onThyroxine': array(['f', 't'], dtype=object),
 'preg': array(['f', 't'], dtype=object),
 'psych': array(['f', 't'], dtype=object),
 'queryHyperthyroid': array(['f', 't'], dtype=object),
 'queryHypothyroid': array(['f', 't'], dtype=object),
 'queryOnThyroxine': array(['f', 't'], dtype=object),
 'refSource': array(['STMW', 'SVHC', 'SVHD', 'SVI', 'other'], dtype=obj
ect),
 'sex': array(['F', 'M', 'None'], dtype=object),
 'sick': array(['f', 't'], dtype=object),
 'thySurg': array(['f', 't'], dtype=object),
 'tumor': array(['f', 't'], dtype=object)}
```

As you can see, most object-type values are binary type except for 'refSource'. So 'refSource' is transformed to a multinomial feature and others are transformed to binary features. In addition, the feature 'TBGInd' is full of single value such that it does not have influence on classification, so it can be removed.

In [418]:
```
for key, value in objects.items():
    for i in range(len(value)):
        data[key].replace(to_replace=value[i],value=i,inplace=True)
data.drop('TBGInd',axis=1,inplace=True)
data_y = pd.get_dummies(data['class']).iloc[:,2]
data.drop('class',axis=1,inplace=True)
```

In [419]:
```
plt.figure(figsize=(16,12))
sns.heatmap(data.corr(),cmap="YlGnBu",annot=True,fmt='.2f')
```

Out[419]: <matplotlib.axes._subplots.AxesSubplot at 0x1a1e8a2fd0>



In [420]:
```
data.drop('T4UInd',axis=1,inplace=True)
```

(a)

In [421]:
```
class myRandomForest(object):
    def __init__(self, nest, criterion, maxDepth, minSamplesLeaf):
        self.nest = nest
        self.criterion = criterion
        self.maxDepth = maxDepth
        self.minSamplesLeaf = minSamplesLeaf
        self.forest = {}
        self.oob_dict = {}
        self.features = {}
        self.oob_score = {}
    def fit(self, trainX, trainY):
        self.labels = trainX.columns.values
        self.m = int(np.sqrt(trainX.shape[0]))
        for b in range(self.nest):
            x_train,y_train = resample(trainX,trainY,replace=True)
            x_test =
trainX.loc[trainX.index.drop(x_train.index.unique())]
            y_test =
trainY.loc[trainY.index.drop(y_train.index.unique())]
            new_labels = resample(self.labels,n_samples=self.m)
            dtc = tree.DecisionTreeClassifier(criterion=self.criterion,
max_depth = self.maxDepth, min_samples_leaf=self.minSamplesLeaf)
            dtc.fit(x_train[new_labels],y_train)
            self.features[b] = new_labels
            self.oob_dict[b] = (x_test,y_test)
            self.oob_score[b] = dtc.score(x_test[new_labels],y_test)
            self.forest[b] = dtc
        return
    def calc_features_importance(self,  B=-1):
        if B == -1:
            B = self.nest
        # calculate the feature importances of the whole random forest
        importance_dict = {}
        for item in self.labels:
            importance_dict[item] = 0.0
        for key in range(B):
            names = self.features[key]
            oobs = self.oob_dict[key]
            old_acc = self.oob_score[key]
            for i in range(len(names)):
                oobs_x = oobs[0].copy()
                oobs_x[names[i]] =
np.random.permutation(oobs_x[names[i]])
                new_acc = self.forest[key].score(oobs_x[names],oobs[1])
                importance_dict[names[i]] = np.mean([importance_dict[nam
es[i]],abs(old_acc-new_acc)])
        return importance_dict
    def calc_oob(self,  B=-1):
        if B == -1:
            B = self.nest
        total = 0.0
        for key in range(B):
            total += self.oob_score[key]
        return total/B
    def predict(self, x, B=-1):
        if B == -1:
            B = self.nest
        pre = []
        for key in range(B):
            pre.append(self.forest[key].predict(x[self.features[key]]))
        nonzeros = np.count_nonzero(pre,axis=0)
        result = []
        for item in nonzeros:
            result.append(1 if item >= (self.nest/2) else 0)
        return result
    def score(self, x, y,  B=-1):
        if B == -1:
            B = self.nest
        result = 0.0
        for key in range(B):
            result += self.forest[key].score(x[self.features[key]],y)
        return result/self.nest
```

In [424]:
```
trainX, testX, trainY, testY = model_selection.train_test_split(data, da
ta_y, test_size=3.0/10)
```

In [440]:
```
nest = 25
criterion = 'gini'
maxDepth = 5
minSamplesLeaf = 5

myforest = myRandomForest(nest, criterion,maxDepth,minSamplesLeaf)
myforest.fit(trainX,trainY)

print 'OOB accuracy:\t', myforest.calc_oob()
print 'test set score:\t', myforest.score(testX,testY)
print 'test set F2 score:\t',
metrics.fbeta_score(testY,myforest.predict(testX),beta=2.0)
```

```
OOB accuracy:   0.984155340424
test set score: 0.988666666667
test set F2 score:      0.792682926829
```

(b)

In [427]:
```
def calc_scores(nest, criterion, x_index, y_index, train_x, train_y):
    result = {}
    for i in range(10,nest):
        result[i] = np.zeros((len(y_index),len(x_index)))

    for j in x_index: # min_samples_leaf = j
        for k in y_index: # max_depth = k
            myForest = myRandomForest(nest, criterion,k,j)
            myForest.fit(train_x,train_y)
            for i in range(10,nest):
                result[i][k-1][j-1] = myForest.calc_oob(i)
    return result
```

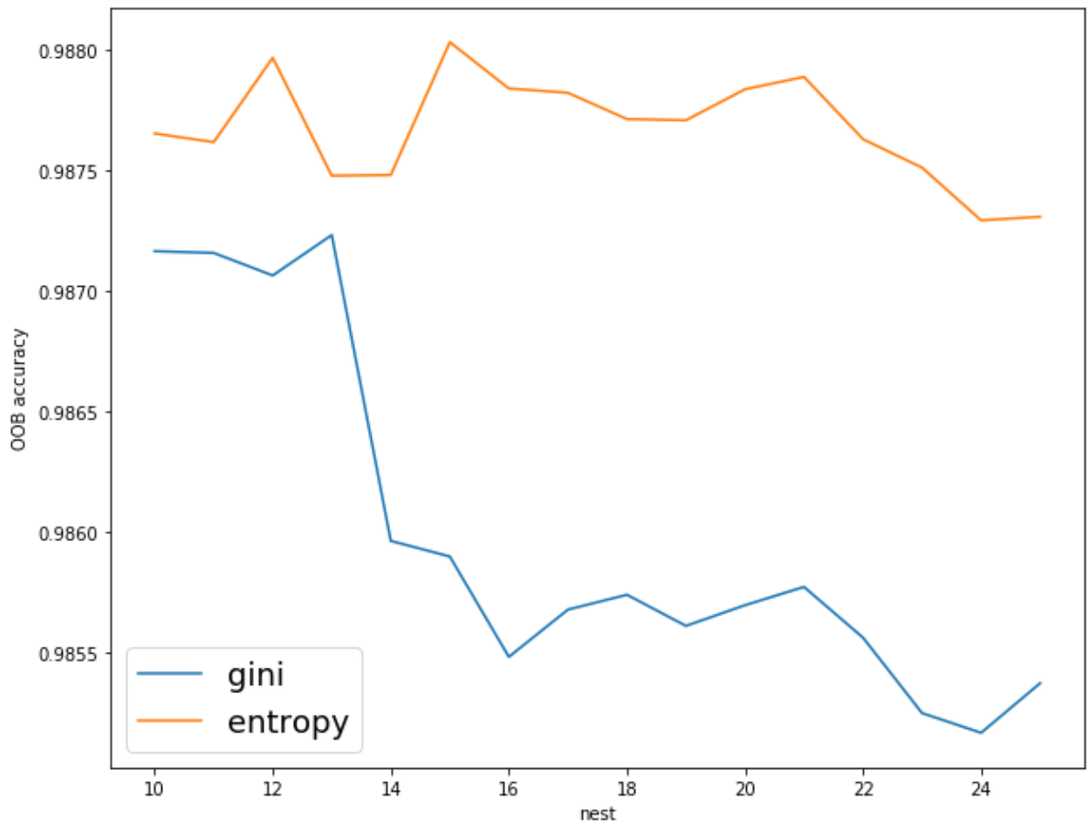
In [428]:
```
x_index = range(1,36)
y_index = range(1,31)
X,Y = np.meshgrid(x_index,y_index)

score_dict_g = calc_scores(26, 'gini', x_index, y_index, trainX, trainY)
score_dict_e = calc_scores(26, 'entropy', x_index, y_index, trainX, trai
nY)
```

In [429]:
```
g_max_arr = []
e_max_arr = []
for i in range(10,26):
    g_max_arr.append(np.max(score_dict_g[i]))
    e_max_arr.append(np.max(score_dict_e[i]))
table = pd.DataFrame(data=[[np.max(g_max_arr),np.argmax(g_max_arr)+10],
[np.max(e_max_arr),np.argmax(e_max_arr)+10]], index=['gini','entropy'],c
olumns=['max_oob_score','optimal nest'])
table.head()
```

Out[429]:

	max_oob_score	optimal nest
gini	0.987232	13
entropy	0.988033	15

In [431]:
```
fig = plt.figure(figsize=(10,8))
plt.plot(range(10,26),g_max_arr,label='gini')
plt.plot(range(10,26),e_max_arr,label='entropy')
plt.ylabel('OOB accuracy')
plt.xlabel('nest')
plt.legend(fontsize=18)
plt.show()
```

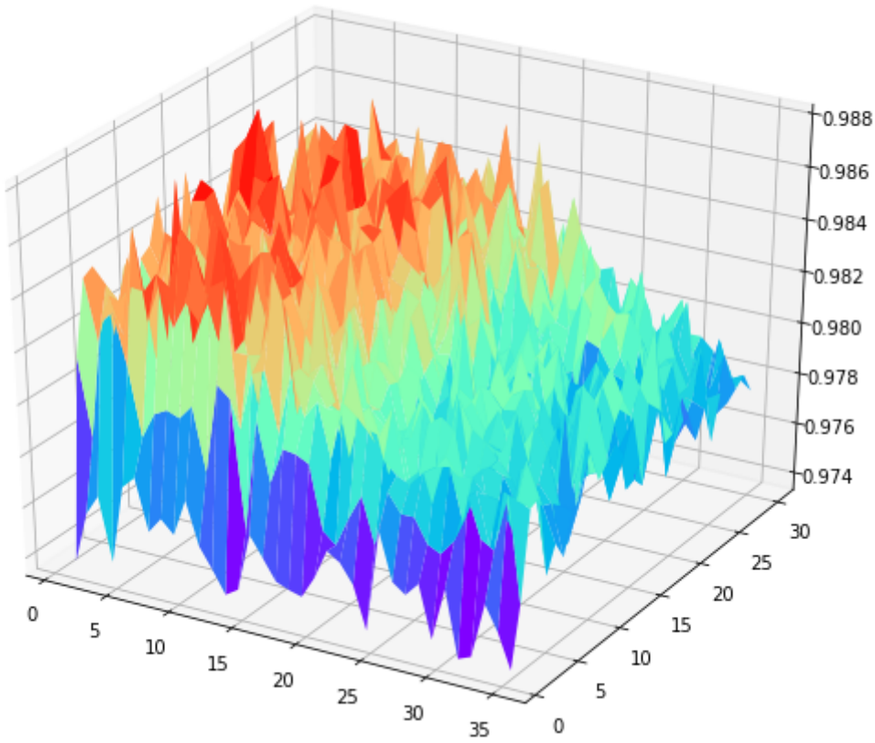


As we can see in the figure above, if we use the **oob sample accuracy** to choose parameters, **the best split criterion must be 'entropy' and the best nest is 15.** Because of the randomness of splits of data set and the features selection of random forest, the result is not the same every time. So for this data set, the entropy is more suitable for this data set and the nest value should not be too big, because excessive 'voters' easily introduce uncertainty and mess such that the entropy increases.

In [432]:
```
print 'Optimal Choices of parameters:'
print 'max_depth\t','min_samples_leaf'
print
np.argmax(np.max(score_dict_e[15],axis=1))+1,'\t\t\t',np.argmax(np.max(s
core_dict_e[15],axis=0))+1
```

```
Optimal Choices of parameters:
max_depth       min_samples_leaf
5                       7
```

In [433]:
```
fig = plt.figure(figsize=(10,8))
ax1 = fig.gca(projection='3d')
ax1.plot_surface(X,Y,score_dict_e[15],rstride=1, cstride=1, cmap='rainbo
w')
fig.show()
```



As we can see from the 3d figure, the optimal min_samples_leaf area is (0,12), the accuracy decreases as the min_samples_leaf increases. In addition, for max depth, there is no explicit trend for accuracy. I think it changes along with the randomness of the data splits.

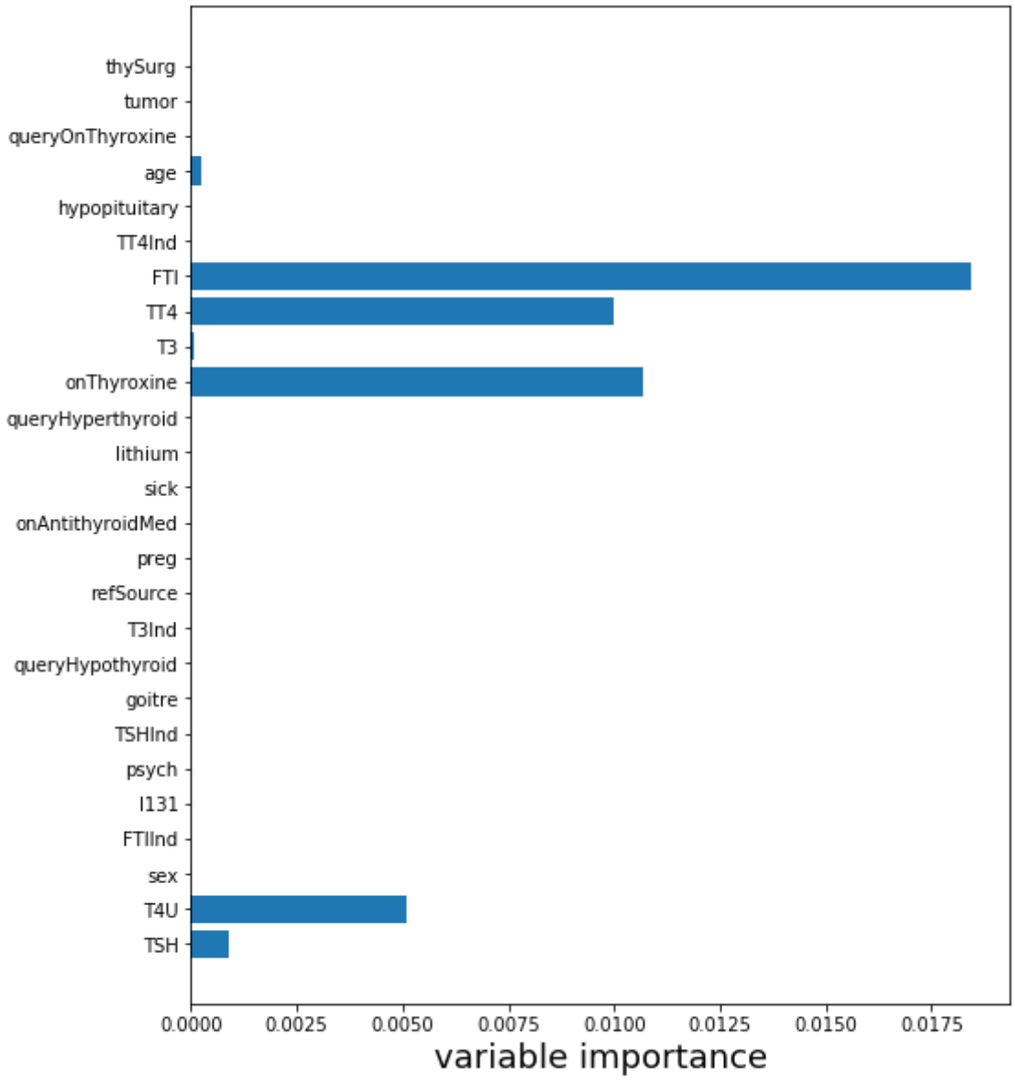
(c)

In [443]:
```
myForest = myRandomForest(15, 'entropy', np.argmax(np.max(score_dict_e[1
5],axis=1))+1,np.argmax(np.max(score_dict_e[15],axis=0))+1)
myForest.fit(trainX,trainY)
test_score = myForest.score(testX,testY)
best_oob = myForest.calc_oob()
print 'test_score \t best_oob \t test set F2 score'
print test_score,'\t',best_oob, metrics.fbeta_score(testY,myforest.predi
ct(testX),beta=2.0)
```

```
test_score       best_oob        test set F2 score
0.988253968254  0.983513077317 0.792682926829
```

(d)

In [438]:
```
importance_dict = myForest.calc_features_importance()
y_pos = range(len(importance_dict.keys()))
fig = plt.figure(figsize=(8,10))
plt.barh(y_pos,importance_dict.values())
plt.yticks(y_pos,importance_dict.keys())
plt.xlabel('variable importance',fontsize=18)
plt.show()
```



From the variable importance figure above, we can know that the most important features is the 'FTI'

Problem 3

(a)(b)

In [390]:
```
'''
    load data from txt file
'''
def load_data(filename):
    f = open(filename, 'r')
    k = 0
    data = f.read()
    f.close()
    data_list = data.split('\n')
    d = {}
    for line in data_list:
        if line != '' :
            arr = line.split(' ')
            d[k] = (arr[0],set(arr[1:]))
            k+=1

    return d
def construct_matrix(data,keys,features):
    y = []
    x = []
    for key in keys:
        y.append(data[key][0])
        temp = np.zeros(len(features))
        for i in range(len(features)):
            if features[i] in data[key][1]:
                temp[i] = 1
        x.append(temp)
    return np.array(x),np.array(y)
def get_data(split_rate):
    origin_d = load_data('spamAssassin.data')
    whole = shuffle(origin_d.keys())
    size = int(len(whole)*0.7)
    train_keys = whole[:size]
    test_keys = whole[size:]
    features = {}
    for key in train_keys:
        for word in origin_d[key][1]:
            try:
                features[word] += 1
            except :
                features[word] = 1
    for key in features.keys():
        if features[key] < 30 :
            del features[key]
    features_arr = features.keys()
    trainX,trainY = construct_matrix(origin_d, train_keys, features_arr)
    testX,testY = construct_matrix(origin_d, test_keys,features_arr)
    trainY = trainY.astype(int)
    np.place(trainY, trainY == 0, -1)
    testY = testY.astype(int)
    np.place(testY, testY == 0, -1)
    return trainX,trainY,testX,testY
```

(c)(e)

In [391]:
```
class perceptron(object):
    def __init__(self, max_epoch = float('inf')):
        self.max_epoch = max_epoch

    def fit(self,x,y,shuffle_flag=False):
        self.mistakes = 0
        self.epochs = 0
        n,p = x.shape
        #x = x.as_matrix()
        self.w = np.ones(p)/(p*1.0)
        self.w0 = 0
        self.w_mean = np.ones(p)/(p*1.0)
        self.w0_mean = 0
        temp_mistakes = -1
        while temp_mistakes != 0:
            temp_mistakes = 0
            if shuffle_flag :
                x,y = shuffle(x,y)
            for i in range(n):
                if y[i]*np.sign(self.w0+np.dot(self.w,x[i])) < 0:
                    temp_mistakes += 1
                    self.w = self.w + y[i]*x[i]
                    self.w0 = self.w0 + y[i]
                self.w_mean = np.add(self.w_mean,self.w)
                self.w0_mean += self.w0
            self.mistakes += temp_mistakes
            self.epochs += 1
            if self.epochs >= self.max_epoch:
                break
        self.w_mean /= (self.epochs*n*1.0)
        self.w0_mean /= (self.epochs*n*1.0)
    def test(self,x,y):
        n = x.shape[0]
        temp_errs = 0
        for i in range(n):
            if y[i]*np.sign(self.w0+np.dot(self.w,x[i])) < 0:
                temp_errs += 1
        return temp_errs*1.0/n
    def avg_test(self,x,y):
        n = x.shape[0]
        temp_errs = 0
        for i in range(n):
            if y[i]*np.sign(self.w0_mean+np.dot(self.w_mean,x[i])) < 0:
                temp_errs += 1
        return temp_errs*1.0/n
```

(d)

In [398]:
```
trainX,trainY,testX,testY = get_data(0.7)
```

In [399]:
```
pct = perceptron()
pct.fit(trainX,trainY)
print 'Stop criterion: no new mistakes in train set'
print 'Mistakes:\t', pct.mistakes
print 'Estimated pridiction error:\t', pct.test(testX,testY)
```

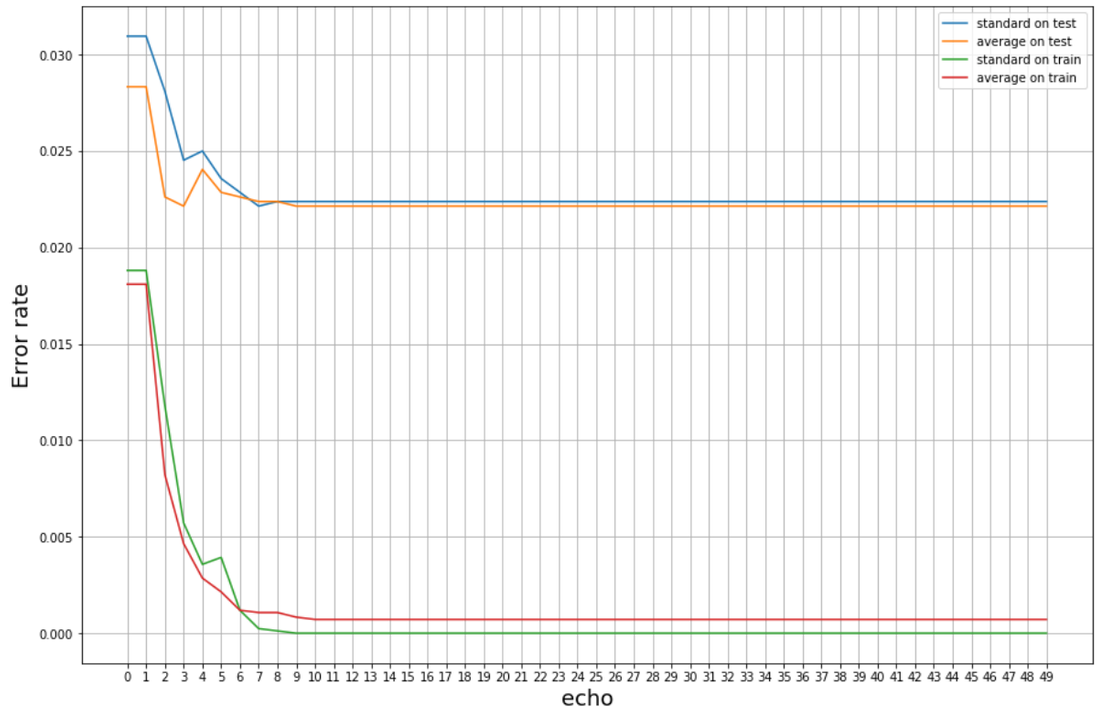
```
Stop criterion: no new mistakes in train set
Mistakes:       471
Estimated pridiction error:     0.015
```

(f)

1.If we do not shuffle data after training through the data each echo, which means the perceptron is trained by a fixed direction such that test error can converge. Although the method without shuffle cannot gaurantee that it can obtain the optimal classifier for the data, it is stable.

2.If we shuffle the data after each epoch. Because there is no fixed order of training sequence, it would not be outfiting to the data such that it can achieve better performance than that of the model without shuffle. However, the random training leads to instability on test error such that some time its performance is worse than that of model without shuffle.

In [400]:
```
epochs = range(50)
std_err = []
avg_err = []
train_std = []
train_avg = []
kf = KFold(n_splits = 3)
for train_index,test_index in kf.split(trainX):
    train_x, test_x = trainX[train_index],trainX[test_index]
    train_y, test_y = trainY[train_index],trainY[test_index]
    temp_std_err = []
    temp_avg_err = []
    temp_train_std = []
    temp_train_avg = []
    for i in epochs:
        pct = perceptron(i)
        pct.fit(train_x,train_y,shuffle_flag=False)
        temp_std_err.append(pct.test(test_x,test_y))
        temp_avg_err.append(pct.avg_test(test_x,test_y))
        temp_train_std.append(pct.test(train_x,train_y))
        temp_train_avg.append(pct.avg_test(train_x,train_y))
    std_err.append(temp_std_err)
    avg_err.append(temp_avg_err)
    train_std.append(temp_train_std)
    train_avg.append(temp_train_avg)
std_err = np.mean(np.array(std_err),axis=0)
avg_err = np.mean(np.array(avg_err),axis=0)
train_std = np.mean(np.array(train_std),axis=0)
train_avg = np.mean(np.array(train_avg),axis=0)

plt.figure(figsize=(15,10))
plt.plot(epochs,std_err, label='standard on test')
plt.plot(epochs,avg_err, label='average on test')
plt.plot(epochs,train_std, label='standard on train')
plt.plot(epochs,train_avg, label='average on train')
plt.xticks(epochs)
plt.ylabel('Error rate',fontsize=18)
plt.xlabel('echo',fontsize=18)
plt.legend()
plt.grid(True)
plt.show()
```



1.It is obvious that the optimal model is **average perceptron**. The average model does not converge to exactly zero so the model does not be overfitting to the train set such that it achieve better performance on test set.

2.As we can see, the optimal echo of the model without shuffle must be **18** because the train error converge to zero and the test error would not change any more. In contrast, the optimal echo of the model with shuffle is **18** because the the train error of both two models converge to zero. After the train error converge to zero, the perceptron can separate the train set. If we shuffle data each echo, the perceptron changes among its 'safe' area of the train set such that the train error does not change but the test error changes. Therefore, I choose 18 as the optimal value of max echo of the model with shuffle.

(g)

In [401]:
```
pct = perceptron(13)
pct.fit(trainX,trainY)
score = pct.avg_test(testX,testY)
print 'Test Error'
print score
```

```
Test Error
0.0138888888889
```

(h)

In [402]:
```
sort_w = np.argsort(pct.w)
top = []
for i in sort_w[-15:][::-1]:
    top.append(features_arr[i])
tail = []
for i in sort_w[:15]:
    tail.append(features_arr[i])
table = pd.DataFrame(data=[top,tail],index=['top 15 positive weights','t
op 15 negative weights'])
table.transpose().head(20)
```

Out[402]:

	top 15 positive weights	top 15 negative weights
0	doubl	compat
1	numberm	yahoo
2	limit	kei
3	those	pleasur
4	local	despit
5	domain	line
6	van	numberbit
7	collector	certainli
8	learn	imag
9	treat	western
10	resolv	take
11	lifetim	ideal
12	degre	anywai
13	block	statist
14	explor	neg

Problem 4

In [341]:
```
data = pd.read_csv('allhyper.data')
data['class'] = data['class'].str.rsplit('.',expand=True)[0]
data.dropna(axis=1, how='all', inplace=True)
label_types = data.dtypes.values
labels = data.columns
```

(a)

In [97]:
```
print 'percentage of class = "hyperthyroid" in the data:\t',
(data[data['class']=='hyperthyroid'].shape[0]*1.0/data.shape[0])*100,'%'
```

```
percentage of class = "hyperthyroid" in the data:       2.21428571429 %
```

Because the value of the class is highly imbalanced such that the class only has 2.21 % of the key value 'hyperthyroid', the misclassification cannot exactly show the performance of models. So F1 score with 'recall' is more suitable for validate the performance of models. Particularly, F2 score may be more expected than F1 score **because it weights recall higher than precision by placing more emphasis on false negatives**.

(b) Preprocessing

In [98]:
```
miss = pd.DataFrame(data.isnull().sum())/data.shape[0]*100
miss = pd.concat([miss,data.dtypes],axis=1)
miss.columns = ['percentage of missing values','data type']
miss[miss['percentage of missing values']>0]
```

Out[98]:

	percentage of missing values	data type
age	0.035714	float64
sex	3.928571	object
TSH	10.142857	float64
T3	20.892857	float64
TT4	6.571429	float64
T4U	10.607143	float64
FTI	10.535714	float64

As you can see from the table above,

1. There are missing values in data set. We handle the missing values according to their typye: (1) using the mean to fill 'float' missing values; (2) using the mode to fill the 'object' value.
2. Because original data are object values, we transform the **object vaues to binary values or multinomial values for convenient computations**.
3. The original class are **multinomial class values, but here we only care about the 'hyperthyproid' and 'negative'**. So we transform **multinomial class values to binary values** such that '1' is 'hyperthyproid' and '0' is others classes including 'negative'.

In [342]:
```
for i in range(len(label_types)-1):
    if label_types[i] == 'float':
        data[labels[i]].fillna(data[labels[i]].mean(), inplace=True)
    else:
        data[labels[i]].fillna(data[labels[i]].mode()[0], inplace=True)
object_names = data.dtypes[data.dtypes=='object'].index.values
objects = {}
for key in object_names[:-1]: # not include 'class' column
    objects[key] = data.groupby(key).sum().index.values
objects
```

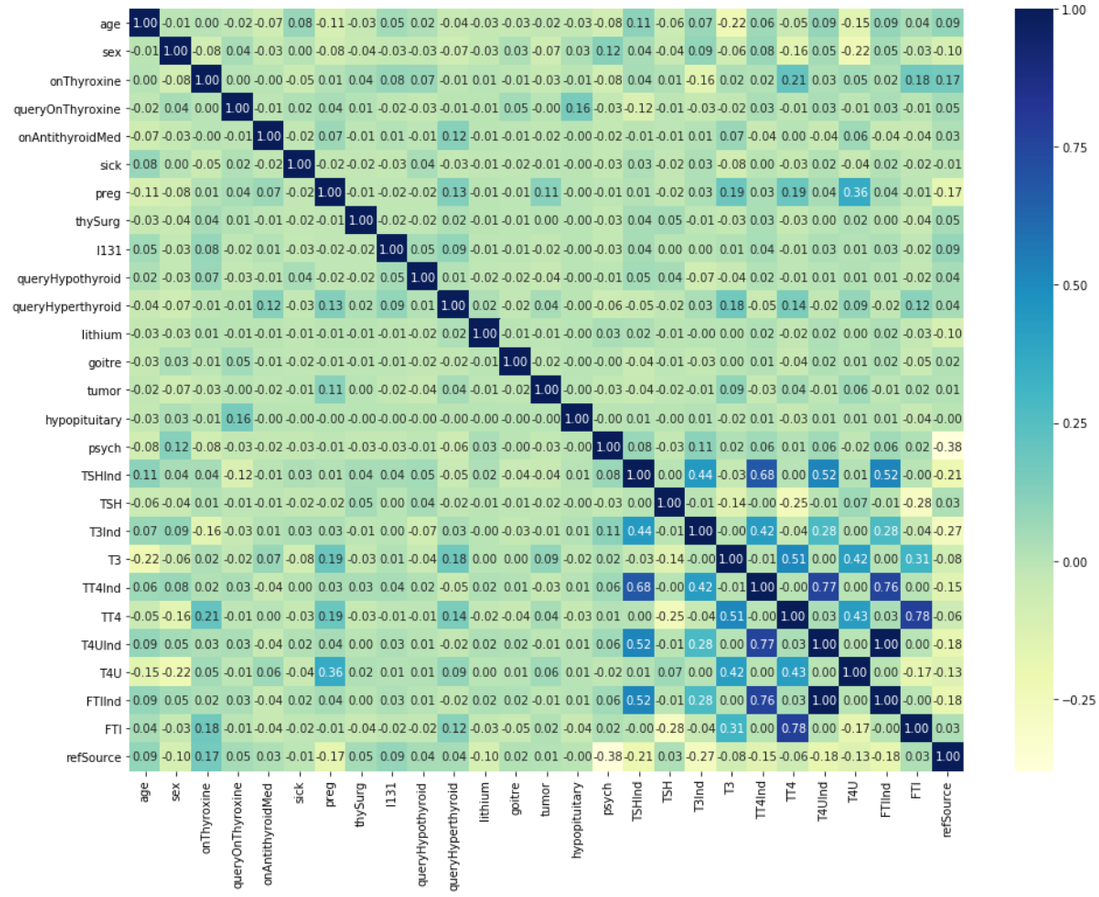
Out[342]:
```
{'FTIInd': array(['f', 't'], dtype=object),
 'I131': array(['f', 't'], dtype=object),
 'T3Ind': array(['f', 't'], dtype=object),
 'T4UInd': array(['f', 't'], dtype=object),
 'TBGInd': array(['f'], dtype=object),
 'TSHInd': array(['f', 't'], dtype=object),
 'TT4Ind': array(['f', 't'], dtype=object),
 'goitre': array(['f', 't'], dtype=object),
 'hypopituitary': array(['f', 't'], dtype=object),
 'lithium': array(['f', 't'], dtype=object),
 'onAntithyroidMed': array(['f', 't'], dtype=object),
 'onThyroxine': array(['f', 't'], dtype=object),
 'preg': array(['f', 't'], dtype=object),
 'psych': array(['f', 't'], dtype=object),
 'queryHyperthyroid': array(['f', 't'], dtype=object),
 'queryHypothyroid': array(['f', 't'], dtype=object),
 'queryOnThyroxine': array(['f', 't'], dtype=object),
 'refSource': array(['STMW', 'SVHC', 'SVHD', 'SVI', 'other'], dtype=obj
ect),
 'sex': array(['F', 'M'], dtype=object),
 'sick': array(['f', 't'], dtype=object),
 'thySurg': array(['f', 't'], dtype=object),
 'tumor': array(['f', 't'], dtype=object)}
```

As you can see, most object-type values are binary type except for 'refSource'. So 'refSource' is transformed to a multinomial feature and others are transformed to binary features. In addition, the feature 'TBGInd' is full of single value such that it does not have influence on classification, so it can be removed.

In [343]:
```
data.drop('TBGInd',axis=1,inplace=True)
objects.pop('TBGInd')
v = [-2,-1,0,1,2]
for key, value in objects.items():
    if key == 'refSource':
        for i in range(len(value)):
            data[key].replace(to_replace=value[i],value=v[i],inplace=Tru
e)
    else:
        data[key].replace(to_replace=value[0],value=-1,inplace=True)
        data[key].replace(to_replace=value[1],value=1,inplace=True)
data_y = pd.get_dummies(data['class']).iloc[:,2]
data.drop('class',axis=1,inplace=True)
```

In [345]:
```
plt.figure(figsize=(16,12))
sns.heatmap(data.corr(),cmap="YlGnBu",annot=True,fmt='.2f')
```

Out[345]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x1a25209910>
```



As we can see, there is a **strong correlation between 'T4UInd' and 'FTIInd'**, so I decide to drop the 'T4UInd' because it also has a correlation with 'TT4Ind'.

In [346]:
```
data.drop('T4UInd',axis=1,inplace=True)
```

Because the **range** of some features are **very different** and the **SVM model are sensitive to the data**, we need to normalize the data. Because most features are binary, I dicide to do **min-max normalization** to [0,1].

In [347]:
```
data_y = np.ravel(data_y)
trainX, testX, trainY, testY = model_selection.train_test_split(data, da
ta_y, test_size=3.0/10)
scaler = preprocessing.StandardScaler()
scaler.fit(trainX)
trainX = scaler.transform(trainX)
testX = scaler.transform(testX)
```

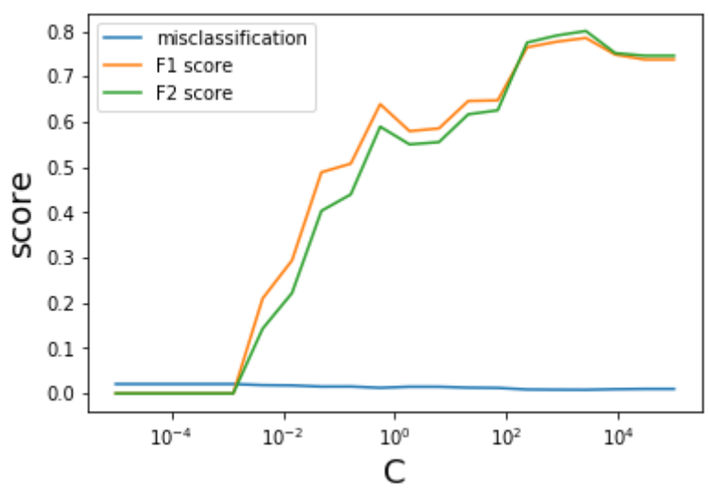
(c)

In [358]:
```
def cv_score(model,X,Y,cv=5):
    kf = KFold(n_splits=cv)
    score = np.zeros(3)
    for train_index,test_index in kf.split(X):
        train_x, test_x = X[train_index],X[test_index]
        train_y, test_y = Y[train_index],Y[test_index]
        model.fit(train_x,train_y)
        pre = model.predict(test_x)
        temp = [1-metrics.accuracy_score(pre,test_y),metrics.f1_score(te
st_y,pre),metrics.fbeta_score(test_y,pre,beta=2.0)]
        score = np.mean([score,temp],axis=0)
    return score
def test_score(model,X,Y,test_x,test_y):
    model.fit(X,Y)
    pre = model.predict(test_x)
    score = [1-metrics.accuracy_score(pre,test_y),metrics.f1_score(pre,t
est_y),metrics.fbeta_score(pre,test_y,beta=2.0)]
    return score
```

For linear SVM, the important parameter must only be the 'C', so here I will use CV to find the optimal value of 'C'.

In [367]:
```
c_arr = np.logspace(-5,5,20)
lin_scores = []
for c in c_arr:
    lin = svm.SVC(C=c,kernel='linear')
    lin_score = cv_score(lin,trainX,trainY)
    lin_scores.append(lin_score)
lin_scores = np.array(lin_scores).transpose()
print 'optimal parameter:'
print 'C = ', c_arr[np.argmax(lin_scores[2])]
print 'F2 score=', np.max(lin_scores[2])
plt.plot(c_arr,lin_scores[0],label='misclassification')
plt.plot(c_arr,lin_scores[1],label='F1 score')
plt.plot(c_arr,lin_scores[2],label='F2 score')
plt.xscale('log')
plt.xlabel('C',fontsize=18)
plt.ylabel('score',fontsize=18)
plt.legend()
plt.show()
```

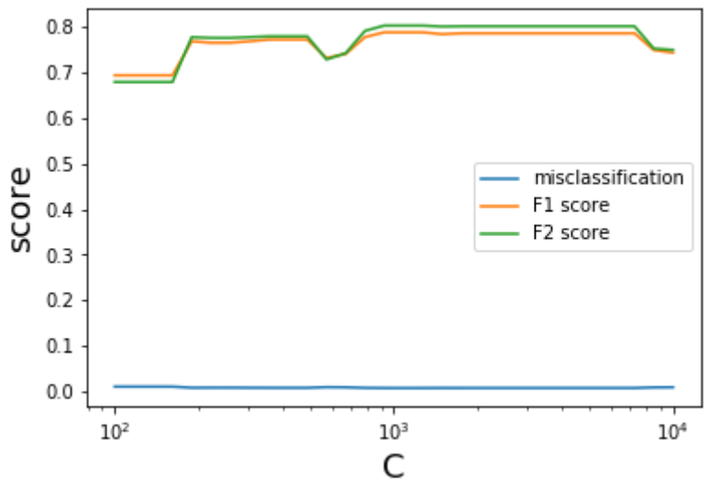
```
optimal parameter:
C =  2636.65089873
F2 score= 0.80095963055
```



Then, according to the figure above, we know that the **optimal area of 'C' is (0.1,1000)**.

In [374]:
```
c_arr = np.logspace(2,4,30)
lin_scores = []
for c in c_arr:
    lin = svm.SVC(C=c,kernel='linear')
    lin_score = cv_score(lin,trainX,trainY)
    lin_scores.append(lin_score)
lin_scores = np.array(lin_scores).transpose()
print 'optimal parameter:'
lin_opt_c = c_arr[np.argmax(lin_scores[2])]
print 'lin_opt_c = ', lin_opt_c
print 'F2 score =', np.max(lin_scores[2])
plt.plot(c_arr,lin_scores[0],label='misclassification')
plt.plot(c_arr,lin_scores[1],label='F1 score')
plt.plot(c_arr,lin_scores[2],label='F2 score')
plt.xscale('log')
plt.xlabel('C',fontsize=18)
plt.ylabel('score',fontsize=18)
plt.legend()
plt.show()
```

```
optimal parameter:
lin_opt_c =  923.670857187
F2 score = 0.802434573431
```



In [375]:
```
lin = svm.SVC(C=lin_opt_c,kernel='linear')
train_scores = test_score(lin,trainX,trainY,trainX,trainY)
test_scores = test_score(lin,trainX,trainY,testX,testY)
table = pd.DataFrame(data=[train_scores,test_scores],index=['train','tes
t'],columns=['Misclassification',' F1 score ', ' F2 score'])
table.head()
```

Out[375]:

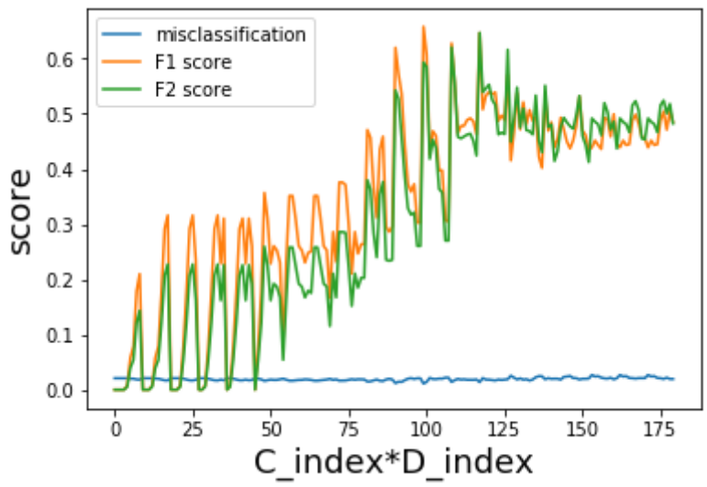
	Misclassification	F1 score	F2 score
train	0.004082	0.894737	0.880829
test	0.014286	0.739130	0.779817

(d)

For polynomial kernel, there are two important parameters **'C' and 'degree'** where **'degree' is related to the power of polynomial kernel**. I use the CV to find the optimal parameters. First, I use a **wide range** of parameters **to check the approximate area** of the optimal parameters.

In [380]:
```
c_arr = np.logspace(-5,5,20)
d_arr = [2,3,4,5,6,7,8,9,10]

poly_scores =[]
for c in c_arr:
    for d in d_arr:
        poly = svm.SVC(C=c,kernel='poly',degree=d)
        score = cv_score(poly,trainX,trainY)
        poly_scores.append(score)
poly_scores = np.array(poly_scores).transpose()

arr = range(len(c_arr)*len(d_arr))
print 'optimal parameter:'
print 'C = ', c_arr[arr[np.argmax(poly_scores[2])]/len(d_arr)], 'C_index
=', arr[np.argmax(poly_scores[2])]/len(d_arr)
print 'Degree = ', d_arr[arr[np.argmax(poly_scores[2])]%len(d_arr)]
print 'F2 score=', np.max(poly_scores[2])
plt.plot(arr,poly_scores[0],label='misclassification')
plt.plot(arr,poly_scores[1],label='F1 score')
plt.plot(arr,poly_scores[2],label='F2 score')
#plt.xscale('log')
plt.xlabel('C_index*D_index',fontsize=18)
plt.ylabel('score',fontsize=18)
plt.legend()
plt.show()
```

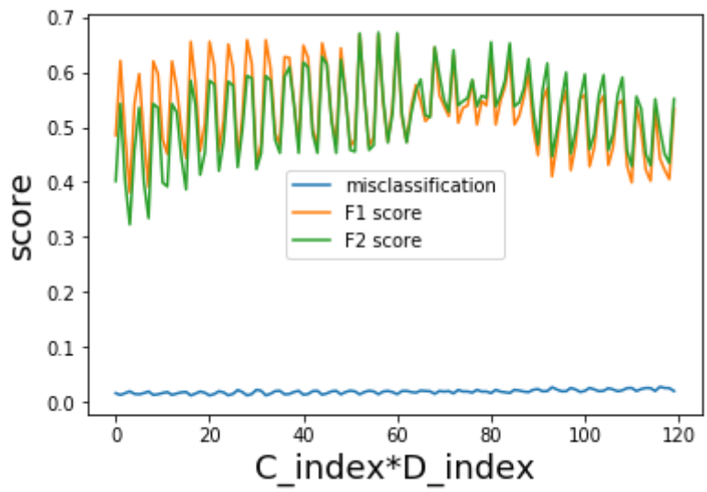
```
optimal parameter:
C =  69.5192796178 C_index= 13
Degree =  2
F2 score= 0.646995022903
```



Then, according to the figure above, we know that the **optimal area of 'C' is (1,1000)**, and the **optimal area of 'degree' is [2,3,4,5]**.

In [381]:
```
c_arr = np.logspace(0,3,30)
d_arr = [2,3,4,5]
poly_scores =[]
for c in c_arr:
    for d in d_arr:
        poly = svm.SVC(C=c,kernel='poly',degree=d)
        score = cv_score(poly,trainX,trainY)
        poly_scores.append(score)
poly_scores = np.array(poly_scores).transpose()

arr = range(len(c_arr)*len(d_arr))
print 'optimal parameter:'
poly_opt_c = c_arr[arr[np.argmax(poly_scores[2])]/len(d_arr)]
poly_opt_d = d_arr[arr[np.argmax(poly_scores[2])]%len(d_arr)]
print 'poly_opt_c = ', poly_opt_c
print 'poly_opt_degree = ', poly_opt_d
plt.plot(arr,poly_scores[0],label='misclassification')
plt.plot(arr,poly_scores[1],label='F1 score')
plt.plot(arr,poly_scores[2],label='F2 score')
#plt.xscale('log')
plt.xlabel('C_index*D_index',fontsize=18)
plt.ylabel('score',fontsize=18)
plt.legend()
plt.show()
```

```
optimal parameter:
poly_opt_c =  28.0721620394
poly_opt_degree =  2
```



In [384]:
```
poly = svm.SVC(C=poly_opt_c,kernel='poly',degree=poly_opt_d)
train_scores = test_score(poly,trainX,trainY,trainX,trainY)
test_scores = test_score(poly,trainX,trainY,testX,testY)
table = pd.DataFrame(data=[train_scores,test_scores],index=['train','tes
t'],columns=['Misclassification',' F1 score ', ' F2 score'])
table.head()
```

Out[384]:

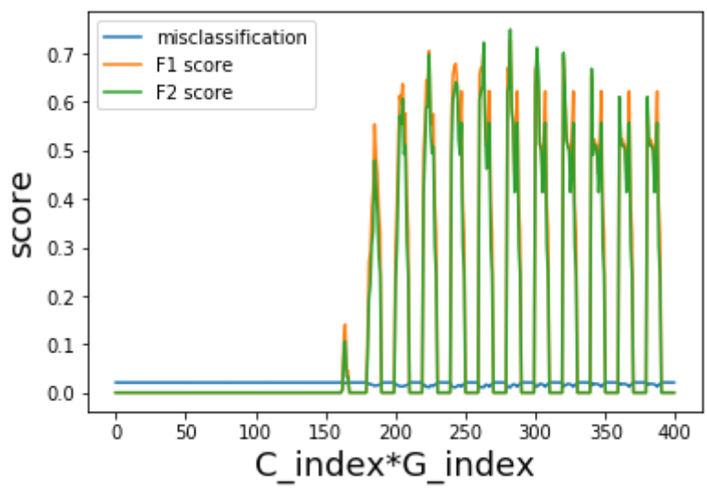
	Misclassification	F1 score	F2 score
train	0.003571	0.904110	0.911602
test	0.019048	0.636364	0.693069

(e)

For polynomial kernel, there are two important parameters **'C' and 'gamma'** where **'gamma' is related to the power of polynomial kernel**. I use the CV to find the optimal parameters. First, I use a **wide range** of parameters **to check the approximate area** of the optimal parameters.

In [362]:
```
c_arr = np.logspace(-5,6,20)
g_arr = np.logspace(-3,3,20)
rbf_scores =[]
for c in c_arr:
    for g in g_arr:
        rbf = svm.SVC(C=c,kernel='rbf',gamma=g)
        score = cv_score(rbf,trainX,trainY)
        rbf_scores.append(score)
rbf_scores = np.array(rbf_scores).transpose()

arr = range(len(c_arr)*len(g_arr))
print 'optimal parameter:'
print 'C = ', c_arr[arr[np.argmax(rbf_scores[2])]/len(g_arr)], 'C_index
=', arr[np.argmax(rbf_scores[2])]/len(g_arr)
print 'Degree = ', g_arr[arr[np.argmax(rbf_scores[2])]%len(g_arr)]
print 'F2 score=', np.max(rbf_scores[2])
plt.plot(arr,rbf_scores[0],label='misclassification')
plt.plot(arr,rbf_scores[1],label='F1 score')
plt.plot(arr,rbf_scores[2],label='F2 score')
#plt.xscale('log')
plt.xlabel('C_index*G_index',fontsize=18)
plt.ylabel('score',fontsize=18)
plt.legend()
plt.show()
```

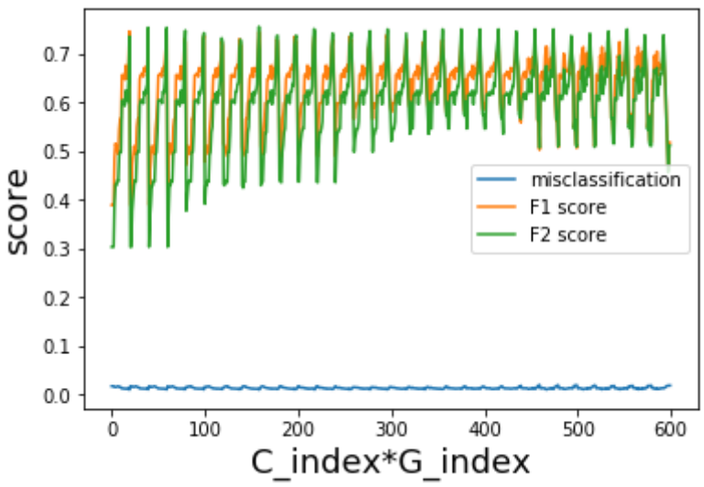
```
optimal parameter:
C =  1274.2749857 C_index= 14
Degree =  0.00428133239872
F2 score= 0.749846888252
```



Then, according to the figure above, we know that the **optimal area of 'C' is (100,10000)**, and the **optimal area of 'gamma' is [10^-4,10^-1]**.

In [365]:
```
c_arr = np.logspace(2,4,30)
g_arr = np.logspace(-4,-2,20)
rbf_scores =[]
for c in c_arr:
    for g in g_arr:
        rbf = svm.SVC(C=c,kernel='rbf',gamma=g)
        score = cv_score(rbf,trainX,trainY)
        rbf_scores.append(score)
rbf_scores = np.array(rbf_scores).transpose()

arr = range(len(c_arr)*len(g_arr))
print 'optimal parameter:'
rbf_opt_c = c_arr[arr[np.argmax(rbf_scores[2])]/len(g_arr)]
rbf_opt_g = g_arr[arr[np.argmax(rbf_scores[2])]%len(g_arr)]
print 'rbf_opt_c = ', rbf_opt_c
print 'rbf_opt_gamma = ', rbf_opt_g
print 'F2 score=', np.max(rbf_scores[2])
plt.plot(arr,rbf_scores[0],label='misclassification')
plt.plot(arr,rbf_scores[1],label='F1 score')
plt.plot(arr,rbf_scores[2],label='F2 score')
#plt.xscale('log')
plt.xlabel('C_index*G_index',fontsize=18)
plt.ylabel('score',fontsize=18)
plt.legend()
plt.show()
```

```
optimal parameter:
rbf_opt_c =  303.919538231
rbf_opt_gamma =  0.00784759970351
F2 score= 0.755325797206
```



In [366]:
```
rbf = svm.SVC(C=rbf_opt_c,kernel='rbf',gamma=rbf_opt_g)
train_scores = test_score(rbf,trainX,trainY,trainX,trainY)
test_scores = test_score(rbf,trainX,trainY,testX,testY)
table = pd.DataFrame(data=[train_scores,test_scores],index=['train','tes
t'],columns=['Misclassification',' F1 score ', ' F2 score'])
table.head()
```

Out[366]:

	Misclassification	F1 score	F2 score
train	0.002551	0.933333	0.925926
test	0.016667	0.708333	0.726496

(f)

In [385]:
```
# after run the cells before, we now have three models with optimal para
meters.
test_arr = []
train_arr = []
train_arr.append(test_score(lin,trainX,trainY,trainX,trainY))
train_arr.append(test_score(poly,trainX,trainY,trainX,trainY))
train_arr.append(test_score(rbf,trainX,trainY,trainX,trainY))
test_arr.append(test_score(lin,trainX,trainY,testX,testY))
test_arr.append(test_score(poly,trainX,trainY,testX,testY))
test_arr.append(test_score(rbf,trainX,trainY,testX,testY))
```

In [386]:
```
print 'Train table'
table = pd.DataFrame(data=train_arr,index=
['linear','polynomial','RBF'],columns=['Misclassification',' F1 score ',
 ' F2 score'])
table.head()
```

```
Train table
```

Out[386]:

	Misclassification	F1 score	F2 score
linear	0.004082	0.894737	0.880829
polynomial	0.003571	0.904110	0.911602
RBF	0.002551	0.933333	0.925926

In [389]:
```
print 'Test table '
table = pd.DataFrame(data=test_arr,index=['linear','polynomial','RBF'],c
olumns=['Misclassification',' F1 score ', ' F2 score'])
table.head()
```

```
Test table
```

Out[389]:

	Misclassification	F1 score	F2 score
linear	0.014286	0.739130	0.779817
polynomial	0.019048	0.636364	0.693069
RBF	0.016667	0.708333	0.726496

In [388]:
```
print 'Parameter Table'

table = pd.DataFrame(data=[[lin_opt_c,0,0],[poly_opt_c,poly_opt_d,0],[rb
f_opt_c,0,rbf_opt_g]],index=['linear','polynomial','RBF'],columns=['Opti
mal C','Optimal Degree', 'Optimal Gamma'])
table.head()
```

```
Parameter Table
```

Out[388]:

	Optimal C	Optimal Degree	Optimal Gamma
linear	923.670857	0	0.000000
polynomial	28.072162	2	0.000000
RBF	303.919538	0	0.007848

Conclusion

1.Because of the imbalanced data set, the three model cannot obtain ideal performance on test set. The models are easily to be overfitting because of the imbalance such that F score cannot reach higher. However, we can also see from the comparison table that F2 Score with high weighted recall is higher than the normal F1 Score. Therefore, for the assessment criterion to the models on imbalanced data, F2 score is more suitable than misclassification and F1 score.

2.From the 'train table' and 'test table', we can see that given the imbalanced data, for the scores of the three model with their optimal parameters, linear model > the RBF kernel with gamma = 0.008 > the polynomial kernel with degree of 2 . Although random splits of data set and CV cause different results of the three models, this relationship between them is almost stable.

3.From the 'Parameter table', we can see that the linear SVM needs the larger C for regularization because it needs larger penalty for 'slacks' to obtain a separable boundary. But the polynomial SVM and RBF needs the smaller C for regularization because they introduce kernels to obtain a boundary in a hyperplane with smaller penalty for 'slacks'.

4.The reason why the linear model is the best on test might be that other two models with kernel are overfitting to the train data (see "Train table") such that they achieve poor performance on test set (see "Test table"). Another possible reason might be the data is imbalanced such that the two kernel models are easy to be overfitting.