CS 671 Homework 1

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I consent to the following agreements.

This assignment represents my own work. I did not work on this assignment with others. All coding was done by myself.

I understand that if I struggle with this assignment that I will reevaluate whether this is the correct class for me to take. I understand that the homework only gets harder.

1 Concepts of Learning

1. A ranking problem. Because we need to predict the 1st, 2nd and 3rd places of the horses.
2. Classification. We are going to classify the galaxies into four types
3. Regression. We should use the 1000 people's data and appropriate algorithms to make predictions on other people.
4. A regression problem. Again predict the pounds of needed vegetables for future.
5. Pattern mining. We need to find correlations between different products.
6. Density estimation.
7. Conditional probability estimation. The measure of "how likely" is probability.
8. Conditional probability estimation.
9. Conditional probability estimation.
10. Clustering. It's unsupervised learning and clustering usually use distance as criterion.

2 Information Theory

2.1

According to Jensen's inequality and $-log_b a$ is a convex function,

$$\begin{aligned}
-KL(P,Q) &= -\sum_{a\in O} P(a)log\frac{P(a)}{Q(a)} \\
&= \sum_{a\in O} P(a)log\frac{Q(a)}{P(a)} \\
&\leq log\left(\sum_{a\in O} P(a)\frac{Q(a)}{P(a)}\right) \\
&= log\left(\sum_{a\in O} Q(a)\right) \\
&= 0
\end{aligned}$$

Therefore,

$$\begin{aligned}
-KL(P,Q) &\leq 0 \\
KL(P,Q) &\geq 0
\end{aligned}$$

2.2

If P and Q subject to the same distribution, then

$$\begin{aligned}
P(a) &= Q(a)\ for\ all\ a \in O \\
\therefore \quad KL(P,Q) &= \sum_{a\in O} P(a)log1 = 0
\end{aligned}$$

2.3

Take $P(a)$ and $Q(a)$ that subject to Bernoulli distribution. Define

$$P(a) = \begin{cases} \frac{1}{2},\ if\ a=1 \\ \frac{1}{2},\ if\ a=0 \end{cases} \quad and \quad Q(a) = \begin{cases} \frac{1}{3},\ if\ a=1 \\ \frac{2}{3},\ if\ a=0 \end{cases}$$

$$\begin{aligned}
KL(P,Q) &= \sum_{a\in O} P(a)log\frac{P(a)}{Q(a)} \\
&= \frac{1}{2}log\frac{\frac{1}{2}}{\frac{1}{3}} + \frac{1}{2}log\frac{\frac{1}{2}}{\frac{2}{3}} \\
&= \frac{1}{2}\left(log\frac{3}{2} + log\frac{3}{4}\right) \\
&= \frac{1}{2}log\frac{9}{4} = log\frac{3}{2}
\end{aligned}$$

$$
\begin{aligned}
KL(Q,P) &= \sum_{a \in O} Q(a) log \frac{Q(a)}{P(a)} \\
&= \frac{1}{3} log \frac{\frac{1}{3}}{\frac{1}{2}} + \frac{2}{3} log \frac{\frac{2}{3}}{\frac{4}{3}} \\
&= \frac{1}{3}\left(log \frac{2}{3} + log \frac{16}{9} \right) \\
&= \frac{1}{3} log \frac{22}{9}
\end{aligned}
$$

Clearly, $KL(P,Q) \neq KL(Q,P)$.

2.4

$$
\begin{aligned}
-KL(J,PQ) &= \sum_{(x,y)\in(X,Y)} J(x,y) log \frac{P(x)Q(y)}{J(x,y)} \\
&= \sum_{(x,y)\in(X,Y)} J(x,y) log \frac{Q(y)}{J(x,y)} + \sum_{(x,y)\in(X,Y)} J(x,y) log P(x) \\
&= \sum_{(x,y)\in(X,Y)} J(x,y) log \frac{Q(y)}{J(x,y)} + \sum_{x \in X} P(x) log P(x) \\
&= H(X|Y) - H(X)
\end{aligned}
$$

$\therefore KL(J,PQ) = H(X) - H(X|Y)$

2.5

Recall 2.4,

$$
\begin{aligned}
-KL(J,PQ) &= \sum_{(x,y)\in(X,Y)} J(x,y) log \frac{P(x)Q(y)}{J(x,y)} \\
&= \sum_{(x,y)\in(X,Y)} J(x,y) log \frac{P(x)}{J(x,y)} + \sum_{(x,y)\in(X,Y)} J(x,y) log Q(y) \\
&= \sum_{(x,y)\in(X,Y)} J(x,y) log \frac{P(x)}{J(x,y)} + \sum_{y \in Y} Q(y) log Q(y) \\
&= H(Y|X) - H(Y) \\
&= -I(X,Y)
\end{aligned}
$$

$\therefore I(X,Y) = KL(J,PQ)$

2.6

$\because 0 < p < 0.5$

$\therefore 0.5 < p < 1$

$\therefore Error(p) = min(p, 1-p) = p$

To find the relationship betweem H and p, compute the derivative of H w.r.t. p.

$$\begin{aligned} H^{'}(p) &= -\left(log_2 p + p\frac{1}{ln2}\right) - \left[-log_2(1-p) + (1-p)\frac{-1}{(1-p)ln2}\right] \\ &= -log_2 p - \frac{1}{ln2} + log_2(1-p) + \frac{1}{ln2} \\ &= log_2 \frac{1-p}{p} = log_2\left(\frac{1}{p} - 1\right) \end{aligned}$$

$\because 0 < p < 0.5$

$\therefore \frac{1}{p} > 2 \Rightarrow \frac{1}{p} - 1 > 1$

$\therefore log\left(\frac{1}{p} - 1\right) > 0$

$\therefore H^{'}(p) > 0$

$\therefore H(p)$ is a increasing function.

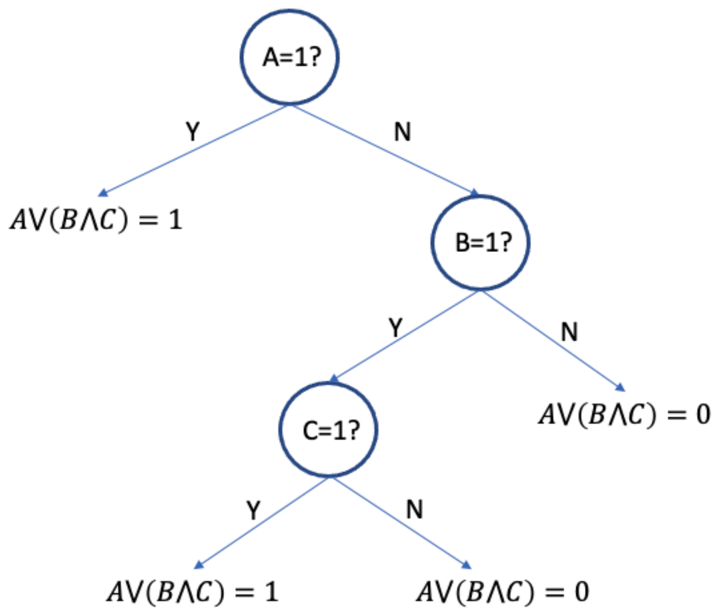
$\therefore$ A smaller entopy H corresponds to a smaller misclassification error p under the $0 < p < 0.5$ setting.

3 Classifiers and Metrics - Coding

See Jupyter Notebook Appendix.

4 Calculate Splits

4.1



4.2

$$GiniIndex(A) = \frac{1}{2} \times 0 + \frac{1}{2} \times \frac{3}{8} = \frac{3}{16}$$
$$GiniIndex(B) = \frac{1}{2}\left[1 - \left(\frac{3}{4}\right)^2 - \left(\frac{1}{4}\right)^2\right] + \frac{1}{2}\left[1 - \left(\frac{1}{2}\right)^2 - \left(\frac{1}{2}\right)^2\right] = \frac{7}{16}$$
$$GiniIndex(C) = \frac{1}{2}\left[1 - \left(\frac{3}{4}\right)^2 - \left(\frac{1}{4}\right)^2\right] + \frac{1}{2}\left[1 - \left(\frac{1}{2}\right)^2 - \left(\frac{1}{2}\right)^2\right] = \frac{7}{16}$$

$\because$ we should choose the node with the smallest Gini index, and follow alphabetical order if encounter ties.

$\therefore$ split with A.

4.3 information gain

The original entropy:

$$H = -\left(\frac{5}{8}log_2\frac{5}{8} + \frac{3}{8}log_2\frac{3}{8}\right) \approx 0.954$$

Entropy after splitting with each feature:

$$Split\ with\ A: H(A) = \frac{1}{2}\left(-log_2 1\right) + \frac{1}{2}\left[-\left(\frac{5}{8}log_2\frac{5}{8} + \frac{3}{8}log_2\frac{3}{8}\right)\right] \approx 0.094$$
$$Split\ with\ B: H(B) = \frac{1}{2}\left[-\left(\frac{3}{4}log_2\frac{3}{4} + \frac{1}{4}log_2\frac{1}{4}\right)\right] + \frac{1}{2}\left[-\left(\frac{1}{2}log_2\frac{1}{2} + \frac{1}{2}log_2\frac{1}{2}\right)\right] \approx 0.906$$
$$Split\ with\ C: H(C) = \frac{1}{2}\left[-\left(\frac{3}{4}log_2\frac{3}{4} + \frac{1}{4}log_2\frac{1}{4}\right)\right] + \frac{1}{2}\left[-\left(\frac{1}{2}log_2\frac{1}{2} + \frac{1}{2}log_2\frac{1}{2}\right)\right] \approx 0.906$$

Information gain after splitting with each feature:

$$Gain(A) = H - H(A) = 0.860$$
$$Gain(B) = H - H(B) = 0.049$$
$$Gain(C) = H - H(C) = 0.049$$

$\because$ We should choose the feature with the largest information gain, and follow alphabetical order if encounter ties.

$\therefore$ Split with feature A, which is the same as splitting with Gini index.

5 Classification with KNN and Decision Trees

See jupyter notebook appendix

6 Consistency and Curse of Dimensionality in K-Nearest Neighbors

6.1

This problem is equivalent to prove the following statement:

If we randomly take a point out of the training set for n times (with putting back), the probability that this point is exactly $NN(x_{test})$ (i.e. $x_{test} = NN(x_{test})$) *for at least once* will be **1** if $n \to \infty$.

Assume the probability that $x_{test} = NN(x_{test})$ is a, i.e. $P(x_{test} = NN(x_{test})) = a$

Then the probability that $x_{test} = NN(x_{test})$ *never happens* during n times will be $(1-a)^n$.

Therefore, the probability that $x_{test} = NN(x_{test})$ *for at least once* will be $1-(1-a)^n$

Since $0 < a < 1$, $1-(1-a)^n \to 1$ *when* $n \to \infty$, which suggests that we will definitely find a point x_{test} that equals to $NN(x_{test})$ if we keep taking points out of the training set for infinity times.

Therefore,

$$lim_{n\to\infty} P(\rho(x_{test}, NN(x_{test})) \leq \epsilon) = 1, \quad \forall \epsilon > 0$$
$$i.e.\ lim_{n\to\infty} P(\rho(x_{test}, NN(x_{test}) > \epsilon)) = 0, \quad \forall \epsilon > 0$$

6.2

Since we proved that $lim_{n\to\infty} P(\rho(x_{test}, NN(x_{test})) > \epsilon) = 1, \quad \forall \epsilon = 0$,

which means x_{test} will finally converge to $NN(x_{test})$ when $n \to \infty$, i.e. $\rho(x_{test}, NN(x_{test})) = 0$ when $n \to \infty$.

According to Lipschitz function,

$$|f(NN(x_{test}) - f(x_{test})| \leq L \cdot \rho(x_{test}, NN(x_{test})) = 0 \quad as\ n \to \infty$$

Therefore,

$$lim_{n\to\infty} |f(NN(x_{test}) - f(x_{test})| = 0$$

6.3

Simplify the problem:

$N_2(\mathbf{x}_{test}) := \{\mathbf{x} \in \{0,1\}^d : \rho(\mathbf{x}_{test}, \mathbf{x}) \leq 2\}$ means given d features and n observation points, there are K' points that have at most 2 features different from that of $\mathbf{x}_{test}$. Denote such event as $\mathbf{A}$

Since $x_1, x_2, \cdots, x_n$ are drawn I.I.D. from the uniform distribution on the d-dimensional hypercube $\{0,1\}^d$, we can write the following equation:

$$
\begin{aligned}
P(\mathbf{A}) = \frac{K'}{n} &= \binom{d}{2}\left(\frac{1}{2}\right)^d + \binom{d}{1}\left(\frac{1}{2}\right)^d + \binom{d}{0}\left(\frac{1}{2}\right)^d \\
&= \left(\frac{1}{2}\right)^d \left(1 + \binom{d}{1} + \binom{d}{2}\right) \\
&= \frac{\left(d^2 + d + 2\right)}{2^{d+1}} \\
\Longrightarrow K' &= \frac{\left(d^2 + d + 2\right) n}{2^{d+1}}
\end{aligned}
$$

6.4

Apparently, as $d \to \infty$, denominator 2^{d+1} converges to infinity exponentially, while the numerator converges to infinity polynomially, which means 2^{d+1} dominates the convergence speed.

Therefore, $lim_{d \to \infty} K' = 0$

6.5

If test set has very high dimensions, then the number of nearest neighbors we could find in a given area will exponentially decrease.

In other words, the searching area Nr should be expanded exponentially to find the same amount of neighbors.

Therefore, the test points we should include will be extremely large, even more than the electrons in the universe when $d > 100$, which, of course, incredibly increases computational complexity and is just unlikely.

Coding Appendix

September 25, 2022

There are double numbers for each question because I also made titles in Jupyter Notebook and exported the .tex version. I apologize for any confusing caused by these problem. But please focus on the latter number assignment and also check the titles.

1 3 Classifiers and Metrics - Coding

1.1 3.1 Calculate the value of g(x) and choose the threshold to minimize misclassification error

[171]:
```
import pandas as pd
import matplotlib.pyplot as plt
import math as mt
import numpy as np
```

[256]:
```
# creat a dataframe with features and labels
data = {'Age': [20, 18, 11, 31, 19, 21, 44, 15, 16, 17],
        'likeRowing': [1, 1, 0, 0, 1, 1, 1, 1, 0, 1],
        'Experience': [0, 1, 1, 0, 1, 0, 0, 1, 1, 0],
        'Income': [20, 33, 21, 18, 7, 10, 23, 16, 15, 6],
        'Y': [0, 0, 1, 1, 1, 0, 1, 0, 1, 0]}
df = pd.DataFrame(data)
```

[173]:
```
# define function g(x) and f(x)
theta = np.array([0.05, -3, 2.1, 0.008])
theta_0 = np.full([1, 10], 0.3)

def g(x):

    result = x @ theta.transpose() + theta_0

    return result.tolist()[0]


def tanh(x):

    result = (mt.exp(x) - mt.exp(-x))/(mt.exp(x) + mt.exp(-x))

    return result
```

```python


def f(x):

    result = tanh(g(x))

    return result
```

[257]:
```python
# calculate g(x)
x = np.array(df.iloc[:, 0:4])
df1 = df
gx = g(x)
df1['g(x)'] = gx
df1
df1_sortby_g = df1.sort_values(by='g(x)', ascending=False)
df1_sortby_g.reset_index()
```

[257]:

	index	Age	likeRowing	Experience	Income	Y	g(x)
0	8	16	0	1	15	1	3.320
1	2	11	0	1	21	1	3.118
2	3	31	0	0	18	1	1.994
3	1	18	1	1	33	0	0.564
4	4	19	1	1	7	1	0.406
5	7	15	1	1	16	0	0.278
6	6	44	1	0	23	1	-0.316
7	0	20	1	0	20	0	-1.540
8	5	21	1	0	10	0	-1.570
9	9	17	1	0	6	0	-1.802

[206]:
```python
# calculate misclassification error for each threshold
def MisClassificationError(df, classifier):  # Note: pass a string to␣
 ↪'classifier'

    df_sorted = df.sort_values(by=classifier, ascending=False)

    mis_errors = []
    f1scores = []
    precisions = []
    recalls = []
    N = df.shape[0]

    for idx in df_sorted.index:

        pred_1 = df_sorted['Y'].iloc[:idx+1]
        pred_0 = df_sorted['Y'].iloc[idx+1:]

        TP = sum(pred_1)
```

```
        FP = len(pred_1) - TP
        FN = sum(pred_0)
        TN = len(pred_0) - FN

        mis_error = (FP + FN) / N
        precision = TP / (TP + FP)
        recall = TP / (TP + FN)
        f1score = 2 * (precision * recall) / (precision + recall)

        mis_errors.append(mis_error)
        f1scores.append(f1score)
        precisions.append(precision)
        recalls.append(recall)

    error_sort = np.sort(mis_errors)
    error_args = np.argsort(mis_errors)

    return error_sort, error_args
```

[211]:
```
df = df1
classifier = 'g(x)'
g_min_err = MisClassificationError(df, classifier)
print('misclassification errors and index using g(x) as classifier:\n',␣
 ↪g_min_err)
g_arg_min_err = g_min_err[1][:3]
thresholds_g = df1_sortby_g['g(x)'].iloc[g_arg_min_err+1]
print('thresholds that will achieve the minimum misclassification error:\n',␣
 ↪thresholds_g)
print('minimum misclassification error:', np.min(g_min_err[0]))
```

```
misclassification errors and index using g(x) as classifier:
 (array([0.2, 0.2, 0.2, 0.3, 0.3, 0.3, 0.3, 0.4, 0.4, 0.5]), array([1, 4, 6, 2,
3, 5, 8, 0, 7, 9]))
thresholds that will achieve the minimum misclassification error:
 3    1.994
7    0.278
0   -1.540
Name: g(x), dtype: float64
minimum misclassification error: 0.2
```

The thresholds (denote as T) that will achieve the minimum classification error are:

$$T = 1.994 \ or \ 0.278 \ or \ -1.540$$

the minimum misclassification error is $\frac{FP+FN}{N} = \frac{2}{10} = 0.2$

[ ]:
```

```

1.2 3.2 Calculate f(x), choose the threshold to minimize misclassification error, and compute its cofusion matrix, precision, recall and F1 score

[258]:
```
df1['f(x)'] = df1['g(x)'].apply(tanh)
df1_sortby_f = df1.sort_values(by='f(x)', ascending=False)
df1_sortby_f
```

[258]:

	Age	likeRowing	Experience	Income	Y	g(x)	f(x)
8	16	0	1	15	1	3.320	0.997389
2	11	0	1	21	1	3.118	0.996092
3	31	0	0	18	1	1.994	0.963601
1	18	1	1	33	0	0.564	0.510939
4	19	1	1	7	1	0.406	0.385071
7	15	1	1	16	0	0.278	0.271053
6	44	1	0	23	1	-0.316	-0.305886
0	20	1	0	20	0	-1.540	-0.912120
5	21	1	0	10	0	-1.570	-0.917026
9	17	1	0	6	0	-1.802	-0.947013

[212]:
```
df = df1
classifier = 'f(x)'
f_min_err = MisClassificationError(df, classifier)
print('misclassification errors and index using f(x) as classifier:\n',␣
 ↪f_min_err)
f_arg_min_err = f_min_err[1][:3]
thresholds_f = df1_sortby_f['f(x)'].iloc[f_arg_min_err+1]
print('thresholds that will achieve the minimum misclassification error:\n',␣
 ↪thresholds_f)
print('minimum misclassification error:', np.min(f_min_err[0]))
```

```
misclassification errors and index using f(x) as classifier:
 (array([0.2, 0.2, 0.2, 0.3, 0.3, 0.3, 0.3, 0.4, 0.4, 0.5]), array([1, 4, 6, 2,
3, 5, 8, 0, 7, 9]))
thresholds that will achieve the minimum misclassification error:
 3    0.963601
7    0.271053
0   -0.912120
Name: f(x), dtype: float64
minimum misclassification error: 0.2
```

The thresholds (denote as T) that will minimize the classification error are:

$$T = 0.9636 \ or \ 0.2720 \ or \ -0.9121$$

the minimum misclassification error is $\frac{FP+FN}{N} = \frac{2}{10} = 0.2$

Take $T = 0.9636$ as an example.

$$TP = 3, \ TN = 5, \ FP = 0, \ FN = 2$$

Confusion matrix:

	$y = 1$	$y = 0$
$\hat{y} = 1$	3	0
$\hat{y} = 0$	2	5

$$Precision = \frac{TP}{predictedpositive} = 1$$
$$Recall = \frac{TP}{Positive} = \frac{3}{5}$$
$$F1score = 2\frac{Precision * Recall}{Precision + Recall} = \frac{3}{4}$$

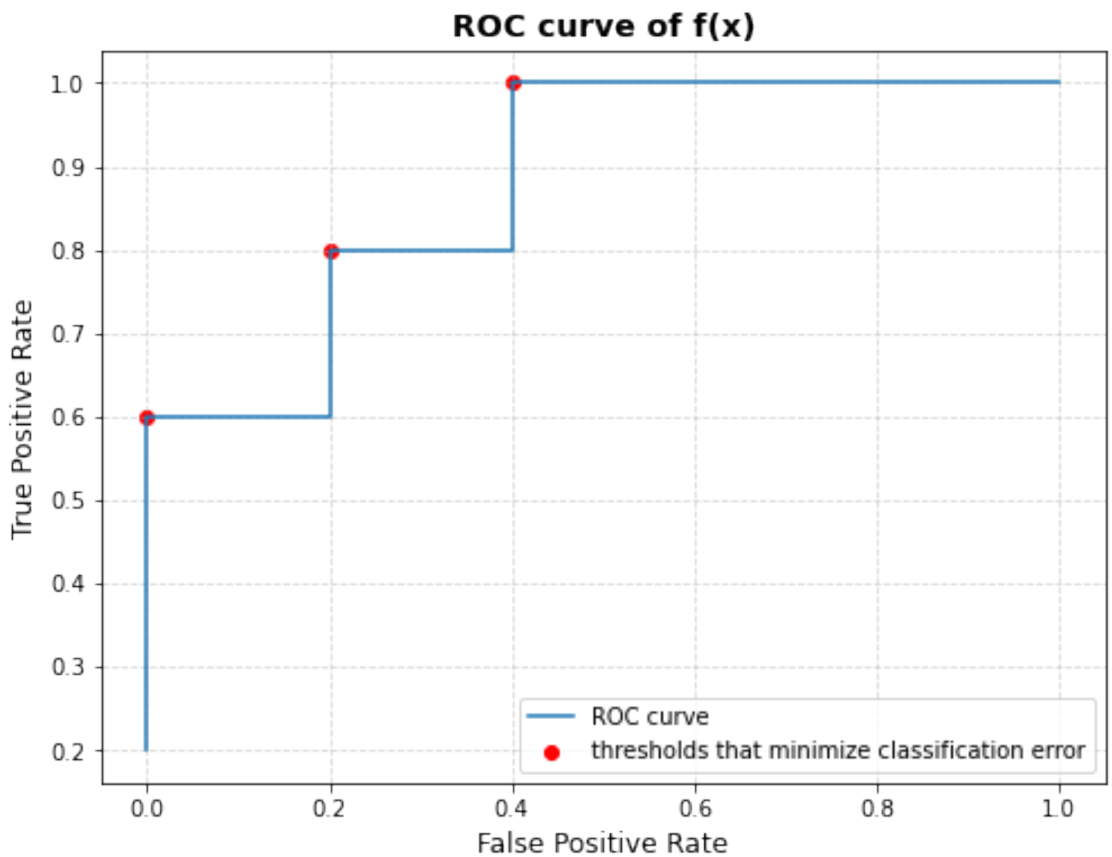
1.3 3.3 Plot ROC curve of f(x) and the points that represent decision points with the minimum classification error.

[260]:
```
df_sorty_reindex = df1_sortby_f.reset_index()

TPR_list = []
FPR_list = []
pos = neg = 5
for i in list(df_sorty_reindex.index):

    TP = sum(df_sorty_reindex['Y'].iloc[:i+1])
    FP = i + 1 - TP
    TPR = TP / pos
    FPR = FP / neg
    TPR_list.append(TPR)
    FPR_list.append(FPR)


print(TPR_list)
print(FPR_list)


plt.figure(figsize=(8,6))
plt.plot(FPR_list, TPR_list);
plt.grid(True, linestyle='--', alpha = .5)
plt.xlabel('False Positive Rate', fontsize=12)
plt.ylabel('True Positive Rate', fontsize=12)
plt.title('ROC curve of f(x)', fontsize=14, fontweight='bold')

# plot the thresholds
fpr_threshold = [0, 0.2, 0.4]
tpr_threshold = [0.6, 0.8, 1]
plt.scatter(fpr_threshold, tpr_threshold, c='r')
```

```
plt.legend(['ROC curve','thresholds that minimize classification error'])
```

```
[0.2, 0.4, 0.6, 0.6, 0.8, 0.8, 1.0, 1.0, 1.0, 1.0]
[0.0, 0.0, 0.0, 0.2, 0.2, 0.4, 0.4, 0.6, 0.8, 1.0]
```

[260]: <matplotlib.legend.Legend at 0x7fd8b47c45b0>



[ ]:

2 5 Classification with KNN and Decision Tree

2.1 5.2 Use two decision tree packages, report F1 score and tune parameter with K-fold cross validation

[52]:
```
from sklearn.preprocessing import OneHotEncoder
from sklearn.tree import DecisionTreeClassifier
from sklearn.metrics import f1_score
from sklearn.model_selection import GridSearchCV
from sklearn.model_selection import KFold
import warnings
warnings.filterwarnings('ignore')
```

[53]:
```
df_train = pd.read_csv(
    '/Users/shaoyutong/Library/Mobile Documents/com~apple~CloudDocs/CS671-ML/HW/
 ↪NEW-HW1/carseats_train.csv')
df_test = pd.read_csv(
    '/Users/shaoyutong/Library/Mobile Documents/com~apple~CloudDocs/CS671-ML/HW/
 ↪NEW-HW1/carseats_test.csv')
```

[54]:
```
df_train.head()
df_train1 = df_train.copy()
```

2.2 step1: encoding

[57]:
```
# data preprocessing--encoding strings with binary variables
# encoding ShelveLoc
encoder = OneHotEncoder(handle_unknown='ignore')
sl_train = np.array(df_train['ShelveLoc']).reshape(-1,1)
sl_test = np.array(df_test['ShelveLoc']).reshape(-1,1)
encoder.fit(sl_train)
encoder.categories_
df_train[['sl_bad','sl_good','sl_medium']]=encoder.transform(sl_train).toarray()
df_test[['sl_bad','sl_good','sl_medium']]=encoder.transform(sl_test).toarray()

# encoding Urban, US
urban_train = pd.get_dummies(df_train['Urban'], prefix='urban')
urban_train.head()
urban_test = pd.get_dummies(df_test['Urban'], prefix='urban')

US_train = pd.get_dummies(df_train['US'], prefix='us')
US_train.head()
US_test = pd.get_dummies(df_test['US'], prefix='us')
```

[222]:
```
us_urban_train = pd.merge(urban_train, US_train, left_index=True,␣
 ↪right_index=True)
train = pd.merge(df_train, us_urban_train, left_index=True, right_index=True)
train1 = train.drop(columns=['ShelveLoc','US','Urban'])
```

```
train1
us_urban_test = pd.merge(urban_test, US_test, left_index=True, right_index=True)
test = pd.merge(df_test, us_urban_test, left_index=True, right_index=True)
test1 = test.drop(columns=['ShelveLoc','US','Urban'])
test1.head()
```

[222]:

```
   Sales  CompPrice  Income  Advertising  Population  Price  Age  Education  \
0      0        117     100            4         466     97   55         14
1      0        141      64            3         340    128   38         13
2      0        115     105            0          45    108   71         15
3      1        136      81           15         425    120   67         10
4      1        107     117           11         148    118   52         18

   sl_bad  sl_good  sl_medium  urban_No  urban_Yes  us_No  us_Yes
0     0.0      0.0        1.0         0          1      0       1
1     1.0      0.0        0.0         0          1      1       0
2     0.0      0.0        1.0         0          1      1       0
3     0.0      1.0        0.0         0          1      0       1
4     0.0      1.0        0.0         0          1      0       1
```

2.3 1. Decision Tree Classifier

[ ]:

```
# training data (df_train)
x_train = train1.drop(columns=['Sales'])
y_train = train1['Sales']
clf = DecisionTreeClassifier()
clf_gini = clf.fit(x_train, y_train)

# prediction
x_test = test1.drop(columns='Sales')
y_test = test1['Sales']
y_pred = clf.predict(x_test)
y_true = y_test

# report f1-score
# f1_score(y_pred, y_true)
```

2.3.1 1.1 Compute F1 score

[261]:

```
def F1Score(y_true, y_pred):

    # initialization
    TP = 0
    FP = 0
    TN = 0
    FN = 0
```

```
    for true in y_true:

        for pred in y_pred:

            if pred == 1:

                if true == 1:
                    TP += 1

                elif true == 0:
                    FP += 1

            if pred == 0:

                if true == 1:
                    FN += 1

                elif true == 0:
                    TN += 1

    confusion_matrix = np.array([[TP, FP],[FN, TN]])
    TPR_recall = TP / (TP + FN)
    precision = TP / (TP + FP)
    f1 = 2 * (precision * TPR_recall) / (precision + TPR_recall)

    return f1


# F1Score(y_true, y_pred)
```

2.3.2 1.2 Parameter tuning for decision tree

[251]:
```
# k-fold Cross validation

def CrossValidation(train_set, test_set, K, max_depths, target_label):

    # initialization
    TP = 0
    FP = 0
    TN = 0
    FN = 0
    f1_score_all = []
    #K-fold
    kf = KFold(n_splits=K)

#     for pname, pvalues in parameters.items(): # interate each parameter and␣
 ↪value list
```

```
#         f1_param_list = []  # create a list to store the f1 score of each␣
↪parameter

    for v in max_depths:  # for each parameter, interate values of that specific␣
↪parameter

        f1_each_depth_list = []  # list of f1 score for each value of one␣
↪parameter

        for train_idx, test_idx in kf.split(train_set):
            # for each value, run k-fold CV

            train = train_set.iloc[train_idx]
            x_train = train.drop(columns=target_label)
            y_train = train[target_label]

            test = train_set.iloc[test_idx]
            x_test = test.drop(columns=target_label)
            y_test = test[target_label]

            Dtree = DecisionTreeClassifier(max_depth=v)  # modify parameter and␣
↪train model
            clf = Dtree.fit(x_train, y_train)

            y_pred = clf.predict(x_test)  # predict with newly-trained model
            y_true = y_test

            f1 = F1Score(y_true, y_pred)  # call the f1 function created above

            f1_each_depth_list.append(f1)
              # store f1 scores in a list for each parameter value

        f1_depth = np.average(f1_each_depth_list) # f1 score of one param value
        f1_score_all.append(f1_depth)   #

    f1_dict = {
        'max_depths': max_depths,
        'f1_score': f1_score_all
    }
    df_f1 = pd.DataFrame(f1_dict)
    arg_best = np.argsort(f1_score_all)[-1]
    best_depth = max_depths[arg_best]
    best_f1 = np.sort(f1_score_all)[-1]

    return best_depth, best_f1, df_f1
```

[262]:
```python
depths = np.arange(2,20)
CrossValidation(train1, test1, 10, max_depths=depths, target_label='Sales')
```

[262]:
```
(19,
 0.3881671769157439,
     max_depths  f1_score
 0            2  0.260535
 1            3  0.291266
 2            4  0.332741
 3            5  0.326365
 4            6  0.366840
 5            7  0.374136
 6            8  0.368940
 7            9  0.386816
 8           10  0.386379
 9           11  0.381974
 10          12  0.366365
 11          13  0.374312
 12          14  0.380966
 13          15  0.363467
 14          16  0.375719
 15          17  0.388074
 16          18  0.385409
 17          19  0.388167)
```

[247]:
```python
# using GridSearchCV to tune parameter
depths = np.arange(0,20,1)
leafs = [1, 5, 10, 15, 20, 50, 75, 100]
param = {'max_depth': depths,
        'min_samples_leaf': leafs}
DT_gscv = GridSearchCV(estimator=clf, param_grid=param, cv=10)
DT_gscv.fit(x_train, y_train)
```

[247]:
```
GridSearchCV(cv=10, estimator=DecisionTreeClassifier(max_depth=3),
             param_grid={'max_depth': array([ 0,  1,  2,  3,  4,  5,  6,  7,  8,
9, 10, 11, 12, 13, 14, 15, 16,
       17, 18, 19]),
                         'min_samples_leaf': [1, 5, 10, 15, 20, 50, 75, 100]})
```

[14]:
```python
print(DT_gscv.best_score_, DT_gscv.best_params_)
```

```
0.737807881773399 {'max_depth': 8, 'min_samples_leaf': 5}
```

2.4 2. Chefboost

[167]:
```python
from chefboost import Chefboost as chef
```

[48]:

```
# cross_validation
def ChefBoostCrossValidation(train_set, test_set, algorithms, K, target_label):

    # initialization
    TP = 0
    FP = 0
    TN = 0
    FN = 0

    f1_score_all = []
    #K-fold
    kf = KFold(n_splits=K)
#     kf.get_n_splits(train_set)

    for algo in algorithms:   # for each algo, run k-fold CV

        config = {'algorithm': algo}

        f1list_each_algo = []

        for train_idx, test_idx in kf.split(train_set):  # run k-fold␣
 ↪cross-validation

            train = train_set.iloc[train_idx]

            x_train = train.drop(columns=target_label)
            y_train = train[target_label]

            test = train_set.iloc[test_idx]
            x_test = test.drop(columns=target_label)
            y_test = test[target_label]

            model_chef = chef.fit(train, config=config, target_label='Sales')
            # for each train set the K-fold selected, apply and fit a new model

            # then for each newly-trained model, run prediction and compute␣
 ↪f1-score
                  # chefboost can only pass one row at a time when predicting
            for index, row in x_test.iterrows():   # for each row in test set
                pred_label = chef.predict(model_chef, row)  # run prediction

                # compute confusion matrix
                if pred_label == 1:

                    if y_test[index] == 1:
                        TP += 1
```

```
                    elif y_test[index] == 0:
                        FP += 1

                if pred_label == 0:

                    if y_test[index] == 1:
                        FN += 1

                    elif y_test[index] == 0:
                        TN += 1

            confusion_matrix = np.array([[TP, FP],[FN, TN]])
            TPR_recall = TP / (TP + FN)
            precision = TP / (TP + FP)
            f1 = 2 * (precision * TPR_recall) / (precision + TPR_recall)
                  # this is the f1-score of one model using a specific algorithm
            f1list_each_algo.append(f1)
                  # store the score in a list

        algo_f1 = np.average(f1list_each_algo)
                  # after completing k-fold CV for one depth, jump out of the␣
↪loop
                  # and compute the average of all f1-scores for that algorithm
        f1_score_all.append(algo_f1)

    f1_dict = {
        'algorithms': algorithms,
        'f1_score': f1_score_all
    }
    df_f1 = pd.DataFrame(f1_dict)
    arg_best = np.argsort(f1_score_all)[-1]
    best_algo = algorithms[arg_best]
    best_f1 = np.sort(f1_score_all)[-1]

    return best_algo, best_f1, df_f1
```

[154]:
```
algorithms = ['C4.5', 'ID3', 'CART']
K=3
target_label = 'Sales'
chef_result = ChefBoostCrossValidation(train1, test1, algorithms, K,␣
↪target_label)
```

```
[INFO]:  4 CPU cores will be allocated in parallel running
WARNING: You set the algorithm to  C4.5  but the Decision column of your data
set has non-object type.
That's why, the algorithm is set to Regression to handle the data set.
Regression  tree is going to be built...
-------------------------
```

```
finished in  3.493199110031128  seconds
-------------------------
Evaluate  train set
-------------------------
MAE:  0.0647163120567376
MSE:  0.05097517730496453
RMSE:  0.22577683075321198
RAE:  0.37540827448129
RRSE:  0.46988560699401155
Mean:  0.3617021276595745
MAE / Mean:  17.8921568627451 %
RMSE / Mean:  62.42065320824095 %
[INFO]:  4 CPU cores will be allocated in parallel running
Regression  tree is going to be built...
-------------------------
finished in  3.073704957962036  seconds
-------------------------
Evaluate  train set
-------------------------
MAE:  0.12677304964539007
MSE:  0.08732269503546099
RMSE:  0.295504137086879
RAE:  0.45877018807904835
RRSE:  0.5997603769110708
Mean:  0.4148936170212766
MAE / Mean:  30.555555555555556 %
RMSE / Mean:  71.22407406709392 %
[INFO]:  4 CPU cores will be allocated in parallel running
Regression  tree is going to be built...
-------------------------
finished in  2.456028938293457  seconds
-------------------------
Evaluate  train set
-------------------------
MAE:  0.0523049645390071
MSE:  0.03679078014184397
RMSE:  0.19180922851063234
RAE:  0.3287444549595729
RRSE:  0.40478696441355394
Mean:  0.3404255319148936
MAE / Mean:  15.364583333333334 %
RMSE / Mean:  56.343960874998245 %
[INFO]:  4 CPU cores will be allocated in parallel running
WARNING: You set the algorithm to  ID3  but the Decision column of your data set
has non-object type.
That's why, the algorithm is set to Regression to handle the data set.
Regression  tree is going to be built...
-------------------------
```

```
finished in  2.865651845932007  seconds
-------------------------
Evaluate  train set
-------------------------
MAE:  0.0647163120567376
MSE:  0.05097517730496453
RMSE:  0.22577683075321198
RAE:  0.37540827448129
RRSE:  0.46988560699401155
Mean:  0.3617021276595745
MAE / Mean:  17.8921568627451 %
RMSE / Mean:  62.42065320824095 %
[INFO]:  4 CPU cores will be allocated in parallel running
Regression  tree is going to be built...
-------------------------
finished in  3.015012741088867  seconds
-------------------------
Evaluate  train set
-------------------------
MAE:  0.12677304964539007
MSE:  0.08732269503546099
RMSE:  0.295504137086879
RAE:  0.45877018807904835
RRSE:  0.5997603769110708
Mean:  0.4148936170212766
MAE / Mean:  30.555555555555556 %
RMSE / Mean:  71.22407406709392 %
[INFO]:  4 CPU cores will be allocated in parallel running
Regression  tree is going to be built...
-------------------------
finished in  2.4575560092926025  seconds
-------------------------
Evaluate  train set
-------------------------
MAE:  0.0523049645390071
MSE:  0.03679078014184397
RMSE:  0.19180922851063234
RAE:  0.3287444549595729
RRSE:  0.40478696441355394
Mean:  0.3404255319148936
MAE / Mean:  15.364583333333334 %
RMSE / Mean:  56.343960874998245 %
[INFO]:  4 CPU cores will be allocated in parallel running
WARNING: You set the algorithm to  CART  but the Decision column of your data
set has non-object type.
That's why, the algorithm is set to Regression to handle the data set.
Regression  tree is going to be built...
-------------------------
```

```
finished in  2.8816869258880615  seconds
-------------------------
Evaluate  train set
-------------------------
MAE:  0.0647163120567376
MSE:  0.05097517730496453
RMSE:  0.22577683075321198
RAE:  0.37540827448129
RRSE:  0.46988560699401155
Mean:  0.3617021276595745
MAE / Mean:  17.8921568627451 %
RMSE / Mean:  62.42065320824095 %
[INFO]:  4 CPU cores will be allocated in parallel running
Regression  tree is going to be built...
-------------------------
finished in  3.1659939289093018  seconds
-------------------------
Evaluate  train set
-------------------------
MAE:  0.12677304964539007
MSE:  0.08732269503546099
RMSE:  0.295504137086879
RAE:  0.45877018807904835
RRSE:  0.5997603769110708
Mean:  0.4148936170212766
MAE / Mean:  30.555555555555556 %
RMSE / Mean:  71.22407406709392 %
[INFO]:  4 CPU cores will be allocated in parallel running
Regression  tree is going to be built...
-------------------------
finished in  2.6229701042175293  seconds
-------------------------
Evaluate  train set
-------------------------
MAE:  0.0523049645390071
MSE:  0.03679078014184397
RMSE:  0.19180922851063234
RAE:  0.3287444549595729
RRSE:  0.40478696441355394
Mean:  0.3404255319148936
MAE / Mean:  15.364583333333334 %
RMSE / Mean:  56.343960874998245 %
```

[157]:
```
chef_result
```

[157]:
```
('C4.5',
 0.6539487607908661,
```

```
  algorithms  f1_score
0       C4.5  0.653949
1        ID3  0.645775
2       CART  0.644683)
```

[ ]:

```

```

2.5 5.3 KNN

2.5.1 Algorithm

1. calculate distance (Euclidean, Manhattan)
2. define K, find K nearest neighbors
3. using voting to define the category

[266]:

```
# caculate didstance for each test points
def distance(train, test, cal_type):

    index = np.arange(test.shape[0])
    distance_dict = {}

    if cal_type == 'Manhattan':

        for i in index: # iterate each row of test set
            distance_list = []
            l_test = test.iloc[i]
            for j in list(train.index):
                # iterate each row of train set and compute distance w.r.t. each␣
↪test point
                l_train = train.iloc[j]
                distance = abs(sum(l_test-l_train))
                distance_list.append(distance)
            distance_dict[i] = distance_list

    elif cal_type == 'Euclidean':

        for i in index:
            distance_list = []
            l_test = test.iloc[i]
            for j in list(train.index):
                l_train = train.iloc[j]
                distance = mt.sqrt(sum(l_train-l_test)**2)
                distance_list.append(distance)
            distance_dict[i] = distance_list

    else:
        return 'Type not found.'
        distance_dict = {np.na}
```

```
    return distance_dict



# find K nearest neighbors according to the defined K parameter
def KNNClassifier(train, test, K, cal_type):

    dis = distance(train, test, cal_type)

    df_distance = pd.DataFrame(dis).T # return distance result as a dataframe
    class_result = []
    # the following lines decide which category gets the most votes and return␣
 ↪results
    for index, row in df_distance.iterrows():

        args = np.argsort(row) # return the argument(index) of the K most␣
 ↪nearest points
        Knns = [train['Sales'].iloc[j] for j in args[:K]]
           #for each index, return the category in training set

        if Knns.count('Yes') >= Knns.count('No'):  # most votes
            result = 1

        else:
            result = 0

        class_result.append(result)

#          class_result[index] = class_each_row
#          df_class_result = pd.DataFrame(class_result).T # transform to dataframe
#          df_class_result['True_Urban'] = test1['urban_Yes']
#          df_class_result['True_US'] = test1['us_Yes']
        # add the actual classification to the last two columns

    return class_result
```

2.5.2 Tuning parameters (K and distance metric)

[267]:
```
def ParamTuning(train, test, K_list, dis_metrics, target_label):

    compare = {}
    y_true = test[target_label]

    for d in dis_metrics:
        inner = {}
```

```
        for k in K_list:
            y_pred = KNNClassifier(train, test, k, d)
            f1 = f1_score(y_true, y_pred)
            inner[f'k={k}'] = f1

        compare[f'distance_metric={d}'] = inner
    df_compare = pd.DataFrame(compare)
    max_f1 = df_compare.max()

    return max_f1
```

[268]:
```
K_list = np.arange(3,7)
dis_metrics = ['Manhattan', 'Euclidean']
knn_best = ParamTuning(train1, test1, K_list, dis_metrics, target_label='Sales')
```

[269]:
```
knn_best
```

[269]:
```
distance_metric=Manhattan    0.666667
distance_metric=Euclidean    0.666667
dtype: float64
```

2.6 5.4 Best preformance

[166]:
```
# Decision Tree
print('DecisionTree:', DT_gscv.best_score_, DT_gscv.best_params_)

# ChefBoost
print('ChefBoost:', chef_result[0], chef_result[1])

# KNN
print('KNN:', knn_best)
```

```
DecisionTree: 0.737807881773399 {'max_depth': 8, 'min_samples_leaf': 5}
ChefBoost: C4.5 0.6539487607908661
KNN: distance_metric=Manhattan    0.666667
distance_metric=Euclidean    0.666667
dtype: float64
```

Therefore, DecisionTreeClassifier performed the best.

2.7 5.5

As its name implies, LOOCV only keeps one point as the validation set while tuning parameters.

If K=n (n=total number of training points), then LOOCV equals K-fold CV.

Disadvantages:

1. High variance compared with k-fold. The training sets of LOOCV greatly overlap with one another. Therefore, the prediction will be highly correlated and interdependent, which increases

variance.

2. Computationally expensive. Every time it needs to train on n-1 datasets and test on one set, which is more time-consuming than k-fold.

2.8 5.6

I think f1 score and accuracy (misclassification error) are both good metrics for this specific dataset. Since f1 score is the Hamonic average of precision and recall, it can better return the prediction preformance on imbalanced dataset. However, in this problem, dataset is balanced (equal number of 1s and 0s in test set), so both f1 and accuracy are plausible.

```
[ ]:
```