Programming Assignment #2 Report

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Code Interpretation:

第一步先匯入資料。python 的 sklearn 裡面就有一些常用到的 datasets,例如 iris、wine 等。若不是用 sklearn 的就要另外從網路上下載並做一些前處理。 之後把 dataset 切割成 training subset 和 validation subset,這裡我是用 sklearn 裡的 train_test_split,test_size = 0.3 就代表 training subset 佔 0.7、validation subset 佔 0.3,random state 可以確保每次分割出來的 subset 不會一樣。

接下來就是實作 decision tree 的部分。這就像是條件比較多的二元樹。先寫一個叫 node 的 class,這個 class 的成員有 feature 陣列、與其對應的 target 陣列、node splitting 條件(attribute bagging、包含一個 feature index 和一個 threshold)、left node、right node。接著寫一個計算 gini 值的函式。這個函式會傳入兩個參數,feature 陣列和對應之 target 陣列。它依次取出每個 feature,將值排序後算出 target-1 個 threshold 值((v1+v2)/2,(v2+v3)/2,...,(vn-1+vn)/2),依照每個 threshold 值切割 target 陣列,算出每個 gini 值。算完後選出最小的 gini 值,選擇此 gini 值對應之 feature 和 threshold 為 node splitting 之條件並回傳。

最後就可以遞迴建出整棵 decision tree 了。先建立 root node 並傳入 training subset 的 feature 陣列和 target 陣列,並將 root 傳入 tree 建構函式。每次遞迴,都用 gini 計算函式算出 splitting 條件,依照此條件分割出 left node 和 right node,再將這兩個 node 遞迴傳入 tree 建構函式,並將 depth 值加 1。若 depth 等於5或是分割出的 node 只有唯一一種 target 就 return。

Random forest 的部分就是建出 20 棵不同的 decision tree,這 20 棵 tree 算法部分完全相同,只是一開始 root 傳入的 feature 陣列、target 陣列不同。每棵樹 傳入的 data 都是在 training subset 中隨機取樣,這裡我一樣用 train_test_split 切 出佔比 0.7 的 data,而每次迴圈的 random_state 不同,確保每次取出的 data 不會完全一致。最後在 prediction 時採取 majority vote 的方式,但每棵樹的一票不完全等值,而是要乘上它的準確率。舉例來說,tree no.3 預測 target 為 2 ,而 tree no.3 預測 2 的準確率為 75%,那麼它的這一票就會是 1*0.75 = 0.75 分。最後 random forest 會選擇最高分的那個 target 為最終的 prediction 結果。

Observation:

我採用了三種 dataset 來做評估,分別是 iris、wine、ecoli。其中 iris 和 wine 是用 sklearn 裡面的,ecoli 是從 UCI Machine Learning Repository 下載的。 我的 decision tree 和 random forest 的 depth 都是 5,其中 random forest 為 20 棵 樹做 tree bagging。算法部分都是照上個部分所述。每個 dataset 都執行三次,以下為執行結果(以 confusion matrix 和 total accuracy 呈現):

Iris:

1	
decision	n free:
GCC1D101	i dicc.

[10 0 0]	[15 0 0]	[16 0 0]
[0 15 3]	[0 9 0]	[0 13 2]
[0 4 13]	[0 4 17]	[0 1 13]
accuracy: 84%	accuracy: 91%	accuracy: 93%

random forest:

accura	ıcy: 89%	accı	irac	y: 93%	accu	racy	7: 98%
[0 3	14]	0]	3	18]	0]	1	13]
[0 1	6 2]	[0	9	0]	0]	15	0]
[10 (0 0]	[15	0	0]	[16	0	0]

Wine:

decision tree:

accuracy: 89%	accuracy: 91%	accuracy: 94%
[0 2 16]	[0 2 14]	[0 1 13]
[1 17 0]	[0 15 0]	[2 22 0]
[15 3 0]	[20 3 0]	[16 0 0]

random forest:

[15 3 0]	[22 1 0]	[16 0 0]
[0 17 1]	[1 14 0]	[0 24 0]
[0 1 17]	[0 2 14]	[0 0 14]
accuracy: 91%	accuracy: 93%	accuracy: 100%

Ecoli:

decision tree:

```
[3 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0] [2 \ 0 \ 0 \ 0 \ 0 \ 0] [3 \ 0 \ 0 \ 0 \ 0 \ 0]
[0 \quad 13 \quad 1 \quad 11 \quad 0 \quad 0 \quad 0 \quad 0] \quad [0 \quad 16 \quad 0 \quad 8 \quad 0 \quad 0 \quad 0 \quad 0] \quad [0 \quad 17 \quad 0 \quad 2 \quad 1
[0 \quad 0 \quad 40 \quad 0 \quad 1 \quad 1 \quad 0 \quad 0] \quad [0 \quad 1 \quad 38 \quad 1 \quad 0 \quad 1 \quad 0 \quad 0] \quad [0 \quad 1 \quad 51 \quad 1 \quad 0 \quad 0]
                                                                                                               0]
                                                        7 0 1 0 0] [0 2 0
\begin{bmatrix} 0 & 0 & 0 \end{bmatrix}
                7 0 0 0 0] [0 1 0
                                                                                               4 0 0
                                                                                                                 0]
                0 0 2 0 0] [0 0 1
                                                       0 2 4 0 0] [0 0 0
                                                                                               0 0 4
                                                                                                                 0]
              0 2 15 0 0] [0 0
                                                 2
                                                     2 4 8 0 0] [0 0
                                                                                         1 0 0 13 0
                                                                                                                 0]
\begin{bmatrix} 0 & 0 & 3 \end{bmatrix}
              0 0 0 0 0
                                       [0 \ 0 \ 0 \ 0 \ 1 \ 0 \ 0 \ 0]
                                                                               \begin{bmatrix} 0 & 0 \end{bmatrix}
                                                                                         0
                                                                                                                 0]
                                                                               [0 \ 0 \ 1 \ 0 \ 0 \ 0]
[0 \ 0 \ 1 \ 0 \ 0 \ 0 \ 0]
                                       [1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0]
                                                                                                                 0]
```

accuracy: 77% accuracy: 72% accuracy: 87%

random forest:

[3	0	0	0	0	0	0	0]	[2	0	0	0	0	0	0	0]	[3	0	0	0	0	0	0	0]
[0	15	1	9	0	0	0	0]	[0	19	0	5	0	0	0	0]	[0	15	0	5	0	0	0	0]
[0	0	41	0	0	1	0	0]	[0	0	40	0	0	1	0	0]	[0	1	52	0	0	0	0	0]
[0	0	0	7	0	0	0	0]	[0	2	0	6	0	1	0	0]	[0	2	0	4	0	0	0	0]
[0	0	0	0	0	2	0	0]	[0	0	1	0	1	5	0	0]	[0	0	0	0	0	4	0	0]
[0	0	3	0	0	17	0	0]	[0	2	3	2	0	9	0	0]	[0	0	1	0	0	13	0	0]
[0	0	1	0	0	0	0	0]	[0	0	0	0	0	1	0	0]	[0	0	0	0	0	0	0	0]
[0	0	1	0	0	0	0	0]	[1	0	0	0	0	0	0	0]	[0	0	0	0	0	1	0	0]
acci	ırac	y: 8	2%					accı	ırac	y: 70	6%					accı	ırac	y: 86	%				

從以上數據可以看出,random forest 的正確率普遍會比 decision tree 還要好一點。不論是樣本數小的 iris,或是樣本數、feature 數都較大的 ecoli 都呈現差不多的趨勢。這證明 random forest 用多棵樹隨機取樣預測並投票是有效果的。但缺點是犧牲了執行的效率,用 20 棵樹預測理論上就要比 decision tree 多花 20 倍的時間。

Experiments and Results:

以下分析之準確率皆為執行5次之平均。

Relative sizes of the training and validation subsets:

透過更改 train_test_split 的 test_size,就可以更改 training 和 validation 的比例。以下為 wine 在不同比例下的正確率:

Training size	Validation size	Decision tree	Random forest
0.9	0.1	94.33%	98%
0.7	0.3	91.33%	94.67%
0.5	0.5	92.67%	95%
0.3	0.7	85%	90.33%

由上表可以看出,當 training size 愈小、validation size 愈大時,正確率大致會下降。此結果符合預期,因為當 training 的資料愈多時, tree 看到的資料就更為全面,也就愈能做出正確的判斷。

Number of trees in the forest:

這次使用 target 和 feature 皆較複雜的 ecoli,較能看出變化:

Number of trees	5	10	15	20
Accuracy	78%	81.2%	83.6%	82.2%

由上表可以看出,用愈多棵樹進行投票,準確率大致會提升。而大概用 15 棵樹就可以達到最高的準確率。再用更多的樹將不會提升準確率,只會使執行效率 更差。

Decision tree's depth:

將深度設為 tree 建構函式遞迴的中止條件可以限制 tree's depth。理論上, tree 深度太小會造成 underfit,而深度過大會造成 overfit。以下為 wine 的 decision tree 在各深度的準確率:

depth	1	2	3	4	5	6	7	8
accuracy	56.4%	84.8%	90.2%	87.6%	90.4%	90.6%	87.8%	88.4%

由上表可看出,depth=1 時會明顯的 underfit,而 depth=2 就能做出很好的 node splitting,但還是稍稍 underfit;到 depth=7,8 時會稍稍 overfit 但不明顯,是因為遞迴中止條件並不只有 depth,還有是當 node splitting 已經完全分出一類,也就是gini 值等於 0 時,其遞迴也會中止。因此其深度根本無法達到太深,depth 超過一個臨界值就等同於無效了。

Rate of majority vote in random forest:

若將 20 棵樹都視為相等的效力,也就是 majority vote 中所謂的「一票」,這樣出來的結果,random forest 的正確率會和 decision tree 差不多、甚至更差,而不是預期的提升。這代表這組資料具有一定的雜亂程度,會容易讓每棵 decision tree 做出不同的選擇。而正確率較差的 tree 會影響到正確率較高的 tree,導致最後投出的 prediction 錯誤。因此,每棵樹不應該票票等值,而是要乘上它預測它要投的那個 target 的正確率。而此正確率可以在樹建出來時就順便算好,例如 tree bagging 時選擇 K 個 sample 進去 train,剩下的,也就是所謂的 out-of-bag samples,就拿來算正確率並存起來,等著 voting 時使用。

Extremely random forest:

每次 node splitting 時都選擇隨機一個 feature。要做到這件事只要將原本迭代 feature 的 for i in range(feature_size)改成 i = random.randint(0, feature_size-1)即可。這對於 feature 較多的 data 例如 ecoli,執行效率上會有大幅度的提升。然而隨機選取 feature 來做 splitting,找到的分法可能不會是最理想的,導致單一個 decision tree 的準確度變差。但 random forest 是所有 decision tree 的投票結果,準確度較差的 decision tree 拿到的票數也會較低,所以綜合來看,extremely

random forest 的準確度和普通 random forest 不會差太多。以下數據為 wine 用 random feature splitting 的準確率:

Decision tree with random feature splitting	79%
Extremely random forest	98%

可以看出,單棵 decision tree 的準確率比起原本的 90 出頭大幅下降到了 79%,然而 random forest 依然能維持高檔的準確率。

Things I Have Learned:

這次作業中,我學會了如何建構一棵完整的 decision tree, 並接著實作出 random forest。包含如何計算 gini、attribute bagging 找到最好的 node splitting 方法、forest 中利用 tree bagging 得出結果。最後是分析及比較各種 dataset、各種數據,並得出結論。

Remaining Questions:

剩下的問題主要是在 node splitting 的地方。我使用的 attribute bagging 方式一次只找一個 attribute,也就是只用一個條件來 splitting。但若是數據量龐大且複雜,有可能一個條件並不足以良好的切割,尤其是在 tree depth 或執行時間上有限制的時候。而若是一次使用多個條件進行 splitting,理論上能更有效率的找到更好的 splitting 方式、使 gini 值更低。

Ideas of Future Investigation:

不是每種 dataset 都能用 decision tree 和 random forest 做出最好的預測。還有許多 training model 可以用來嘗試,每種 dataset 都能依照其 feature、target 特性,找到一種最適合的 model。通常 training 需要大量的經驗和嘗試,才能讓準確率稍微上升一點點。而我們學習的目標就是能在盡量短的時間內找到最理想、能符合我們預期的 model。

Appendix:

```
import numpy as np
import pandas as pd
from sklearn import datasets, metrics
from sklearn.model selection import train test split
from sklearn.metrics import confusion_matrix
from sklearn.metrics import classification report
import random
# iris data
def iris():
     iris = datasets.load iris()
     # splitting data to training set and validation set
     x train, x test, y train, y test = train test split(iris.data, iris.target, test size=0.3)
     return x_train, x_test, y_train, y_test
# wine data
def wine():
     wine = datasets.load wine()
     x_train, x_test, y_train, y_test = train_test_split(wine.data, wine.target, test_size=0.3)
     return x_train, x_test, y_train, y_test
# ecoli data
def ecoli():
   # data preprocessing
     ecoli = pd.read_csv('ecoli.data', header=None)
     ecoli data = []
     ecoli_target = []
     for i in range(len(ecoli)):
          a = ecoli[0][i].split()
          li = [float(i) \text{ for } i \text{ in } a[1:8]]
          ecoli data.append(li)
          ecoli target.append(a[8])
     ecoli_data = np.array(ecoli_data)
     echoli_target_t = list(set(ecoli_target))
     e = []
     for i in ecoli_target:
```

```
for j in range(len(echoli target t)):
               if echoli_target_t[j] == i:
                     e.append(j)
                    break
     ecoli target = np.array(e)
     x_train, x_test, y_train, y_test = train_test_split(ecoli_data, ecoli_target, test_size=0.3)
     return x_train, x_test, y_train, y_test
x_train, x_test, y_train, y_test = wine()
                                              # choose which dataset to use
feature size = len(x train[0])
                                              # get number of feature
target size = len(set(y train))
                                              # get number of target
# tree node
class node:
     def __init__(self,feature,target):
          self.feature=feature
          self.target=target
          self.attr ind=-1
          self.attr val=-1
          self.left=None
          self.right=None
          self.attr=-1
     def get_attr(self):
        # calculate which target has the most samples in this node,
        # this node represent this target in prediction
          global target size
          cnt = []
          for i in range(target_size):
               cnt.append(self.target.tolist().count(i))
          m = -1
          ind = -1
          for i in range(len(cnt)):
               if cnt[i] > m:
                    m = cnt[i]
                    ind = i
```

```
self.attr = ind
     def is_terminate(self):
        # if this node doesn't need to split (gini == 0), terminate
          global target_size
          cnt = []
          for i in range(target size):
                cnt.append(self.target.tolist().count(i))
          if cnt.count(0) == len(cnt) - 1:
                for i in range(len(cnt)):
                     if cnt[i] != 0:
                          self.attr = i
                          break
                return True
          return False
def calc_gini(li,li_y):
   # do attribute bagging, try all feature and threshold, calculate and return the splitting condition
     global feature_size
     1 = len(li y)
     g min = 10000
     g ind = -1
     g m = 10000
     if li.size == 0:
          return 0,0
     \#i = \text{random.randint}(0, \text{feature size-1})
                                                   # extremely random forest, select attribute randomly
                                                  # random forest, iterate all attribute
     for i in range(feature size):
          attr = li[:,i]
          tmp_attr = sorted(attr)
          m li = []
          for j in range(len(attr)-1):
```

```
m_li.append((tmp_attr[j]+tmp_attr[j+1])/2) # sort and calculate all threshold
                                                       # splitting and calculate gini
                                                       for m in m li:
                                                                                  y_right = []
                                                                                 y_left = []
                                                                                  for j in range(1):
                                                                                                             if li[j][i] > m:
                                                                                                                                        y_right.append(li_y[j])
                                                                                                             else:
                                                                                                                                        y_left.append(li_y[j])
                                                                                  gini right = 0
                                                                                  gini_left = 0
                                                                                  if len(y right) != 0:
                                                                                                             gini\_right = 1 - ((y\_right.count(0)/len(y\_right))**2 + (y\_right.count(1)/len(y\_right))**2 + (y\_right.count(1)/len(y\_righ
(y_right.count(2)/len(y_right))**2)
                                                                                  else:
                                                                                                              continue
                                                                                  if len(y_left) != 0:
                                                                                                              gini_left = 1 - ((y_left.count(0)/len(y_left))**2 + (y_left.count(1)/len(y_left))**2 + (y_left.count(1)/len(y_left))**2
(y_left.count(2)/len(y_left))**2)
                                                                                  else:
                                                                                                              continue
                                                                                  gini = len(y_right) * gini_right + len(y_left) * gini_left
                                                                                  if gini < g min:
                                                                                                             g min = gini
                                                                                                             g_ind = i
                                                                                                              g m = m
                           return g ind, g m
                                                                                                                                                         # return splitting condition (attribute and threshold)
# tree construction
def tree(n,depth):
                           if n.is terminate(): # terminate condition: gini == 0
                                                       return
                                                                                                                                 # terminate condition: depth
                           if depth == 5:
                                                       n.get_attr()
```

```
return
```

```
x = n.feature
     y = n.target
     a,m = calc_gini(x,y) # get splitting condition
     n.attr ind = a
     n.attr_val = m
     # node splitting
     y_right = []
     x_right = []
     y_left = []
     x_left = []
     for i in range(len(y)):
          if x[i][a] > m:
               y_right.append(y[i])
               x_right.append(x[i])
          else:
               y_left.append(y[i])
               x_left.append(x[i])
     x_{left} = np.array(x_{left})
     y_left = np.array(y_left)
     x_right = np.array(x_right)
     y_right = np.array(y_right)
     node left = node(x left, y left)
     node_right = node(x_right,y_right)
     n.left = node left
     n.right = node right
     # recursive call tree construction (construct left and right subtrees)
     tree(n.left, depth+1)
     tree(n.right, depth+1)
root = node(x_train,y_train)
tree(root,0)
# predict a value
def evaluation(root,t):
```

```
curr = root
     ans = -1
     while curr != None:
          if t[curr.attr_ind] > curr.attr_val:
               ans = curr.attr
               curr = curr.right
          else:
               ans = curr.attr
               curr = curr.left
     return ans
correct = 0
pred = []
for i in range(len(y test)): # put all validation data into prediction: decision tree
     result = evaluation(root,x_test[i])
     pred.append(result)
     if result == y_test[i]:
          correct += 1
print('Decision Tree:')
print(confusion_matrix(y_test, pred))
print(classification_report(y_test, pred))
# calculate rate of vote
def confusion matrix element precision(cm, i):
     try:
          cm2 = cm[i].tolist()
     except:
          return 0
     acc = 0
     if sum(cm2) != 0:
          acc = cm2[i]/sum(cm2)
     return acc
# random forest tree bagging
trees = []
ac_score = []
```

```
# construct 20 trees in a forest
for i in range (20):
   # randomly select 0.7 from training subset
     num = random.randint(1,1000)
     x_train1, x_test1, y_train1, y_test1 = train_test_split(x_train, y_train, test_size=0.3, random_state=num)
     root = node(x train1, y train1)
     tree(root,0)
     trees.append(root)
     pred = []
     for j in range(len(y_test1)):
          result = evaluation(root,x test1[i])
          pred.append(result)
     # calculate out-of-bag and store rate of voting
     cm = confusion matrix(y test1, pred)
     ele = []
     for j in range(target size):
          ele.append(confusion matrix element precision(cm, j))
          ac_score.append(ele)
# put all validation data into prediction: random forest
rf pred = []
for i in range(len(y_test)):
     vote = []
     for r in trees:
                       # voting
          res = evaluation(r,x test[i])
          vote.append(res)
     #rf_pred.append(max(vote)) # majority vote
     # majority vote with different rate
     k = [0] * target size
     for j in range(target_size):
          for v in range(20):
               if vote[v] == j:
                    k[j] += ac\_score[v][j]
     m = -1
     ind = -1
     for j in range(target_size):
          if k[j] > m:
               m = k[j]
```

```
ind = j
rf\_pred.append(ind)
```

```
print('Random Forest:')
print(confusion_matrix(y_test, rf_pred))
print(classification_report(y_test, rf_pred))
```