大家好，这篇是有关台大机器学习课程作业七的详解。

我的github地址：
https://github.com/Doraemonzzz

个人主页：
http://doraemonzzz.com/

作业地址:
https://www.csie.ntu.edu.tw/~htlin/course/ml15fall/

参考资料:
https://blog.csdn.net/a1015553840/article/details/51085129
http://www.vynguyen.net/category/study/machine-learning/page/6/
http://book.caltech.edu/bookforum/index.php
http://beader.me/mlnotebook/
https://blog.csdn.net/qian1122221/article/details/50130093
https://acecoooool.github.io/blog/

Problem 1

$$\begin{aligned}1-\mu_+^2-\mu_-^2&=1-\mu_+^2-(1-\mu_+)^2\\&=1-\mu_+^2-\mu_+^2+2\mu_+-1\\&=-2\mu_+^2+2\mu_+\\&=-2(\mu_+-\frac{1}{2})^2+\frac{1}{2}\end{aligned}$$

因为$\mu_+\in[0,1]$，所以$1-\mu_+^2-\mu_-^2\in[0,\frac{1}{2}]$，最大值为$\frac{1}{2}$。

Problem 2

$$\begin{aligned}\mu_+(1-(\mu_+-\mu_-))^2+\mu_-(-1-(\mu_+-\mu_-))^2&=\mu_+[1-2(\mu_+-\mu_-)+(\mu_+-\mu_-)^2]+\mu_-[1+2(\mu_+-\mu_-)+(\mu_+-\mu_-)^2]\\&=\mu_++\mu_-+(\mu_++\mu_-)(\mu_+-\mu_-)^2-2(\mu_+-\mu_-)(\mu_+-\mu_-)\\&=1+(\mu_+-\mu_-)^2-2(\mu_+-\mu_-)^2\\&=1-(\mu_+-\mu_-)^2\\&=1-(2\mu_+-1)^2\\&=4\mu_+-4\mu_+^2\end{aligned}$$

根据Problem 1以及正规化错误的定义可知

$$\text{normalized Gini index}=(-2\mu_+^2+2\mu_+)/(\frac{1}{2})=4\mu_+-4\mu_+^2$$

所以

$$\text{normalized Gini index}=\text{normalized squared regression error}$$

Problem 3

回顾课件可知，一个数据不被选择的概率为

$$(1-\frac{1}{N})^{N'}=(1-\frac{1}{N})^{pN}=[(1-\frac{1}{N})^{N}]^{p}\approx e^{-p}$$

因为一共有N组数据，所以没有被选择的数据数量大概为

$$e^{-p}N$$

Problem 4

根据下一题可知

$$E_{\text{out}}(G)\le\frac{2}{3+1}(0.15+0.25+0.35)=0.375$$

显然

$$E_{\text{out}}(G)\ge 0$$

所以

$$E_{\text{out}}(G)\in[0,0.375)$$

Problem 5

根据Random Forest的算法，我们知道如果要把一个点误分，那么K个binary classification trees中必然至少要$\frac{K+1}{2}$个分类器犯错，假设一共有N个点，那么一共有$(\sum_{k=1}^{K}e_k)N$个分类错误，所以被Random Forest算法分类错误的点最多为

$$(\sum_{k=1}^{K}e_k)N/\frac{K+1}{2}$$

因此$E_{\text{out}}(G)$最多为

$$(\sum_{k=1}^{K}e_k)N/(\frac{K+1}{2}N)=\frac{2}{K+1}\sum_{k=1}^{K}e_k$$

Problem 6

计算公式为

$$U_{t+1}=2U_t\sqrt{\epsilon_t(1-\epsilon_t)}$$

具体的推导过程可以看作业6的22题，这里直接带入

$$U_3=2U_2\sqrt{\epsilon_2(1-\epsilon_2)}=4U_1\sqrt{\epsilon_2(1-\epsilon_2)}\sqrt{\epsilon_1(1-\epsilon_1)}$$

注意$(u_1,\ldots,u_N)=(\frac{1}{N},\ldots,\frac{1}{N})$，所以$U_1=1$

$$U_3=2U_2\sqrt{\epsilon_2(1-\epsilon_2)}=4U_1\sqrt{\epsilon_2(1-\epsilon_2)}\sqrt{\epsilon_1(1-\epsilon_1)}=4\sqrt{\epsilon_2(1-\epsilon_2)}\sqrt{\epsilon_1(1-\epsilon_1)}$$

Problem 7

结合题目以及课件17页可知

$$\eta\text{为使得 }\frac{1}{N}\sum_{n=1}^{N}\Big((y_n-s_n)-\eta g_1(x_n)\Big)^2\text{ 最小的值}$$

对上式关于η求偏导可得

$$-\frac{2}{N}\sum_{n=1}^{N}g_1(x_n)\Big((y_n-s_n)-\eta g_1(x_n)\Big)=0$$

此处$g_1(x_n)=2,s_n=0$带入可得

$$\sum_{n=1}^{N}2\Big((y_n-0)-2\eta\Big)=0$$

$$\eta=\frac{1}{2N}\sum_{n=1}^{N}y_n$$

由于更新规则为$\alpha_1=\eta$，$s_n=\alpha_1g_1(x_n)$，所以

$$s_n=\alpha_1g_1(x_n)=\frac{1}{2N}\sum_{n=1}^{N}y_n\times 2=\sum_{n=1}^{N}y_n$$

Problem 8

回顾课件19页可知

$$\alpha_t = \eta = \frac{\sum_{n=1}^{N} g_t(x_n)(y_n - s_n)}{\sum_{n=1}^{N} g_t^2(x_n)}$$
$$\sum_{n=1}^{N} g_t(x_n)(y_n - s_n) = \alpha_t \sum_{n=1}^{N} g_t^2(x_n)$$
$$\sum_{n=1}^{N} g_t(x_n)s_n = \sum_{n=1}^{N} g_t(x_n)y_n - \alpha_t \sum_{n=1}^{N} g_t^2(x_n)$$

Problem 9

OR运算的特点是只有当每个值都为False，结果才为False，结合这个特点可以取

$$w_0 = d - \frac{1}{2}, w_i = 1(i = 1, \ldots, d)$$

Problem 10

由Problem 21，D的最小值为5，具体过程见Problem 21

Problem 11

初始的$w_{ij}^{(l)}$都为0，所以前向传播之后$s_j^{(l)} = 0, (l = 1, \ldots, L)$

回顾反向传播的更新规则

$$\frac{\partial e_n}{\partial w_{ij}^{(l)}} = \delta_j^{(l)}\left(x_i^{(l-1)}\right)$$
$$\delta_j^{(L)} = -2\left(y_n - s_j^{(L)}\right)$$
$$\delta_j^{(l)} = \sum_k \left(\delta_k^{(l+1)}\right)\left(w_{jk}^{(l+1)}\right)\tanh'(s_j^{(l)})(l = 0, \ldots, L-1)$$

所以根据上式，

$$\delta_j^{(l)} = 0, (l = 0, \ldots, L-1)$$

因为原始的$w_{ij}^{(l)}$都为0，所以根据更新规则

$$w_{ij}^{(l)} = w_{ij}^{(l)} - \eta\delta_j^{(l)} x_i^{(l-1)}$$

可知

$$w_{ij}^{(l)} = 0(l = 0, \ldots, L-1)$$

Problem 12

初始的$w_{ij}^{(l)}$都为1，假设输入为$x_1,\ldots,x_d$，偏置项为$x_0=1$，那么

$$s_i^{(1)}=\sum_{i=0}^{d}w_{ij}^{(l)}x_i=\sum_{i=0}^{d}x_i$$

说明第一个隐藏层的$s_i^{(1)}$都相等，根据递推公式

$$x_i^{(l-1)}=\tanh(s_i^{(l)})$$

$$s_i^{(l)}=\sum_{i=0}^{d^{(l-1)}}w_{ij}^{(l)}x_i^{(l-1)}$$

我们知道每个隐藏层的$s_i^{(l)},x_i^{(l)}$都相等，从而$\delta_j^{(L)}=-2\Big(y_n-s_j^{(L)}\Big)$都相等，根据反向传播的更新公式

$$\delta_j^{(l)}=\sum_k\Big(\delta_k^{(l+1)}\Big)\Big(w_{jk}^{(l+1)}\Big)\Big(\tanh'(s_j^{(l)})\Big)$$

可得，对于固定的l，$\delta_j^{(l)}$都相等，特别的，第一层的$\delta_j^{(1)}$都相等，根据更新规则

$$w_{ij}^{(1)}=w_{ij}^{(1)}-\eta\delta_j^{(1)}x_i^{(0)}$$

以及初始的$w_{ij}^{(l)}$都为1可得

$$w_{ij}^{(1)}=w_{i(j+1)}^{(1)}$$

Problem 13

略过

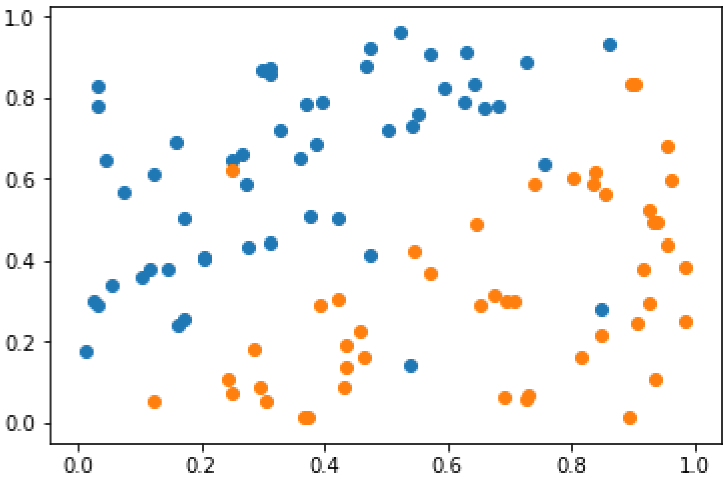
Problem 14

读取数据并作图。

```
import numpy as np
import matplotlib.pyplot as plt

#读取数据并作图
train = np.genfromtxt('hw7_train.dat')
X_train, y_train = train[:, :-1], train[:, -1]
test = np.genfromtxt('hw7_test.dat')
X_test, y_test = test[:, :-1], test[:, -1]

#作图
plt.scatter(train[:, 0][train[:, 2] == -1], train[:, 1][train[:, 2] == -1])
plt.scatter(train[:, 0][train[:, 2] == 1], train[:, 1][train[:, 2] == 1])
plt.show()
```



定义Gini index

```
#Gini index
def Gini(y):
    '''
    二分类gini系数
    '''
    if(len(y) == 0):
        return 1
    t = np.mean(y == -1)
    return 1 - t**2 - (1 - t)**2
```

定义impurty

```python
#定义impurty
def lossfunc(theta, X, y):
    '''
    d为数据的维度，theta为decision stump的阈值
    '''
    y1 = y[X < theta]
    y2 = y[X >= theta]
    Gini1 = Gini(y1)
    Gini2 = Gini(y2)
    #print(len(y1), len(y2))
    return len(y1) * Gini1 + len(y2) * Gini2
```

在d个维度上分别利用decision stump计算，找到损失函数的最小值，返回维度以及阈值

```python
def Generate_theta(X):
    """
    生成阈值
    """
    X = np.sort(X)
    theta = (X[1:] + X[:-1]) / 2
    theta = np.r_[[X[0] - 1], theta]
    theta = np.r_[theta, [X[-1] + 1]]

    return theta

#在d个维度上分别利用decision stump计算，找到损失函数的最小值，返回维度以及阈值
def Decision_stump(X, y):
    """
    对d个维度使用Decision_stump
    """
    #获得数据维度
    n, d = X.shape
    #最终结果
    Theta = 0
    D = 0
    Score = n
    for i in range(d):
        #取第d维的数据
        x = X[:, i]
        #计算阈值
        theta = Generate_theta(x)
        #遍历
        for theta_ in theta:
            #计算损失函数
            score = lossfunc(theta_, x, y)
            if score < Score:
                Score = score
                Theta = theta_
                D = i

    return D, Theta, Score
```

构造学习函数

```python
def isstop(X, y):
    '''
    判断是否停止，有两种情形，X全相同，另一种是所有数据都为一类
    '''
    n = X.shape[0]
    #n1 = np.sum(y==-1)
    n1 = np.sum(y!=y[0])
    n2 = np.sum(X!=X[0, :])
    return n1 == 0 or n2 == 0

#构造树类
class DTree:
    def __init__(self, theta, d, value=None):
        #阈值
        self.theta = theta
        #维度
        self.d = d
        #当前节点对应的值
        self.value = value
        #左右节点
        self.left = None
        self.right = None

NUM = 0
#构造学习函数
def learntree(X, y):
    global NUM
    NUM += 1
    if isstop(X, y):
        #print(X.shape, y)
        return DTree(None, None, y[0])
    else:
        d, theta, score = Decision_stump(X, y)
        #print(d, theta, score)
        tree = DTree(theta, d)
        #划分数据
        i1 = X[:, d] < theta
        X1 = X[i1]
        #print("X1", X1.shape)
        y1 = y[i1]
        i2 = X[:, d] >= theta
        X2 = X[i2]
        y2 = y[i2]
        #学习左树
        leftTree = learntree(X1, y1)
        #学习右树
        rightTree = learntree(X2, y2)
        #返回
        tree.left = leftTree
        tree.right = rightTree
```

```
        return tree
```

预测函数

```
#预测函数
def pred(tree, x):
    #if tree.left == None and tree.right == None:
    if tree.value != None:
        return tree.value
    if x[tree.d] < tree.theta:
        return pred(tree.left, x)
    else:
        return pred(tree.right, x)
```

计算误差

```
#计算误差
def error(tree, X, y):
    ypred = [pred(tree, x) for x in X]
    return np.mean(ypred!=y)
```

训练数据

```
dtree = learntree(X_train, y_train)
#14
print(error(dtree, X_train, y_train))
```

```
0.0
```

Problem 15

```
#15
print(error(dtree, X_test, y_test))
```

```
0.126
```

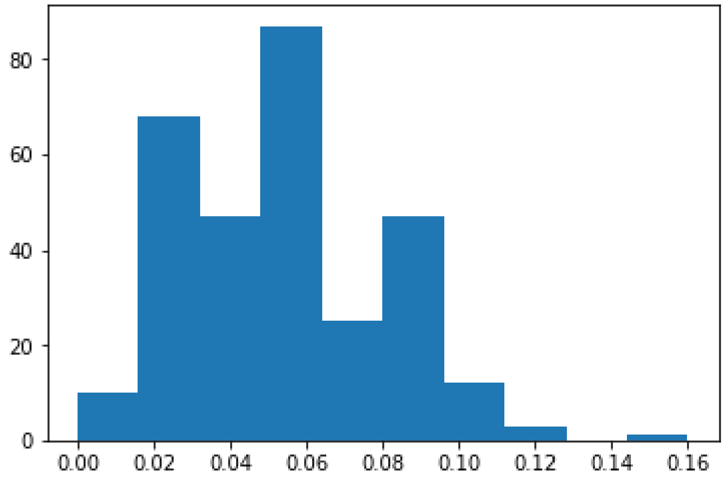
Problem 16

求出30000棵树对应的$E_{\text{in}}(g_t)$，为了减少运算量，这里取300棵。

```
#16
N = 300
Ein = np.array([])
tree = []
m, n = train.shape
```

```
for i in range(N):
    index = np.random.randint(0, m, (m))
    X1 = X_train[index, :]
    y1 = y_train[index]
    dtree = learntree(X1, y1)
    tree.append(dtree)
    Ein = np.append(Ein, error(dtree, X_train, y_train))

plt.hist(Ein)
plt.show()
```




```
print("Ein = {}".format(np.mean(Ein)))
```

```
Ein = 0.05319999999999999
```

Problem 17

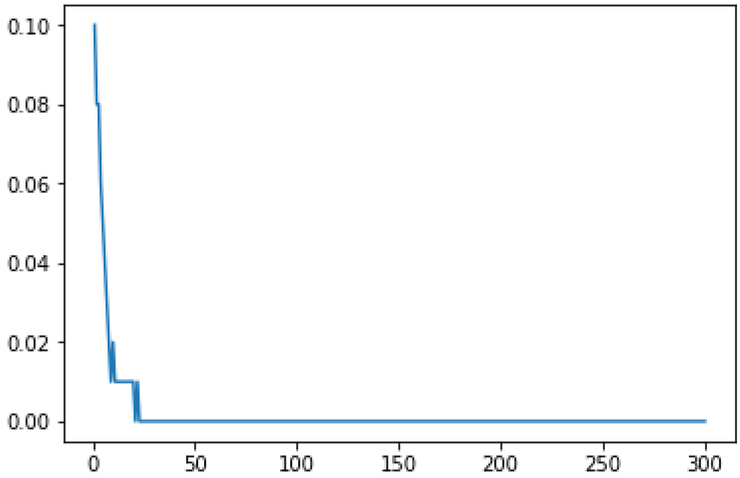
每次取前t棵数构成随机森林，计算结果并作图。

```
#17
def random_forest_error(tree, X, y):
    """
    利用前k个树计算结果
    """
    Error = np.array([])
    N = len(tree)
    for i in range(N):
        E = []
        for j in range(1+i):
            E.append([pred(tree[j], x) for x in X])
        E = np.array(E)
        #0视为1
        ypred = np.sign(E.sum(axis=0) + 0.5)
```

```
        error = np.mean(ypred!=y)
        Error = np.append(Error, error)
    return Error

Ein_G = random_forest_error(tree, X_train, y_train)

plt.plot(np.arange(1, N+1), Ein_G)
plt.show()
```



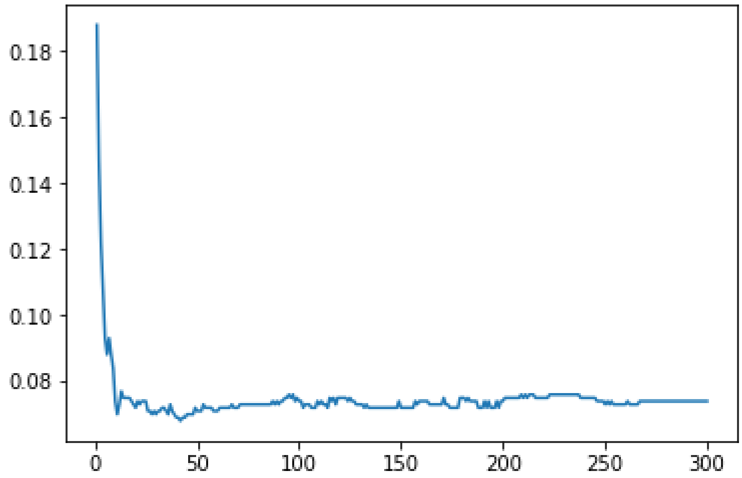

```
print("Ein = {}".format(np.mean(Ein_G)))
```

```
Ein = 0.002
```

Problem 18

```
#18
Eout_G = random_forest_error(tree, X_test, y_test)

plt.plot(np.arange(1, N+1), Eout_G)
plt.show()
```




```
print("Eout = {}".format(np.mean(Eout_G)))
```

```
Eout = 0.07453666666666665
```

Problem 19

依旧取前t棵数构成随机森林，但是没棵树只有一个branch，即每棵树对应了二元分类。

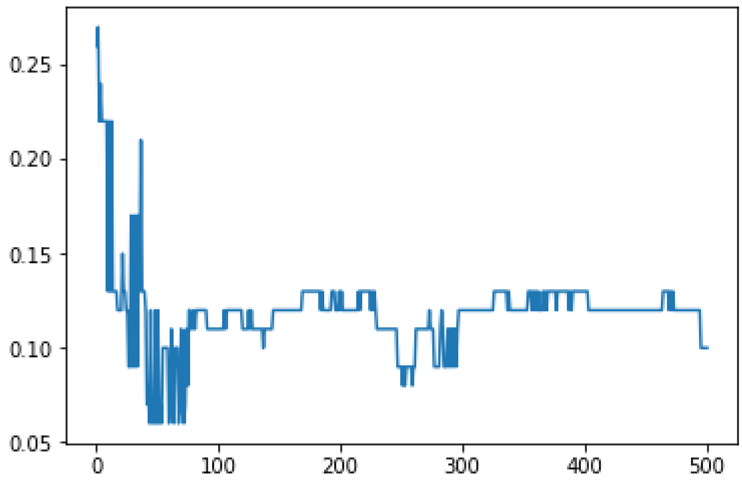
```
#19
def learntree_new(X, y):
    d, theta, score = Decision_stump(X, y)
    tree = DTree(theta, d)
    #划分数据
    i1 = X[:, d] < theta
    X1 = X[i1]
    y1 = y[i1]
    i2 = X[:, d] >= theta
    X2 = X[i2]
    y2 = y[i2]
    #学习左树
    leftTree = learntree(X1, y1)
    #学习右树
    rightTree = learntree(X2, y2)

    #左树
    k1 = np.sign(np.sum(y1) + 0.5)#+0.5是为了防止出现0
    leftTree = DTree(None, None, k1)
    #右树
    k2 = np.sign(np.sum(y2) + 0.5)
    rightTree = DTree(None, None, k2)
    #返回
    tree.left = leftTree
    tree.right = rightTree
    return tree
```

```python
N = 500
newtree = []
m, n = train.shape
for i in range(N):
    index = np.random.randint(0, m, (m))
    X1 = X_train[index, :]
    y1 = y_train[index]
    dtree = learntree_new(X1, y1)
    newtree.append(dtree)

newEin_G = random_forest_error(newtree, X_train, y_train)

plt.plot(np.arange(1, N+1), newEin_G)
plt.show()
```



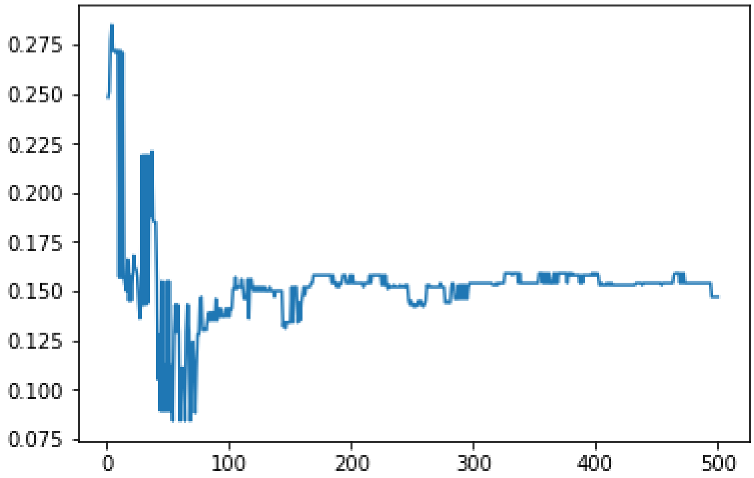

```python
print("Ein = {}".format(np.mean(newEin_G)))
```

```
Ein = 0.11872000000000002
```

Problem 20

```python
#20
newEout_G = random_forest_error(newtree, X_test, y_test)

plt.plot(np.arange(1, N+1), newEout_G)
plt.show()
```




```
print("Eout = {}".format(np.mean(newEout_G)))
```

```
Eout = 0.15301599999999999
```

Problem 21

由之前讨论可以知道，我们可以利用$\text{sign}(s)$表示NOT,AND逻辑，从而第一层可以表示如下逻辑关系

$$\prod_{i=d_1}^{d_n} x_i^t, x_i^t \in \{x_i, \overline{x}_i\}(1 \le d_1 \le \ldots \le d_n \le d)$$

第二层我们利用这种逻辑关系来表达$\text{XOR}\left(x_1, x_2, \ldots, x_d\right)$，给出以下命题：

$$\text{记 } x_1, \ldots, x_d \text{为} d \text{个逻辑单元，}$$
$$z_j = \prod_{i=a_1}^{a_{s_j}} x_i^t, x_i^t \in \{x_i, \overline{x}_i\}(1 \le a_1 \le \ldots \le a_{s_j} \le d)$$
$$f_m = \sum_{j=1}^{m} z_j^t, \text{其中} z_j^t \in \{z_j, \overline{z}_j\}$$
$$\text{那么存在 } f_d = \text{XOR}\left(x_1, x_2, \ldots, x_d\right)\text{，且 } d \text{为表达异或逻辑的神经元数量的最小值}$$

证明：

关于d利用数学归纳法。

这里的基础情况为$d=2$，因为1个逻辑单元无法表示异或逻辑，回顾课件可知

$$f_2 = \overline{x}_1 x_2 + x_1 \overline{x}_2$$

可以表示异或逻辑，所以$d=2$时结论成立。

假设$d=k$时结论，现在证$d=k+1$时结论也成立。假设逻辑单元为$x_1,\ldots,x_k,x_{k+1}$，根据归纳假设，存在

$$f_k=\sum_{j=1}^{k}z_j^t,\text{其中}z_j^t\in\{z_j,\overline{z}_j\}$$

$$z_j=\prod_{i=a_1}^{a_{s_j}}x_i^t,x_i^t\in\{x_i,\overline{x}_i\}(1\le a_1\le\ldots\le a_{s_j}\le k)$$

$$f_k=\mathrm{XOR}\Big(x_1,\ldots,x_k\Big)$$

$$k\text{表达异或逻辑的神经元数量的最小值}$$

根据异或的定义，有如下关系

$$\mathrm{XOR}\Big(x_1,x_2,\ldots,x_k,x_{k+1}\Big)=\mathrm{XOR}\Big(\mathrm{XOR}\Big(x_1,\ldots,x_d\Big),x_{k+1}\Big)=\mathrm{XOR}\Big(f_k,x_{k+1}\Big)$$

因为f_k也为逻辑单元，所以表示$\mathrm{XOR}\Big(f_k,x_{k+1}\Big)$至少需要关于$f_k,x_{k+1}$的2个逻辑单元，可以表示如下

$$\mathrm{XOR}\Big(f_k,x_{k+1}\Big)=\overline{f}_kx_{k+1}+f_k\overline{x}_{k+1}$$

根据逻辑运算规则，

$$\overline{f_k}=\prod_{j=1}^{k}\overline{z}_j^t$$

$$z_j=\prod_{i=a_1}^{a_{s_j}}x_i^t,x_i^t\in\{x_i,\overline{x}_i\}(1\le a_1\le\ldots\le a_{s_j}\le k)$$

从而$\overline{f_k}$为一个逻辑单元，将$f_k=\sum_{j=1}^{k}z_j^t$一起带入可得

$$\begin{aligned}\mathrm{XOR}\Big(x_1,x_2,\ldots,x_k,x_{k+1}\Big)&=\mathrm{XOR}\Big(f_k,x_{k+1}\Big)\\&=\overline{f}_kx_{k+1}+f_k\overline{x}_{k+1}\\&=x_{k+1}\prod_{j=1}^{k}\overline{z}_j^t+\left(\sum_{j=1}^{k}z_j^t\right)\overline{x}_{k+1}\end{aligned}$$

由逻辑学知识可知，NOT,AND逻辑可以表达所有的逻辑，从而$x_{k+1}\prod_{j=1}^{k}\overline{z}_j^t,z_j^t\overline{x}_{k+1}$可以表达为

$$\prod_{i=1}^{a_{s_{j+1}}}\overline{x}_i^t\text{或}\overline{\prod_{i=1}^{a_{s_{j+1}}}\overline{x}_i^t},\text{其中}x_i^t\in\{x_i,\overline{x}_i\}$$

记$z_j^{'}=\prod_{i=1}^{a_{s_{j+1}}}x_i^t,x_i^t\in\{x_i,\overline{x}_i\}(1\le a_1\le\ldots\le a_{s_{j+1}}\le k+1)$，那么

$$\mathrm{XOR}\Big(x_1, x_2, \ldots, x_k, x_{k+1}\Big) = \sum_{j=1}^{k+1} z_j'^{t}$$

$$其中\, z_j'^{t} \in \{z_j', \overline{z}_j'\}$$

所以结论对于$d = k + 1$也成立，从而结论得证。

Problem 22

直接给出结论，最小值为

$$1 + [\log_2 n]$$

方法很巧妙，可以参考以下两篇文献，主要是文献2，文献已经下载在文件夹中。

[Neural network computation with DNA strand displacement cascades]

[The Realization of Symmetric Switching Functions with Linear-Input Logical Elements]