

1 K-Nearest Neighbour Algorithm

1.1 Basic Method

The K-Nearest Neighbour Algorithm is an intuitive algorithm. Given an unknown sample, we compute its **Minkowski distance**

$$d(v_i, v_j) = \left(\sum_{k=1}^n (v_i^{(k)} - v_j^{(k)})^p \right)^{\frac{1}{p}} \quad (1)$$

to elements in our training set, and use the average features of the K nearest elements picked out to predict the unknown one.

1.2 Implementation

Algorithm 1 K-NN Algorithm (S, Vec)

Require: training set: S , sample vector $Vec = \{v_1, v_2, \dots, v_n\}$, hashmap H

for $s_i \in S$ **do**

$d_i \leftarrow \sqrt{\sum_{j=1}^n ((s_i)_j - v_j)^2}$ (Using Euclidean distance)

$H[s_i] = d_i$

end for

sort H with key

$array \leftarrow s_i | H[s_i] \text{ are K nearest}$

$Vec.label = \sum_{s_i \in array} \epsilon_i \cdot s_i.label, \epsilon_i = H[s_i] / \sum_{s_j \in array} H[s_j]$

1.3 Performance Analysis

Assume that \mathbf{x} is our testing vector, and the nearest training vector is \mathbf{z} . Then the generalization error is

$$P_{\text{err}} = 1 - \sum_{c \in \mathcal{Y}} P(c|\mathbf{x})P(c|\mathbf{z}) \quad (2)$$

where \mathcal{Y} is the label set. Then assume that the training set is dense enough, such that $\forall \mathbf{x}, \exists \delta, \mathbf{z} \in \mathbf{x} + \delta$. The condition gives

$$\begin{aligned}
 P_{\text{err}} &= 1 - \sum_{c \in \mathcal{Y}} P(c|\mathbf{x})P(c|\mathbf{z}) \\
 &\approx 1 - \sum_{c \in \mathcal{Y}} P^2(c|\mathbf{x}) \\
 &= 1 - \left(\arg \max_{c \in \mathcal{Y}} P(c|\mathbf{x}) \right)^2 \\
 &= \left(1 - \arg \max_{c \in \mathcal{Y}} P(c|\mathbf{x}) \right) \left(1 + \arg \max_{c \in \mathcal{Y}} P(c|\mathbf{x}) \right) \leq 2 - 2 \arg \max_{c \in \mathcal{Y}} P(c|\mathbf{x})
 \end{aligned} \tag{3}$$

This manifests that the error rate of K-NN will not exceed the double of the one of the Bayes optimal classifier.

1.4 Code (with Python)

Listing 1: K-NN.py

```

1 import numpy as np
2 from numpy import *
3
4 def fileToMatrix(filename):
5     file = open(filename)
6     arrayOfLines = file.readlines()
7     numOfLines = len(arrayOfLines)
8     returnMat = np.zeros([numOfLines, 3], dtype = double)
9     labelVector = []
10    index = 0
11    for line in arrayOfLines:
12        line = line.strip()
13        lineList = line.split('\t')
14        returnMat[index,...] = lineList[0:3]
15        labelVector.append( int(lineList[-1]))
16        index += 1
17    return returnMat, labelVector
18
19 def normalize(dataMat): #normalize the dataset
20     colMinVal = dataMat.min(0)
21     colMaxVal = dataMat.max(0)
22     interval = colMaxVal - colMinVal
23     normDataMat = np.zeros(shape(dataMat))
24     colLength = shape(dataMat)[0]
25     normDataMat = dataMat - np.tile(colMinVal, (colLength, 1))
26     np.seterr(invalid = 'ignore')

```

```

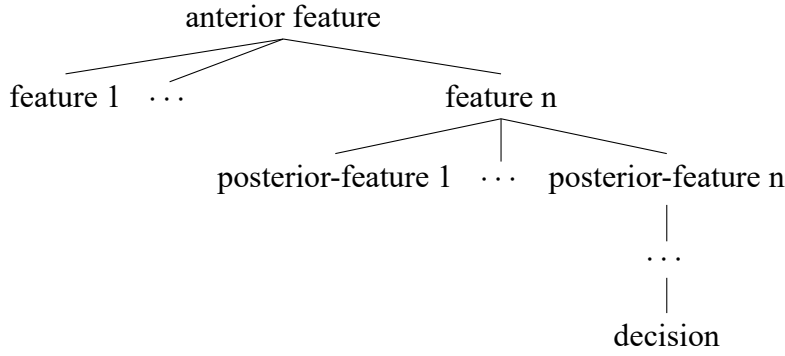
27     normDataMat = np.divide(normDataMat, np.tile(interval, (colLength, 1)))
28     return normDataMat
29
30 def classify(sampleVec, dataSet, labelVec, K):
31     dataSetSize = dataSet.shape[0]
32     diffMat = np.tile(sampleVec, (dataSetSize, 1)) - dataSet
33     sqDiffMat = diffMat ** 2
34     sqDistances = sqDiffMat.sum(axis = 1) #calculate the distance to each element in the dataset
35     distances = sqDistances ** (1/2)
36     disIndices = distances.argsort() #replace the distances with their ranks
37     totalDistance = 0
38     dis, vote = {}, {}
39     for i in range(dataSetSize):
40         if disIndices[i] < K:
41             dis[disIndices[i]] = (distances[i], i)
42     for d in dis:
43         totalDistance += dis[d][0]
44     for i in dis:
45         weight = dis[i][0] / totalDistance
46         if labelVec[dis[i][-1]] in vote:
47             vote[labelVec[dis[i][-1]]] += weight
48         else:
49             vote[labelVec[dis[i][-1]]] = weight
50     sortedVoteCount = sorted({v : k for k, v in vote.items()}.items(), reverse = True)
51     return sortedVoteCount[0][1]
52
53 def K_NN(sampleVec, K, dataSet, labelVec):
54     return classify(normalize(sampleVec), normalize(dataSet), labelVec, K)

```

2 Decision Tree

2.1 Basic Model

We tend to enable machines to do decision-making like humans. The data structure we use is the decision tree, where each internal node corresponds to a characteristic testing a_i , and each leaf node denotes a final decision y_i . The core manipulation is to build up optimal classification at each node. Every top-down process on analyzing a sample corresponds to a testing sequence.



2.2 Partition Scenario

Shannon Entropy

For a decision set D , the **information size** $H_0(D)$ which denotes the number of bits needed to encode elements in D is $H_0(D) = \log_2 |D|$. Let $\mathbf{D} = (D, p)$ be a discrete probability space, where $D = \{D_1, D_2, \dots, D_n\}$ is a finite set, with D_i corresponds to probability p_i under definite discrete characteristic. Then the **Shannon entropy** of \mathbf{D} is

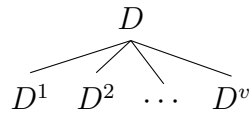
$$\text{Ent}(D) = - \sum_{i=1}^n p_i \log_2 p_i \quad (4)$$

Since $-\log_2 x$ is convex, we give an upper-bound for the entropy where

$$-\log_2 \left(\sum_{i=1}^n \frac{1}{p_i} p_i \right) \leq \sum_{i=1}^n p_i \left(-\log_2 \frac{1}{p_i} \right) = -\text{Ent}(D) \longrightarrow \text{Ent}(D) \leq \log_2 n \quad (5)$$

Information Gain

Given a partition criterion $a = \{a^1, a^2, \dots, a^v\}$ where $a^i \in a$ is the possible value. For sample set D , we split it into subsets D^1, D^2, \dots, D^v where D^i is the subset determined by criterion a^i .



Then the **information gain** we obtain from this partition is

$$\text{Gain}(D, a) = \text{Ent}(D) - \sum_{i=1}^v \frac{|D^i|}{|D|} \text{Ent}(D^i) \quad (6)$$

In ID3 Algorithm, the **optimal class partition** a_* for A with sample D is defined as

$$a_* = \arg \max_{a \in A} \text{Gain}(D, a) \quad (7)$$

while for C4.5 Algorithm, the optimal one is defined as

$$a_* = \arg \max_{a \in A} \text{GainRatio}(D, a), \quad \text{GainRatio}(D, a) = \text{Gain}(D, a) / \text{Ent}(D) \quad (8)$$

2.3 Implementation

Assume that training sample set $D = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \dots, (\mathbf{x}_n, y_n)\}$, where \mathbf{x}_i is the class characteristics, and y_i is the decision, eventually treated as leafnode. Possible partition criterion for D is $A = \{a_1, a_2, \dots, a_d\}$, where a_i denotes a possible partition.

Algorithm 2 treeGenerate(D, A)

Require: Training set D , Partition criterion set A

```

initialize node
if  $\forall D_i, D_j \in D, i \neq j, D_i = D_j$  then
    node = leafnode, node  $\leftarrow D.y$ 
return
end if
if  $A = \emptyset$  or  $\forall a_i, a_j \in A, i \neq j, \text{Gain}(D, a_i) = \text{Gain}(D, a_j)$  then
    node = leafnode, node  $\leftarrow \arg \max_y (|N|, N = \{y | (\mathbf{x}, y) \in D\})$ 
end if
 $a_* \leftarrow \arg \max_{a \in A} \text{Gain}(D, a)$ 
for  $a_*^v \in a_*$  do
    initialize node.branch $^v$ ,  $D_v$  be the subset split with  $a_*^v$ 
    if  $D_v = \emptyset$  then
        node.branch $^v$  = leafnode, node.branch $^v \leftarrow \arg \max_y (|N|, N = \{y | (\mathbf{x}, y) \in D_v\})$ 
    else
        node.branch $^v$  = treeGenerate( $D_v, A - \{a_*\}$ )
    end if
end for

```

2.4 Code

Listing 2: decisionTree.py

```

1 from math import log
2
3 class decisionNode( object): # tree organized by decision tree data structure
4     def __init__(self, label):
5         self.label = label
6         self.branches = []
7         self.decision = ""
8     def assignDecision(self, decision):
9         self.decision += decision
10    def addBranch(self, newNode):

```

```
11     newNode.assignDecision(self.decision)
12     self.branches.append(newNode)
13     def visualize(self, treeNode, layer): # Visualize manipulation displays the layer an label belongs
        to and its anterior choice
14         print("{}{}: {}".format(layer, treeNode.decision, treeNode.label))
15         for s in treeNode.branches:
16             self.visualize(s, layer + 1)
17
18 def shannonEntropy(dataset):
19     entriesNum = len(dataset)
20     labelCount = {}
21     for dataVec in dataset:
22         dataLabel = dataVec[-1] # The last element in the vector is our decision
23         if dataLabel not in labelCount:
24             labelCount[dataLabel] = 0
25             labelCount[dataLabel] += 1
26     shannonEntropy = 0.000
27     for label in labelCount:
28         probability = labelCount[label] / entriesNum
29         shannonEntropy -= probability * log(probability, 2)
30     return shannonEntropy
31
32 def splitDataset(dataset, index, expectValue): # Search the dataset with specified index and return the
        reduced dataset
33     retDataset = []
34     for lineVec in dataset:
35         if lineVec[index] == expectValue:
36             reducedVec = lineVec[:index]
37             reducedVec += lineVec[index+1:]
38             retDataset.append(reducedVec)
39     return retDataset
40
41 def optimalPartition(dataset): # ID3 Algotihm
42     featureNums = len(dataset[0]) - 1
43     originalEntropy = shannonEntropy(dataset)
44     bestFeature = -1
45     maxInfoGain = 0.00
46     for featureIndex in range(featureNums):
47         labelVec = set([dataset[i][featureIndex] for i in range(len(dataset))])
48         extraEntropy = 0.00
49         for label in labelVec:
50             reducedSet = splitDataset(dataset, featureIndex, label)
51             extraEntropy += len(reducedSet) / float(len(dataset)) * shannonEntropy(reducedSet)
52         if originalEntropy - extraEntropy > maxInfoGain:
53             maxInfoGain = originalEntropy - extraEntropy
54             bestFeature = featureIndex
```

```

55     return bestFeature
56
57 def majorityCount(classList):
58     classNum = {}
59     for member in classList:
60         if member not in classNum:
61             classNum[member] = 0
62             classNum[member] += 1
63     reverseDict = {v:k for k, v in classNum.items()}
64     orderList = sorted(reverseDict)
65     return reverseDict[ max(orderList)]
66
67
68 def createTree(dataset, labels):
69     classList = [data[-1] for data in dataset]
70     if classList.count(classList[0]) == len(classList):
71         return decisionNode(classList[0])
72     if len(dataset[0]) == 1:
73         return decisionNode(majorityCount(classList))
74     bestPartition = optimalPartition(dataset)
75     bestPartitionLabel = labels[bestPartition]
76     newTree = decisionNode(bestPartitionLabel)
77     uniqueVal = set([data[bestPartition] for data in dataset])
78     del(labels[bestPartition])
79     for value in uniqueVal:
80         subLabels = labels[:]
81         branchNode = createTree(splitDataset(dataset, bestPartition, value), subLabels)
82         branchNode.assignDecision(value)
83         newTree.addBranch(branchNode)
84     return newTree

```

3 Naive Bayes Algorithm

3.1 Principle and Method

Given that the input vector $X \subseteq \mathbb{R}^n$, where $X = \begin{bmatrix} X^{(1)} & X^{(2)} & \dots & X^{(n)} \end{bmatrix}^T$, and the relevant output class label set $Y \in \{c_1, c_2, \dots, c_K\}$. The joint distribution $P(X, Y)$ generates the data outcome

$$T = \{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\} \quad (9)$$

Applying Bayes rule we construct the algorithm for determining the label for an arbitrary new input.

Assume that the input vector is $x = [x^{(1)} \ x^{(2)} \ \dots \ x^{(n)}]$, the probable label set is $\mathbf{c} = \{c_1, c_2, \dots, c_K\}$, then for $c_i \in \mathbf{c}$

$$P(X = x|Y = c_i) = P(X^{(1)} = x^{(1)}, X^{(2)} = x^{(2)}, \dots, X^{(n)} = x^{(n)}|Y = c_i) \quad (10)$$

Assume that the variables in X are mutually independent, then the posteriori distribution is

$$P(Y = c_i|X = x) = \frac{P(X = x|Y = c_i)P(Y = c_i)}{\sum_i P(X = x|Y = c_i)P(Y = c_i)} = \frac{\prod_j P(X^{(j)} = x^{(j)}|Y = c_i)P(Y = c_i)}{\sum_i \prod_j P(X^{(j)} = x^{(j)}|Y = c_i)P(Y = c_i)}$$

The optimal choice for c_i is

$$\begin{aligned} y = f(x) = \arg \max_{c_i} P(Y = c_i|X = x) &= \arg \max_{c_i} \frac{\prod_j P(X^{(j)} = x^{(j)}|Y = c_i)P(Y = c_i)}{\sum_i \prod_j P(X^{(j)} = x^{(j)}|Y = c_i)P(Y = c_i)} \\ &= \arg \max_{c_i} \prod_j P(X^{(j)} = x^{(j)}|Y = c_i)P(Y = c_i) \end{aligned} \quad (11)$$

Assume that $x^{(j)} \in \mathbf{a}_j = \{a_{j,1}, a_{j,2}, \dots, a_{j,S_j}\}$, where \mathbf{a}_j is the probable value set, then the apriori probability is

$$\begin{aligned} P(Y = c_i) &= \frac{\sum_{k=1}^N I(y_k = c_i)}{N} \\ P(X^{(j)} = a_{j,l}|Y = c_i) &= \frac{\sum_{k=1}^N I(x_k^{(j)} = a_{j,l}, y_k = c_i)}{\sum_{k=1}^N I(y_k = c_i)} \quad 1 \leq l \leq S_j, 1 \leq j \leq n, 1 \leq i \leq K \end{aligned}$$

3.2 Laplace Smoothing

When calculating the conditional probability, some special cases might annihilate the indicator random variable, where

$$I(x_k^{(j)} = a_{j,l}, y_k = c_i) = 0 \quad (12)$$

Then we use a coefficient λ to prevent. Redefine the probabilities as

$$\begin{aligned} P(Y = c_i) &= \frac{\sum_{k=1}^N I(y_k = c_i) + \lambda}{N + K\lambda} \\ P(X^{(j)} = a_{j,l}|Y = c_i) &= \frac{\sum_{k=1}^N I(x_k^{(j)} = a_{j,l}, y_k = c_i) + \lambda}{\sum_{k=1}^N I(y_k = c_i) + S_j\lambda} \end{aligned} \quad (13)$$

When $\lambda = 1$, it is called **Laplace Smoothing**.

3.3 Code

Listing 3: Naive Bayes Method.py

```

1 def posterioriProb(inputVec, trainData, smoothCoef): # Laplacian smooth coefficient is used to prevent
    possibility annihilation
2     labels = trainData[-1]
3     uniqueLabels = set(labels)
4     labelClasses = len(set(labels))
5     trainData = trainData[:-1]
6     totalSample = len(trainData[0])
7     characterList = []
8     labelDict = {}
9     posterioriProbList = []
10    for i in labels:
11        if i not in labelDict:
12            labelDict[i] = 1
13        else:
14            labelDict[i] += 1
15    for character in trainData:
16        singleCharacter = len(set(character))
17        characterDict = {}
18        for j in range(totalSample):
19            if (character[j], labels[j]) not in characterDict:
20                characterDict[(character[j], labels[j])] = 1
21            else:
22                characterDict[(character[j], labels[j])] += 1
23        for j in characterDict:
24            characterDict[j] = (characterDict[j] + smoothCoef) /
                float(labelDict[j[-1]] + singleCharacter*smoothCoef)
25        characterList.append(characterDict)
26    for label in labelDict:
27        probability = (labelDict[label] + smoothCoef) / (totalSample + smoothCoef * labelClasses)
28        for i in range(len(trainData)):
29            layerCharacter = characterList[i]
30            probability *= layerCharacter[(inputVec[i], label)]
31        posterioriProbList.append(probability)
32    posterioriIndex = posterioriProbList.index(max(posterioriProbList))
33    return list(uniqueLabels)[posterioriIndex]

```

4 Logistic Regression

4.1 Logistic Distribution

If random variable X follows logistic distribution, i.e. $X \sim \text{logistic}(\mu, \gamma)$, then

$$F_X(x) = \frac{1}{1 + e^{-(x-\mu)/\gamma}} \quad f_X(x) = \frac{e^{-(x-\mu)/\gamma}}{\gamma(1 + e^{-(x-\mu)/\gamma})^2} \quad (14)$$

where μ is denotes the translation, and γ is the scale factor.

4.2 Multi-nominal Logistic Regression Model

For sample data x , we tend to build up estimator for $f(x)$, such that

$$\hat{f}(x) = \arg \max_k \Pr(Y = k|x) \quad (15)$$

The core of logistic regression is to build up **linear separating hyperplane** for classes $Y \in \{1, 2, \dots, K\}$. Then we expand x from \mathbb{R}^n to \mathbb{R}^{n+1} ,

$$\mathbf{w}_k = \begin{bmatrix} w_k^{(0)} \\ w_k^{(1)} \\ \vdots \\ w_k^{(n)} \end{bmatrix} = \begin{bmatrix} b \\ w_k^{(1)} \\ \vdots \\ w_k^{(n)} \end{bmatrix}, \quad \mathbf{x}_k = \begin{bmatrix} x_k^{(0)} \\ x_k^{(1)} \\ \vdots \\ x_k^{(n)} \end{bmatrix} = \begin{bmatrix} 1 \\ x_k^{(1)} \\ \vdots \\ x_k^{(n)} \end{bmatrix} \quad (16)$$

where b is the bias.

Then if two classes intersect, we take the class K as the reference, then

$$\log \frac{\Pr(Y = k|x)}{\Pr(Y = K|x)} = \mathbf{w}_k^T \mathbf{x} \rightarrow \Pr(Y = k|x) = \Pr(Y = K|x) \exp(\mathbf{w}_k^T \mathbf{x}) \quad (17)$$

Apply the normalized characteristic of probability, we have

$$\sum_{k=1}^K \Pr(Y = k|x) = \Pr(Y = K|x) \sum_{k=1}^K \exp(\mathbf{w}_k^T \mathbf{x}) \rightarrow \Pr(Y = K|x) = \frac{1}{\sum_{k=1}^K \exp(\mathbf{w}_k^T \mathbf{x})} \quad (18)$$

Since $\mathbf{w}_K^T \mathbf{x} = 0$, then

$$\Pr(Y = k|x) = \frac{\exp(\mathbf{w}_k^T \mathbf{x})}{1 + \sum_{k=1}^{K-1} \exp(\mathbf{w}_k^T \mathbf{x})} \quad \Pr(Y = K|x) = \frac{1}{1 + \sum_{k=1}^{K-1} \exp(\mathbf{w}_k^T \mathbf{x})} \quad (19)$$

With training set $T = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \dots, (\mathbf{x}_N, y_N)\}$, the likelihood function is

$$L(\mathbf{w}_0, \mathbf{w}_1, \dots, \mathbf{w}_n) = \prod_{i=1}^K \Pr\{Y = y_i | \mathbf{x}_i\} = \prod_{i=1}^K \frac{\exp(\mathbf{w}_{y_i}^T \mathbf{x}_i)}{1 + \sum_{k=1}^{K-1} \exp(\mathbf{w}_k^T \mathbf{x}_i)} \quad (20)$$

If $K = 2$, then the model degrades to a binomial LR model with 0 – 1 label. We take

$$\Pr(Y = 0|x) = \frac{\exp(\mathbf{w}^T \mathbf{x})}{1 + \exp(\mathbf{w}^T \mathbf{x})} = \pi(\mathbf{x}) \quad \Pr(Y = 1|x) = \frac{1}{1 + \exp(\mathbf{w}^T \mathbf{x})} = 1 - \pi(\mathbf{x}) \quad (21)$$

Then the likelihood function is

$$\begin{aligned} L(\mathbf{w}) &= \prod_{i=1}^N [\pi(x_i)]^{y_i} [1 - \pi(x_i)]^{1-y_i} \rightarrow \frac{\partial}{\partial w^{(j)}} \log L(\mathbf{w}) = \frac{\partial}{\partial w^{(j)}} \sum_{i=1}^N y_i (\mathbf{w}^T \mathbf{x}_i) - \log[1 + \exp(\mathbf{w}^T \mathbf{x}_i)] \\ &= \sum_{i=1}^N \left[y_i - \frac{\exp(\sum_{k=0}^n w^{(k)} x_i^{(k)})}{1 + \exp(\sum_{k=0}^n w^{(k)} x_i^{(k)})} \right] x_i^{(j)} \end{aligned}$$

Or

$$\frac{\partial}{\partial \mathbf{w}} \log L(\mathbf{w}) = \sum_{i=1}^N \mathbf{x}_i \left(y_i - \frac{1}{1 + \exp(-\mathbf{w}^T \mathbf{x}_i)} \right) = 0 \quad (22)$$

4.3 Gradient Descent Algorithm

4.3.1 Method

If we give estimator $\hat{\mathbf{w}}$ for weight vector \mathbf{w} , then the **Loss Function** is defined as

$$L(\mathbf{w}, \mathbf{x}, y) = f(\mathbf{w}^T \mathbf{x}, y) \quad (23)$$

Where $f : \mathbb{R} \mapsto \mathbb{R}$ maps the loss outcome to quantity that corresponds to the form of y .

The Gradient Descent algorithm use iteration to approach the optimal choice with **step width** η for \mathbf{w}

Algorithm 3 gradientDescent($\mathbf{X} = [\mathbf{x}_1 \ \mathbf{x}_2 \ \cdots \ \mathbf{x}_N]$, $\mathbf{Y} = [y_1 \ y_2 \ \cdots \ y_N]$)

Require: $\mathbf{w}_1 = 0$

for $t = 1$ **to** T **do**

$$\hat{\mathbf{Y}} = \mathbf{w}_t^T \mathbf{X}$$

evaluate $L = f(\mathbf{w}_t, \mathbf{X}, \mathbf{Y})$

$$\mathbf{w}_t := \mathbf{w}_t - \eta \nabla_{\mathbf{w}} L(\mathbf{w}_t, \mathbf{X}, \mathbf{Y})$$

end for

return \mathbf{w}_T

4.3.2 Widrow-Hoff Algorithm

If we reasonably choose the loss function to simplify the calculation. The Widrow-Hoff algorithm choose the euclidean distance as the loss function mapping, i.e. $L(\mathbf{w}, \mathbf{x}, y) = 1/2 \cdot (\mathbf{w}^T \mathbf{x} - y)^2$. Then

$$\begin{aligned} \nabla_{\mathbf{w}} \frac{1}{2} (\mathbf{w}^T \mathbf{x} - y)^2 &= \sum_{j=0}^n \frac{\partial}{\partial w^{(j)}} \frac{1}{2} \left(\sum_{k=0}^n w^{(k)} x^{(k)} - y \right)^2 \\ &= \sum_{j=0}^n \left(\sum_{k=0}^n w^{(k)} x^{(k)} - y \right) x^{(j)} \\ &= (\mathbf{w}^T \mathbf{x} - y) \mathbf{x} \end{aligned} \quad (24)$$

Then the recurrence equation becomes

$$\mathbf{w}_t := \mathbf{w}_t - \eta (\mathbf{w}_t^T \mathbf{X} - \mathbf{Y}) \mathbf{X} \quad (25)$$

4.3.3 Logistic Algorithm

We have derived that

$$\nabla_w \log L(w) = \sum_{i=1}^N x_i \left(y_i - \frac{1}{1 + \exp(-w^T x_i)} \right) \quad (26)$$

then substitute it into gradient descent algorithm as the loss function. We have

$$w_t := w_t - \eta \sum_{i=1}^N x_i \left(y_i - \frac{1}{1 + \exp(-w^T x_i)} \right) \quad (27)$$

Or

$$w_t := \begin{bmatrix} w_t^{(0)} \\ w_t^{(1)} \\ \vdots \\ w_t^{(n)} \end{bmatrix} - \eta \begin{bmatrix} x_1 & x_2 & \cdots & x_N \end{bmatrix} \begin{bmatrix} y_1 - \frac{1}{1 + \exp(-w^T x_1)} \\ y_2 - \frac{1}{1 + \exp(-w^T x_2)} \\ \vdots \\ y_N - \frac{1}{1 + \exp(-w^T x_N)} \end{bmatrix} \quad (28)$$

4.4 Code

Listing 4: logisticRegression.py

```

1 import numpy as np
2 import matplotlib.pyplot as plt
3
4 def loadDataset(filename):
5     dataMat = []; labelMat = []
6     file = open(filename)
7     fileString = file.readlines()
8     for line in fileString:
9         lineArray = line.strip().split()
10        dataMat.append([1.0] + [float(i) for i in lineArray[:-1]])
11        labelMat.append([int(float(i)) for i in lineArray[-1:]])
12    dataMat = np.asarray(dataMat)
13    labelMat = np.asarray(labelMat)
14    return dataMat, labelMat
15
16 def sigmoid(X):
17     return 1.00/(1+np.exp(-X))
18
19 def sigmoidClassify(X):
20     if 1 / (1 + float(np.exp(-X))) > 0.5:
21         return 1
22     else:
23         return 0

```

```

24
25 def gradAscent(dataMat, labelMat, iterTimes, stepLength):
26     row, column = np.shape(dataMat)
27     weights = np.ones((column, 1))
28     for i in range(iterTimes):
29         h = sigmoid(dataMat.dot(weights))
30         error = labelMat - h
31         weights = weights + stepLength * (dataMat.transpose().dot(error))
32     return weights
33
34 def plotFit(weights, filename): # Plot the two-dimensional model
35     dataMat, labelMat = loadDataset(filename)
36     col = np.shape(dataMat)[0]
37     x1, y1, x2, y2 = [], [], [], []
38     for i in range(col):
39         if labelMat[i] == 1:
40             x1.append(dataMat[i, 1])
41             y1.append(dataMat[i, 2])
42         else:
43             x2.append(dataMat[i, 1])
44             y2.append(dataMat[i, 2])
45     figure = plt.figure()
46     plt.scatter(x1, y1, c = 'red')
47     plt.scatter(x2, y2, c = 'green')
48     x = np.arange(-4, 4, 0.1)
49     y = (-weights[0] - weights[1] * x) / weights[2]
50     plt.plot(x, y)
51     plt.xlabel('Type 1')
52     plt.ylabel('Type 2')
53     plt.show()

```

5 Support Vector Machine

5.1 Constraint Condition for Linear SVM

Consider **binary label** sample $T = \{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\}$, where $x \in \mathcal{X} = \mathbb{R}^n$, $y \in \{-1, +1\}$. We assume that the optimal hyperplane separating data pairs into binary classes is

$$w^T x + b = 0 \quad (29)$$

Relevant decision function is the **Heaviside step function**

$$f(x) = \text{sign}(w^T x + b) \quad (30)$$

For each data pair $(\mathbf{x}_i, y_i) \in T$, the **geometric margin** is defined as

$$\gamma_i = y_i(\mathbf{w}^T \mathbf{x}_i + b) / \|\mathbf{w}\| \quad (31)$$

Since the confidence we have in the separate hyperplane is positive proportional to the geometric margin, then we define the geometric margin between the hyperplane (\mathbf{w}, b) and dataset T as

$$\gamma = \min_{1 \leq i \leq N} \gamma_i = \min_{1 \leq i \leq N} \frac{y_i(\mathbf{w}^T \mathbf{x}_i + b)}{\|\mathbf{w}\|} \quad (32)$$

The core implementation of SVM is to maximize the geometric margin, i.e. to find

$$\arg \max_{\mathbf{w}, b} \left(\min_{1 \leq i \leq N} \frac{y_i(\mathbf{w}^T \mathbf{x}_i + b)}{\|\mathbf{w}\|} \right) \quad (33)$$

If the minimum function margin $(= \min_{1 \leq i \leq N} y_i(\mathbf{w}^T \mathbf{x}_i + b))$ is fixed to 1, then the preposition is equivalent to

$$\arg \max_{\mathbf{w}, b} \left(\min_{1 \leq i \leq N} \frac{y_i(\mathbf{w}^T \mathbf{x}_i + b)}{\|\mathbf{w}\|} \right) \Big|_{\gamma=1} \sim \arg \max_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|^2, \text{ s.t. } \gamma_i = y_i(\mathbf{w}^T \mathbf{x}_i + b) \geq \min_{1 \leq i \leq N} \gamma_i = 1$$

Take Lagrange multiplier matrix $\boldsymbol{\alpha} = [\alpha_1 \ \alpha_2 \ \cdots \ \alpha_n]^T$, then the Lagrange function is

$$L(\mathbf{w}, \boldsymbol{\alpha}, b) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^N \alpha_i y_i (\mathbf{w}^T \mathbf{x}_i + b) + \sum_{i=1}^N \alpha_i \quad (34)$$

The Lagrange dual problem gives

$$\arg \max_{\boldsymbol{\alpha}} \min_{\mathbf{w}, b} L(\mathbf{w}, \boldsymbol{\alpha}, b) \quad (35)$$

We firstly consider internal minimization, where

$$\begin{aligned} \nabla_{\mathbf{w}} L(\mathbf{w}, \boldsymbol{\alpha}, b) &= \sum_{j=1}^n \frac{\partial}{\partial w^{(j)}} \left(\frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^N \alpha_i y_i (\mathbf{w}^T \mathbf{x}_i + b) + \sum_{i=1}^N \alpha_i \right) \\ &= \sum_{j=1}^n \left(w^{(j)} - \sum_{i=1}^N \alpha_i y_i x_i^{(j)} \right) = \mathbf{w} - \sum_{i=1}^N \alpha_i y_i \mathbf{x}_i = 0 \end{aligned} \quad (36)$$

$$\nabla_b L(\mathbf{w}, \boldsymbol{\alpha}, b) = - \sum_{i=1}^N \alpha_i y_i = 0 \quad (37)$$

Then the original function becomes

$$\begin{aligned} L(\mathbf{w}, \boldsymbol{\alpha}, b) &= \frac{1}{2} \left(\sum_{i=1}^N \alpha_i y_i \mathbf{x}_i \right)^T \left(\sum_{i=1}^N \alpha_i y_i \mathbf{x}_i \right) - \sum_{i=1}^N \alpha_i y_i \left(\left(\sum_{i=1}^N \alpha_i y_i \mathbf{x}_i \right)^T \mathbf{x}_i + b \right) + \sum_{i=1}^N \alpha_i \\ &= -\frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle + \sum_{i=1}^N \alpha_i \end{aligned} \quad (38)$$

The terminal target function is

$$\arg \min_{\alpha} \left(\frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle - \sum_{i=1}^N \alpha_i \right) = \arg \min_{\alpha} W(\alpha) \quad \text{s.t.} \quad \sum_{i=1}^N \alpha_i y_i = 0 \quad (39)$$

Once the iteration has reached equilibrium state, denoted as α^* , then we can solve the corresponding parameters \mathbf{w}^* and b^* , where

$$\mathbf{w}^* = \sum_{i=1}^n \alpha_i^* y_i \mathbf{x}_i \quad (40)$$

$$y_j (\langle \mathbf{w}^*, \mathbf{x}_j \rangle + b^*) = 1 \rightarrow b^* = y_j - \sum_{i=1}^n \alpha_i^* y_i \langle \mathbf{x}_i, \mathbf{x}_j \rangle \quad (41)$$

5.2 Constraint Condition under Soft Margin Assumption

The above constraint condition is derived under the condition that dataset T is linearly separable. For dataset that is not linearly separable, i.e. **the convex hulls determined by two classes of data points have intersecting edges**.

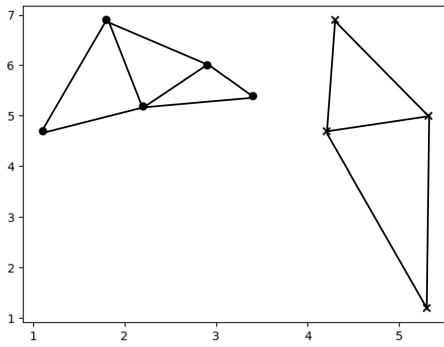


Fig. 1: Separable

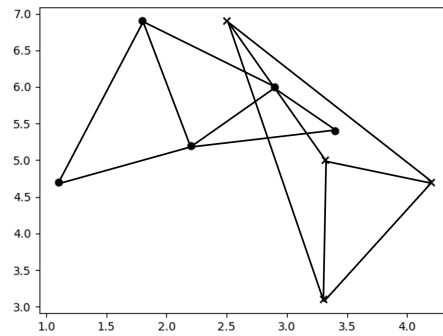


Fig. 2: Not Separable

To cancel out the effect of some specific data points, we introduce **slack variable** ξ_i for each data pair (\mathbf{x}_i, y_i) , and define the **soft geometric margin** as

$$\gamma = \frac{y_i(\mathbf{w}^T \mathbf{x}_i + b) + \xi_i}{\|\mathbf{w}\|} \quad (42)$$

Then for each slack variable, the target function gains a relevant penalty $C\xi_i$. Then the equivalent problem is

$$\begin{aligned} \arg \max_{\alpha} \min_{\mathbf{w}, \xi, b} & \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^N \xi_i \\ \text{s.t.} & y_i(\mathbf{w}^T \mathbf{x}_i + b) \geq 1 - \xi_i, \quad \xi_i \geq 0, \end{aligned} \quad (43)$$

Lagrange function with double multipliers (α, μ) is

$$L(\alpha, \mathbf{w}, \xi, b) = \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^N \xi_i - \sum_{i=1}^N \alpha_i (y_i(\mathbf{w}^T \mathbf{x}_i + b) - 1 + \xi_i) - \sum_{i=1}^N \mu_i \xi_i \quad (44)$$

with the dual problem

$$\arg \max_{\alpha} \min_{\mathbf{w}, \xi, b} L(\alpha, \mathbf{w}, \xi, b) \quad \text{s.t. } \alpha_i \geq 0, \mu_i \geq 0 \quad (45)$$

then

$$\frac{\partial}{\partial \mathbf{w}} L = \frac{\partial}{\partial \mathbf{x}_i} L = \frac{\partial}{\partial b} L = 0 \longrightarrow \begin{cases} \mathbf{w} = \sum_{i=1}^N \alpha_i y_i \mathbf{x}_i \\ \sum_{i=1}^N \alpha_i y_i = 0 \\ C - \alpha_i - \mu_i = 0, \alpha_i \geq 0, \mu_i \geq 0 \rightarrow 0 \leq \alpha_i \leq C \end{cases} \quad (46)$$

Likewise, we obtain a new **quadratic programming** target

$$\begin{aligned} \arg \min_{\alpha} \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle - \sum_{i=1}^N \alpha_i \\ \text{s.t. } \sum_{i=1}^N \alpha_i y_i = 0, 0 \leq \alpha_i \leq C \end{aligned} \quad (47)$$

5.3 Hinge Loss Function

We can give an equivalent description of the original optimizing problem. The minimizing part gives

$$\arg \min_{\mathbf{w}, \xi, b} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^N \xi_i, \quad \text{s.t. } y_i(\mathbf{w}^T \mathbf{x}_i + b) \geq 1 - \xi_i, \xi_i \geq 0 \quad (48)$$

If we take

$$[1 - y_i(\mathbf{w}^T \mathbf{x}_i + b)]_+ = \xi_i \quad \left(f(x)_+ = \begin{cases} f(x) & f(x) > 0 \\ 0 & x \leq 0 \end{cases} \right) \quad (49)$$

Then if $1 - y_i(\mathbf{w}^T \mathbf{x}_i + b) > 0$, then $y_i(\mathbf{w}^T \mathbf{x}_i + b) = 1 - \xi_i$. If $1 - y_i(\mathbf{w}^T \mathbf{x}_i + b) \leq 0$, then $\xi_i = 0$. It meets the condition that $y_i(\mathbf{w}^T \mathbf{x}_i + b) \geq 1 - \xi_i$. Hence, the minimization can be rewritten as

$$\arg \min_{\mathbf{w}, \xi, b} \frac{1}{2C} \|\mathbf{w}\|^2 + \sum_{i=1}^N \xi_i \xrightarrow{\lambda=1/2C} \arg \min_{\mathbf{w}, b} \lambda \|\mathbf{w}\|^2 + \sum_{i=1}^N [1 - y_i(\mathbf{w}^T \mathbf{x}_i + b)]_+ \quad (50)$$

Then loss function $[1 - y_i(\mathbf{w}^T \mathbf{x}_i + b)]_+$ on the RHS is defined as the **hinge loss function**, which requires a higher standard for sample studying.

5.4 Kernel Trick for Non-linear SVM

The linear separable and linear inseparable sample can be split using a hyperplane. Whereas non-linear samples require a hypersurface for partition.

5.4.1 Kernel Function

Assume input space is \mathcal{X} and characteristic space \mathcal{H} , there exists a mapping $\phi(x)$, where

$$\phi(x) : \mathcal{X} \mapsto \mathcal{H} \quad (51)$$

such that $\forall x, y \in \mathcal{X}$,

$$K(x, y) = \langle \phi(x), \phi(y) \rangle \quad (52)$$

then $K(x, y)$ is the kernel function, and $\phi(x)$ is the mapping function. For a given kernel $K(x, y)$, the selection for characteristic space and mapping function is not unique.

In non-linear SVM, we take the place of inner function in the optimization by the kernel function, i.e.

$$\begin{aligned} \arg \min_{\alpha} \quad & \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j) - \sum_{i=1}^N \alpha_i \\ \text{s.t.} \quad & \sum_{i=1}^N \alpha_i y_i = 0, \quad 0 \leq \alpha_i \leq C \end{aligned} \quad (53)$$

5.4.2 Positive Definite Kernel Function

The following will give the necessary and sufficient condition for $K(x, y)$ to be **positive definite kernel**. We first consider mapping function

$$\phi : x \mapsto K(\cdot, x) \quad (54)$$

Then $\forall x_i \in \mathcal{X}, \alpha_i \in \mathbb{R}$, define linear mapping

$$f(\cdot) = \sum_{i=1}^N \alpha_i K(\cdot, x_i) \quad (55)$$

the space \mathcal{S} is determined by mapping ϕ . Define operation $\langle f, g \rangle$ in space \mathcal{S} for f, g , where

$$f(\cdot) = \sum_{i=1}^N \alpha_i K(\cdot, x_i), \quad g(\cdot) = \sum_{j=1}^N \beta_j K(\cdot, y_j) \quad (56)$$

$$\langle f, g \rangle = \sum_{i=1}^N \sum_{j=1}^N \alpha_i \beta_j K(x_i, y_j) \quad (57)$$

Lemma 1 The operation is a inner product of \mathcal{S} .

$$\sum_{i=1}^N \sum_{j=1}^N C \alpha_i \beta_j K(x_i, y_j) = C \sum_{i=1}^N \sum_{j=1}^N \alpha_i \beta_j K(x_i, y_j) \longrightarrow \langle Cf, g \rangle = C \langle f, g \rangle \quad (58)$$

$$\langle f, g \rangle = \langle g, f \rangle \quad (\text{trivial}) \quad (59)$$

$$\begin{aligned} \sum_{i=1}^N \sum_{j=1}^N ((\alpha_i + \beta_i) \gamma_j K(y_i, z_j)) &= \sum_{i=1}^N \sum_{j=1}^N \alpha_i \gamma_j K(x_i, z_j) + \sum_{i=1}^N \sum_{j=1}^N \beta_i \gamma_j K(y_i, z_j) \\ &\rightarrow \langle f + g, h \rangle = \langle f, h \rangle + \langle g, h \rangle \end{aligned} \quad (60)$$

$$\langle f, f \rangle = \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j K(x_i, x_j) = \boldsymbol{\alpha}^T G_x \boldsymbol{\alpha} \geq 0 \quad (61)$$

The following will give the proof that $\langle f, f \rangle = 0$ if and only if $f(\cdot) = 0$. Necessity is trivial. It is evident that \mathcal{S} is a closure, then $\forall f, g \in \mathcal{S}, \lambda \in \mathbb{R}, f + \lambda g \in \mathcal{S}$. Then

$$\begin{aligned} \langle f + \lambda g, f + \lambda g \rangle &= \langle f, f \rangle + 2\lambda \langle f, g \rangle + \lambda^2 \langle g, g \rangle \geq 0 \\ \Delta &= 4(|\langle f, f \rangle|^2 - \langle f, f \rangle \langle g, g \rangle) \leq 0 \rightarrow |\langle f, f \rangle|^2 - \langle f, f \rangle \langle g, g \rangle \leq 0 \end{aligned} \quad (62)$$

then

$$\forall x \in \mathcal{X}, \langle K(\cdot, x), f(\cdot) \rangle = \sum_{i=1}^N \alpha_i \langle K(\cdot, x), K(\cdot, x_i) \rangle = f(x) \quad (63)$$

with the inequality above,

$$|\langle K(\cdot, x), f(\cdot) \rangle|^2 \leq \langle K(\cdot, x), K(\cdot, x) \rangle \langle f(\cdot), f(\cdot) \rangle \quad (64)$$

Where

$$\langle K(\cdot, x), K(\cdot, x) \rangle = K(x, x) \quad (65)$$

then

$$|f(x)|^2 \leq K(x, x) \langle f(\cdot), f(\cdot) \rangle \quad (66)$$

then if $\langle f, f \rangle = 0$, $f(x) = 0$ must holds for all x . We can conclude that operation $\langle f, g \rangle$ on f, g is a well-defined inner product.

Define norm $\|f\|$ for all $f \in \mathcal{S}$ as follows

$$\|f\| = \sqrt{\langle f, f \rangle} \quad (67)$$

then \mathcal{S} is completed as an Hilbert space \mathcal{H} , named **reproducing kernel Hilbert space**, for kernel K has reproducibility, i.e. $\langle K(\cdot, x), f \rangle = f(x)$, $\langle K(\cdot, x), K(x, \cdot) \rangle = K(x, x)$. We can conclude that

Any kernel function K implicitly defines a reproducing kernel Hilbert space

Lemma 2 Kernel K is a positive definite kernel if and only if the Gram matrix of K is half positive definite.

Necessity: If G_K is half positive definite for arbitrary \mathbf{x} , then as shown above, K determines a RKHS, that is, $\langle K(\cdot, x), f \rangle = f(x)$, $\langle K(\cdot, x), K(x, \cdot) \rangle = K(x, x)$ holds. a mapping $\phi : x \mapsto K(\cdot, x) \leftrightarrow \mathcal{H}$ can be built up by defining

$$K(x, y) = \langle \phi(x), \phi(y) \rangle \quad (68)$$

Sufficiency: If K is a positive definite kernel, then $K(x, y) = \langle \phi(x), \phi(y) \rangle$. Hence $\forall \alpha \in \mathbb{R}^N$,

$$\alpha^T G_K \alpha = \sum_{i=1}^N \alpha_i \sum_{j=1}^N \alpha_j \langle \phi(x_i), \phi(y_j) \rangle = \left\langle \sum_{i=1}^N \alpha_i \phi(x_i), \sum_{j=1}^N \alpha_j \phi(y_j) \right\rangle \geq 0 \quad (69)$$

then G_K is half positive definite. QED

5.4.3 Normally-used Kernel Function

Linear/Polynomial Kernel

$$K(x, y) = \langle x, y \rangle^d \quad (70)$$

Gaussian/Laplacian Kernel

$$K(x, y) = -\frac{\|x - y\|^2}{2\sigma^2} \Bigg/ -\frac{\|x - y\|}{\sigma} \quad (71)$$

Sigmoid Kernel

$$K(x, y) = \tanh(\beta \langle x, y \rangle + \theta) \quad (72)$$

5.5 Coordinate Descent

One basic algorithm to search for the lagrange multiplier matrix is the coordinate descent. The following gives the iteration

Algorithm 4 coordinateDescent(α)**while** not converge **do** **for** $i = 0$ **to** N **do** $\alpha_i := \arg \min_{\hat{\alpha}_i} W(\alpha_1, \alpha_2, \dots, \alpha_{i-1}, \hat{\alpha}_i, \alpha_{i+1}, \dots, \alpha_N)$ s.t. $\hat{\alpha}_i = -\sum_{j \neq i} \alpha_j$ **end for****end while**

The inner loop search the minima of W with one variable α_i at one time.

5.6 Sequential Minimization Optimization

5.6.1 Mathematical Model

If we deal with two variables α_i, α_j chosen at random on optimizing the convex optimization (due to the constraint condition). Apart from the pivot (α_i, α_j) we have other variables fixed. Then (α_i, α_j) constructs a partition for the original quadratic programming problem. Then the constraint condition is expanded to

$$\arg \min_{\alpha_i, \alpha_j} \frac{1}{2} \alpha_i^2 K(x_i, x_i) + \frac{1}{2} \alpha_j^2 K(x_j, x_j) + \alpha_i \alpha_j y_i y_j K(x_i, x_j) - (\alpha_i + \alpha_j) + \alpha_i y_i \sum_{k \neq i, j} \alpha_k y_k K(x_i, x_k) + \alpha_j y_j \sum_{k \neq i, j} \alpha_k y_k K(x_j, x_k) - \sum_{k \neq i, j} \alpha_k \quad (73)$$

$$\text{s.t. } \alpha_i y_i + \alpha_j y_j = - \sum_{k \neq i, j}^N \alpha_k y_k = \zeta, \quad 0 \leq \alpha_i, \alpha_j \leq C \quad (74)$$

Then constraint condition is shown as

$$\begin{cases} \alpha_i + \alpha_j = \zeta / y_i & y_i = y_j \\ \alpha_i - \alpha_j = \zeta / y_i & y_i \neq y_j \end{cases} \quad (75)$$

And in the optimizing iteration the equality

$$\alpha_i^{\text{new}} y_i + \alpha_j^{\text{new}} y_j = \zeta = \alpha_i^{\text{old}} y_i + \alpha_j^{\text{old}} y_j \quad (76)$$

then the constraint condition for α_j^{new} is

$$L \leq \alpha_j^{\text{new}} \leq H, \quad (L, H) = \begin{cases} (\max(0, \alpha_j^{\text{old}} - \alpha_i^{\text{old}}), \min(C, C + \alpha_j^{\text{old}} - \alpha_i^{\text{old}})) & y_i = y_j \\ (\max(0, \alpha_j^{\text{old}} + \alpha_i^{\text{old}} - C), \min(C, \alpha_j^{\text{old}} + \alpha_i^{\text{old}})) & y_i \neq y_j \end{cases} \quad (77)$$

With $\alpha_i y_i = \zeta - \alpha_j y_j \rightarrow \alpha_i = y_i(\zeta - \alpha_j y_j)$, target expands to

$$\begin{aligned} & \arg \min_{\alpha_j} W(\alpha_j) \\ &= \frac{1}{2} \alpha_i^2 K(x_i, x_j) + \frac{1}{2} \alpha_j^2 K(x_j, x_j) + \alpha_i \alpha_j y_i y_j K(x_i, x_j) - (\alpha_i + \alpha_j) + \alpha_i y_i v_i + \alpha_j y_j v_j \end{aligned} \quad (78)$$

$$\text{where } v_t = \sum_{k \neq i, j} \alpha_k y_k K(x_t, x_k) \quad (79)$$

then

$$\frac{\partial}{\partial \alpha_j} W(\alpha_j) = 0 \rightarrow \alpha_j = y_j \frac{y_j - y_i + \zeta(K(x_i, x_i) - K(x_i, x_j)) + v_i - v_j}{K(x_i, x_i) + K(x_j, x_j) - 2K(x_i, x_j)} \quad (80)$$

Take

$$E_t = \left(\sum_{k=1}^N \alpha_k y_k K(x_k, x_t) + b \right) - y_t = v_t + \alpha_i y_i K(x_i, x_t) + \alpha_j y_j K(x_j, x_t) + b - y_t \quad (81)$$

as prediction bias. Then α_j^{new} expands to

$$\alpha_j^{\text{new}} = \alpha_j^{\text{old}} + \frac{(E_i - E_j) y_j}{K(x_i, x_i) + K(x_j, x_j) - 2K(x_i, x_j)} = \alpha_j^{\text{old}} + \frac{(E_i - E_j) y_j}{\|\phi(x_i) - \phi(x_j)\|^2} \quad (82)$$

Also α_j^{new} requires truncation when exceeds the feasible region, hence

$$\alpha_j^{\text{new-truncated}} = \begin{cases} L & \alpha_j^{\text{new}} \leq L \\ \alpha_j^{\text{new}} & L < \alpha_j^{\text{new}} \leq H \\ H & H < \alpha_j^{\text{new}} \end{cases} \quad (83)$$

then from α_j^{new} , $\alpha_i^{\text{new}} = \alpha_i^{\text{old}} + y_i y_j (\alpha_j^{\text{old}} - \alpha_j^{\text{new}})$. Every time in the optimizing iteration, the sample dataset is checked to see if Karush-Kuhn-Tucker Conditions is violated, i.e.

$$\begin{aligned} \alpha_i = 0 & \leftrightarrow y_i \left(\sum_{j=1}^N \alpha_j y_j K(x_i, x_j) + b \right) \geq 1 \\ 0 < \alpha_i < C & \leftrightarrow y_i \left(\sum_{j=1}^N \alpha_j y_j K(x_i, x_j) + b \right) = 1 \\ \alpha_i = C & \leftrightarrow y_i \left(\sum_{j=1}^N \alpha_j y_j K(x_i, x_j) + b \right) \leq 1 \end{aligned} \quad (84)$$

Then if $0 < \alpha_i^{\text{new}} < C$ bias E and value b are

$$b_i^{\text{new}} = y_i - \sum_{k=1}^N \alpha_k y_k K(x_i, x_k) = -E_i + \alpha_i^{\text{old}} y_i K(x_i, x_i) + \alpha_j^{\text{old}} y_j K(x_i, x_j) + b^{\text{old}} \quad (85)$$

Likewise,

$$b_j^{\text{new}} = y_j - \sum_{k=1}^N \alpha_k y_k K(x_j, x_k) = -E_j + \alpha_j^{\text{old}} y_j K(x_i, x_j) + \alpha_j^{\text{old}} y_j K(x_j, x_j) + b^{\text{old}} \quad (86)$$

Updated value of b depends on the consistence of α_i/α_j with KKT conditions. If both values are valid, take $b^{\text{new}} = (b_i^{\text{new}} + b_j^{\text{new}})/2$. The loop ends with updating bias E as

$$E_i^{\text{new}} = \sum_{k=1}^N \alpha_k y_k K(x_i, x_k) + b^{\text{new}} - y_i \quad (87)$$

5.6.2 Implementation

Algorithm 5 SMO Algorithm

Require: Input dataset $T = \{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\}$, $x_i \in \mathcal{X}, y_i \in \mathcal{H} = \{-1, 1\}$

initialize $k \leftarrow 0, \alpha^{(k)} \leftarrow \mathbf{0}$

while halt condition not met **do**

 search $\alpha_i^{(k)}$

 search $\arg \min_{\alpha_j^{(k)}} E$ under $\alpha_i^{(k)}$

 calculate optimization $(\alpha_i^{(k+1)}, \alpha_j^{(k+1)})$, update E, b

$(\alpha_i^{(k)}, \alpha_j^{(k)}) \leftarrow (\alpha_i^{(k+1)}, \alpha_j^{(k+1)}), k \leftarrow k + 1$

end while

return $\alpha^{(k+1)}$
