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E.E 511 :- Homework 5

Problem 1:-

I have read and understood the general instructions at the top of HW5 and I formally declare that all work I turn in for everything in this course will not contain or involve any cheating at all.

Problem 2:-

a) Note that all printed evaluation metrics are w/o matching

(i) Please refer to the end of this pdf for this qn.

(ii) Please refer to the end of this pdf for this qn.

b) For the MNIST dataset with 10 classes & 10

(i) clusters, there are $(10 \times 9 \times 8 \times 7 \times 6 \times 5 \times 4 \times 3 \times 2 \times 1) = 10!$
$= 3628800$ matchings possible.
(The above can be deduced by matching clusters to a class 1 by 1.
First, match cluster 1 to a class (there are 10 possible classes) then cluster 2 which would have 9 possibles till cluster 10, which would have only 1 class remaining.)

There are 2 parts of the Hungarian algorithm that are responsible for its worst case complexity :- equality graph construction & augmented path search.

The equality graph construction assigns labels to rows & columns of the cost matrix, and has a worst case complexity of $O(n^2)$ per iteration. The same also applies to the ~~aug~~ path search in the E_G, using BFS/DFS.

∴ the net worst case complexity would be $O(n^2 \times n)$, where n is the number of tasks/workers in the Hungarian algo..

⇒ net worst case time complexity $= O(n^3)$.

(ii) Please refer to the end of this pdf for this qn.

c) (i) Please refer to the end of this pdf for this qn.

(ii) Yes, spectral clustering improves the accuracy of K-means from $\simeq 50\%$ → $\simeq 60\%$.

This is mostly because spectral clustering is good at representing complex relationships b/w data & transforming data from a high dimensional manifold to a low dimensions one with these relationships.
K-means on the other hand is biased towards spherical relationships and so does not handle datasets like MNIST as well.

d) (i) Please refer to the end of this pdf for this qn.

(ii) The random sampled X_s ~~dataset~~ performs the worst, which is expected as doing any form of clustering would give you better reference points for K-NN than random sampling.

However, spectral KNN show a strange pattern:—

→ K=1 → KNN performs better
→ K=3 → Similar perf.
→ K=5 → Spectral performs better

My ~~mod~~ intuition says this is because spectral takes a more nuanced approach to representing relationships amongst various points in the dataset, that make it better for higher ks, as it more thorough in its "clustering analysis". However, for lower ks (like k=1) this level of thorough analysis in the data generalises it too much, which is why K-NN performs better

Problem 3:—

a) Please ~~update this~~ refer to the end of this pdf for this qn.

b) Please refer to the end of this pdf for this qn.

c) Please refer to the end of this pdf for this qn.

d) Please refer to the end of this pdf for this qn.

e) (next page)

Validation Accuracy:-

Logistic Regression	Random Forest	K-NN	Multilayer Perceptron
0.90264	0.01565	0.9418	0.9664

Overall, it seems like ~~K-NN~~ MLP > ~~MLP~~ KNN > Logistic > RF.

Unfortunately, in RF's, I suspect it's an implementation issue causing a poor accuracy. For the others, I like to view MLP as a complex version of logistic regression in a way. Since the given dataset is also complex & likely has ~~not~~ a ~~not~~ complex decision boundary, MLP performs better than the logistic regressions. K-NN also has a tendency to simplify decision boundaries and so, MLP outperforms K-NN in this dataset. Further, while K-NN may not ~~give~~ generate as complex decision boundaries as MLP, logistic regression tends to stay closer to a linear form, while K-NN is still good at representing non-linear boundaries. ∴ KNN outperforms the logistic regression in this dataset, which clearly has complex non-linear decision boundaries.

f) As MLP performed best in my previous runs, I chose MLP as the classifier for this run. I used sklearn to implement it & tuned its hyperparameters in 3d) (which I reused in 3f) using GridSearchCV. Please find the .txt file in the submission & the code in the attached .mpynb files.

wuicpnd8q

March 16, 2024

[1]:
```
# always import
import sys
from time import time

# numpy & scipy
import numpy as np
import scipy

# sklearn
from sklearn.cluster import KMeans
from sklearn.decomposition import PCA
from sklearn.preprocessing import scale
from sklearn import metrics
from sklearn.metrics import confusion_matrix
from sklearn.metrics import pairwise_distances_argmin, pairwise_distances
from sklearn.metrics.cluster import homogeneity_score, completeness_score,␣
 ↪v_measure_score, adjusted_rand_score, adjusted_mutual_info_score
from sklearn import neighbors
from sklearn.model_selection import train_test_split

# Hungarian algorithm
from munkres import Munkres
from scipy.optimize import linear_sum_assignment

# visuals
import matplotlib.pyplot as plt
from matplotlib import offsetbox
from sklearn.manifold import Isomap, TSNE

# maybe
from numba import jit
```

[2]:
```
# load MNIST data and normalization
from sklearn.datasets import fetch_openml
X, y = fetch_openml('mnist_784', version=1, return_X_y=True, data_home='mnist/')
y = np.asarray(list(map(int, y)))
X = np.asarray(X.astype(float))
```

```
X = scale(X)
n_digits = len(np.unique(y))
```

[3]:
```
# TODO: Hungarian algorithm
def calculate_hungarian_cost_matrix(y_true, y_pred, K) :
    conf_mat = confusion_matrix(y_true, y_pred, labels=range(K))
    #print(conf_mat.max())
    cost_matrix = (conf_mat.max() - conf_mat)/conf_mat.max()
    return cost_matrix

def accuracy(pred, y):
    dataset_size = y.size
    correct_predictions = 0
    #print(pred)
    #print(y)
    for i in range(dataset_size):
        if y[i] == (pred[i]):
            correct_predictions += 1
    precision = (correct_predictions/dataset_size)*100
    return precision
```

[4]:
```
# TODO: Kmeans
def get_distance_matrix(X, C):
    return (np.sqrt(((X[:,np.newaxis,:] - C) ** 2).sum(axis=2)))

def calculate_cost(centroids, X, min_index_matrix):
    return ((X - centroids[min_index_matrix]) ** 2).sum()

def run_kmeans(K, initial_centroids, X):
    num_samples, num_features = X.shape
    #print(centroids[0])
    #print(centroids.shape)
    centroids = initial_centroids.copy()
    distance_matrix = get_distance_matrix(X, centroids)
    max_iter = 300
    epsilon = 0.00001
    iter = 0
    old_cost = 0
    min_index_matrix = np.argmin(distance_matrix, axis = 1)
    new_cost = calculate_cost(centroids, X, min_index_matrix)
    #print("New Cost : " + str(new_cost))
    while iter <= max_iter and abs(new_cost-old_cost) >= epsilon :
        #print("Iteration : " + str(iter))
        #print(centroids)
        for j in range(K):
            jcluster_indices = np.array(min_index_matrix == j)
            jcluster = X[jcluster_indices, :]
```

```
            if jcluster.shape[0] > 0 :
                centroids[j,:] = jcluster.sum(axis=0)/jcluster.shape[0]
        distance_matrix = get_distance_matrix(X, centroids)
        min_index_matrix = np.argmin(distance_matrix, axis = 1)
        old_cost = new_cost
        new_cost = calculate_cost(centroids, X, min_index_matrix)
        iter = iter + 1
    return [centroids, new_cost]


#print ("NOTE : THESE VALUES DO NOT CORRESPOND TO ANY ANSWER AND WERE SIMPLY␣
 ↪USED FOR TESTING K-MEANS")
num_samples, num_features = X.shape
K = 10
'''
#Using the Forgy seed method for initialisation : take K random datapoints from␣
 ↪the dataset
initial_centroid_indices = np.random.choice(num_samples, K, replace=False)
centroids = X[initial_centroid_indices][:]
#print(initial_centroid_indices)
[final_kmeans_centroids, new_cost] = run_kmeans(K, centroids, X)
#print(final_kmeans_solution[0])
distance_matrix = get_distance_matrix(X, final_kmeans_centroids)
y_pred = np.argmin(distance_matrix, axis = 1)
homogeneity_score = metrics.homogeneity_score(y, y_pred)
print("Homogeneity Score (using Forgy method): " + str(homogeneity_score))
completeness_score = metrics.completeness_score(y, y_pred)
print("Completeness Score (using Forgy method): " + str(completeness_score))
vmeasure_score = metrics.v_measure_score(y, y_pred)
print("V-Measure Score (using Forgy method): " + str(vmeasure_score))
adjusted_rand_score = metrics.adjusted_rand_score(y, y_pred)
print("Adjusted Rand Score (using Forgy method): " + str(adjusted_rand_score))
adjusted_mutual_info_score = metrics.adjusted_mutual_info_score(y, y_pred)
print("Adjusted Rand Score (using Forgy method): " +␣
 ↪str(adjusted_mutual_info_score))
cost_matrix = calculate_hungarian_cost_matrix(y, y_pred, K)
#print(cost_matrix)
cluster_to_class_matching = {}
row_ind, col_ind = linear_sum_assignment(cost_matrix)
for row, column in zip(row_ind, col_ind):
    print(f"Cluster {row} assigned to Class {column} ")
    cluster_to_class_matching[row] = column
for original_value, new_value in cluster_to_class_matching.items():
    y_pred[y_pred == original_value] = new_value + 10
y_pred = y_pred - 10
cm = confusion_matrix(y, y_pred, labels=range(K))
print(cm)
```

```
acc = accuracy(y_pred, y)
print("Accuracy : " + str(acc))
print ("NOTE : THESE VALUES DO NOT CORRESPOND TO ANY ANSWER AND WERE SIMPLY␣
 ↪USED FOR TESTING K-MEANS")
'''
```

[4]:
```
'\n#Using the Forgy seed method for initialisation : take K random datapoints
from the dataset\ninitial_centroid_indices = np.random.choice(num_samples, K,
replace=False)\ncentroids = X[initial_centroid_indices][:]\n#print(initial_centr
oid_indices)\n[final_kmeans_centroids, new_cost] = run_kmeans(K, centroids,
X)\n#print(final_kmeans_solution[0])\ndistance_matrix = get_distance_matrix(X,
final_kmeans_centroids)\ny_pred = np.argmin(distance_matrix, axis =
1)\nhomogeneity_score = metrics.homogeneity_score(y, y_pred)\nprint("Homogeneity
Score (using Forgy method): " + str(homogeneity_score))\ncompleteness_score =
metrics.completeness_score(y, y_pred)\nprint("Completeness Score (using Forgy
method): " + str(completeness_score))\nvmeasure_score =
metrics.v_measure_score(y, y_pred)\nprint("V-Measure Score (using Forgy method):
" + str(vmeasure_score))\nadjusted_rand_score = metrics.adjusted_rand_score(y,
y_pred)\nprint("Adjusted Rand Score (using Forgy method): " +
str(adjusted_rand_score))\nadjusted_mutual_info_score =
metrics.adjusted_mutual_info_score(y, y_pred)\nprint("Adjusted Rand Score (using
Forgy method): " + str(adjusted_mutual_info_score))\ncost_matrix =
calculate_hungarian_cost_matrix(y, y_pred,
K)\n#print(cost_matrix)\ncluster_to_class_matching = {}\nrow_ind, col_ind =
linear_sum_assignment(cost_matrix)\nfor row, column in zip(row_ind, col_ind):\n
print(f"Cluster {row} assigned to Class {column} ")\n
cluster_to_class_matching[row] = column\nfor original_value, new_value in
cluster_to_class_matching.items():\n    y_pred[y_pred == original_value] =
new_value + 10\ny_pred = y_pred - 10\ncm = confusion_matrix(y, y_pred,
labels=range(K))\nprint(cm)\nacc = accuracy(y_pred, y)\nprint("Accuracy : " +
str(acc))\nprint ("NOTE : THESE VALUES DO NOT CORRESPOND TO ANY ANSWER AND WERE
SIMPLY USED FOR TESTING K-MEANS")\n'
```

[5]:
```
print("Section 2 a/b) - I")
pca = PCA(n_components=K)
pca.fit(X)
centroids = pca.components_
[final_kmeans_centroids, new_cost] = run_kmeans(K, centroids, X)
#print(final_kmeans_solution[0])
distance_matrix = get_distance_matrix(X, final_kmeans_centroids)
y_pred = np.argmin(distance_matrix, axis = 1)
homogeneity_score = metrics.homogeneity_score(y, y_pred)
print("Homogeneity Score (using top K principal eigenvectors of PCA): " +␣
 ↪str(homogeneity_score))
completeness_score = metrics.completeness_score(y, y_pred)
print("Completeness Score (using top K principal eigenvectors of PCA): " +␣
 ↪str(completeness_score))
```

```
vmeasure_score = metrics.v_measure_score(y, y_pred)
print("V-Measure Score (using top K principal eigenvectors of PCA): " +␣
 ↪str(vmeasure_score))
adjusted_rand_score = metrics.adjusted_rand_score(y, y_pred)
print("Adjusted Rand Score (using top K principal eigenvectors of PCA): " +␣
 ↪str(adjusted_rand_score))
adjusted_mutual_info_score = metrics.adjusted_mutual_info_score(y, y_pred)
print("Adjusted Rand Score (using top K principal eigenvectors of PCA): " +␣
 ↪str(adjusted_mutual_info_score))
cost_matrix = calculate_hungarian_cost_matrix(y, y_pred, K)
#print(cost_matrix)
cluster_to_class_matching = {}
row_ind, col_ind = linear_sum_assignment(cost_matrix)
print("Class to Cluster Assignments based on Hungarian Algorithm")
for row, column in zip(row_ind, col_ind):
    print(f"Class {row} assigned to Cluster {column} ")
    cluster_to_class_matching[column] = row
for original_value, new_value in cluster_to_class_matching.items():
    y_pred[y_pred == original_value] = new_value + 10
y_pred = y_pred - 10
print("Confusion Matrix on predictions post matching : ")
cm = confusion_matrix(y, y_pred, labels=range(K))
print(cm)
acc = accuracy(y_pred, y)
print("Accuracy : " + str(acc))
```

```
Section 2 a/b) - I
Homogeneity Score (using top K principal eigenvectors of PCA):
0.4197975269152666
Completeness Score (using top K principal eigenvectors of PCA):
0.4419190420959369
V-Measure Score (using top K principal eigenvectors of PCA): 0.43057433880263696
Adjusted Rand Score (using top K principal eigenvectors of PCA):
0.32075816979535976
Adjusted Rand Score (using top K principal eigenvectors of PCA):
0.4304273983543338
Class to Cluster Assignments based on Hungarian Algorithm
Class 0 assigned to Cluster 0
Class 1 assigned to Cluster 4
Class 2 assigned to Cluster 2
Class 3 assigned to Cluster 5
Class 4 assigned to Cluster 9
Class 5 assigned to Cluster 8
Class 6 assigned to Cluster 3
Class 7 assigned to Cluster 7
Class 8 assigned to Cluster 6
Class 9 assigned to Cluster 1
```

```
Confusion Matrix on predictions post matching :
[[3876   35  118 1356   13  658  351    6  480   10]
 [   0 7638   13   27    8  159   16    5   10    1]
 [  40  827 2380  726  185   85  862   29 1815   41]
 [  10  577  734 4097  200  118   88   95 1117  105]
 [  55  536   73    5 3968  948  128  741   27  343]
 [  33  467  246 2131  311 2709  102   93  158   63]
 [ 282  561  423  109   27  133 5323    1   12    5]
 [  20  516   16    9 1580  134    3 4086   13  916]
 [  45 1171  205 2589  355 2096   31  182   78   73]
 [  44  331   23  124 3487  131    5 2368   14  431]]
Accuracy : 49.40857142857143
```

[6]:
```
print("Section 2 a/b) - II")
d = 30
pca = PCA(n_components=d)
X_pca = pca.fit_transform(X)
#print(X_pca.shape)
no_of_runs = 10
cost = 100000000
final_centroids = np.zeros((K, d))
for i in range(no_of_runs) :
    #Using the Forgy seed method for initialisation : take K random datapoints␣
 ↪from PCA-applied dataset
    rs = 5*i
    np.random.seed(rs)
    initial_centroid_indices = np.random.choice(num_samples, K, replace=False)
    centroids = X_pca[initial_centroid_indices][:]
    #print(centroids.shape)
    [final_kmeans_centroids, new_cost] = run_kmeans(K, centroids, X_pca)
    if cost > new_cost :
        cost = new_cost
        final_centroids = final_kmeans_centroids.copy()
distance_matrix = get_distance_matrix(X_pca, final_centroids)
y_pred = np.argmin(distance_matrix, axis = 1)
homogeneity_score = metrics.homogeneity_score(y, y_pred)
print("Homogeneity Score (using PCA for dimensionality reduction to d = 30): "␣
 ↪+ str(homogeneity_score))
completeness_score = metrics.completeness_score(y, y_pred)
print("Completeness Score (using PCA for dimensionality reduction to d = 30): "␣
 ↪+ str(completeness_score))
vmeasure_score = metrics.v_measure_score(y, y_pred)
print("V-Measure Score (using PCA for dimensionality reduction to d = 30): " +␣
 ↪str(vmeasure_score))
adjusted_rand_score = metrics.adjusted_rand_score(y, y_pred)
print("Adjusted Rand Score (using PCA for dimensionality reduction to d = 30):␣
 ↪" + str(adjusted_rand_score))
```

```
adjusted_mutual_info_score = metrics.adjusted_mutual_info_score(y, y_pred)
print("Adjusted Rand Score (using PCA for dimensionality reduction to d = 30):␣
 ↪" + str(adjusted_mutual_info_score))
cost_matrix = calculate_hungarian_cost_matrix(y, y_pred, K)
#print(cost_matrix)
cluster_to_class_matching = {}
row_ind, col_ind = linear_sum_assignment(cost_matrix)
print("Class to Cluster Assignments based on Hungarian Algorithm")
for row, column in zip(row_ind, col_ind):
    print(f"Class {row} assigned to Cluster {column} ")
    cluster_to_class_matching[column] = row
for original_value, new_value in cluster_to_class_matching.items():
    y_pred[y_pred == original_value] = new_value + 10
y_pred = y_pred - 10
cm = confusion_matrix(y, y_pred, labels=range(K))
print("Confusion Matrix on predictions post matching : ")
print(cm)
acc = accuracy(y_pred, y)
print("Accuracy : " + str(acc))
```

```
Section 2 a/b) - II
Homogeneity Score (using PCA for dimensionality reduction to d = 30):
0.4222313136385659
Completeness Score (using PCA for dimensionality reduction to d = 30):
0.4439863964506075
V-Measure Score (using PCA for dimensionality reduction to d = 30):
0.43283566527794587
Adjusted Rand Score (using PCA for dimensionality reduction to d = 30):
0.32192715104290953
Adjusted Rand Score (using PCA for dimensionality reduction to d = 30):
0.43268938916389627
Class to Cluster Assignments based on Hungarian Algorithm
Class 0 assigned to Cluster 7
Class 1 assigned to Cluster 1
Class 2 assigned to Cluster 5
Class 3 assigned to Cluster 6
Class 4 assigned to Cluster 0
Class 5 assigned to Cluster 2
Class 6 assigned to Cluster 4
Class 7 assigned to Cluster 9
Class 8 assigned to Cluster 8
Class 9 assigned to Cluster 3
Confusion Matrix on predictions post matching :
[[3965   35   82  942   20  658  763    7  418   13]
 [   0 7621   13   29    5  173   16    7   12    1]
 [  42  839 2588  775  165   92  673   42 1717   57]
 [  11  678  219 4440  187  152   97   91 1141  125]
```

```
 [  50  543   49    3 3938  905  159  677   25  475]
 [  35  529  128 2061  326 2798  129   70  157   80]
 [ 240  504  774   53   37  132 5120    1    9    6]
 [  19  552    7   14 1584  114    3 4072   17  911]
 [  48 1348   96 2220  398 2297   53  180   78  107]
 [  42  361   15  106 3502  118    6 2275   15  518]]
Accuracy : 50.197142857142865
```

[7]:
```
# TODO: Spectral clustering
def spectral_clustering_analysis(X_pca):
    # k is number of nearest neighbours in the KNN model, K is the number of␣
 ↪clusters in k_means
    k = 500
    H = neighbors.NearestNeighbors(n_neighbors=k, algorithm='kd_tree',␣
 ↪metric='euclidean').fit(X_pca).kneighbors_graph(mode='distance')
    #print(E.shape)
    sigma = H.sum()/H.nnz
    H = H.power(2)
    E = -H.multiply(1.0/(2*sigma*sigma))
    #print("norm done")
    #print(E)
    #print(scipy.sparse.issparse(E))
    E.data = np.exp(E.data)
    #print("exp done")
    #print(E)
    E.setdiag(values=0)
    #print(E)
    #total_sum = E.sum()
    #E = E.multiply(1.0/total_sum)
    row_sums = E.sum(axis=1)
    row_sums = np.ravel(row_sums)
    row_sums_reciprocal = np.reciprocal(row_sums, where=row_sums!=0)
    E = E.multiply(row_sums_reciprocal[:, np.newaxis])
    E.setdiag(values=1)
    #print(E)
    E_transpose = E.transpose()
    E = (E + E_transpose)
    E = E.multiply(0.5)
    #print(E)
    D = scipy.sparse.csr_array((E.shape))
    D.setdiag(E.sum(axis=1))
    #print(D)
    D_L = D.sqrt()
    D_L = scipy.sparse.linalg.inv(D_L)
    L = -D_L @ E @ D_L
    L_r, L_c = L.shape
    L = scipy.sparse.identity(L_r, format='csr') + L
```

```
    #print(L.shape)
    #print(L)
    no_of_eigenvectors = 20
    #print("Start Eigen Analysis")
    eigenvalues, eigenvectors = scipy.sparse.linalg.eigs(L,␣
 ↪k=no_of_eigenvectors, which='SR')
    #print(eigenvectors)
    idx = np.argsort(eigenvalues.real)
    sorted_eigen_values = eigenvalues[idx]
    sorted_eigen_vectors = eigenvectors.real[:,idx]
    k_eigen_vectors = sorted_eigen_vectors[:,1:]
    return [sorted_eigen_values, k_eigen_vectors]

print("Spectral Clustering Results :")
[sorted_eigen_values, k_eigen_vectors] = spectral_clustering_analysis(X_pca)
y_pred = KMeans(init='k-means++', n_clusters=10, n_init=10).
 ↪fit_predict(k_eigen_vectors)
homogeneity_score = metrics.homogeneity_score(y, y_pred)
print("Homogeneity Score (using spectral clustering): " +␣
 ↪str(homogeneity_score))
completeness_score = metrics.completeness_score(y, y_pred)
print("Completeness Score (using spectral clustering): " +␣
 ↪str(completeness_score))
vmeasure_score = metrics.v_measure_score(y, y_pred)
print("V-Measure Score (using spectral clustering): " + str(vmeasure_score))
adjusted_rand_score = metrics.adjusted_rand_score(y, y_pred)
print("Adjusted Rand Score (using spectral clustering): " +␣
 ↪str(adjusted_rand_score))
adjusted_mutual_info_score = metrics.adjusted_mutual_info_score(y, y_pred)
print("Adjusted Rand Score (using spectral clustering): " +␣
 ↪str(adjusted_mutual_info_score))
cost_matrix = calculate_hungarian_cost_matrix(y, y_pred, 10)
#print(cost_matrix)
#print(sorted_eigen_values)
#print(k_eigen_vectors.shape)
cluster_to_class_matching = {}
row_ind, col_ind = linear_sum_assignment(cost_matrix)
print("Class to Cluster Assignments based on Hungarian Algorithm")
for row, column in zip(row_ind, col_ind):
    print(f"Class {row} assigned to Cluster {column} ")
    cluster_to_class_matching[column] = row
for original_value, new_value in cluster_to_class_matching.items():
    y_pred[y_pred == original_value] = new_value + 10
y_pred = y_pred - 10
print("Confusion Matrix on predictions post matching : ")
cm = confusion_matrix(y, y_pred, labels=range(10))
```

```
print(cm)
acc = accuracy(y_pred, y)
print("Accuracy : " + str(acc))
```

```
Spectral Clustering Results :

/Users/prateek/anaconda3/envs/AnacondaTest/lib/python3.11/site-
packages/scipy/sparse/_index.py:146: SparseEfficiencyWarning: Changing the
sparsity structure of a csr_matrix is expensive. lil_matrix is more efficient.
  self._set_arrayXarray(i, j, x)
/Users/prateek/anaconda3/envs/AnacondaTest/lib/python3.11/site-
packages/scipy/sparse/linalg/_dsolve/linsolve.py:394: SparseEfficiencyWarning:
splu converted its input to CSC format
  warn('splu converted its input to CSC format', SparseEfficiencyWarning)
/Users/prateek/anaconda3/envs/AnacondaTest/lib/python3.11/site-
packages/scipy/sparse/linalg/_dsolve/linsolve.py:285: SparseEfficiencyWarning:
spsolve is more efficient when sparse b is in the CSC matrix format
  warn('spsolve is more efficient when sparse b '

Homogeneity Score (using spectral clustering): 0.5987127729924084
Completeness Score (using spectral clustering): 0.6694485180155375
V-Measure Score (using spectral clustering): 0.6321078894912106
Adjusted Rand Score (using spectral clustering): 0.4677415369830309
Adjusted Rand Score (using spectral clustering): 0.6320129377410119
Class to Cluster Assignments based on Hungarian Algorithm
Class 0 assigned to Cluster 9
Class 1 assigned to Cluster 6
Class 2 assigned to Cluster 1
Class 3 assigned to Cluster 0
Class 4 assigned to Cluster 7
Class 5 assigned to Cluster 3
Class 6 assigned to Cluster 8
Class 7 assigned to Cluster 2
Class 8 assigned to Cluster 4
Class 9 assigned to Cluster 5
Confusion Matrix on predictions post matching :
[[6475    3   70   70    0    0   22    1  233   29]
 [   0 4396   28   21 3333    0    7    1   62   29]
 [  57   35 5861  362   12    0   44   38  473  108]
 [  11   10  185 6049   53    0    1   47  603  182]
 [   3   28  116   23   29    1   11   10   50 6553]
 [  44    4 1542 1803    8    0   19    6 2631  256]
 [ 104   12   95   29    7    0 3639    0 2939   51]
 [  10   88   44   38   43    1    0 4150   29 2890]
 [  47   40  351  945   28    0    3    6 5149  256]
 [  20   10   32   97   31    0    0   96   70 6602]]
Accuracy : 60.5
```

[8]:
```
# TODO: Clustering + KNN
def euclidean_distance(row1, row2):
    distance = np.linalg.norm(row1 - row2)
    return distance

def knn(X_train, y_train, X_test, kvalue):
    y_pred = []
    for x in X_test :
        distances = [euclidean_distance(x, x_train) for x_train in X_train]
        k_indices = np.argsort(distances)[:kvalue]
        k_nearest_labels = [y_train[i] for i in k_indices]
        most_common = np.argmax(np.bincount(k_nearest_labels))
        y_pred.append(most_common)
    return np.array(y_pred)

no_of_runs = 10
cost = 100000000
K_d_cluster_size=100
k_values = [1,3,5]
final_centroids = np.zeros((K, d))
for i in range(no_of_runs) :
    #Using the Forgy seed method for initialisation : take K random datapoints␣
 ↪from PCA-applied dataset
    rs = 5*i
    np.random.seed(rs)
    initial_centroid_indices = np.random.choice(num_samples, K_d_cluster_size,␣
 ↪replace=False)
    centroids = X_pca[initial_centroid_indices][:]
    #print(centroids.shape)
    [final_kmeans_centroids, new_cost] = run_kmeans(K_d_cluster_size,␣
 ↪centroids, X_pca)
    #print(cost)
    if cost > new_cost :
        cost = new_cost
        final_centroids = final_kmeans_centroids.copy()
distance_matrix = get_distance_matrix(X_pca, final_centroids)
min_row_indices = np.argmin(distance_matrix, axis=0)
final_knn_train_X = X_pca[min_row_indices][:]
final_knn_train_y = y[min_row_indices][:]
final_knn_test_X = np.delete(X_pca, min_row_indices, axis=0)
final_knn_test_y = np.delete(y, min_row_indices, axis=0)

train_accuracies = []
test_accuracies = []
# We loop over the different values of k and calculate the accuracy for each␣
 ↪value of k.
for kvalue in k_values:
```

```
    # Predict labels for train set and test set
    y_pred_train = knn(final_knn_train_X, final_knn_train_y, final_knn_train_X,␣
 ↪kvalue)
    y_pred_test = knn(final_knn_train_X, final_knn_train_y, final_knn_test_X,␣
 ↪kvalue)
    # Calculate accuracy
    train_accuracies.append(accuracy(final_knn_train_y, y_pred_train))
    test_accuracies.append(accuracy(final_knn_test_y, y_pred_test))

print("Kmeans + kNN Results :")
print("Training Accuracy for Kmeans+knn for k = 1 : " +␣
 ↪str(train_accuracies[0]))
print("Testing Accuracy for Kmeans+knn for k = 1 : " + str(test_accuracies[0]))
print("Training Accuracy for Kmeans+knn for k = 3 : " +␣
 ↪str(train_accuracies[1]))
print("Testing Accuracy for Kmeans+knn for k = 3 : " + str(test_accuracies[1]))
print("Training Accuracy for Kmeans+knn for k = 5 : " +␣
 ↪str(train_accuracies[2]))
print("Testing Accuracy for Kmeans+knn for k = 5 : " + str(test_accuracies[2]))
```

```
Kmeans + kNN Results :
Training Accuracy for Kmeans+knn for k = 1 : 100.0
Testing Accuracy for Kmeans+knn for k = 1 : 82.00286123032903
Training Accuracy for Kmeans+knn for k = 3 : 93.0
Testing Accuracy for Kmeans+knn for k = 3 : 77.81545064377683
Training Accuracy for Kmeans+knn for k = 5 : 88.0
Testing Accuracy for Kmeans+knn for k = 5 : 76.03290414878397
```

[12]:
```
cost = 100000000
[sorted_eigen_values, k_eigen_vectors] = spectral_clustering_analysis(X_pca)
for i in range(no_of_runs) :
    #Using the Forgy seed method for initialisation : take K random datapoints␣
 ↪from PCA-applied dataset
    rs = 5*i
    np.random.seed(rs)
    initial_centroid_indices = np.random.choice(num_samples, K_d_cluster_size,␣
 ↪replace=False)
    centroids = k_eigen_vectors[initial_centroid_indices][:]
    #print(centroids.shape)
    [final_kmeans_centroids, new_cost] = run_kmeans(K_d_cluster_size,␣
 ↪centroids, k_eigen_vectors)
    #print(cost)
    if cost > new_cost :
        cost = new_cost
        final_centroids = final_kmeans_centroids.copy()
distance_matrix = get_distance_matrix(k_eigen_vectors, final_centroids)
```

```
min_row_indices = np.argmin(distance_matrix, axis=0)
final_knn_train_X = k_eigen_vectors[min_row_indices][:]
final_knn_train_y = y[min_row_indices][:]
final_knn_test_X = np.delete(k_eigen_vectors, min_row_indices, axis=0)
final_knn_test_y = np.delete(y, min_row_indices, axis=0)

train_accuracies = []
test_accuracies = []
# We loop over the different values of k and calculate the accuracy for each␣
 ↪value of k.
for kvalue in k_values:
    # Predict labels for train set and test set
    y_pred_train = knn(final_knn_train_X, final_knn_train_y, final_knn_train_X,␣
 ↪kvalue)
    y_pred_test = knn(final_knn_train_X, final_knn_train_y, final_knn_test_X,␣
 ↪kvalue)
    # Calculate accuracy
    train_accuracies.append(accuracy(final_knn_train_y, y_pred_train))
    test_accuracies.append(accuracy(final_knn_test_y, y_pred_test))

print("Spectral Clustering + kNN Results :")
print("Training Accuracy for Spectral+Kmeans+knn for k = 1 : " +␣
 ↪str(train_accuracies[0]))
print("Testing Accuracy for Spectral+Kmeans+knn for k = 1 : " +␣
 ↪str(test_accuracies[0]))
print("Training Accuracy for Spectral+Kmeans+knn for k = 3 : " +␣
 ↪str(train_accuracies[1]))
print("Testing Accuracy for Spectral+Kmeans+knn for k = 3 : " +␣
 ↪str(test_accuracies[1]))
print("Training Accuracy for Spectral+Kmeans+knn for k = 5 : " +␣
 ↪str(train_accuracies[2]))
print("Testing Accuracy for Spectral+Kmeans+knn for k = 5 : " +␣
 ↪str(test_accuracies[2]))
```

```
/Users/prateek/anaconda3/envs/AnacondaTest/lib/python3.11/site-
packages/scipy/sparse/_index.py:146: SparseEfficiencyWarning: Changing the
sparsity structure of a csr_matrix is expensive. lil_matrix is more efficient.
  self._set_arrayXarray(i, j, x)
/Users/prateek/anaconda3/envs/AnacondaTest/lib/python3.11/site-
packages/scipy/sparse/linalg/_dsolve/linsolve.py:394: SparseEfficiencyWarning:
splu converted its input to CSC format
  warn('splu converted its input to CSC format', SparseEfficiencyWarning)
/Users/prateek/anaconda3/envs/AnacondaTest/lib/python3.11/site-
packages/scipy/sparse/linalg/_dsolve/linsolve.py:285: SparseEfficiencyWarning:
spsolve is more efficient when sparse b is in the CSC matrix format
  warn('spsolve is more efficient when sparse b '
```

```
Spectral Clustering + kNN Results :
Training Accuracy for Spectral+Kmeans+knn for k = 1 : 100.0
Testing Accuracy for Spectral+Kmeans+knn for k = 1 : 78.8483547925608
Training Accuracy for Spectral+Kmeans+knn for k = 3 : 81.0
Testing Accuracy for Spectral+Kmeans+knn for k = 3 : 77.46638054363376
Training Accuracy for Spectral+Kmeans+knn for k = 5 : 80.0
Testing Accuracy for Spectral+Kmeans+knn for k = 5 : 76.13590844062948
```

[10]:
```python
row_indices = np.random.choice(num_samples, K_d_cluster_size, replace=False)
final_knn_train_X = X_pca[row_indices][:]
final_knn_train_y = y[row_indices][:]
final_knn_test_X = np.delete(X_pca, row_indices, axis=0)
final_knn_test_y =np.delete(y, row_indices, axis=0)

train_accuracies = []
test_accuracies = []
# We loop over the different values of k and calculate the accuracy for each␣
 ↪value of k.
for kvalue in k_values:
    # Predict labels for train set and test set
    y_pred_train = knn(final_knn_train_X, final_knn_train_y, final_knn_train_X,␣
 ↪kvalue)
    y_pred_test = knn(final_knn_train_X, final_knn_train_y, final_knn_test_X,␣
 ↪kvalue)
    # Calculate accuracy
    train_accuracies.append(accuracy(final_knn_train_y, y_pred_train))
    test_accuracies.append(accuracy(final_knn_test_y, y_pred_test))

print("Random Sampling + kNN Results :")
print("Training Accuracy for RS+knn for k = 1 : " + str(train_accuracies[0]))
print("Testing Accuracy for RS+knn for k = 1 : " + str(test_accuracies[0]))
print("Training Accuracy for RS+knn for k = 3 : " + str(train_accuracies[1]))
print("Testing Accuracy for RS+knn for k = 3 : " + str(test_accuracies[1]))
print("Training Accuracy for RS+knn for k = 5 : " + str(train_accuracies[2]))
print("Testing Accuracy for RS+knn for k = 5 : " + str(test_accuracies[2]))
```

```
Random Sampling + kNN Results :
Training Accuracy for RS+knn for k = 1 : 100.0
Testing Accuracy for RS+knn for k = 1 : 73.03719599427754
Training Accuracy for RS+knn for k = 3 : 87.0
Testing Accuracy for RS+knn for k = 3 : 68.42346208869814
Training Accuracy for RS+knn for k = 5 : 83.0
Testing Accuracy for RS+knn for k = 5 : 67.6752503576538
```

os7jzrfx0

March 16, 2024

[1]:
```
import argparse
import os
import random

import numpy as np
import numpy.matlib

import matplotlib.pyplot as plt
import pickle

from sklearn.model_selection import GridSearchCV, PredefinedSplit
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import GridSearchCV, train_test_split
from sklearn.preprocessing import StandardScaler
from sklearn.pipeline import make_pipeline
```

0.1 Dataset overview

In this problem we are building 15-way multi-class classifiers for a fruit classification task. The training and validation sets are stored in the .pkl files provided. See the hw5.pdf file we have provided for details.

In each dataset, we provide the following: - 'images': the raw RGB images - 'feats': 15 dimensional condensed representations of each image (that were precomputed by using a pretrained vision transformer + PCA) - 'labels': an integer value between 0 and 14. The integer to class mapping is provided below in the variable 'idx_to_class'.

We first create a simple python dictionary that maps integers to textual class labels that can be useful for debugging.

[2]:
```
idx_to_class = {0: 'Apple', 1: 'Banana', 2: 'Carambola', 3: 'Guava', 4: 'Kiwi',␣
↪5: 'Mango', 6: 'Orange', 7: 'Peach', 8: 'Pear', 9: 'Persimmon', 10:␣
↪'Pitaya', 11: 'Plum', 12: 'Pomegranate', 13: 'Tomatoes', 14: 'Muskmelon'}
print(idx_to_class)
```

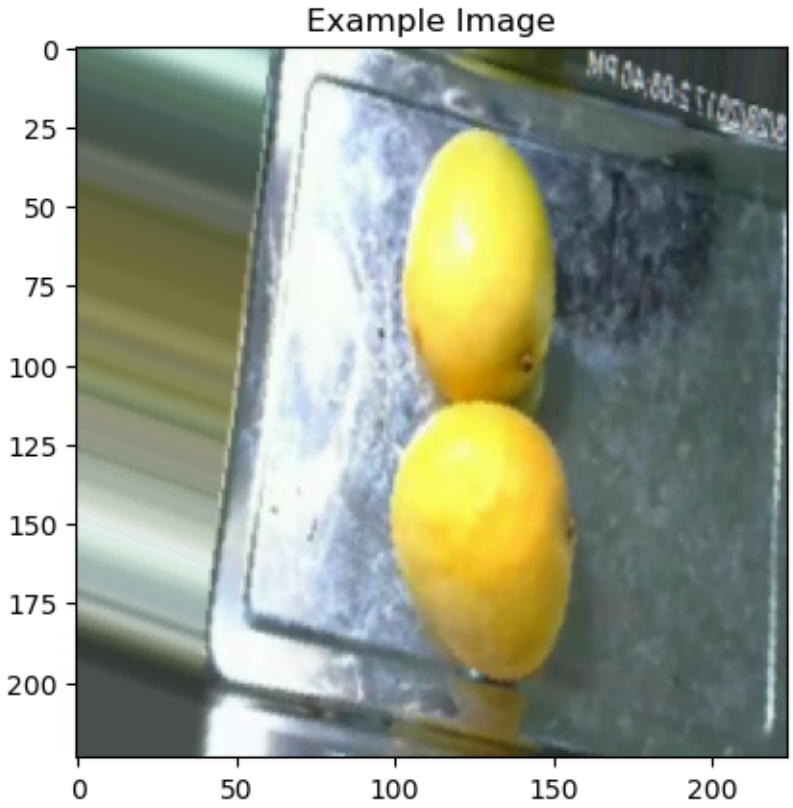
```
{0: 'Apple', 1: 'Banana', 2: 'Carambola', 3: 'Guava', 4: 'Kiwi', 5: 'Mango', 6:
'Orange', 7: 'Peach', 8: 'Pear', 9: 'Persimmon', 10: 'Pitaya', 11: 'Plum', 12:
'Pomegranate', 13: 'Tomatoes', 14: 'Muskmelon'}
```

Next, we load the .pkl files that load as python dictionaries.

[3]:
```
with open('datasets/train.pkl', 'rb') as f:
    train_dataset = pickle.load(f)
```

[4]:
```
with open('datasets/val.pkl', 'rb') as f:
    val_dataset = pickle.load(f)
```

[5]:
```
# We can plot the images this way. This will be quite useful for debugging.
plt.figure()
plt.title('Example Image')
plt.imshow(train_dataset['images'][0])
plt.show()
```



[6]:
```
print("Examples Features shape:", train_dataset['feats'][0].shape)
```

```
Examples Features shape: (15,)
```

[7]:
```
print("Example image label:", idx_to_class[train_dataset['labels'][0]])
```

```
Example image label: Mango
```

[8]:
```
print(train_dataset['feats'][0])
print(np.array(train_dataset['labels']).shape)
print(np.array(train_dataset['images']).reshape(np.
  ↪array(train_dataset['labels']).size,150528).shape)
```

```
[-0.73493075  0.35717848  1.3297853   0.16270295  1.7608238  -1.1582989
  0.5272275  -0.54177004  0.27921718 -0.02514401  0.66478443  0.25313285
  0.15742105  0.21063007 -0.09196111]
(9876,)
(9876, 150528)
```

0.2 Part 2(a): Logistic Regression

Implement Logistic Regression from scratch and report your classifier's accuracy on the training and validation sets. **You should use your implementation from prior homeworks and turn it in again with updates, if any.**

[9]:
```
y_train = np.array(train_dataset['labels'])
X_train = np.array(train_dataset['feats'])
y_val = np.array(val_dataset['labels'])
X_val = np.array(val_dataset['feats'])

print(X_val.shape)
```

```
(2116, 15)
```

[10]:
```
# TODO: Implement multinomial logistic regression
# TODO: stochastic gradient descent (SGD) for Logistic regression
from sklearn.base import BaseEstimator, ClassifierMixin

class LogRegMine(BaseEstimator, ClassifierMixin):
    # encode integer labels to binary vectors
    def yMatrix(self, y, num_class):
        Y = np.zeros((len(y), num_class))
        Y[range(len(y)), y] = 1
        return Y

    # minibatch iterator
    def iterate_minibatches(self, X, y, Y, batchsize, shuffle=False):
        assert X.shape[0] == y.shape[0]
        if shuffle:
            indices = np.arange(X.shape[0])
            np.random.shuffle(indices)
        for start_idx in range(0, X.shape[0] - batchsize + 1, batchsize):
            if shuffle:
                excerpt = indices[start_idx:start_idx + batchsize]
            else:
                excerpt = slice(start_idx, start_idx + batchsize)
```

```
            yield X[excerpt], y[excerpt], Y[excerpt]

    def softmax(self, x):
        e = np.exp(x - np.max(x))  # prevent overflow
        if e.ndim == 1:
            return e / np.sum(e, axis=0)
        else:
            return e / np.array([np.sum(e, axis=1)]).T

    def __init__(self, batch_size = 100, lr = 1.0e-1, eta = 0.3, eps = 0.0005,
                           max_epoch = 500, print_epoch = 20, lr_epoch = 10,␣
↪stop_epoch = 20,
                           bias = True, shuffle = True, verbose = True):
        self.batch_size = batch_size
        self.lr = lr
        self.eta = eta
        self.eps = eps
        self.max_epoch = max_epoch
        self.print_epoch = print_epoch
        self.lr_epoch = lr_epoch
        self.stop_epoch = stop_epoch
        self.bias = bias
        self.shuffle = shuffle
        self.verbose = verbose
        self.W = np.zeros(1)
        self.b = np.zeros(1)

    # stochastic gradient descent (SGD) for Logistic regression
    def fit(self, X, y):
        ncvg = True
        epoch = 0
        n, d = X.shape
        loss = []
        num_class = len(np.unique(y))
        Y = self.yMatrix(y, num_class)
        self.W = np.zeros((d, num_class))

        if self.bias:
            X = np.concatenate([X, np.ones((n, 1))], axis=1)
            self.W = np.concatenate([self.W, np.ones((1, num_class))], axis = 0)

        # optimization loop
        while ncvg and epoch < self.max_epoch:

            loss_epoch = 0.0
            for Xb, yb, Yb in self.iterate_minibatches(X, y, Y, self.
↪batch_size, self.shuffle):
```

```
                # minibatch gradient descent
                nb = len(yb)
                logits = self.softmax(np.matmul(Xb, self.W))
                grad = np.matmul(Xb.T, Yb - logits) - self.eta * self.W
                self.W = self.W + (self.lr / float(nb)) * grad
                loss_epoch += -np.sum(np.log(logits[range(nb), yb]))

            loss.append(loss_epoch / float(n))

            # half lr if not improving in lr_epoch epochs
            if epoch > self.lr_epoch:
                if loss[epoch - self.lr_epoch] <= loss[epoch] - self.eps:
                    self.lr *= 0.5
                    print('halfing learning rate to', self.lr)

            # stop if not improving in stop_epoch epochs
            if epoch > self.stop_epoch:
                if loss[epoch - self.stop_epoch] <= loss[epoch] - self.eps or␣
 ↪abs(loss[epoch] - loss[epoch-1]) <= self.eps:
                    ncvg = False
                    break

            epoch += 1

        #print('epoch', epoch-1, ': loss =', loss[-1])

        if self.bias:
            self.b = self.W[-1]
            self.W = self.W[:d]
        else:
            self.b = np.zeros(num_class)

    def predict(self, X):
        if self.bias:
            pred = np.argmax(np.matmul(X, self.W) + self.b, axis = 1)
        else:
            pred = np.argmax(np.matmul(X, self.W), axis = 1)
        return pred
```

[11]:
```
# TODO: Report accuracy on training and validation sets
def precision(pred, y):
    return sum(np.equal(pred, y)) / float(len(y))

# Define the parameter space for the GridSearch
param_grid = {
    'batch_size': [1,20,50,100,500,1000],
```

```
    'lr': [0.001, 0.01, 0.1],
    'eta': [0.001, 0.01, 0.1, 1, 10, 100, 1000],
    'max_epoch': [500],
    'print_epoch': [500],
    'lr_epoch':[20, 50, 100],
    'stop_epoch':[20],
    'bias':[True],
    'shuffle':[False],
    'verbose':[False]
}

X = np.concatenate((X_train, X_val), axis=0)
y = np.concatenate((y_train, y_val), axis=0)

# Create the split index (-1 for training set, 0 for validation set)
test_fold = [-1 for _ in range(X_train.shape[0])] + [0 for _ in range(X_val.
 ↪shape[0])]
ps = PredefinedSplit(test_fold=test_fold)
# Initialize your custom model
my_model = LogRegMine()

# Setup GridSearchCV
grid_search = GridSearchCV(estimator=my_model, param_grid=param_grid, cv=ps,␣
 ↪scoring='accuracy', return_train_score=True, verbose=0)

# Fit GridSearchCV
grid_search.fit(X, y)
print("Best parameters:", grid_search.best_params_)
```

```
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:7
4: RuntimeWarning: divide by zero encountered in log
  loss_epoch += -np.sum(np.log(logits[range(nb), yb]))
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:7
2: RuntimeWarning: overflow encountered in multiply
  grad = np.matmul(Xb.T, Yb - logits) - self.eta * self.W
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:2
6: RuntimeWarning: invalid value encountered in subtract
  e = np.exp(x - np.max(x))  # prevent overflow
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:7
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```

```
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:7
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/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:2
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/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:7
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  grad = np.matmul(Xb.T, Yb - logits) - self.eta * self.W
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:2
6: RuntimeWarning: invalid value encountered in subtract
  e = np.exp(x - np.max(x))  # prevent overflow
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:7
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/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:7
2: RuntimeWarning: overflow encountered in multiply
  grad = np.matmul(Xb.T, Yb - logits) - self.eta * self.W
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:2
6: RuntimeWarning: invalid value encountered in subtract
  e = np.exp(x - np.max(x))  # prevent overflow
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:7
4: RuntimeWarning: divide by zero encountered in log
  loss_epoch += -np.sum(np.log(logits[range(nb), yb]))
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:7
2: RuntimeWarning: overflow encountered in multiply
  grad = np.matmul(Xb.T, Yb - logits) - self.eta * self.W
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:2
6: RuntimeWarning: invalid value encountered in subtract
  e = np.exp(x - np.max(x))  # prevent overflow
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:7
4: RuntimeWarning: divide by zero encountered in log
  loss_epoch += -np.sum(np.log(logits[range(nb), yb]))
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:7
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4: RuntimeWarning: divide by zero encountered in log
  loss_epoch += -np.sum(np.log(logits[range(nb), yb]))
```

```
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:7
2: RuntimeWarning: overflow encountered in multiply
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  e = np.exp(x - np.max(x))  # prevent overflow
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:3
0: RuntimeWarning: invalid value encountered in divide
  return e / np.array([np.sum(e, axis=1)]).T
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:7
4: RuntimeWarning: divide by zero encountered in log
  loss_epoch += -np.sum(np.log(logits[range(nb), yb]))
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:3
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4: RuntimeWarning: divide by zero encountered in log
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/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:3
0: RuntimeWarning: invalid value encountered in divide
  return e / np.array([np.sum(e, axis=1)]).T
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:7
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  loss_epoch += -np.sum(np.log(logits[range(nb), yb]))
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:7
4: RuntimeWarning: divide by zero encountered in log
  loss_epoch += -np.sum(np.log(logits[range(nb), yb]))
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:3
0: RuntimeWarning: invalid value encountered in divide
  return e / np.array([np.sum(e, axis=1)]).T
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:7
4: RuntimeWarning: divide by zero encountered in log
  loss_epoch += -np.sum(np.log(logits[range(nb), yb]))
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:3
0: RuntimeWarning: invalid value encountered in divide
  return e / np.array([np.sum(e, axis=1)]).T
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:7
4: RuntimeWarning: divide by zero encountered in log
  loss_epoch += -np.sum(np.log(logits[range(nb), yb]))
```

```
/var/folders/c9/3q_3q36n4k9_t4gnwrhyd7s80000gn/T/ipykernel_49908/1574790776.py:3
0: RuntimeWarning: invalid value encountered in divide
  return e / np.array([np.sum(e, axis=1)]).T
```

```
Best parameters: {'batch_size': 50, 'bias': True, 'eta': 0.001, 'lr': 0.1,
'lr_epoch': 20, 'max_epoch': 500, 'print_epoch': 500, 'shuffle': False,
'stop_epoch': 20, 'verbose': False}
```

[12]:
```
# Access the best score and corresponding training score
best_validation_score = grid_search.best_score_
best_index = grid_search.best_index_
best_training_score = grid_search.cv_results_['mean_train_score'][best_index]

print(f"Best Validation Score: {best_validation_score}")
print(f"Corresponding Training Score: {best_training_score}")
```

```
Best Validation Score: 0.9026465028355387
Corresponding Training Score: 0.9141352774402592
```

0.3 Part 2(b): Random Forest/GBDT

Implement a random forest or GBDT from scratch and report your classifier's accuracy on the training and validation sets. **You should use your implementation from prior homeworks and turn it in again with updates, if any.**

[58]:
```
class loss(object):
    '''Loss class for mse. As for mse, pred function is pred=score.'''
    def pred(self,X_test,trees,log_threshold):
        return 0
    def g(self, y_true, pred):
        return 0
    def h(self, pred):
        return 0

class logistic(loss):
    '''Loss class for log loss. As for log loss, pred function is logistic␣
 ↪transformation.'''
    def pred(self,X_test,trees,log_threshold):
        predictions = []
        #print(len(trees))
        for test in X_test:
            temp = np.zeros(len(trees))
            for i in range(len(trees)):
                tree = trees[i]
                curr_node = tree.root_node
                while(curr_node.is_leaf == False):
                    curr_node = curr_node.forward(test)
                temp[i] = curr_node.weight
```

```
            min = np.min(temp)
            max = np.max(temp)
            #print(min)
            #print(max)
            if max != min :
                temp = (temp - min)/(max - min)
            temp = np.rint(temp)
            unique, counts = np.unique(temp, return_counts=True)
            #print(unique)
            if(unique.size > 1):
                if counts[1] > counts[0] :
                    predictions.append(1.0)
                else :
                    predictions.append(0.0)
            else :
                predictions.append(unique[0])
        return predictions

    def g(self, y_true, pred):
        return ((((1-y_true)*np.exp(pred)) - y_true)/(np.exp(pred) + 1))

    def h(self, y_true, pred):
        return (np.exp(pred)/((np.exp(pred) + 1)*(np.exp(pred) + 1)))*np.
 ↪ones(y_true.shape)

# TODO: class of a node on a tree
class TreeNode(object):
    '''
    Data structure that are used for storing a node on a tree.

    A tree is presented by a set of nested TreeNodes,
    with one TreeNode pointing two child TreeNodes,
    until a tree leaf is reached.

    A node on a tree can be either a leaf node or a non-leaf node.
    '''

    #TODO
    def __init__(self, X1, X2, index_y, threshold, value_y, is_leaf):
        self.is_leaf = is_leaf
        self.left_child = X1
        self.right_child = X2
        self.feature_index = index_y
        self.threshold = threshold
        self.weight = value_y

    def forward(self, x):
```

```
        #print(self.weight)
        #print(self.feature_index)
        #print(self.threshold)
        #print(self.is_leaf)
        #print(self.left_child.is_leaf)
        #print(self.right_child.is_leaf)
        if self.is_leaf == True :
            raise RuntimeError('This is a leaf node and you cannot forward from␣
 ↪it')
        elif x[self.feature_index] < self.threshold:
            #print(self.left_child.is_leaf)
            return self.left_child
        else :
            #print(self.right_child.is_leaf)
            return self.right_child

# TODO: class of single tree
class Tree(object):
    '''
    Class of a single decision tree in GBDT

    Parameters:
        n_threads: The number of threads used for fitting and predicting.
        max_depth: The maximum depth of the tree.
        min_sample_split: The minimum number of samples required to further␣
 ↪split a node.
        lamda: The regularization coefficient for leaf prediction, also known␣
 ↪as lambda.
        gamma: The regularization coefficient for number of TreeNode, also know␣
 ↪as gamma.
        rf: rf*m is the size of random subset of features, from which we select␣
 ↪the best decision rule,
            rf = 0 means we are training a GBDT.
    '''

    def __init__(self, root_node = None, n_threads = None,
                 max_depth = 3, min_sample_split = 10,
                 lamda = 1, gamma = 0, pred = 0):
        self.n_threads = n_threads
        self.max_depth = max_depth
        self.min_sample_split = min_sample_split
        self.root_node = root_node
        self.lamda = lamda
        self.gamma = gamma
        self.pred = pred
        self.treenodes = []
```

```
    def fit(self, X, y, loss):
        '''
        train is the training data matrix, and must be numpy array (an n_train x m matrix).
        g and h are gradient and hessian respectively.
        '''
        g = loss.g(y, self.pred)
        h = loss.h(y, self.pred)
        #print(g)
        #print(h)
        self.root_node = self.construct_tree(X, y, g, h, 0)
        #print(self.root_node.weight)
        return self

    def split_dataset(self, X, y, feature_index, threshold):
        left_mask = X[:, feature_index] < threshold
        right_mask = X[:, feature_index] >= threshold
        return X[left_mask], X[right_mask], y[left_mask], y[right_mask]

    def calculate_gain(self, g_l, h_l, g_r, h_r):
        G_l_tot = g_l.sum()
        G_r_tot = g_r.sum()
        H_l_tot = h_l.sum()
        H_r_tot = h_r.sum()
        gain = (0.5)*(((G_l_tot)*(G_l_tot)/(H_l_tot + self.lamda)) +
↪((G_r_tot)*(G_r_tot)/(H_r_tot + self.lamda)) -
↪(((G_l_tot+G_r_tot)*(G_l_tot+G_r_tot))/(H_l_tot + H_r_tot+ self.lamda))) -
↪self.gamma
        return gain

    def find_threshold(self, g, h, X, y, feature_index):
        '''
        Given a particular feature $p_j$,
        return the best split threshold $\tau_j$ together with the gain that is
↪achieved.
        '''
        best_gain = 0
        best_threshold = 0
        thresholds = np.unique(X[:, feature_index])
        for threshold in thresholds:
            X_left, X_right, y_left, y_right = self.split_dataset(X, y,
↪feature_index, threshold)
            if len(y_left) == 0 or len(y_right) == 0:
                continue
            left_mask = X[:, feature_index] < threshold
            right_mask = X[:, feature_index] >= threshold
```

```
            gain = self.calculate_gain(g[left_mask], h[left_mask],␣
↪g[right_mask], h[right_mask])
            #print("Gain : " +str(gain))
            if gain > best_gain:
                best_gain = gain
                best_threshold = threshold
        return [threshold, best_gain]

    def construct_tree(self, X, y, g, h, current_depth):
        '''
        Node Addition, which is recursively used to grow a tree.
        First we should check if we should stop further splitting.

        The stopping conditions include:
            1. tree reaches max_depth $d_{max}$
            2. The number of sample points at current node is less than␣
↪min_sample_split, i.e., $n_{min}$
            3. gain <= 0
        '''
        if current_depth > self.max_depth or y.size < self.min_sample_split :
            return None
        best_feature, threshold, best_gain = self.find_best_decision_rule(X, y,␣
↪g, h)
        #print("best_feature : " + str(best_feature))
        #print("threshold : " + str(threshold))
        #print("best_gain : " + str(best_gain))
        if best_gain == 0 :
            return None
        #print(X[:, best_feature])
        left_mask = X[:, best_feature] < threshold
        right_mask = X[:, best_feature] >= threshold
        node_left = self.construct_tree(X[left_mask], y[left_mask],␣
↪g[left_mask], h[left_mask], current_depth + 1)
        node_right = self.construct_tree(X[right_mask], y[right_mask],␣
↪g[right_mask], h[right_mask], current_depth + 1)
        h_val = h.sum()
        weight = -(g.sum()/(h_val + self.lamda))
        is_leaf = False
        if node_left is None and node_right is not None :
            node_left = TreeNode(None, None, 0, 0, weight, True)
        elif node_right is None and node_left is not None :
            node_right = TreeNode(None, None, 0, 0, weight, True)
        elif node_right is None and node_left is None :
            is_leaf = True
        node = TreeNode(node_left, node_right, best_feature, threshold, weight,␣
↪is_leaf)
```

```
        self.treenodes.append(node)
        #print(node)
        return node

    def find_best_decision_rule(self, X, y, g, h):
        '''
        Return the best decision rule [feature, treshold], i.e., $(p_j,␣
↪\tau_j)$ on a node j,
        train is the training data assigned to node j
        g and h are the corresponding 1st and 2nd derivatives for each data␣
↪point in train
        g and h should be vectors of the same length as the number of data␣
↪points in train

        for each feature, we find the best threshold by find_threshold(),
        a [threshold, best_gain] list is returned for each feature.
        Then we select the feature with the largest best_gain,
        and return the best decision rule [feature, treshold] together with its␣
↪gain.
        '''
        best_gain = 0
        best_threshold = 0
        best_feature = 0
        for feature_index in range(X.shape[1]):
            #print("Feature " + str(feature_index))
            threshold, gain = self.find_threshold(g, h, X, y, feature_index)
            if gain > best_gain:
                best_gain = gain
                best_threshold = threshold
                best_feature = feature_index
        return best_feature, threshold, best_gain

# TODO: class of Random Forest
class RF(object):
    '''
    Class of Random Forest

    Parameters:
        n_threads: The number of threads used for fitting and predicting.
        loss: Loss function for gradient boosting.
            'mse' for regression task and 'log' for classfication task.
            A child class of the loss class could be passed to implement␣
↪customized loss.
        max_depth: The maximum depth d_max of a tree.
        min_sample_split: The minimum number of samples required to further␣
↪split a node.
```

```
        lamda: The regularization coefficient for leaf score, also known as␣
↪lambda.
        gamma: The regularization coefficient for number of tree nodes, also␣
↪know as gamma.
        rf: rf*m is the size of random subset of features, from which we select␣
↪the best decision rule.
        num_trees: Number of trees.
    '''
    def __init__(self,log_threshold = 0.5,
        n_threads = 0, loss = 'mse',
        max_depth = 3, min_sample_split = 10,
        lamda = 1, gamma = 0,
        rf = 0.99, num_trees = 100):
        self.log_threshold = log_threshold
        self.n_threads = n_threads
        self.loss = logistic()
        self.max_depth = max_depth
        self.min_sample_split = min_sample_split
        self.lamda = lamda
        self.gamma = gamma
        self.rf = rf
        self.num_trees = num_trees
        self.trees = []

    def fit(self, X, y):
        # X is n x m 2d numpy array
        # y is n-dim 1d array
        num_samples, num_features = X.shape
        for i in range(self.num_trees):
            #print ("Tree : " + str(i))
            m_rf = (int)(np.ceil(self.rf*num_features))
            m_rf_indices = np.random.choice(num_features, m_rf, replace=False)
            n_rf_indices = np.random.choice(num_samples, num_samples,␣
↪replace=True)
            XTree = X[n_rf_indices][:,m_rf_indices]
            #print(XTree.shape)
            yTree = y[n_rf_indices]
            prediction = 0
            tree = Tree(None, self.n_threads, self.max_depth, self.
↪min_sample_split,self.lamda, self.gamma, prediction)
            tree = tree.fit(XTree, yTree, self.loss)
            self.trees.append(tree)
        return self

    # test is the input to the model
    def predict(self, X_test):
        return self.loss.pred(X_test, self.trees, self.log_threshold)
```

[65]:
```
# TODO: Report accuracy on training and validation sets
def accuracy(pred, y):
    dataset_size = y.size
    correct_predictions = 0
    #print(pred)
    #print(y)
    for i in range(dataset_size):
        if y[i] == (pred[i]):
            correct_predictions += 1
    precision = (correct_predictions/dataset_size)*100
    return precision

RF_regression = RF(log_threshold = 0.5, n_threads = 0, loss = 'class',␣
 ↪max_depth = 6, min_sample_split = 10, lamda = 1, gamma = 1,rf = 0.5,␣
 ↪num_trees = 30)
RF_regression = RF_regression.fit(np.array(X_train[1:3000]), np.array(y_train[1:
 ↪3000]))
pred_train = RF_regression.predict(X_train)
pred_test = RF_regression.predict(X_val)
acc_test = accuracy(pred_test, y_val)
acc_train = accuracy(pred_train, y_train)
print("Training Accuracy of the Random Forest Method for the Fruit␣
 ↪Classification Dataset is : ", acc_train)
print("Validation Accuracy of the Random Forest Method for the Fruit␣
 ↪Classsification Dataset is : ", acc_test)
```

```
Training Accuracy of the Random Forest Method for the Fruit Classification
Dataset is :  4.56535334584115
Validation Accuracy of the Random Forest Method for the Fruit Classsification
Dataset is :  4.489603024574669
```

0.4 Part 2(c): K-NN

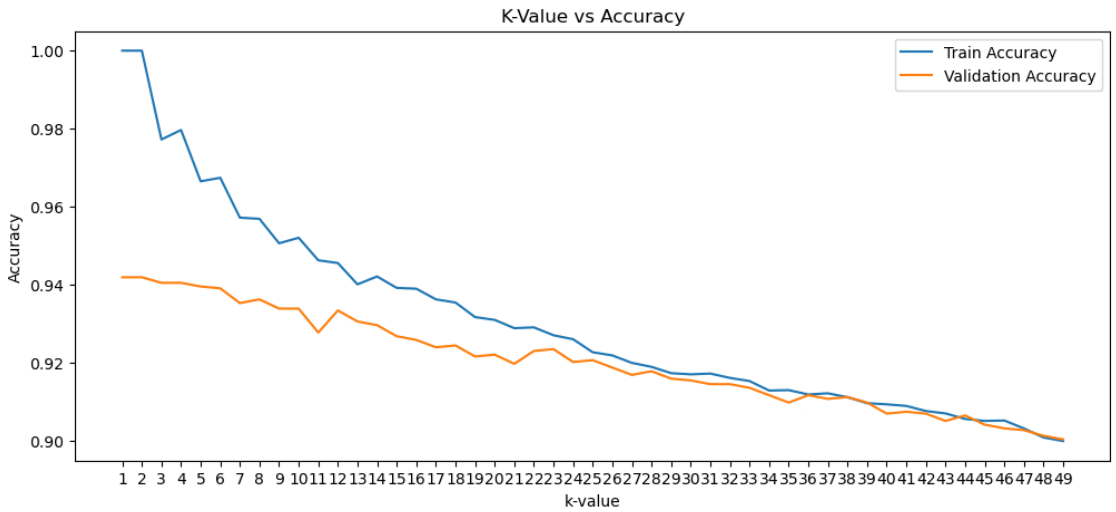
Implement a K-NN classifier from scratch and report your classifier's accuracy on the training and validation sets. **You should use your implementation from prior homeworks and turn it in again with updates, if any.**

[72]:
```
# TODO: Implement a kNN classifier
class KNN:
    def _init_():
        pass
    def fit(X, y):
        pass
    def predict(X):
        pass

    def knn_still_faster(X_train, y_train, X_test, kvalue):
```

```
        tree = KDTree(X_train)
        y_pred_knn = []

        for test_point in X_test:
            # Query the k nearest neighbors
            dists, indices = tree.query([test_point], k=kvalue)  # Ensure␣
↪k_nearest_labels is always an array
            if kvalue == 1:
                k_nearest_labels = [y_train[indices[0]]]
            else:
                k_nearest_labels = y_train[indices[0]]
            most_common = Counter(k_nearest_labels).most_common(1)
            y_pred_knn.append(most_common[0][0])

        return np.array(y_pred_knn)

    train_accuracies = []
    val_accuracies = []
    y_train = np.array(train_dataset['labels'])
    X_train = np.array(train_dataset['feats'])
    y_val = np.array(val_dataset['labels'])
    X_val = np.array(val_dataset['feats'])
    k_values = range(1, 50, 1)

    knn = knn_still_faster

    for kvalue in tqdm(k_values, position=0, desc='k-values Progress'):
        y_pred_train = knn(X_train, y_train, X_train, kvalue)
        y_pred_test = knn(X_train, y_train, X_val, kvalue)

        # Calculate accuracy
        train_accuracy = accuracy_score(y_train, y_pred_train)
        test_accuracy = accuracy_score(y_val, y_pred_test)
        train_accuracies.append(train_accuracy)
        val_accuracies.append(test_accuracy)

        #print(f'Training Accuracy for {kvalue} is {train_accuracy}')
        #print(f'Testing Accuracy for {kvalue} is {test_accuracy}')

    print('----------------------------------------------------------------------')

    # We plot the results of our KNN classifier to see how the accuracy changes␣
↪with the value of kvalue on both
    # training and test data sets, and see where the underfitting and␣
↪overfitting regions are.
    # Plotting
    plt.figure(figsize=(12, 5))
```

```
    plt.plot(k_values, train_accuracies, label='Train Accuracy')
    plt.plot(k_values, val_accuracies, label='Validation Accuracy')
    plt.legend()
    plt.title('K-Value vs Accuracy')
    plt.xlabel('k-value')
    plt.ylabel('Accuracy')
    plt.xticks(list(k_values))  # Ensure that x-axis ticks match k values
    plt.show()

    # Print the k value and accuracy associated with the best performance on␣
↪the test set
    max_accuracy_index = np.argmax(val_accuracies)
    best_k = k_values[max_accuracy_index]
    max_accuracy = val_accuracies[max_accuracy_index]

    print('Best k-value:', best_k)
    print('Max Validation accuracy:', max_accuracy)
    print('Max Training accuracy:', train_accuracies[max_accuracy_index])

    print('-----------------------------------------------------------------------')
    print('-----------------------------------------------------------------------␣
↪\n')
```

```
k-values Progress: 100%|      | 49/49 [00:32<00:00,  1.53it/s]

-----------------------------------------------------------------------
```




```
Best k-value: 1
Max Validation accuracy: 0.9418714555765595
```

```
Max Training accuracy: 1.0
------------------------------------------------------------------
------------------------------------------------------------------
```

0.5 Part 2(d): MLP

Train an MLP classifier and report your classifier's accuracy on the training and validation sets. **You are allowed to use sklearn.neural_network.MLPClassifier for this section.** Make sure to run in all code you used to train and test your MLP classifier. See https://scikit-learn.org/stable/modules/generated/sklearn.neural_network.MLPClassifier.html for details.

[18]:
```
from sklearn.neural_network import MLPClassifier

parameter_space = {
    'hidden_layer_sizes': [(50,50,50), (50,100,50), (100,), (20,50,30),␣
 ↪(30,100,50)],
#    'hidden_layer_sizes':[(100,)],
    'activation': ['tanh', 'relu'],
    'solver': ['sgd', 'adam'],
    'alpha': [0.0001, 0.01, 0.05],
    'learning_rate': ['constant','adaptive'],
}

mlp = MLPClassifier(max_iter=100, random_state=42)
# Create the split index (-1 for training set, 0 for validation set)
test_fold = [-1 for _ in range(X_train.shape[0])] + [0 for _ in range(X_val.
 ↪shape[0])]
ps = PredefinedSplit(test_fold=test_fold)

# Setup GridSearchCV
grid_search = GridSearchCV(estimator=mlp, param_grid=parameter_space, cv=ps,␣
 ↪scoring='accuracy', return_train_score=True, verbose=0)

# Fit GridSearchCV
grid_search.fit(X, y)
print("Best parameters:", grid_search.best_params_)

# Access the best score and corresponding training score
best_validation_score = grid_search.best_score_
best_index = grid_search.best_index_
best_training_score = grid_search.cv_results_['mean_train_score'][best_index]

print(f"Best Validation Score: {best_validation_score}")
print(f"Corresponding Training Score: {best_training_score}")
# TODO: Train an MLPClassifier and report training and validation set accuracies
```

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```

```
Best parameters: {'activation': 'tanh', 'alpha': 0.01, 'hidden_layer_sizes':
(50, 100, 50), 'learning_rate': 'constant', 'solver': 'adam'}
Best Validation Score: 0.9664461247637051
Corresponding Training Score: 0.995240988254354
```

```
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0.6 Part 2(f): Bakeoff: Choose the best Classifier

For this section, you are free to use a classifier of your choice (you are allowed to use any libraries of your choice). You are also free to use the training and validation sets in any way you choose i.e. you can merge them and perform k-fold cross validation.

To evaluate your classifier, we will on March 15th provide you with a pickle file ('test.pkl') that will be in the same format as the 'train.pkl' and 'val.pkl' but **will not contain the labels**. You will need to generate predictions for each of the inputs we provide in 'test.pkl' in a text file.

For your submission, you will need to provide us with a **test_predictions.txt** file containing the class predictions of your classifier. We will compute the accuracy of the predictions you provide for your evaluation.

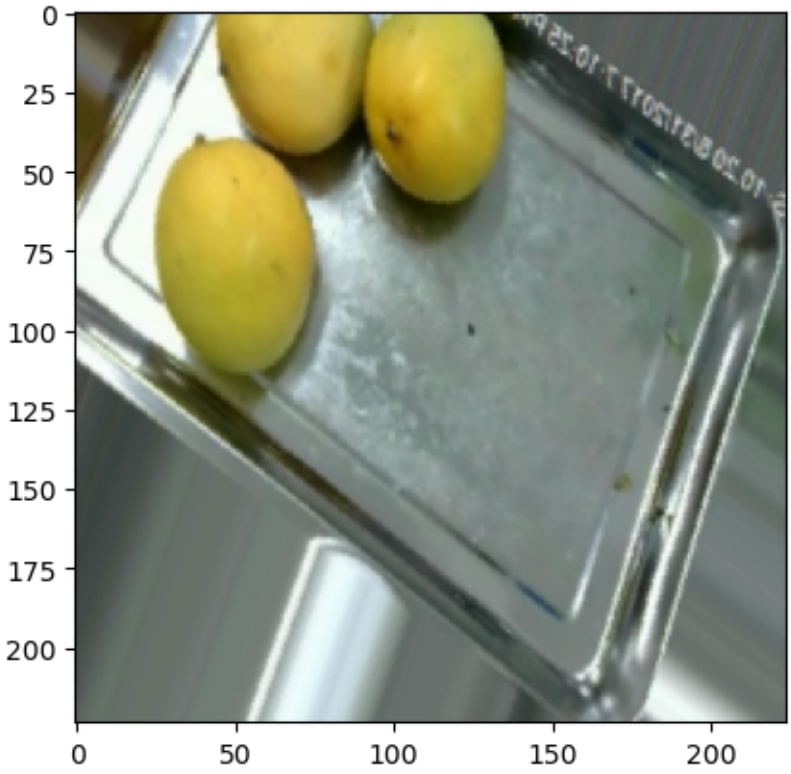
[36]:
```
from sklearn.model_selection import cross_val_score
from sklearn.neural_network import MLPClassifier
from sklearn.datasets import make_classification
from sklearn.model_selection import KFold

#pred = []
with open('datasets/test_data.pkl', 'rb') as f:
    test_dataset = pickle.load(f)
#print(X.shape)
#print(y.shape)
mlp_classifier = MLPClassifier(activation='tanh', alpha=0.05,␣
 ↪hidden_layer_sizes=(50, 100, 50), learning_rate='constant', solver='adam',␣
 ↪max_iter=500, random_state=40)
'''
kfold = KFold(n_splits=5, shuffle=True, random_state=42)
accuracies = []
for train_index, test_index in kfold.split(X):
    X_train, X_test = X[train_index], X[test_index]
    y_train, y_test = y[train_index], y[test_index]

    mlp_classifier.fit(X_train, y_train)
    predictions = mlp_classifier.predict(X_test)
    accuracy = accuracy_score(y_test, predictions)
    accuracies.append(accuracy)

print(f"Accuracy scores for each fold: {accuracies}")
print(f"Mean accuracy: {np.mean(accuracies)}")
'''
print(X.shape)
print(y.shape)
mlp_classifier.fit(X,y)
pred = mlp_classifier.predict(np.array(test_dataset['feats']))
print(pred.shape)
print(pred)

# TODO: Train a classifier and generate predictions on the test set and put␣
 ↪your predictions in pred.
# ...

# Make sure that pred contains a 1-dimensional integer array of class labels␣
 ↪for the test set and make sure that
# every integer is in the range 0 through 14. If you have an entry in this␣
 ↪array outside of the integer
# range of 0 through 14, it will be assumed to be an error. Also, if your array␣
 ↪is not the length of the test
# set that will be assumed to be an error. Specifically, suppose n_mine is the␣
 ↪length of the array of integers
```

```
# you turn in. If the test set has n_test images (meaning
# it is an n_test X m matrix), then if your array is less than n_test long (so␣
 ↪n_mine < n_test, then any missing
# images will be assumed to be an error, so there will be n_test - n_mine␣
 ↪errors. If your array is longer than
# n_test images long, so that n_mine > n_test, then we will take the final␣
 ↪n_mine - n_test images, whatever
# your predictions are for those images, and assume that those n_mine - n_test␣
 ↪images are in error. Bottom line:
# make sure your array is exactly the right length, meaning you should have␣
 ↪n_mine == n_test. Meaning,
# the array pred should be a one-dimensional integer array with integers in the␣
 ↪0-14 range
# of length n_mine. You can make sure that pred is of integer type by doing␣
 ↪`pred = pred.astype(np.int32)` but
# after you do this, make sure to examine the result to ensure that they are␣
 ↪integers in the right range.
#
# Note that the saved text file should have one prediction per ASCII line (this␣
 ↪can be done by ensuring that pred
# is of shape (n_test,) and then simply using np.savetxt).
#
#np.savetxt('test_predictions.txt', pred)
```

```
(11992, 15)
(11992,)
(2116,)
[3 9 3 … 5 4 9]
```

[51]:
```
print(np.transpose(pred))
plt.imshow(test_dataset['images'][-3])
np.savetxt('test_predictions.txt', pred, fmt='%d')
```

```
[3 9 3 … 5 4 9]
```


0
25
50
75
100
125
150
175
200
0
50
100
150
200

[ ]: