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CS 441 - HW1: Instance-based Methods

Complete the sections below. You do not need to fill out the checklist.

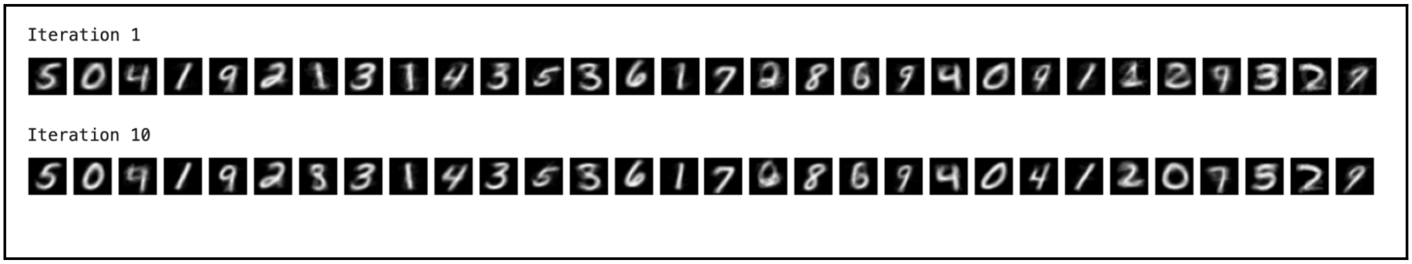
Total Points Available	**[ ] / 145**
1. Retrieval, K-means, 1-NN on MNIST	
a. Retrieval	[ ] / 5
b. K-means	[ ] / 15
c. 1-NN	[ ] / 10
2. Make it fast	
a. K-means plot	[ ] / 15
b. 1-NN error plots	[ ] / 8
c. 1-NN time plots	[ ] / 7
d. Most confused label	[ ] / 5
3. Temperature Regression	
a. RMSE Tables	[ ] / 20
4. Conceptual questions	[ ] / 15
5. Stretch Goals	
a. Evaluate effect of K for MNIST	[ ] / 15
b. Evaluate effect of K for Temp Reg.	[ ] / 15
c. Compare Kmeans more iterations vs. restarts	[ ] / 15

1. Retrieval, K-means, 1-NN on MNIST

a. What index is returned for x_test[1]?

28882

b. Paste the display of clusters after the 1st and 10th iteration for K=30.

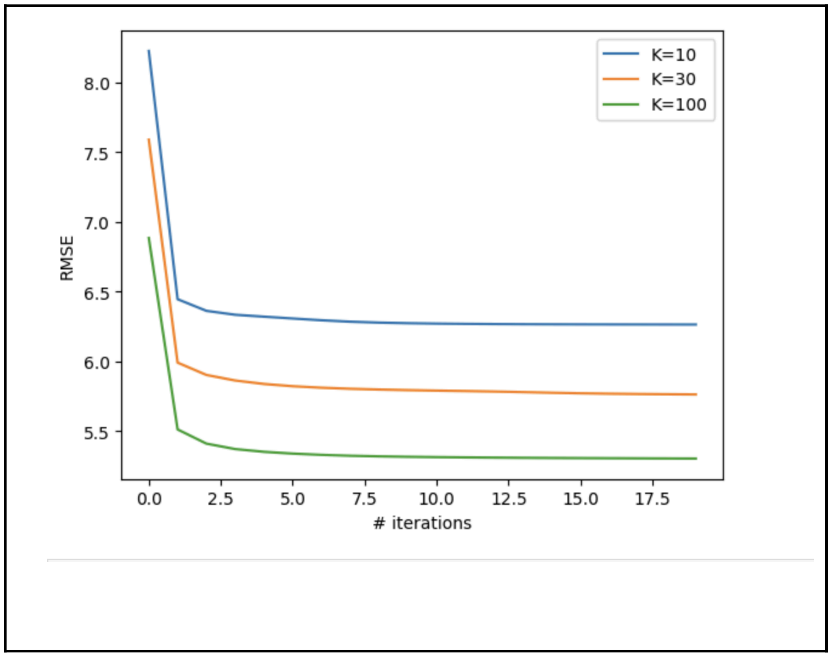


c. Error rate for first 100 test samples, using first 10,000 training samples (x.x%)

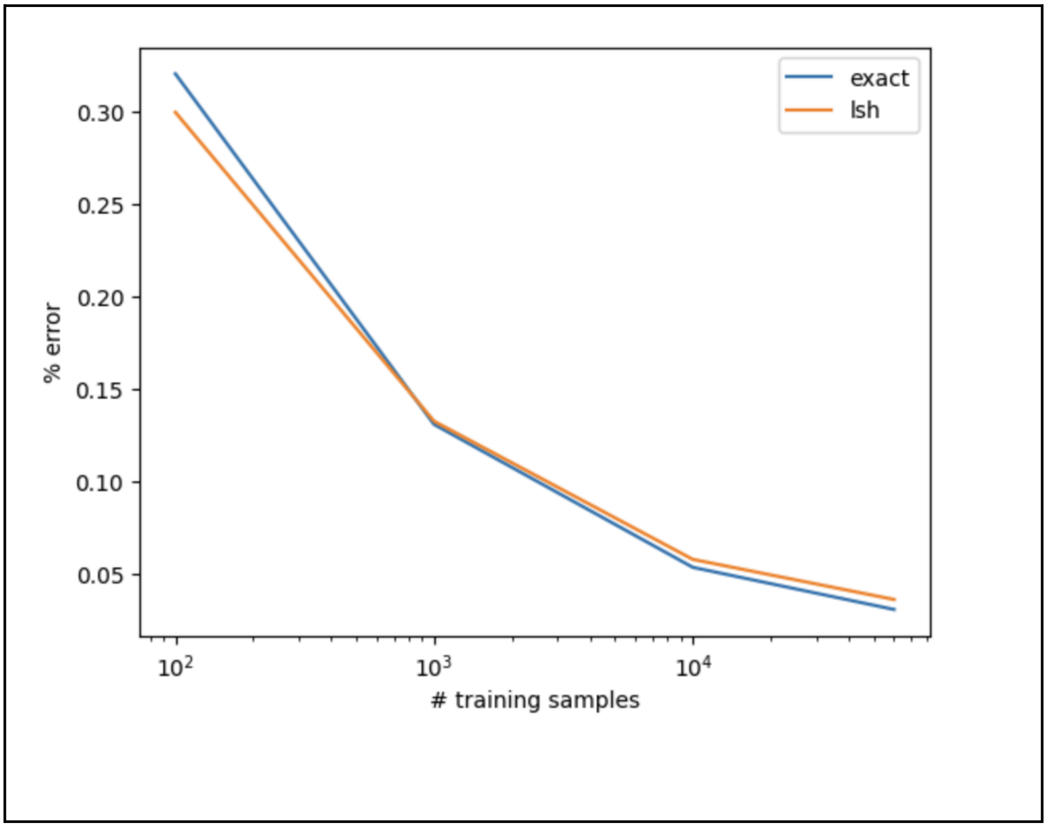
8.0%

2. Make it fast

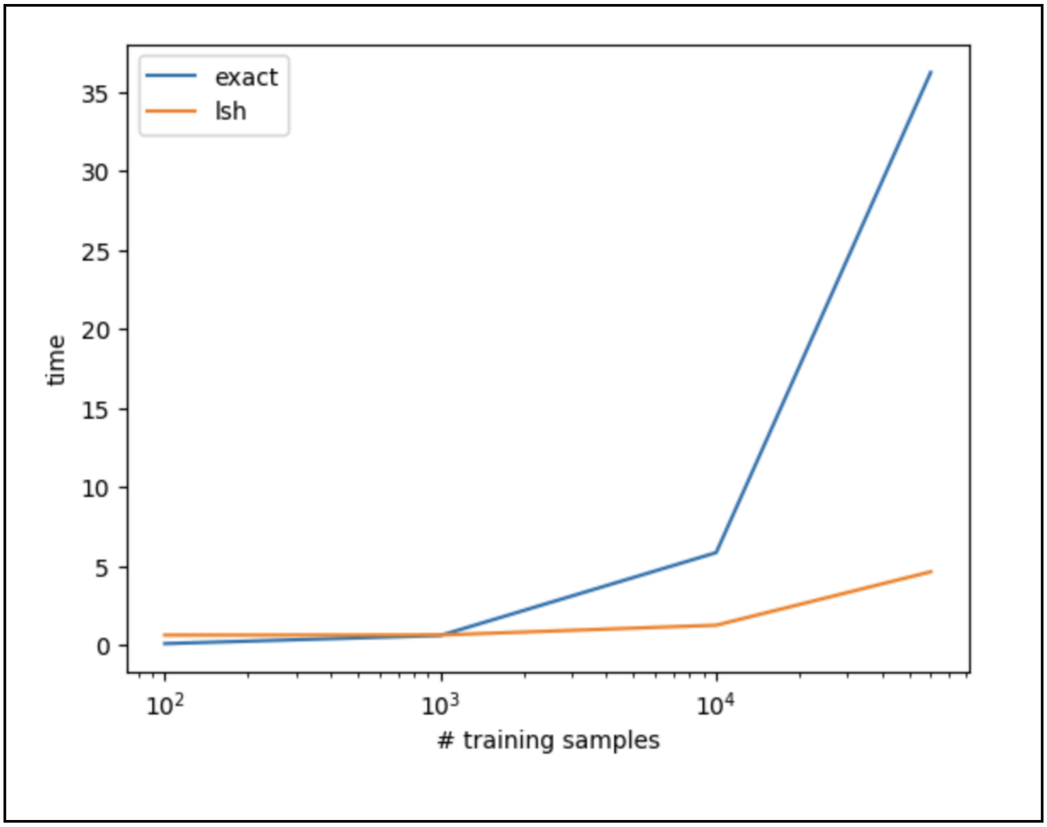
a. KMeans plot of RMSE vs iterations for K=10, 30, 100



b. Nearest neighbor error vs training size plot



c. Nearest neighbor time vs training size plot



d. What label is most commonly confused with '2'?

7

3. Temperature Regression

a. Table of RMSE for KNN with K=5 (x.xx)

	KNN (K=5)
Original Features	3.25
Normalized Features	2.93

4. Test your understanding

Fill in the letter corresponding to the answer. If you're not sure, you can sometimes run small experiments to check.

1. Is K-means guaranteed to decrease RMSE between nearest cluster and samples at each iteration until convergence?

a. Yes
b. No

a

2. If you increase K, is K-means expected or guaranteed to achieve lower RMSE?
   a. Guaranteed
   b. Expected but not guaranteed
   c. Not expected

b

3. In K-NN regression, for training labels y, what is the lowest target value that can possibly be predicted for any query?
   a. Min(y)
   b. Mean(y)
   c. Can't be determined

a

4. Would you expect the "training error" for 1-NN to be higher or lower than 3-NN for classification? Training error is the error if you test on the training data.
   a. Higher
   b. Lower
   c. It's problem-dependent

b

5. Would you expect the test error for 1-NN to be higher or lower than for 3-NN for regression?
   a. Higher
   b. Lower
   c. It's problem-dependent

a

5. Stretch Goals (optional)

a. Select best K parameter for K-NN MNIST classification in K=1, 3, 5, 11, 25. (x.xx)

Validation Set Performance	K=1	K=3	K=5	K=11	K=25

% error	2.88	2.80	2.82	3.08	3.82

Best K:

3

Test % error (x.xx)

2.95

b. Select best K parameter for K-NN temperature regression in K=1, 3, 5, 11, 25. (x.xx)

Validation Set RMSE	K=1	K=3	K=5	K=11	K=25
Original Features	4.33	3.23	3.10	3.06	3.06
Normalized Features	3.87	3.17	3.03	2.89	2.91

Best Setting (K, feature type):

11, Normalized Features

Test RMSE (x.xx)

2.77

c. Kmeans, MNIST: compare average and standard deviation RMSE based on number of iterations and number of restarts

(4 digit precision)

K=30	RMSE avg	RMSE std
20 iterations, 1 restart	5.786	0.007645
4 iterations, 5 restarts	5.823	0.01214
50 iterations, 1 restart	5.777	0.005488
10 iterations, 5 restarts	5.788	0.003718

Acknowledgments / Attribution

List any outside sources for code or ideas or “None”.

CS441_SP24_HW1_Starter

February 5, 2024

0.1 CS441: Applied ML - HW 1

0.1.1 Parts 1-2: MNIST

Include all the code for generating MNIST results below

[2]:
```
# initialization code
import numpy as np
from keras.datasets import mnist
%matplotlib inline
from matplotlib import pyplot as plt
from scipy import stats
import faiss
import time


def load_mnist():
  '''
  Loads, reshapes, and normalizes the data
  '''
  (x_train, y_train), (x_test, y_test) = mnist.load_data() # loads MNIST data
  x_train = np.reshape(x_train, (len(x_train), 28*28))  # reformat to 768-d␣
↪vectors
  x_test = np.reshape(x_test, (len(x_test), 28*28))
  maxval = x_train.max()
  x_train = x_train/maxval  # normalize values to range from 0 to 1
  x_test = x_test/maxval
  return (x_train, y_train), (x_test, y_test)

def display_mnist(x, subplot_rows=1, subplot_cols=1):
  '''
  Displays one or more examples in a row or a grid
  '''
  if subplot_rows>1 or subplot_cols>1:
    fig, ax = plt.subplots(subplot_rows, subplot_cols, figsize=(15,15))
    for i in np.arange(len(x)):
      ax[i].imshow(np.reshape(x[i], (28,28)), cmap='gray')
      ax[i].axis('off')
  else:
```

```
    plt.imshow(np.reshape(x, (28,28)), cmap='gray')
    plt.axis('off')
plt.show()
```

```
2024-02-05 14:55:46.910061: E
external/local_xla/xla/stream_executor/cuda/cuda_dnn.cc:9261] Unable to register
cuDNN factory: Attempting to register factory for plugin cuDNN when one has
already been registered
2024-02-05 14:55:46.910141: E
external/local_xla/xla/stream_executor/cuda/cuda_fft.cc:607] Unable to register
cuFFT factory: Attempting to register factory for plugin cuFFT when one has
already been registered
2024-02-05 14:55:46.912560: E
external/local_xla/xla/stream_executor/cuda/cuda_blas.cc:1515] Unable to
register cuBLAS factory: Attempting to register factory for plugin cuBLAS when
one has already been registered
2024-02-05 14:55:46.922567: I tensorflow/core/platform/cpu_feature_guard.cc:182]
This TensorFlow binary is optimized to use available CPU instructions in
performance-critical operations.
To enable the following instructions: AVX2 FMA, in other operations, rebuild
TensorFlow with the appropriate compiler flags.
2024-02-05 14:55:47.603859: W
tensorflow/compiler/tf2tensorrt/utils/py_utils.cc:38] TF-TRT Warning: Could not
find TensorRT
```

[3]:
```
# example of using MNIST load and display  functions
(x_train, y_train), (x_test, y_test) = load_mnist()
display_mnist(x_train[:10],1,10)
print('Total size: train={}, test ={}'.format(len(x_train), len(x_test)))
```

```
Total size: train=60000, test =10000
```

[3]:
```
display_mnist(x_test[:10],1,10)
```

[4]:
```
x_train[0]
```

[4]:
```
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```

1. Retrieval, Clustering, and NN Classification

[4]:
```python
# Retrieval

def get_nearest(X_query, X):
    ''' Return the index of the sample in X that is closest to X_query according
      to L2 distance '''
    dist = np.square(X_query - X).sum(axis=-1)
    return np.argmin(dist)


j = get_nearest(x_test[0], x_train)
print(j)

j = get_nearest(x_test[1], x_train)
print(j)
```

```
53843
28882
```

[5]:
```python
# K-means

def kmeans(X, K, niter=10):
  '''
  Starting with the first K samples in X as cluster centers, iteratively assign␣
 ↪each
  point to the nearest cluster and compute the mean of each cluster.
  Input: X[i] is the ith sample, K is the number of clusters, niter is the␣
 ↪number of iterations
  Output: K cluster centers
```

```
  '''
  # TO DO -- add code to display cluster centers at each iteration also
  centers = X[:K].copy()
  for i in range(1,1+niter):
    print(f"Iteration {i}")
    clusters = [[] for _ in range(K)]
    for x in X:
      idx = get_nearest(x, centers)
      clusters[idx].append(x)
    for c in range(K):
      centers[c] = np.stack(clusters[c]).mean(axis=0)
    display_mnist(centers, 1, K)

K=30
centers = kmeans(x_train[:1000], K)
```

```
Iteration 1
```

```
Iteration 2
```

```
Iteration 3
```

```
Iteration 4
```

```
Iteration 5
```

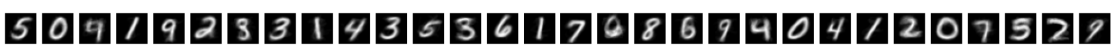
Iteration 6

Iteration 7

Iteration 8

Iteration 9

Iteration 10



[6]:
```python
# 1-NN
errors = []
for i,x in enumerate(x_test[:100]):
  idx = get_nearest(x, x_train[:10000])
  errors.append(y_train[idx] != y_test[i])
print(np.mean(errors))
```

0.08

2. Make it fast

[11]:
```python
# install libraries you need for part 2
!apt install libomp-dev
!pip install faiss-cpu
import faiss
import time
```

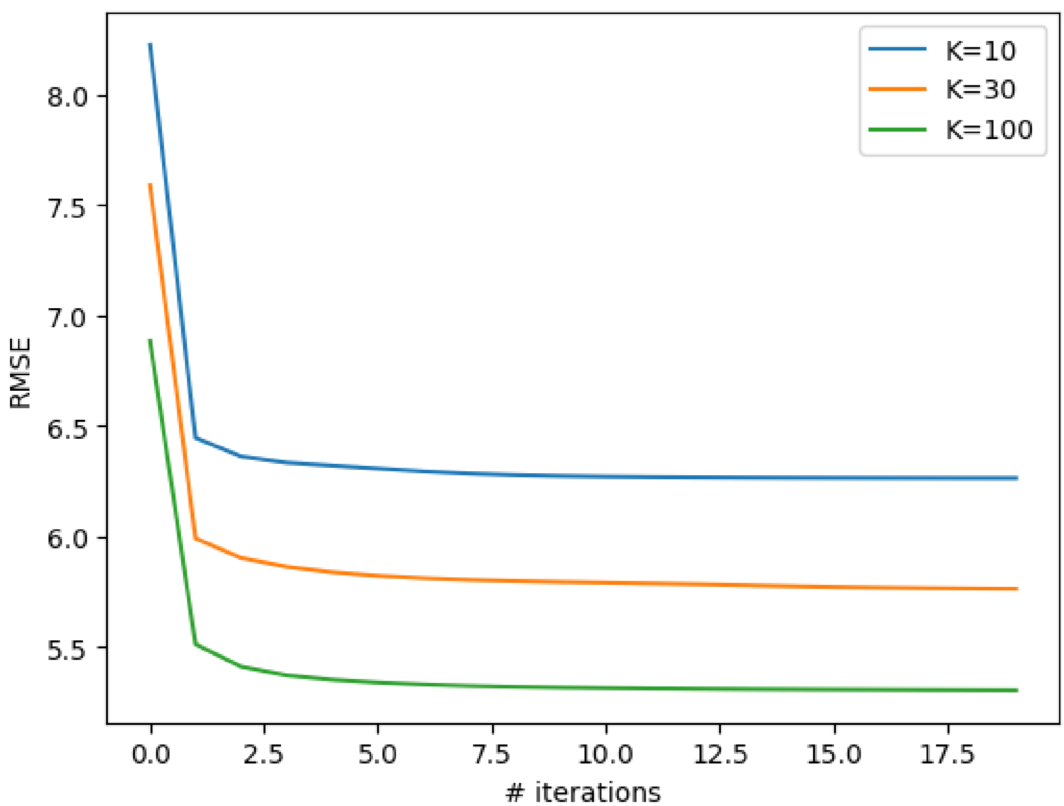
```
E: Could not open lock file /var/lib/dpkg/lock-frontend - open (13:
Permission denied)
E: Unable to acquire the dpkg frontend lock (/var/lib/dpkg/lock-
frontend), are you root?
Defaulting to user installation because normal site-packages is not writeable
Collecting faiss-cpu
  Downloading
faiss_cpu-1.7.4-cp311-cp311-manylinux_2_17_x86_64.manylinux2014_x86_64.whl (17.6
MB)
                            17.6/17.6 MB
21.9 MB/s eta 0:00:0000:0100:01
Installing collected packages: faiss-cpu
Successfully installed faiss-cpu-1.7.4
```

[6]:
```
  # retrieval

# TO DO (check that you're using FAISS correctly)
index = faiss.IndexFlatL2(x_train.shape[1])
index.add(x_train) # add the data
dist, idx = index.search(x_test[:2],1)
print(idx)
```

```
[[53843]
 [28882]]
```

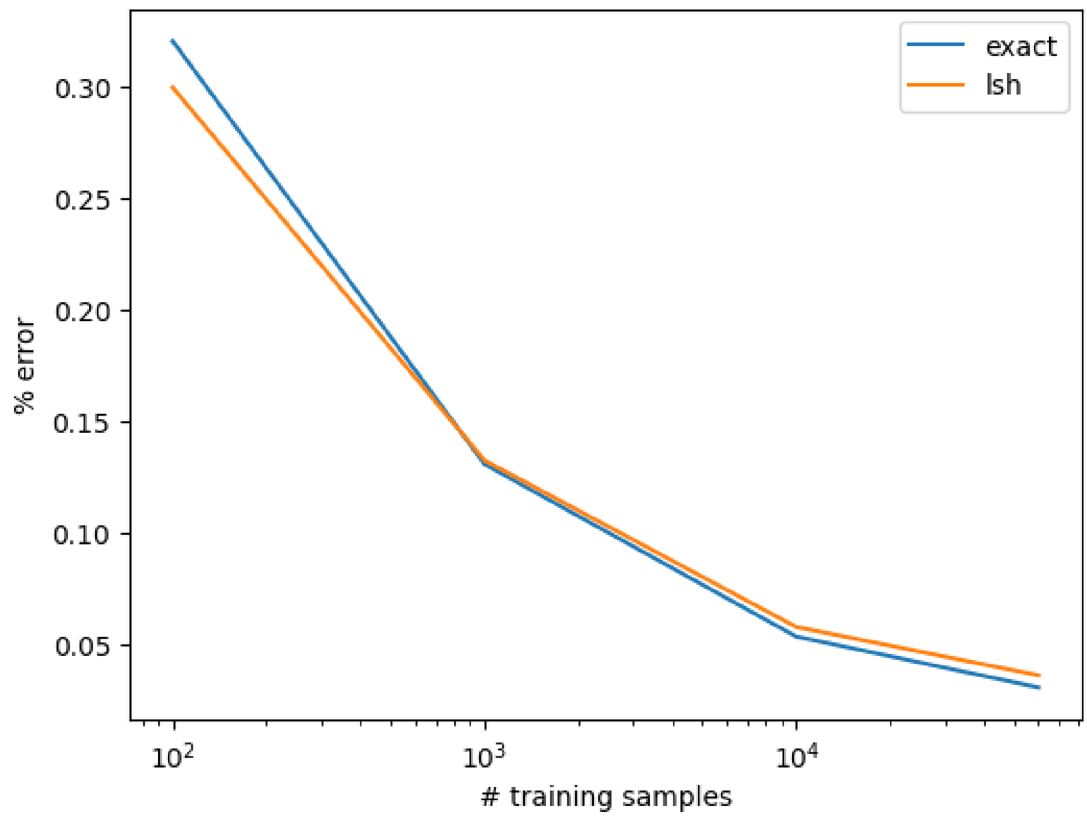
[7]:
```
import faiss
import numpy as np
import matplotlib.pyplot as plt

def kmeans_fast(X, K, niter=10):
    X = X.astype(np.float32)
    d = X.shape[1]
    cluster_centers = X[:K].copy()
    index = faiss.IndexFlatL2(d)

    rmse_list = []

    for i in range(niter):
        index.reset()
        index.add(cluster_centers)
        D, I = index.search(X, 1)  # D is the squared distances
        rmse = np.sqrt(np.mean(D))  # Compute the RMSE from the squared
 ↪distances
        rmse_list.append(rmse)

        for k in range(K):
            points_in_cluster = X[I.squeeze() == k]
```

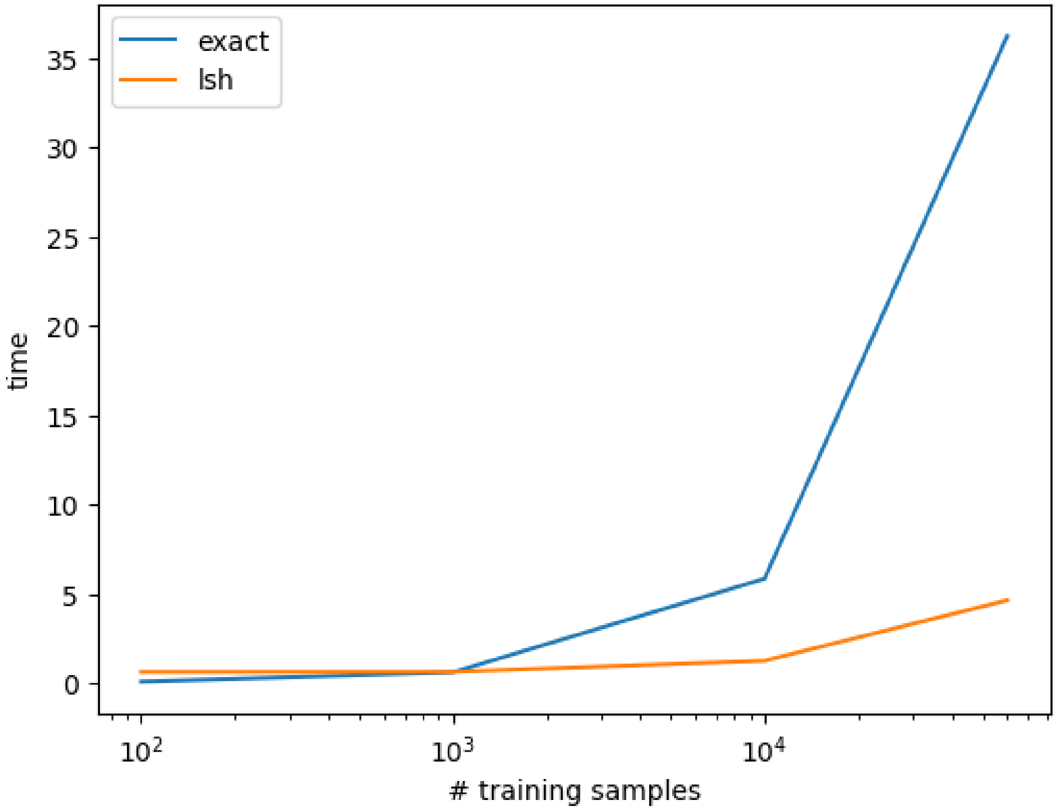
```python
            if len(points_in_cluster) > 0:
                cluster_centers[k] = np.mean(points_in_cluster, axis=0)

    return cluster_centers, rmse_list

# Assuming x_train is defined and is the correct input data
# You can now run the kmeans_fast function and plot the results
K = 10
centers, rmse = kmeans_fast(x_train, K, niter=20)
plt.plot(np.arange(len(rmse)), rmse, label='K=10')

K=30
centers, rmse = kmeans_fast(x_train, K, niter=20)
plt.plot(np.arange(len(rmse)), rmse, label='K=30')

K=100
centers, rmse = kmeans_fast(x_train, K, niter=20)
plt.plot(np.arange(len(rmse)), rmse, label='K=100')
plt.legend(), plt.ylabel('RMSE'), plt.xlabel('# iterations')
plt.show()
```



[8]:

```python
# 1-NN

nsample = [100, 1000, 10000, 60000]

acc_exact = []
timing_exact = []
timing_lsh = []
acc_lsh = []

for s in nsample:
  start = time.time()
  index = faiss.IndexFlatL2(x_train.shape[1])
  index.add(x_train[:s])
  dist, idx = index.search(x_test,1)
  pred = y_train[idx.squeeze()]
  acc = (pred == y_test).mean()
  acc_exact.append(acc)
  timing_exact.append(time.time() - start)

for s in nsample:
  start = time.time()
  dim = x_train.shape[1]
  index = faiss.IndexLSH(dim, dim)
  index.add(x_train[:s])
  dist, idx = index.search(x_test,1)
  pred = y_train[idx.squeeze()]
  acc = (pred == y_test).mean()
  acc_lsh.append(acc)
  timing_lsh.append(time.time() - start)

acc_exact = np.array(acc_exact)
acc_lsh = np.array(acc_lsh)

plt.semilogx(nsample, 1-acc_exact, label='exact')
plt.semilogx(nsample, 1-acc_lsh, label='lsh')
plt.legend(), plt.ylabel('% error'), plt.xlabel('# training samples')
plt.show()

plt.semilogx(nsample, timing_exact, label='exact')
plt.semilogx(nsample, timing_lsh, label='lsh')
plt.legend(), plt.ylabel('time'), plt.xlabel('# training samples')
plt.show()
```


exact
lsh
0.30
0.25
0.20
0.15
0.10
0.05
% error
10^2
10^3
10^4
training samples



[9]:
```
# Confusion matrix
import sklearn
from sklearn.metrics import confusion_matrix


index = faiss.IndexFlatL2(x_train.shape[1])
index.add(x_train[:s])
dist, idx = index.search(x_test,1)
pred = y_train[idx.squeeze()]

C = confusion_matrix(y_test,pred)
print(C)
print(C[:, 2])




# TO DO
```

```
[[ 973    1    1    0    0    1    3    1    0    0]
 [   0 1129    3    0    1    1    1    0    0    0]
 [   7    6  992    5    1    0    2   16    3    0]
```

```
 [  0   1   2 970   1  19   0   7   7   3]
 [  0   7   0   0 944   0   3   5   1  22]
 [  1   1   0  12   2 860   5   1   6   4]
 [  4   2   0   0   3   5 944   0   0   0]
 [  0  14   6   2   4   0   0 992   0  10]
 [  6   1   3  14   5  13   3   4 920   5]
 [  2   5   1   6  10   5   1  11   1 967]]
[  1   3 992   2   0   0   0   6   3   1]
```

0.2 Part 3: Temperature Regression

Include all your code used for part 2 in this section.

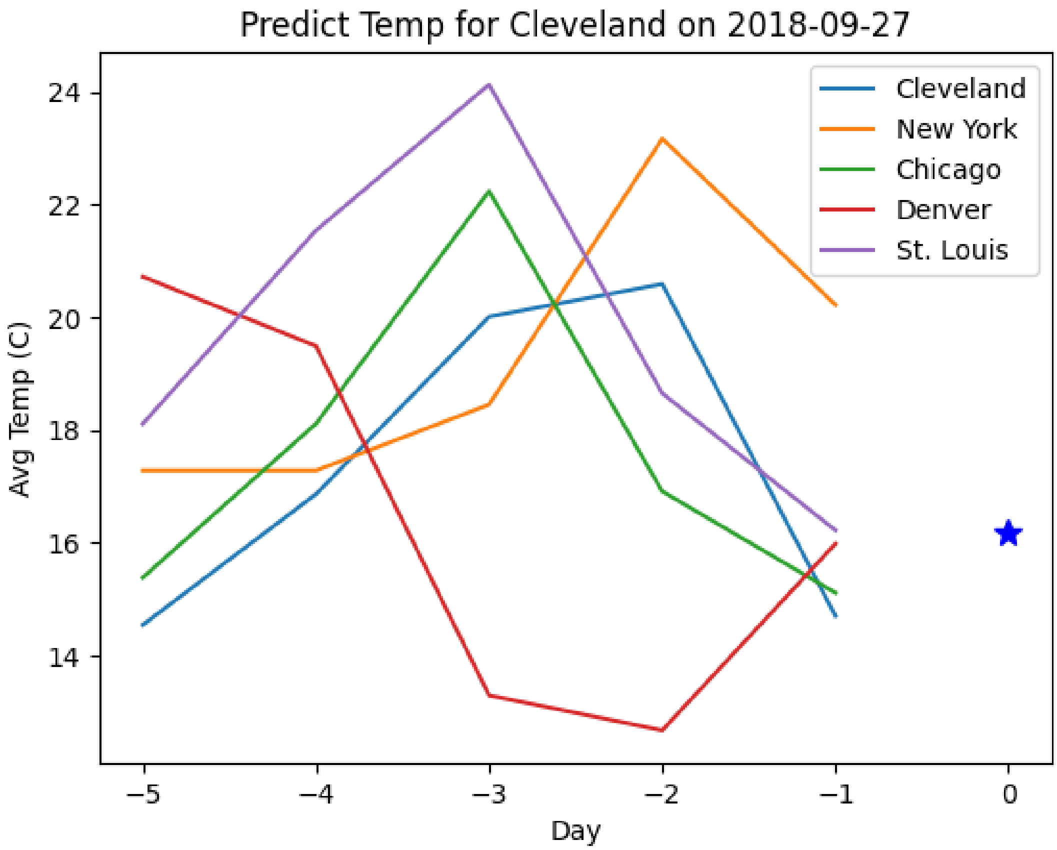
[7]:
```
import numpy as np
# from google.colab import drive
%matplotlib inline
from matplotlib import pyplot as plt
from sklearn.linear_model import Ridge
from sklearn.linear_model import Lasso

# load data (modify to match your data directory or comment)
def load_temp_data():
  # drive.mount('/content/drive')
  # datadir = "/content/drive/My Drive/CS441/24SP/hw1/"
  datadir = "./"
  T = np.load(datadir + 'temperature_data.npz')
  x_train, y_train, x_val, y_val, x_test, y_test, dates_train, dates_val,␣
 ↪dates_test, feature_to_city, feature_to_day = \
  T['x_train'], T['y_train'], T['x_val'], T['y_val'], T['x_test'], T['y_test'],␣
 ↪T['dates_train'], T['dates_val'], T['dates_test'], T['feature_to_city'],␣
 ↪T['feature_to_day']
  return (x_train, y_train, x_val, y_val, x_test, y_test, dates_train,␣
 ↪dates_val, dates_test, feature_to_city, feature_to_day)

# plot one data point for listed cities and target date
def plot_temps(x, y, cities, feature_to_city, feature_to_day, target_date):
  nc = len(cities)
  ndays = 5
  xplot = np.array([-5,-4,-3,-2,-1])
  yplot = np.zeros((nc,ndays))
  for f in np.arange(len(x)):
    for c in np.arange(nc):
      if cities[c]==feature_to_city[f]:
        yplot[feature_to_day[f]+ndays,c] = x[f]
  plt.plot(xplot,yplot)
  plt.legend(cities)
  plt.plot(0, y, 'b*', markersize=10)
  plt.title('Predict Temp for Cleveland on ' + target_date)
```

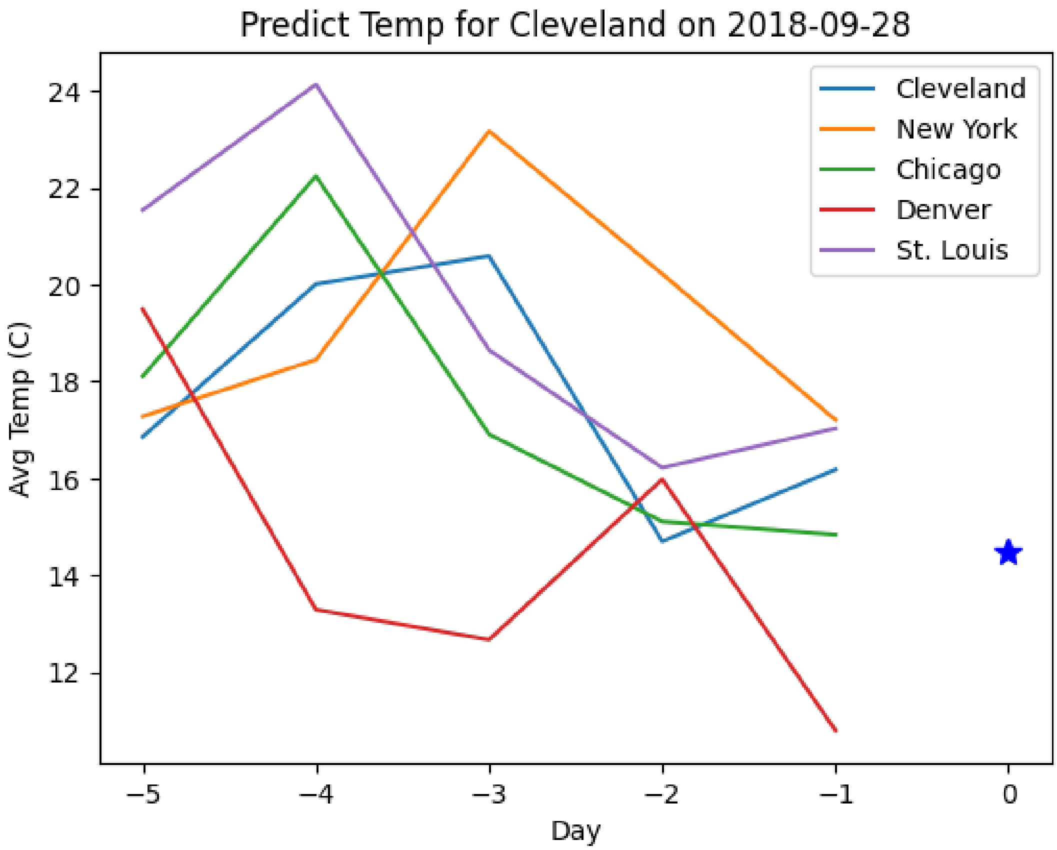
```python
plt.xlabel('Day')
plt.ylabel('Avg Temp (C)')
plt.show()
```

[8]:

```python
# load data
(x_train, y_train, x_val, y_val, x_test, y_test, dates_train, dates_val,␣
↪dates_test, feature_to_city, feature_to_day) = load_temp_data()
''' Data format:
      x_train, y_train: features and target value for each training sample␣
↪(used to fit model)
      x_val, y_val: features and target value for each validation sample (used␣
↪to select hyperparameters, such as regularization and K)
      x_test, y_test: features and target value for each test sample (used to␣
↪evaluate final performance)
      dates_xxx: date of the target value for the corresponding sample
      feature_to_city: maps from a feature number to the city
      feature_to_day: maps from a feature number to a day relative to the␣
↪target value, e.g. -2 means two days before
      Note: 361 is the temperature of Cleveland on the previous day
'''
f = 361
print('Feature {}: city = {}, day= {}'.format(f,feature_to_city[f],␣
↪feature_to_day[f]))
baseline_rmse = np.sqrt(np.mean((y_val[1:]-y_val[:-1])**2)) # root mean squared␣
↪error example
print('Baseline - prediction using previous day: RMSE={}'.format(baseline_rmse))

# plot first two x/y for val
plot_temps(x_val[0], y_val[0], ['Cleveland', 'New York', 'Chicago', 'Denver',␣
↪'St. Louis'], feature_to_city, feature_to_day, dates_val[0])
plot_temps(x_val[1], y_val[1], ['Cleveland', 'New York', 'Chicago', 'Denver',␣
↪'St. Louis'], feature_to_city, feature_to_day, dates_val[1])
```

```
Feature 361: city = Cleveland, day= -1
Baseline - prediction using previous day: RMSE=3.460601246750482
```


Predict Temp for Cleveland on 2018-09-27
Cleveland
New York
Chicago
Denver
St. Louis
Avg Temp (C)
Day
24
22
20
18
16
14
−5
−4
−3
−2
−1
0



[9]:
```
# K-NN Regression

def regress_KNN(X_trn, y_trn, X_tst, K=1):
    '''
    Predict the target value for each data point in X_tst using a
    K-nearest neighbor regressor based on (X_trn, y_trn), with L2 distance.
    Input: X_trn[i] is the ith training data. y_trn[i] is the ith training label.␣
 ↪K is the number of closest neighbors to use.
    Output: return y_pred, where y_pred[i] is the predicted ith test value
    '''
    index = faiss.IndexFlatL2(X_trn.shape[1])
    index.add(X_trn)
    dist, idx = index.search(X_tst,K)
    pred = y_trn[idx]
    pred = pred.mean(axis=1)
    return pred

def normalize_features(x, y, fnum):
    ''' Normalize the features in x and y.
        For each data sample i:
```

```
        x2[i] = x[i]-x[i,fnum]
        y2[i] = y[i]-x[i,fnum]
  '''
  xnorm = x - np.expand_dims(x[:,fnum],1)
  ynorm = y - x[:,fnum]
  return xnorm,ynorm
  # TO DO


k=5

# KNN with original features
y_pred = regress_KNN(x_train,y_train,x_test, K=k)
print(np.square(y_pred - y_test).mean()**0.5)
# TO DO

# KNN with normalized features
fnum = 361 # previous day temp in Cleveland

# TO DO
xnorm_train,ynorm_train = normalize_features(x_train,y_train,fnum)
xnorm_test, ynorm_test = normalize_features(x_test,y_test,fnum)


y_pred = regress_KNN(xnorm_train,ynorm_train,xnorm_test, K=k)

print(np.square(y_pred - ynorm_test).mean()**0.5)
```

```
3.249556245363484
2.9324389176041588
```

0.3 Part 5: Stretch Goals

Include all your code used for part 5 in this section. You can copy-paste code from parts 1-3 if it is re-usable.

[3]:
```
from scipy.stats import mode
# Stretch: KNN classification (Select K)
(x_train, y_train), (x_test, y_test) = load_mnist()

for K in [1, 3, 5, 11, 25]:
  index = faiss.IndexFlatL2(x_train.shape[1])
  index.add(x_train[:50000])
  dist, idx = index.search(x_train[50000:], K)
  pred = y_train[:50000][idx]
  mode_result, mode_count = mode(pred, axis=1)
  error = (mode_result != y_train[50000:]).mean()
  print(f"{K}: {error}")
```

```
1: 0.0288
3: 0.028
5: 0.0282
11: 0.0308
25: 0.0382
```

[5]:

```
# test
K=3
index = faiss.IndexFlatL2(x_train.shape[1])
index.add(x_train)
dist, idx = index.search(x_test, K)
pred = y_train[idx]
mode_result, mode_count = mode(pred, axis=1)
error = (mode_result != y_test).mean()
print(f"{K}: {error}")
```

```
3: 0.0295
```

[14]:

```
(x_train, y_train, x_val, y_val, x_test, y_test, dates_train, dates_val,␣
 ↪dates_test, feature_to_city, feature_to_day) = load_temp_data()



for k in [1, 3, 5, 11, 25]:
  print(f"k: {k}")
  # KNN with original features
  y_pred = regress_KNN(x_train,y_train,x_val, K=k)
  print(np.square(y_pred - y_val).mean()**0.5)

  # KNN with normalized features
  fnum = 361 # previous day temp in Cleveland

  xnorm_train,ynorm_train = normalize_features(x_train,y_train,fnum)
  xnorm_val, ynorm_val = normalize_features(x_val,y_val,fnum)


  y_pred = regress_KNN(xnorm_train,ynorm_train,xnorm_val, K=k)

  print(np.square(y_pred - ynorm_val).mean()**0.5)

print("Optimal:")
xnorm_train,ynorm_train = normalize_features(x_train,y_train,fnum)
xnorm_test, ynorm_test = normalize_features(x_test,y_test,fnum)
y_pred = regress_KNN(xnorm_train,ynorm_train,xnorm_test, K=11)
print(np.square(y_pred - ynorm_test).mean()**0.5)
```

```
k: 1
4.330006390580244
3.8669564684344615
```

```
k: 3
3.2266843182278797
3.174005914679923
k: 5
3.095887258575192
3.032493865875963
k: 11
3.055782885507432
2.8908415810941466
k: 25
3.060219056497986
2.9103974575813334
Optimal:
2.7671311757775685
```

[28]:

```python
# Stretch: K-means (more iters vs redos)
(x_train, y_train), (x_test, y_test) = load_mnist()

ps = [(20,1),(4,5),(50,1),(10,5)]
for (ni,nr) in ps:
  print(ni,nr)
  res = []
  for i in range(5):
    kmeans = faiss.Kmeans(x_train.shape[1], 30, niter=ni, nredo=nr, seed=int(i))
    kmeans.train(x_train)
    dist, idx = kmeans.index.search(x_train, 1)
    rmse = np.sqrt(np.sum(dist) / x_train.shape[0])
    res.append(rmse)
  print(np.mean(res),np.std(res))
  print()
```

```
20 1
5.786271422463997 0.007644752654037744

4 5
5.822844075465655 0.012136287784838528

50 1
5.777090880990907 0.005488117925290951

10 5
5.787613203649412 0.0037177425483455743
```

[ ]:

```python
# from https://gist.github.com/jonathanagustin/b67b97ef12c53a8dec27b343dca4abba
# For use in Colab.  For local, just use jupyter nbconvert directly
```

```python
import os
# @title Convert Notebook to PDF. Save Notebook to given directory
NOTEBOOKS_DIR = "/content/drive/My Drive/CS441/24SP/hw1" # @param {type:"string"}
NOTEBOOK_NAME = "CS441_SP24_HW1_Solution.ipynb" # @param {type:"string"}
#------------------------------------------------------------------------------#
from google.colab import drive
drive.mount("/content/drive/", force_remount=True)
NOTEBOOK_PATH = f"{NOTEBOOKS_DIR}/{NOTEBOOK_NAME}"
assert os.path.exists(NOTEBOOK_PATH), f"NOTEBOOK NOT FOUND: {NOTEBOOK_PATH}"
!apt install -y texlive-xetex texlive-fonts-recommended texlive-plain-generic > /dev/null 2>&1
!jupyter nbconvert "$NOTEBOOK_PATH" --to pdf > /dev/null 2>&1
NOTEBOOK_PDF = NOTEBOOK_PATH.rsplit('.', 1)[0] + '.pdf'
assert os.path.exists(NOTEBOOK_PDF), f"ERROR MAKING PDF: {NOTEBOOK_PDF}"
print(f"PDF CREATED: {NOTEBOOK_PDF}")
```