CorreaSydney

September 18, 2018

```
##
CSCI E-82
##
HW 1 Dimensionality Reduction
###
Due: Sept 17, 2018 11:59pm EST
```

Note that this is an individual homework to be completed without collaborations except through Piazza.

We encourage you to make progress this weekend since the second homework will likely come out in a week before this one is due.

0.0.1 Your name: Sydney Correa

```
In [163]: import numpy as np
import sklearn as sk
```

0.0.2 **Problem 1 (5 points)**

$$\mathbf{X} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$$
$$\mathbf{Y} = \begin{bmatrix} 1 & 2 & 1 \\ 2 & 1 & 2 \end{bmatrix}$$

Compute XYT. The answer can be computed by hand and written in Markdown like the above matrices, or computed in python. Either way is acceptable.

0.0.3 Problem 2

This problem goes through a combination of python data manipulations as well as the full math projection using PCA. We have divided the problem into multiple parts.

0.0.4 Problem 2a (5 points)

Download and load in the data set from the UCI archive https://archive.ics.uci.edu/ml/machine-learning-databases/ecoli/. Print the dimensions and the first few rows to demonstrate a successful load.

```
In [165]: import numpy as np
          import pandas as pd
          import matplotlib.pyplot as plt
          # Remember to use inline to get your plots in the notebook
          %matplotlib inline
          # special matplotlib command for global plot configuration
          from matplotlib import rcParams
          import matplotlib.cm as cm
          import matplotlib as mpl
          import matplotlib.style
          from matplotlib.colors import ListedColormap
          dark2_colors = ['#1b9e77','#d95f02','#7570b3','#e7298a','#66a61e','#e6ab02','#a6761d
          dark2_cmap = ListedColormap(dark2_colors)
          def set_mpl_params():
              rcParams['figure.figsize'] = (10, 6)
              rcParams['figure.dpi'] = 100
              rcParams['axes.prop_cycle'].by_key()['color'][1]
              rcParams['lines.linewidth'] = 2
              rcParams['axes.facecolor'] = 'white'
              rcParams['font.size'] = 12
              rcParams['patch.edgecolor'] = 'white'
              rcParams['patch.facecolor'] = dark2_colors[0]
              rcParams['font.family'] = 'StixGeneral'
          set_mpl_params()
          mpl.style.use('seaborn-dark-palette')
          import seaborn as sns #If you don't have seaborn, use - conda install seaborn
          current_palette = sns.color_palette()
          sns.palplot(current_palette)
```



```
In [183]: #import dataset
          url = 'https://archive.ics.uci.edu/ml/machine-learning-databases/ecoli/ecoli.data'
          #name columns
          eColiCols = ['N_ecoli', 'mcg', 'gvh', 'lip', 'chg', 'aac', 'alm1', 'alm2', 'type']
          #read table into dataset
          eColiData = pd.read_table(url, sep='\s+', header= None, names = eColiCols)
          #print few rows
          #print (eColiData.head())
          eColiData.describe()
          #print dimensions of array
          #eColiData.shape
          #split data into data and values for Ecoli Dataset
          eColiData_num = eColiData.iloc[:,1:8]
          eColiData_class = eColiData.iloc[:,8]
          #print data
          print ('EColi Data: \n%s', eColiData_num.head())
          #print class
          print ('EColi Class Data: \n%s', eColiData_class.head())
          #print dataset for two dimensions alm2, alm1
          ax = plt.gca()
          ax.axis([0, 1, 0, 1])
          #ax.scatter(eColiData.iloc[:,6], eColiData.iloc[:,5], s=10)
          ax.scatter(eColiData.alm2, eColiData.alm1, s=10)
          ax.set_title('Raw Data')
          ax.grid(True)
          #cible_border()
          plt.show()
```

TimeoutError

Traceback (most recent call last)

~\Anaconda3\lib\urllib\request.py in do_open(self, http_class, req, **http_conn_args)
1317 h.request(req.get_method(), req.selector, req.data, headers,

```
-> 1318
                                  encode_chunked=req.has_header('Transfer-encoding'))
                    except OSError as err: # timeout error
   1319
    ~\Anaconda3\lib\http\client.py in request(self, method, url, body, headers, encode_chu
                """Send a complete request to the server."""
   1238
                self. send request(method, url, body, headers, encode chunked)
-> 1239
   1240
    ~\Anaconda3\lib\http\client.py in _send_request(self, method, url, body, headers, enco
                    body = _encode(body, 'body')
   1284
                self.endheaders(body, encode_chunked=encode_chunked)
-> 1285
   1286
    ~\Anaconda3\lib\http\client.py in endheaders(self, message_body, encode_chunked)
                    raise CannotSendHeader()
   1233
-> 1234
                self._send_output(message_body, encode_chunked=encode_chunked)
   1235
    ~\Anaconda3\lib\http\client.py in _send_output(self, message_body, encode_chunked)
                del self._buffer[:]
   1025
-> 1026
                self.send(msg)
   1027
    ~\Anaconda3\lib\http\client.py in send(self, data)
    963
                   if self.auto_open:
--> 964
                        self.connect()
    965
                    else:
    ~\Anaconda3\lib\http\client.py in connect(self)
                    self.sock = self._context.wrap_socket(self.sock,
   1399
-> 1400
                                                           server_hostname=server_hostname)
   1401
                    if not self._context.check_hostname and self._check_hostname:
    ~\Anaconda3\lib\ssl.py in wrap_socket(self, sock, server_side, do_handshake_on_connect
    406
                                 server_hostname=server_hostname,
--> 407
                                 _context=self, _session=session)
    408
    ~\Anaconda3\lib\ssl.py in __init__(self, sock, keyfile, certfile, server_side, cert_real
    813
                                raise ValueError("do_handshake_on_connect should not be sp
```

```
--> 814
                            self.do_handshake()
    815
    ~\Anaconda3\lib\ssl.py in do_handshake(self, block)
                        self.settimeout(None)
   1067
-> 1068
                    self. sslobj.do handshake()
   1069
                finally:
    ~\Anaconda3\lib\ssl.py in do_handshake(self)
                """Start the SSL/TLS handshake."""
    688
--> 689
                self._sslobj.do_handshake()
                if self.context.check_hostname:
    690
    TimeoutError: [WinError 10060] A connection attempt failed because the connected party
During handling of the above exception, another exception occurred:
    URLError
                                               Traceback (most recent call last)
    <ipython-input-183-ca107e279a21> in <module>()
      4 eColiCols = ['N_ecoli', 'mcg', 'gvh', 'lip', 'chg', 'aac', 'alm1', 'alm2', 'type']
      5 #read table into dataset
----> 6 eColiData = pd.read_table(url, sep='\s+', header= None, names = eColiCols)
      7 #print few rows
      8 #print (eColiData.head())
    ~\Anaconda3\lib\site-packages\pandas\io\parsers.py in parser_f(filepath_or_buffer, sep
    676
                            skip_blank_lines=skip_blank_lines)
    677
--> 678
                return _read(filepath_or_buffer, kwds)
    679
    680
            parser_f.__name__ = name
    ~\Anaconda3\lib\site-packages\pandas\io\parsers.py in _read(filepath_or_buffer, kwds)
            compression = _infer_compression(filepath_or_buffer, compression)
    422
            filepath_or_buffer, _, compression, should_close = get_filepath_or_buffer(
    423
                filepath_or_buffer, encoding, compression)
--> 424
            kwds['compression'] = compression
    425
    426
```

```
~\Anaconda3\lib\site-packages\pandas\io\common.py in get_filepath_or_buffer(filepath_or_buffer)
    193
    194
            if _is_url(filepath_or_buffer):
--> 195
                req = _urlopen(filepath_or_buffer)
                content encoding = req.headers.get('Content-Encoding', None)
    196
    197
                if content_encoding == 'gzip':
    ~\Anaconda3\lib\urllib\request.py in urlopen(url, data, timeout, cafile, capath, cadef
    221
            else:
    222
                opener = _opener
--> 223
            return opener.open(url, data, timeout)
    224
    225 def install_opener(opener):
    ~\Anaconda3\lib\urllib\request.py in open(self, fullurl, data, timeout)
                    req = meth(req)
    524
    525
--> 526
                response = self._open(req, data)
    527
    528
                # post-process response
    ~\Anaconda3\lib\urllib\request.py in _open(self, req, data)
    542
                protocol = req.type
    543
                result = self._call_chain(self.handle_open, protocol, protocol +
--> 544
                                           '_open', req)
    545
                if result:
    546
                    return result
    ~\Anaconda3\lib\urllib\request.py in _call_chain(self, chain, kind, meth_name, *args)
    502
                for handler in handlers:
    503
                    func = getattr(handler, meth name)
                    result = func(*args)
--> 504
                    if result is not None:
    505
    506
                        return result
    ~\Anaconda3\lib\urllib\request.py in https_open(self, req)
                def https_open(self, req):
   1359
   1360
                    return self.do_open(http.client.HTTPSConnection, req,
                        context=self._context, check_hostname=self._check_hostname)
-> 1361
   1362
   1363
                https_request = AbstractHTTPHandler.do_request_
```

URLError: <urlopen error [WinError 10060] A connection attempt failed because the connection

0.0.5 **Problem 2b (10 points)**

Compute and print the covariance matrix for all columns excluding the first and last. Rather than use the built-in function, compute this using python code for practice. The following equation will suffice for this.

```
Cov(X, Y) = (Xi - X)(Yi - Y) / N
```

```
In [168]: from sklearn.preprocessing import StandardScaler
          #standardize the data
          X_std = StandardScaler().fit_transform(eColiData_num)
          eColiData_num = eColiData.iloc[:,1:8].values
          #find means for dimensions
          eColiData_mean = np.mean(eColiData_num, axis=0)
          cov_mat = (X_std - eColiData_mean).T.dot((X_std - eColiData_mean)) / (X_std.shape[0]
          print('Covariance matrix \n%s' %cov_mat)
          #validate cov matrix
          print('Covariance matrix validate\n%s' %np.cov(X_std.T))
Covariance matrix
[[1.25379105 0.70693901 0.39578701 0.32199783 0.47214889 0.64902932
  0.41822671]
 [0.70693901 \ 1.25373134 \ 0.29241285 \ 0.27001367 \ 0.3207939 \ 0.42484554
 0.13005389]
 [0.39578701 0.29241285 1.24921456 0.56209934 0.31889194 0.34463989
  0.19060217]
 [0.32199783 \ 0.27001367 \ 0.56209934 \ 1.2552261 \ 0.20664813 \ 0.24390583
 0.19901358]
 [0.47214889 0.3207939 0.31889194 0.20664813 1.25376119 0.53116752
  0.50405568]
 [0.64902932 0.42484554 0.34463989 0.24390583 0.53116752 1.25391048
  1.06244095]
```

[0.41822671 0.13005389 0.19060217 0.19901358 0.50405568 1.06244095

```
1.25346276]]
Covariance matrix validate
0.16758494]
-0.12055805]
-0.057742331
[0.07047535 \ 0.01852114 \ 0.31288221 \ 1.00298507 \ -0.04485938 \ -0.00767652
 -0.052344231
[ \ 0.22135784 \ \ 0.07003271 \ \ 0.07039954 \ -0.04485938 \ \ 1.00298507 \ \ 0.28031677
 0.25342882]
[ \ 0.39816364 \ \ 0.17400972 \ \ 0.09607353 \ -0.00767652 \ \ 0.28031677 \ \ 1.00298507 ]
 0.81173951]
1.00298507]]
```

0.0.6 **Problem 2c (10 points)**

Compute the decomposition of the covariance matrix using singular value decomposition. Using a python function is definitely the way to go here.

```
In [169]: #qet cov matrix
         eColiData_cov = np.cov(X_std.T)
         #print Cov dataset
         #print ('Cov dataset')
         #print(eColiData_cov)
         #check value of determinant >=0
         print ('value of Det(Cov)')
         print(np.linalg.det(eColiData_cov))
         #get eigenvalues, eigenvectors
         eigenvalues, eigenvectors = np.linalg.eigh(eColiData_cov)
         print('Unsorted eign values: \n%s', eigenvalues)
         print('Unsorted eign values: \n%s', eigenvectors)
value of Det(Cov)
0.13729373206325216
Unsorted eign values:
%s [0.12680082 0.48008494 0.671441 0.85971779 1.20508931 1.46555238
2.21220928]
Unsorted eign values:
-0.43301833]
  \begin{bmatrix} -0.18599716 & -0.60363588 & 0.05019625 & -0.14655068 & -0.55288668 & 0.47029644 \end{bmatrix} 
 -0.22398568]
```

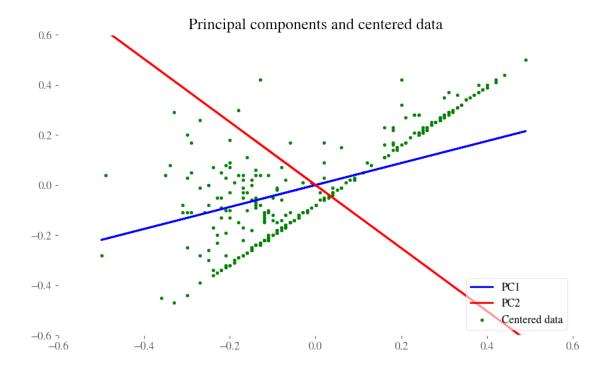
```
 \begin{bmatrix} -0.10478843 & -0.10724976 & -0.67128037 & 0.20125402 & 0.49223261 & 0.48177748 \end{bmatrix} 
     -0.10951653]
   [ 0.01462969 - 0.03639389 \ 0.67163159 - 0.20553058 \ 0.5451792 \ 0.45560856
     -0.01816912]
   [ 0.01385432 -0.09557701  0.29459176  0.88426143 -0.00818155 -0.04745278
     -0.345907221
    \begin{smallmatrix} 0.70393508 & -0.16949665 & -0.09365082 & -0.24341844 & 0.11045841 & -0.16428058 \end{smallmatrix} 
     -0.6070701 ]
   [-0.67219322 -0.08867463 \ 0.01396843 -0.22384663 \ 0.23907035 -0.4135461
     -0.5116792411
In [170]: #sort eigenvalues to get higher values
                           idx = np.argsort(-eigenvalues)
                            #apply index to sort eigenvalues
                           eigenvalues = eigenvalues[idx]
                           print('Sorted eigen values: ', eigenvalues)
                            #sort eigenvectors
                           eigenvectors = eigenvectors[idx]
                            #print ('Eigen vector shape: ', eigenvectors.shape)
                            #print ('Sorted Eigenvectors: ', eigenvectors)
                            #calculate Singular value decomp
                           S = eigenvalues*np.eye(7)
                           U = eigenvectors
                           V = U
                           D = np.dot(U, np.dot(S,V.T))
                            #print ('D value: ')
                            #print(D)
                            #validate SVD results using np svd function
                           U1, S1, V1 = np.linalg.svd(X_std.T)
                           print('Validate U1 value: ')
                           print(U1)
Sorted eigen values: [2.21220928 1.46555238 1.20508931 0.85971779 0.671441 0.48008494
  0.126800827
Validate U1 value:
[[-0.43301833 0.37265574 -0.29219921 0.06707282 0.00490985 0.75965086
        0.08154845]
  [-0.22398568 \quad 0.47029644 \quad -0.55288668 \quad 0.14655068 \quad -0.05019625 \quad -0.60363588 \quad -0.05019625 \quad -
        0.185997167
   \begin{bmatrix} -0.10951653 & 0.48177748 & 0.49223261 & -0.20125402 & 0.67128037 & -0.10724976 \end{bmatrix} 
        0.10478843]
    \begin{bmatrix} -0.01816912 & 0.45560856 & 0.5451792 & 0.20553058 & -0.67163159 & -0.03639389 \end{bmatrix} 
     -0.01462969]
   [-0.34590722 -0.04745278 -0.00818155 -0.88426143 -0.29459176 -0.09557701
```

0.0.7 **Problem 2d (10 points)**

Compute the projection of the raw data onto the appropriate two eigenvectors. Consider which

Answer: Considering the last two feature vectors alm2, alm1 to be projected

```
In [171]: #finding orientation for axes
          h1 = (eigenvectors[6][0]/eigenvectors[5][0])*eColiData_0.alm2
          h2 = (eigenvectors[6][1]/eigenvectors[5][1])*eColiData_0.alm2
In [172]: #ploting the PCA
          ax = plt.gca()
          ax.plot(eColiData_0.alm2, h1, color='blue', label='PC1')
          ax.plot(eColiData_0.alm2, h2, color='red', label='PC2')
          ax.axis([-0.6, 0.6, -0.6, 0.6])
          ax.scatter(eColiData_0.alm2, eColiData_0.alm1, s=10, c='green', label='Centered data
          ax.set_title('Principal components and centered data')
          ax.grid(True)
          #cible_border()
          legend = ax.legend(loc=4,frameon=True,framealpha=0.6, scatterpoints=1)
          rect = legend.get_frame()
          #rect.set_facecolor(light_grey)
          rect.set_linewidth(0.6)
          plt.show()
```



In []:

0.0.8 **Problem 2e (10 points)**

Plot the projected points such that the 8 different classes can be visually identified. Be sure to label the classes and axes. Commont on the quality of the separation of the different classes using PCA.

```
#cible_border()
legend = ax.legend(loc=4,frameon=True,framealpha=0.6, scatterpoints=1)
rect = legend.get_frame()
#rect.set_facecolor(light_grey)
rect.set_linewidth(0.6)
plt.show()
```

0.0.9 **Problem 2f (10 points)**

The PCA that you have just completed takes each data point and projects it using a weighted sum of features. One could also do the opposite to map the features as a weighted sum of the data entries. How could this be done? What is a potential issue? Describe these in a few sentences (do not code it).

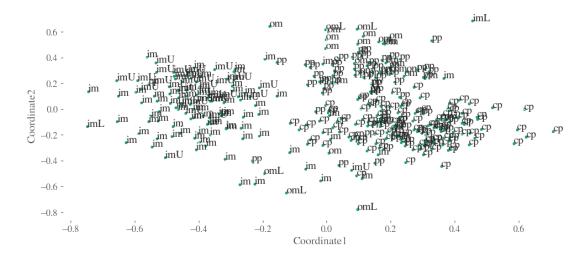
Answer: To map features as weighted sum of data entries we would need to transpose each of the EColi variation into a feature. For this we would need to transpose each row of the data to a feature vector and then apply the same steps of PCA. However by doing it this way we end up with very high number of features and data would be more localized. This may not help with analysis of the overall protien localization for entire dataset.

0.0.10 Problem 3 MDS (10 points)

For the same data set, repeat 2e using sklearn's Multidimensional scaling algorithm.

```
In [174]: from sklearn.metrics.pairwise import cosine_similarity, euclidean_distances
          from sklearn.manifold import MDS
          #qet eculidean dist
          Euclid_dist = euclidean_distances(eColiData_num)
          #Default metric = True, for NonMetric set metric=False
          mds = MDS(n_components=2, dissimilarity="precomputed", random_state=99)
          mds_fit = mds.fit_transform(Euclid_dist) # shape (n_samples, n_components)
In [175]: \#plot the MDS fit
          x1 = mds_fit[:,0]
          y1 = mds_fit[:,1]
          n = eColiData.iloc[:,8:9]
          fig, ax = plt.subplots(figsize=(12,5))
          dark2_colors = ['#1b9e77','#d95f02','#7570b3','#e7298a','#66a61e','#e6ab02','#a6761d
          shade_black = '#262626'
          ax.scatter(x1, y1, s=10, zorder=0, c=dark2_colors[0])
          for i, txt in enumerate(n.values):
              ax.annotate(txt[0], (x1[i],y1[i]), zorder=1, size=14, color=shade_black)
```

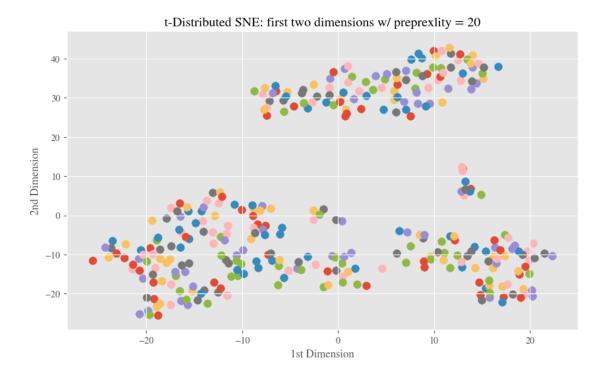
```
ax.set_xlabel('Coordinate1')
ax.set_ylabel('Coordinate2');
```



0.0.11 Problem 4a t-SNE (5 points)

Repeat 2e using a t-SNE plot with the default settings.

Answer: Running t-SNE with components=2 and preplexity=20



0.0.12 Problem 4b t-SNE perplexity (5 points)

Try out a few t-SNE plots by varying the perplexity. State the best perplexity for separating the 8 different classes and describe your rationale in a sentence or two. Report the average calculation time for the t-SNE projection over a number of iterations.

Answer: Looking at the below points, preplexity <20 can be used for more localized visualizations and analysis. Having preplexity >20 helps with more distinct clusters and helps with more higher level (global) analysis for the 8 different classes.

Also looking at times taken, it is a less than 10 seconds for preplexity = 0 and 10 and then staying constant after prelexity >=20

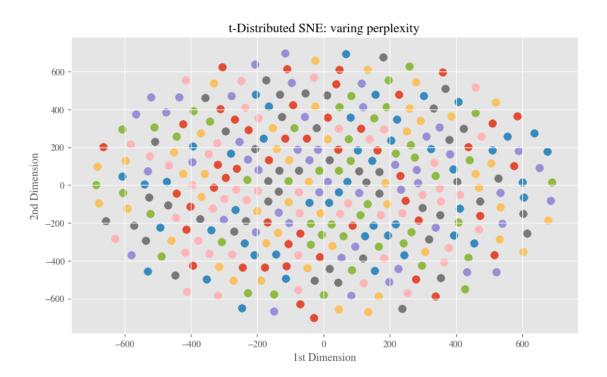
```
In [179]: import timeit
```

```
for iCounter in range(0,60,10):
    start = timeit.default_timer()
    for nloop in range(11):
        X_embedded = TSNE(n_components=2, perplexity=iCounter, verbose=0).fit_transfers
    stop = timeit.default_timer()
    print('Time taken: ', round((stop - start)/nloop,2), 'in seconds, varing preplex

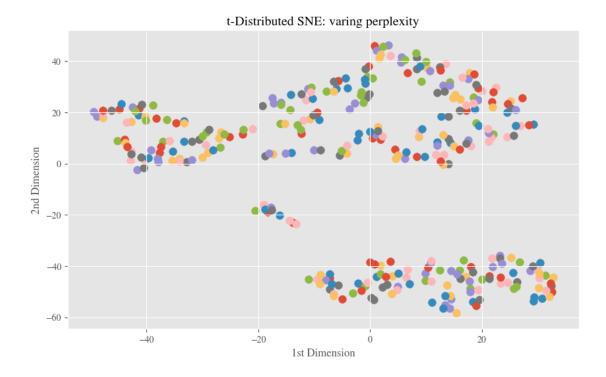
#plotting the t-SNE
    mpl.style.use('ggplot')
    plt.figure(figsize=(10,6))
    for i in range(X_embedded.shape[0]):
        plt.scatter(X_embedded[i,0], X_embedded[i,1], s = 70, zorder=0)
```

```
plt.ylabel('2nd Dimension')
plt.xlabel('1st Dimension')
plt.title('t-Distributed SNE: varing perplexity')
plt.show()
```

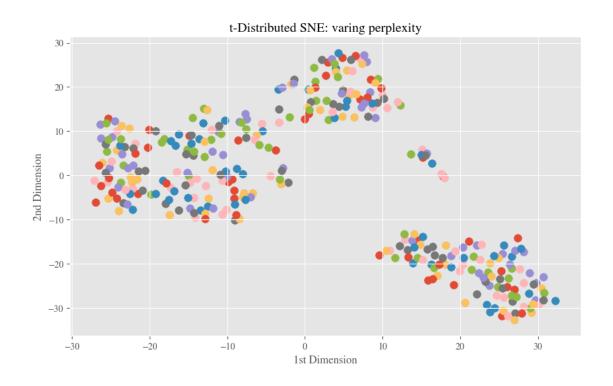
Time taken: 2.5 in seconds, varing preplexity = 0 and 10 iterations



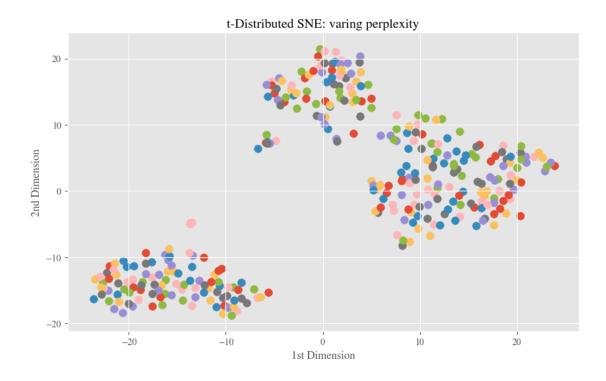
Time taken: 5.0 in seconds, varing preplexity = 10 and 10 iterations



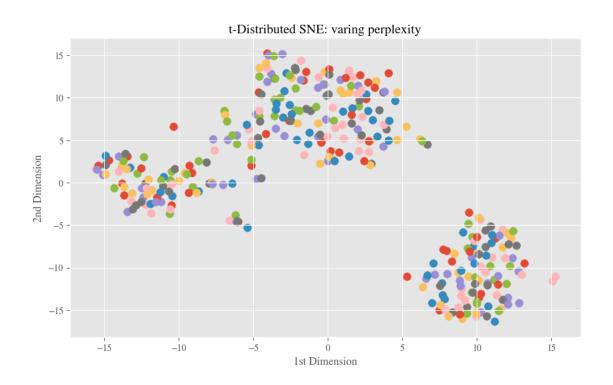
Time taken: 6.65 in seconds, varing preplexity = 20 and 10 iterations

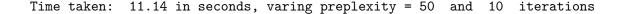


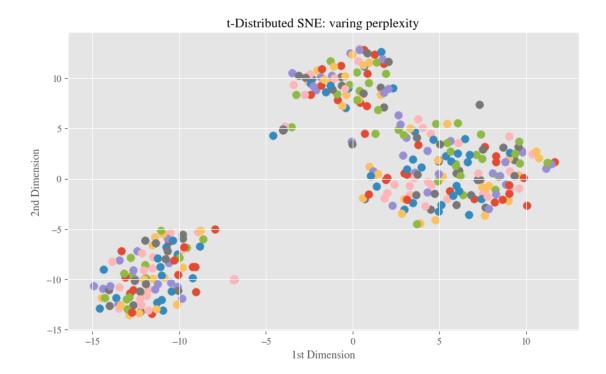
Time taken: 8.6 in seconds, varing preplexity = 30 and 10 iterations



Time taken: 11.04 in seconds, varing preplexity = 40 and 10 iterations







0.0.13 Problem 4c t-SNE randomization (10 points)

The S of t-SNE means stochastic or random, usually as a function of time. Explore whether you can reproduce the result in 4b through a second projection and plot.

0.1 Problem 4d t-SNE Barnes-Hut (5 points)

The default t-SNE method of 4b uses the Barnes-Hut approximation. Keeping the other parameters the same as 4b, plot the t-SNE result using the exact method. Which method do you prefer? Compare the average calculation time for the exact method over a number of iterations.

Answer: Looking at the iteration times for 10 iterations, we see using method exact increased run time by 3 times. This can be a potential problem for very large datasets.

```
In [181]: import timeit

start = timeit.default_timer()

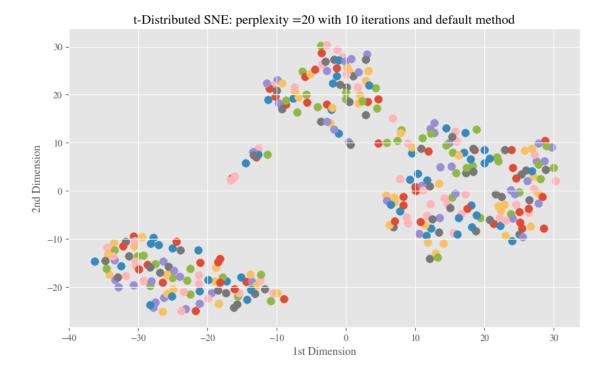
for nloop in range(11):
     X_embedded_20 = TSNE(n_components=2, perplexity=20, verbose=0).fit_transform(eComponents=2)
```

```
stop = timeit.default_timer()
print('Time: ', stop - start, 'seconds')

mpl.style.use('ggplot')

plt.figure(figsize=(10,6))
for i in range(X_embedded_20.shape[0]):
    plt.scatter(X_embedded_20[i,0], X_embedded_20[i,1], s = 70, zorder=0)
plt.ylabel('2nd Dimension')
plt.xlabel('1st Dimension')
plt.title('t-Distributed SNE: perplexity =20 with 10 iterations and default method')
plt.show()
```

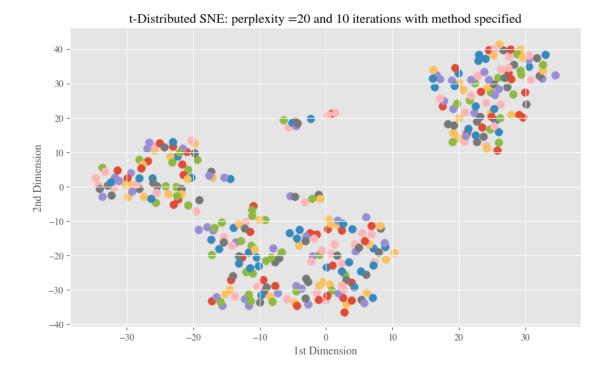
Time: 68.4031629940655 seconds



```
#plot tSNE
mpl.style.use('ggplot')

plt.figure(figsize=(10,6))
for i in range(X_embedded_20_s.shape[0]):
    plt.scatter(X_embedded_20_s[i,0], X_embedded_20_s[i,1], s = 70, zorder=0)
plt.ylabel('2nd Dimension')
plt.xlabel('1st Dimension')
plt.title('t-Distributed SNE: perplexity =20 and 10 iterations with method specified plt.show()
```

Total Time: 87.99440425306966 seconds



0.1.1 How many hours did this homework take?

This will not affect your grade. We will be monitoring time spent on homework to be sure that we are not over-burdening students.

In []: 6 Hrs

0.1.2 Last step (5 points)

Save this notebook as LastnameFirstnameHW1.ipynb such as MuskElonHW1.ipynb. Create a pdf of this notebook named similarly. Submit both the python notebook and the pdf version to the Canvas dropbox. We require both versions.