M11 Visualizing high dimensional data

```
In [1]: import matplotlib.pyplot as plt
import pandas as pd
import seaborn as sns
import numpy as np
import scipy.stats as ss

sns.set_style('white')

%matplotlib inline
```

Scatterplot matrix for low-high dimensional data

In many cases, the number of dimensions is not too large. For instance, the "Iris" dataset (https://en.wikipedia.org/wiki/Iris_flower_data_set) contains four dimensions of measurements on the three types of iris flower species. It's more than two dimensions, yet still manageable.

```
In [2]: iris = sns.load_dataset('iris')
  iris.head(2)
```

Out[2]:

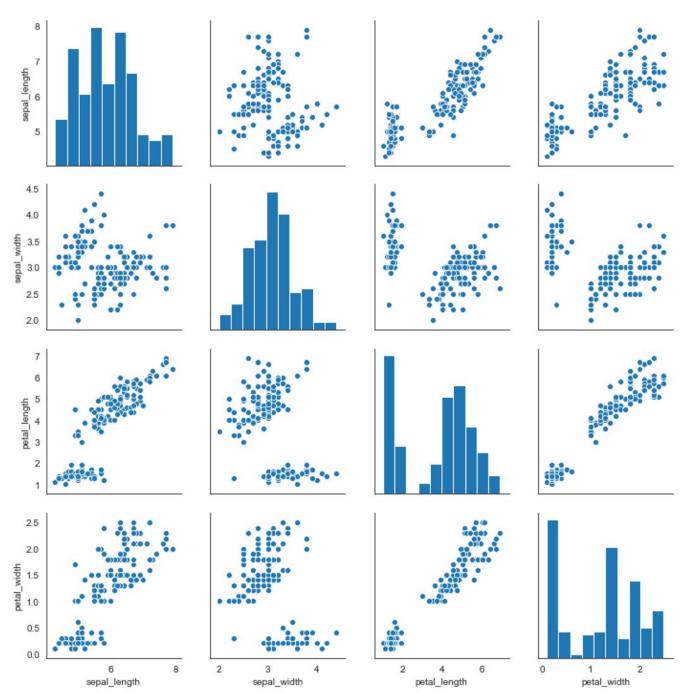
	sepal_length	sepal_width	petal_length	petal_width	species
0	5.1	3.5	1.4	0.2	setosa
1	4.9	3.0	1.4	0.2	setosa

We get four dimensions (sepal_length, sepal_width, petal_length, petal_width). One direct way to visualize them is to have a scatter plot for each pair of dimensions. We can use the <u>pairplot()</u>

(http://stanford.edu/~mwaskom/software/seaborn/generated/seaborn.pairplot.html) function in seaborn to do this.

In [3]: sns.pairplot(iris)

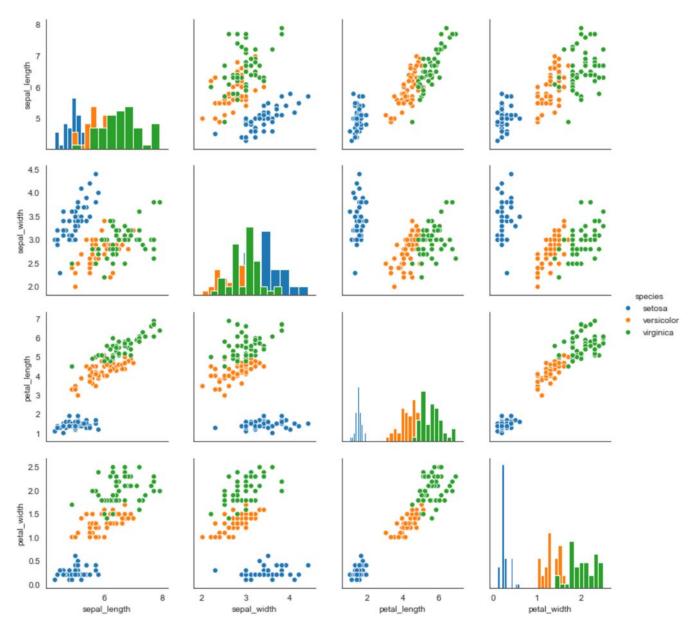
Out[3]: <seaborn.axisgrid.PairGrid at 0x1da14d10be0>



By using colors, you can get a much more useful plot.

In [9]: sns.pairplot(iris, hue='species', diag_kind='hist')

Out[9]: <seaborn.axisgrid.PairGrid at 0x1da1ebde630>



Seaborn also lets us to specify what to put in the diagonal. Let's try KDE. see https://seaborn.pydata.org/generated/seaborn.pairplot.html (<a href="https://seaborn.pydata.org/generated/seaborn.pydata.

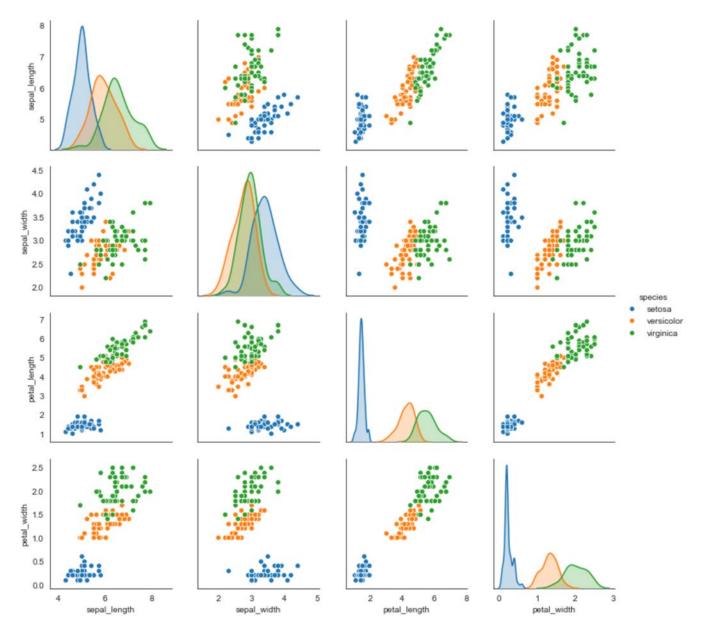
Q: draw a pairplot with KDE on the diagonal

In [8]: sns.pairplot(iris, diag_kind='kde', hue='species')

C:\Users\yyezeret\AppData\Local\Continuum\Anaconda2\envs\dviz\lib\site-packages\scipy\s tats\stats.py:1713: FutureWarning: Using a non-tuple sequence for multidimensional inde xing is deprecated; use `arr[tuple(seq)]` instead of `arr[seq]`. In the future this wil l be interpreted as an array index, `arr[np.array(seq)]`, which will result either in a n error or a different result.

return np.add.reduce(sorted[indexer] * weights, axis=axis) / sumval

Out[8]: <seaborn.axisgrid.PairGrid at 0x1da1df88588>



We can use altair to create an interactive scatterplot matrix. Can you create a scatterplot matrix of iris dataset by consulting https://altair-viz.github.io/gallery/scatter_matrix.html? (https://altair-viz.github.io/gallery/scatter_matrix.html?

Q: Draw an interactive scatterplot matrix for iris dataset in altair

```
In [48]: import altair as alt
from vega_datasets import data
alt.renderers.enable('notebook')
```

Out[48]: RendererRegistry.enable('notebook')

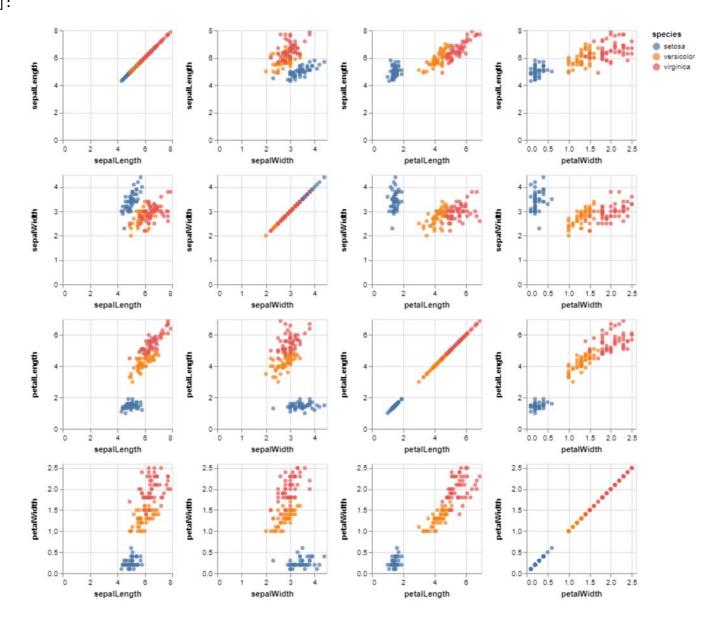
In [46]: iris= data.iris()
 iris.head()

Out[46]:

	petalLength	petalWidth	sepalLength	sepalWidth	species
0	1.4	0.2	5.1	3.5	setosa
1	1.4	0.2	4.9	3.0	setosa
2	1.3	0.2	4.7	3.2	setosa
3	1.5	0.2	4.6	3.1	setosa
4	1.4	0.2	5.0	3.6	setosa

```
In [47]: alt.Chart(iris).mark_circle().encode(
    alt.X(alt.repeat("column"), type='quantitative'),
    alt.Y(alt.repeat("row"), type='quantitative'),
    color='species:N'
).properties(
    width=150,
    height=150
).repeat(
    row=['sepalLength' ,'sepalWidth', 'petalLength','petalWidth'],
    column=['sepalLength' ,'sepalWidth', 'petalLength','petalWidth']
).interactive()
```

Out[47]:



Parallel coordinates

Another useful visualization you can create with not-so-high-dimensional datasets is parallel coordinate visualization. Actually pandas supports parallel coordinate plots as well as "Andrews curve" (you can think of it as a smooth version of parallel coordinate.

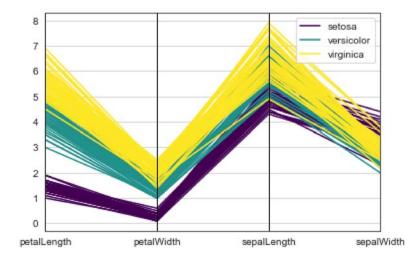
- https://pandas.pydata.org/pandas-docs/stable/visualization.html#parallel-coordinates (https://pandas.pydata.org/pandas-docs/stable/visualization.html#parallel-coordinates)
- https://pandas.pydata.org/pandas-docs/stable/visualization.html#andrews-curves (https://pandas.pydata.org/pandas-docs/stable/visualization.html#andrews-curves)

Q: Can you draw a parallel coordinate plot and a andrews curve plot of iris dataset? (I'm using viridis and winter colormap btw)

```
In [57]: from pandas.plotting import parallel_coordinates

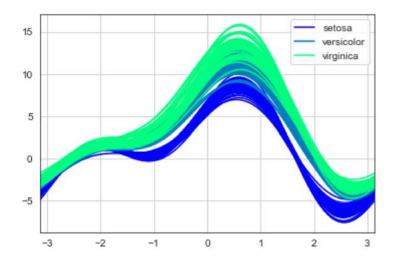
plt.figure()
parallel_coordinates(iris, 'species', colormap='viridis')
```

Out[57]: <matplotlib.axes._subplots.AxesSubplot at 0x1da219a1f98>



```
In [61]: from pandas.plotting import andrews_curves
    plt.figure()
    andrews_curves(iris, 'species', colormap='winter')
```

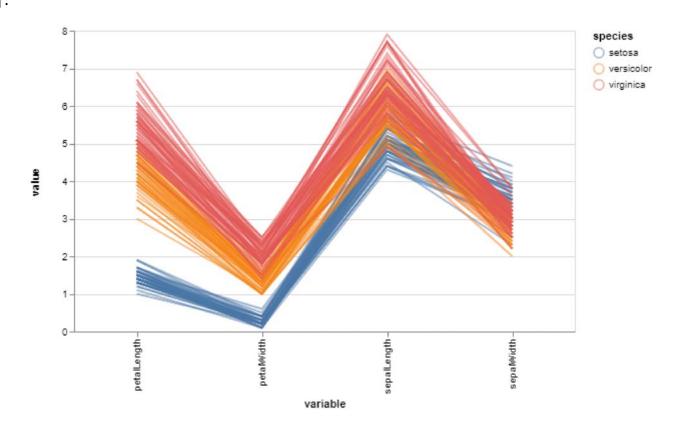
Out[61]: <matplotlib.axes._subplots.AxesSubplot at 0x1da2202c400>



We can also use altair.

```
In [65]: iris_transformed = iris.reset_index().melt(['species', 'index'])
    alt.Chart(iris_transformed).mark_line().encode(
        x='variable:N',
        y='value:Q',
        color='species:N',
        detail='index:N',
        opacity=alt.value(0.5),
    ).properties(width=500)
```

Out[65]:



Q: can you explain how iris_transformed is different from the original iris dataset and why do we need to transform in this way?

Since we would like the index to be available to the chart, we can explicitly turn it into a column using the reset_index() method of Pandas dataframes https://altair-viz.github.io/user_guide/data.html?highlight=reset_index%20melt). In addition, for converting wide-form data to the long-form data used by Altair, the melt method of dataframes was used, in which species and index are used as identifiers.

PCA

The <u>principal component analysis (PCA) (http://setosa.io/ev/principal-component-analysis/)</u> is the most basic dimensionality reduction method. For example, in the Iris dataset we have four variables (sepal_length, sepal_width, petal_length, petal_width). If we can reduce the number of variables to two, then we can easily visualize them in two dimensions.

PCA is already implemented in the <u>scikit-learn (http://scikit-learn.org/stable/)</u> package, a machine learning library in Python, which should have been included in Anaconda. If you don't have it, install it with:

conda install scikit-learn

or

pip install scikit-learn

In [66]: iris.head(2)

Out[66]:

	petalLength	petalWidth	sepalLength	sepalWidth	species
0	1.4	0.2	5.1	3.5	setosa
1	1.4	0.2	4.9	3.0	setosa

This is a four dimensional data. To run the PCA we want to isolate only the numerical columns.

```
In [68]: features = ['sepalLength', 'sepalWidth', 'petalLength', 'petalWidth']
   iris_only_features = iris[features]
   iris_only_features.head()
```

Out[68]:

	sepalLength	sepalWidth	petalLength	petalWidth
0	5.1	3.5	1.4	0.2
1	4.9	3.0	1.4	0.2
2	4.7	3.2	1.3	0.2
3	4.6	3.1	1.5	0.2
4	5.0	3.6	1.4	0.2

We should first create a PCA object and specify the number of components to obtain. Note that you can obtain more than two principal components.

```
In [75]: from sklearn.decomposition import PCA
pca = PCA(n_components=2) # set the number of components to 2
```

Now you can run fit() method to identify principal components.

```
In [76]: pca_iris_fitted = pca.fit(iris_only_features)
```

An important set of numbers that you want to look at is the explained variance ratio.

```
In [77]: pca_iris_fitted.explained_variance_ratio_
Out[77]: array([0.92461872, 0.05306648])
```

It tells you how much of the variance in the original dataset is explained by the principal components that you obtained. It seems like the first two components capture more than 95% of the variance in original dataset. This means that the PCA is very effective on this dataset and just using two principal components is a very good approximation to use all dimensions. Now you can use the result to transform the original dataset.

A convenient way to do both fitting and transforming is

You can see that this transformed matrix has two columns. Each column corresponds to the "loading" for one of the principal components.

Out[115]:

	PC1	PC2
0	-2.684126	0.319397
1	-2.714142	-0.177001
2	-2.888991	-0.144949
3	-2.745343	-0.318299
4	-2.728717	0.326755

Let's add the species information to the dataframe.

Q: add species column to iris_pca_df.

```
In [98]: iris_species = pd.DataFrame(data=iris.species, index=range(len(iris.species)))
    iris_species.head()
```

Out[98]:

	species
0	setosa
1	setosa
2	setosa
3	setosa
4	setosa

```
In [116]: # add a new column
    iris_pca_df['species']=iris.species
    iris_pca_df.head()
```

Out[116]:

	PC1	PC2	species
0	-2.684126	0.319397	setosa
1	-2.714142	-0.177001	setosa
2	-2.888991	-0.144949	setosa
3	-2.745343	-0.318299	setosa
4	-2.728717	0.326755	setosa

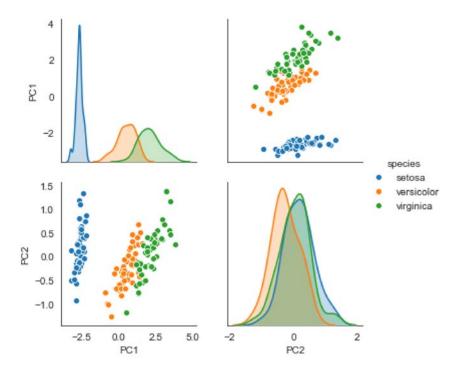
Now we can produce a scatterplot based on the two principal components. Well, let's just draw a pairplot.

In [119]: | sns.pairplot(iris_pca_df, hue='species')

C:\Users\yyezeret\AppData\Local\Continuum\Anaconda2\envs\dviz\lib\site-packages\scipy\s tats\stats.py:1713: FutureWarning: Using a non-tuple sequence for multidimensional inde xing is deprecated; use `arr[tuple(seq)]` instead of `arr[seq]`. In the future this wil l be interpreted as an array index, `arr[np.array(seq)]`, which will result either in a n error or a different result.

return np.add.reduce(sorted[indexer] * weights, axis=axis) / sumval

Out[119]: <seaborn.axisgrid.PairGrid at 0x1da23dafe80>



The PC1 seems to capture inter-species variation while PC2 seems to capture intra-species variation. (2) Interesting!

PCA with faces

Let's play with PCA with some faces. (2) (iii) (iii)

4096

```
In [120]: from sklearn.datasets import fetch_olivetti_faces

dataset = fetch_olivetti_faces(shuffle=True)
faces = dataset.data

downloading Olivetti faces from https://ndownloader.figshare.com/files/5976027 to C:\Us
```

downloading Olivetti faces from https://ndownloader.figshare.com/files/5976027 to C:\Us
ers\yyezeret\scikit_learn_data

So, this dataset contains 400 faces, and each of them has 4096 features (=pixels). Let's look at the first face:

It's an one-dimensional array with 4096 numbers. But a face should be a two-dimensional picture, right? Use numpy's reshape() (http://docs.scipy.org/doc/numpy/reference/generated/numpy.reshape.html) function as well as matplotlib's imshow() (<a href="http://matplotlib.org/api/pyplot_api.html#matplotlib.pyplot.imshow) function, transform this one-dimensional array into an appropriate 2-D matrix and draw it to show the face. You probably want to use plt.cm.gray as colormap.

Be sure to play with different shapes (e.g. 2 x 2048, 1024 x 4, 128 x 32, and so on) and think about why they look like what they look like. What is the right shape of the array?

Q: reshape the one-dimensional array into an appropriate two dimensional array and show the face

```
In [139]: # TODO: draw faces[0] with various shapes. Find the correct dimension.
# image_shape = (?, ?)
# plt.imshow( faces[0].reshape(image_shape), cmap=plt.cm.gray, interpolation='gaussian'
)

#sqrt(4096)=64 therefore the porper image will be around 64X64

imFace = np.array([[64,64],[2,2048],[1024,4],[128,32]])
for i, imgSize in enumerate(imFace, 1):
    plt.subplot( 2, 2, i)
    plt.imshow(faces[0].reshape(imgSize), cmap=plt.cm.gray, interpolation='gaussian')
    plt.xticks(())
    plt.yticks(())
```





Let's perform PCA on this dataset.

```
In [131]: from sklearn.decomposition import PCA
```

Set the number of components to 6:

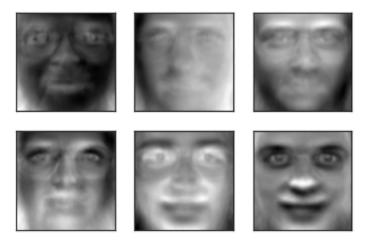
```
In [132]: n_components=6
    pca = PCA(n_components=n_components)
```

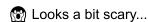
Fit the faces data:

PCA has an attribute called components_. It is a n_components \times n_features matrix, in our case 6×4096 . Each row is a component.

We can display the 6 components as images:

```
In [32]: for i, comp in enumerate(pca.components_, 1):
    plt.subplot(2, 3, i)
    plt.imshow(comp.reshape(image_shape), cmap=plt.cm.gray, interpolation='gaussian')
    plt.xticks(())
    plt.yticks(())
```





They are the "principal faces", which means that, by adding up these images with some appropriate weights, we can get a close approximation of the 400 images in the dataset!

We can get the coordinates of the 6 components to understand how each face is composed with the components.

```
In [140]: faces_pca_transformed = pca.transform(faces)
In [141]: faces_pca_transformed.shape
Out[141]: (400, 6)
```

faces_r is a 400×6 matrix. Each row corresponds to one face, containing the coordinates of the 6 components. For instance, the coordinates for the first face is

It seems that the second component (with coordinate 4.14403343) contributes the most to the first face. Let's display them together and see how similar they are:

```
In [143]: # display the first face image
    plt.subplot(1, 2, 1)
    plt.imshow(faces[0].reshape(image_shape), cmap=plt.cm.gray, interpolation='gaussian')
    plt.xticks(())
    plt.yticks(())

# display the second component
    plt.subplot(1, 2, 2)
    plt.imshow(pca.components_[1].reshape(image_shape), cmap=plt.cm.gray, interpolation='gaussian')
    plt.xticks(())
    plt.yticks(())
```

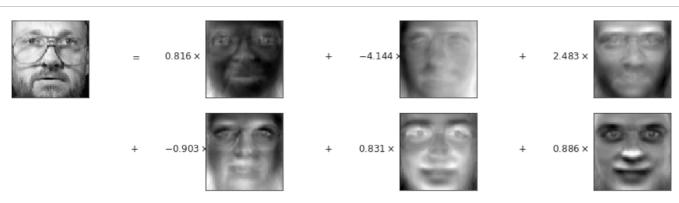
Out[143]: ([], <a list of 0 Text yticklabel objects>)





We can display the composition of faces in an "equation" style:

```
In [146]: from matplotlib import gridspec
          def display_image(ax, image):
              ax.imshow(image, cmap=plt.cm.gray, interpolation='nearest')
              ax.set xticks(())
              ax.set_yticks(())
          def display_text(ax, text):
              ax.text(.5, .5, text, size=12)
              ax.axis('off')
          face_idx = 0
          plt.figure(figsize=(16,4))
          gs = gridspec.GridSpec(2, 10, width_ratios=[5,1,1,5,1,1,5,1,1,5])
          # display the face
          ax = plt.subplot(gs[0])
          display_image(ax, faces[face_idx].reshape(image_shape))
          # display the equal sign
          ax = plt.subplot(gs[1])
          display_text(ax, r'$=$')
          # display the 6 coordinates
          for coord_i, gs_i in enumerate( [2,5,8,12,15,18] ):
              ax = plt.subplot(gs[gs_i])
              display_text( ax, r'$%.3f \times $' % faces_pca_transformed[face_idx][coord_i] )
          # display the 6 components
          for comp_i, gs_i in enumerate( [3,6,9,13,16,19] ):
              ax = plt.subplot(gs[gs_i])
              display_image( ax, pca.components_[comp_i].reshape(image_shape) )
          # display the plus sign
          for gs_i in [4,7,11,14,17]:
              ax = plt.subplot(gs[gs_i])
              display_text(ax, r'$+$')
```



We can directly see the results of this addition.













It becomes more and more real, although quite far with only several components.

NMF

There is another pretty cool dimensionality reduction method called NMF (Non-negative matrix factorization). It is widely used in many domains, such as identifying topics in documents, identifying key components in images, and so on. The key idea is by forcing every element in the decomposed matrices positive, NMF breaks something into **parts** that we can add together.



As you can see here, each 'component' of NMF picks up a certain part of the face (light area), such as eyes, chin, nose, and so on. Very cool.

Q: Can you show the reconstructed faces using the first n components, as we did for the PCA?

















Unlike PCA that keeps superposing positive and negative images, NMF tends to gradually add multiple parts to the image. This is why it is widely used for many decomposing tasks such as detecting topics from documents.

t-SNE, Isomap, and MDS

Isomap, t-SNE, and MDS are nonlinear dimensionality reduction methods. Isomap preserves only the local relationships, MDS tries to preserve everything, and t-SNE is more flexible. t-SNE is very popular especially in machine learning.

Let's try t-SNE out with the iris data.

Q: Fit-transform the iris data with t-SNE and create a scatterplot of it.

```
In [161]: from sklearn.manifold import TSNE
    from sklearn.manifold import Isomap
    from sklearn.manifold import MDS
    from sklearn.datasets import load_iris

    iris = load_iris()

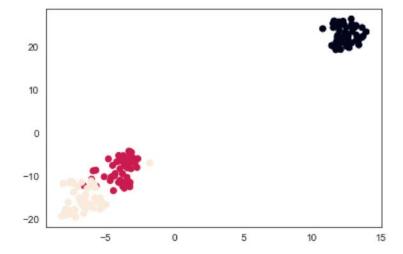
    n_components=2

    X = iris.data[:1000]
    y = iris.target[:1000]

    tsne = TSNE(n_components=n_components, random_state=0, perplexity=30.0)
    X_2d = tsne.fit_transform(X)

# Visualize the data
plt.scatter(X_2d[:, 0], X_2d[:, 1], c=y)
```

Out[161]: <matplotlib.collections.PathCollection at 0x1da2661d518>



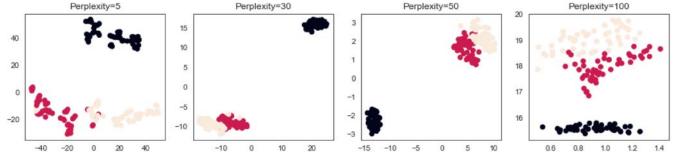
The hyperparameter perplexity determines how to balance attention between local and global aspects of your data. Changing this parameter (default is 30) may cause drastic changes in the output. Play with multiple values of perplexity.

```
In [176]: plt.figure(figsize=(15,3))
    plt.xlim(0, 10)
    plt.ylim(0, 10)

perplexities = [5, 30, 50, 100]
    for i, perplexity in enumerate(perplexities,1):
        plt.subplot(1, 4, i)
        tsne = TSNE(n_components=n_components, perplexity=perplexity)
        X_2d = tsne.fit_transform(X)

    plt.title("Perplexity=%d" % perplexity)

# Visualize the data
    plt.scatter(X_2d[:, 0], X_2d[:, 1], c=y)
```



If you want to learn more about t-SNE, play with https://distill.pub/2016/misread-tsne/ (https://experiments.withgoogle.com/visualizing-high-dimensional-space (<a href="https://experiments.withgoogle.com/

Visualizing the Digits dataset

This is a classic dataset of images of handwritten digits. It contains 1797 images with (8*8=64) pixels each.

digits.data stores the images:

```
In [178]: | digits.data[0]
                                              0.,
Out[178]: array([ 0.,
                      0.,
                           5., 13.,
                                    9.,
                                        1.,
                                                            0., 13., 15., 10.,
                                                   0.,
                                                       0.,
                15., 5.,
                               0.,
                                    3., 15.,
                                              2.,
                                                   0., 11.,
                                                                 0., 0.,
                           0.,
                                                            8.,
                      0.,
                               8.,
                                         0., 0.,
                                                  5., 8.,
                           0.,
                                    8.,
                                                            0.,
                                                                 0.,
                                                            0.,
                      0., 4., 11.,
                                    0.,
                                         1., 12.,
                                                 7.,
                                                      0.,
                                                                 2., 14.,
                10., 12., 0., 0.,
                                    0.,
                                         0., 6., 13., 10.,
                                                            0.,
```

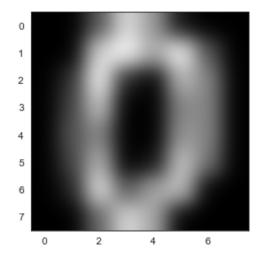
and digits target is the classes (or labels) that the images belong to. There are 10 classes in total.

```
In [179]: digits.target
Out[179]: array([0, 1, 2, ..., 8, 9, 8])
```

Q: use imshow to display the first image.

```
In [188]: image_shape = (8,8)
    plt.imshow(digits.data[0].reshape(image_shape), cmap=plt.cm.gray, interpolation='gaussia
    n' )
```

Out[188]: <matplotlib.image.AxesImage at 0x1da253c2cc0>



Let's first reorder the data points according to the handwritten numbers. We can use np.vstack (np.hstack (https://docs.scipy.org/doc/numpy/reference/generated/numpy.hstack.html).

Then initialize a tsne model. For the meaning of the parameters see here (http://scikit-learn.org/stable/modules/generated/sklearn.manifold.TSNE.html).

```
In [190]: # Implement
tsne = TSNE(n_components=n_components, random_state=0)
```

Fit the model on the data.

```
In [191]: digits_proj = tsne.fit_transform(X)
```

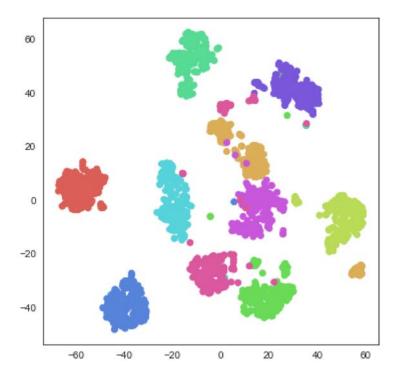
Plot the results. Seaborn's http://seaborn.hls_palette) palatte provides evenly spaced colors in HLS hue space, we can divide it into 10 colors.

```
In [192]: palette = np.array(sns.color_palette("hls", 10))
```

Make a scatter plot of the first component against the second component, with color based on the numbers.

```
In [193]: plt.figure(figsize = (6,6))
  plt.scatter(digits_proj[:,0], digits_proj[:,1],c=palette[y])
```

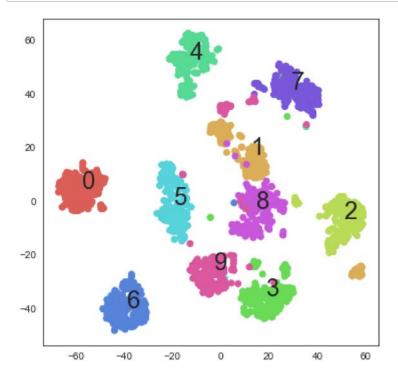
Out[193]: <matplotlib.collections.PathCollection at 0x1da2675e710>



We can add some text for each cluster. The place of the text can be the center of the cluster. We can use np.median to find the centers. To simplify things, we can make the code into a function.

```
In [194]: def plot_scatter(projection):
    plt.figure(figsize = (6,6))
    plt.scatter(projection[:,0], projection[:,1],c=palette[y])
    for i in range(10):
        # Position of each label.
        xtext, ytext = np.median(projection[y == i, :], axis=0)
        txt = plt.text(xtext, ytext, str(i), fontsize=24)
```

In [195]: plot_scatter(digits_proj)

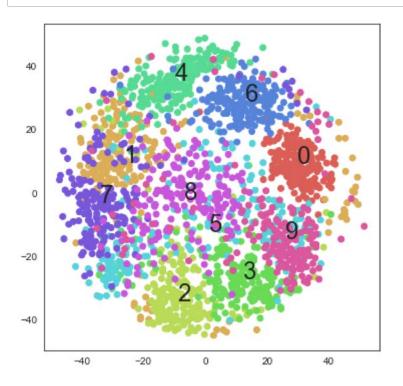


Comparison with Isomap and MDS

We talked about MDS and Isomap in class as two other manifold learning methods. Sklearn also has implementations for this two algorithms: MDS (http://scikit-learn.org/stable/modules/generated/sklearn.manifold.MDS.html) and Isomap.httml), so the usage is very similar. Examples for using this methods can be found http://scikit-learn.org/stable/auto_examples/manifold/plot_lle_digits.html).

Can you make another two plots with these two methods? You only need to change the models and call the plot_scatter function,

In [196]: # Implement MDS
 projection = MDS(n_components=n_components, random_state=0).fit_transform(X)
 plot_scatter(projection)



In [198]: # Implement Isomap
 projection = Isomap(n_components=n_components).fit_transform(X)
 plot_scatter(projection)

