Summer 2020 CX4641/CS7641 Homework 3

Instructor: Dr. Mahdi Roozbahani

Deadline: July 10th, Friday, 11:59 pm

- No unapproved extension of the deadline is allowed. Late submission will lead to 0 credit.
- Discussion is encouraged on Piazza as part of the Q/A. However, all assignments should be done individually.

Instructions for the assignment

- In this assignment, we have programming and writing questions.
- To switch between cell for code and for markdown, see the menu -> Cell -> Cell Type
- You could directly type the Latex equations in the markdown cell.
- Typing with Latex\markdown is required for all the written questions. Handwritten answers would not be accepted.
- If a question requires a picture, you could use this syntax $"< imgsrc ="" style =" width: 300px; " / >"$ to include them within your ipython notebook.
- Questions marked with **[P]** are programming only and should be submitted to the autograder. Questions marked with **[W]** may required that you code a small function or generate plots, but should **NOT** be submitted to the autograder. It should be submitted on the writing portion of the assignment on gradescope
- The outline of the assignment is as follows:
  - Q1 [20 pts] > Naive Bayes classification. **[W]** items 1.1 | **[P]** items 1.2
  - Q2 [30 pts] > Image compression with PCA **[W]** 2.2 and 2.3 | **[P]** items 2.1
  - Q3 [Undergrad: 55+20 (bonus) pts| Grad: 75 pts] > Regression and regularization **[W]** items 3.2, 3.3, 3.4 and 3.5 | **[P]** items 3.1
  - Q4 [20 pts] > Understanding PCA **[W]** items 4.1 and 4.2 | **[P]** None
  - Q5 [Bonus for all][30 pts] > Manifold learning with Isomap **[W]** items 5.2 | **[P]** items 5.1

Using the autograder

- You will find two assignments on Gradescope that correspond to HW3: "HW3 - Programming" and "HW3 - Non-programming".
- You will submit your code for the autograder on "HW3 - Programming" in the following format:
  - nb.py
  - imgcompression.py
  - regression.py
  - isomap.py
- All you will have to do is to copy your implementations of the classes "NaiveBayes", "ImgCompression", "Regression", "Isomap" onto the respective files. We provided you different .py files and we added libraries in those files please DO NOT remove those lines and add your code after those lines. Note that these are the only allowed libraries that you can use for the homework.
- You are allowed to make as many submissions until the deadline as you like. Additionally, note that the autograder tests each function separately, therefore it can serve as a useful tool to help you debug your code if you are not sure of what part of your implementation might have an issue.
- **For the "HW3 - Non-programming" part, you will download your jupyter notbook as HTML, print it as a PDF from your browser and submit it on Gradescope. To download the notebook as html, click on "File" on the top left corner of this page and select "Download as > HTML". The non-programming part corresponds to Q2, Q3.3 (both your response and the generated images with your implementation) and Q4.2.**

In [1]:
```
import numpy as np
import json
from matplotlib import pyplot as plt
from sklearn.feature_extraction import text
from sklearn.datasets import load_boston, load_diabetes, load_digits, load_breast_cancer, load_iris, load_wine
from scipy.sparse import csr_matrix
from scipy.sparse.csgraph import floyd_warshall
%matplotlib inline
```

1. Naive Bayes Classification [20pts]

Processing math: 100%

In Bayesian classification, we're interested in finding the probability of a label given some observed feature vector $x = [x_1, . . , x_d]$, which we can write as $P(y \mid x_1, . . , x_d)$. Bayes's theorem tells us how to express this in terms of quantities we can compute more directly:

$$P(y \mid x_1, . . , x_d) = \frac{P(x_1, . . , x_d \mid y)P(y)}{P(x_1, . . , x_d)}$$

The main assumption in Naive Bayes is that, given the label, the observed features are conditionally independent i.e.

$$P(x_1, . . , x_d \mid y) = P(x_1 \mid y) \times . . \times P(x_d \mid y)$$

Therefore, we can rewrite Bayes rule as

$$P(y \mid x_1, . . , x_d) = \frac{P(x_1 \mid y) \times . . \times P(x_d \mid y)P(y)}{P(x_1, . . , x_d)}$$

Training Naive Bayes

One way to train a Naive Bayes classifier is done using frequentist approach to calculate probability, which is simply going over the training data and calculating the frequency of different observations in the training set given different labels. For example,

$$P(x_1 = i \mid y = j) = \frac{P(x_1 = i, y = j)}{P(y = j)} = \frac{\text{Number of times in training data } x_1 = i \text{ and } y = j}{\text{Total number of times in training data } y = j}$$

Testing Naive Bayes

During the testing phase, we try to estimate the probability of a label given an observed feature vector. We combine the probabilities computed from training data to estimate the probability of a given label. For example, if we are trying to decide between two labels y_1 and y_2, then we compute the ratio of the posterior probabilities for each label:

$$\frac{P(y_1 \mid x_1, . . , x_d)}{P(y_2 \mid x_1, . . , x_d)} = \frac{P(x_1, . . , x_d \mid y_1)}{P(x_1, . . , x_d \mid y_2)} \frac{P(y_1)}{P(y_2)} = \frac{P(x_1 \mid y_1) \times . . \times P(x_d \mid y_1)P(y_1)}{P(x_1 \mid y_2) \times . . \times P(x_d \mid y_2)P(y_2)}$$

All we need now is to compute $P(x_1 | y_i), . . , P(x_d \mid y_i)$ and $P(y_i)$ for each label by pluging in the numbers we got during training. The label with the higher posterior probabilities is the one that is selected.

1.1 Supermarket [5pts] **[W]**

A local supermarket specializing in breakfast cereals decides to analyze the buying patterns of its customers. They make a small survey asking 6 randomly chosen people their age (older or younger than 60 years) and which of the breakfast cereals (Cornflakes, Frosties, Sugar Puffs, Branflakes) they like. Each respondent provides a vector with entries 1 or 0 corresponding to whether they like or dislike the cereal. Thus a respondent with (1101) would like Cornflakes, Frosties and Branflakes, but not Sugar Puffs. The older than 60 years respondents provide the following data (1000), (1001), (1111), (0001). The younger than 60 years old respondents responded (0110), (1110). A new customer comes into the supermarket and says she only likes Frosties and Sugar Puffs. Using naive Bayes, Is the new customer older than 60?

Processing math: 100%

Answer:

The survey results for people >60 are:

Cornflakes	Frosties	Sugar Puffs	Branflakes
1	0	0	0
1	0	0	1
1	1	1	1
0	0	0	1

The survey results for people <60 are:

Cornflakes	Frosties	Sugar Puffs	Branflakes
0	1	1	0
1	1	1	0

We have the overall probabilities of being old or young as:

$$P(Old) = \frac{2}{3}; P(Young) = \frac{1}{3}$$

From the above tables, we can derive the following maximum likelihood estimates given an old customer:

$$P(C = 1 \mid Old) = \frac{3}{4}; P(F = 1 \mid Old) = \frac{1}{4}; P(S = 1 \mid Old) = \frac{1}{4}; P(B = 1 \mid Old) = \frac{3}{4}$$

Given a young customer, we get:

$$P(C = 1 \mid Young) = \frac{1}{2}; P(F = 1 \mid Young) = 1; P(S = 1 \mid Young) = 1; P(B = 1 \mid Young) = 0$$

Now, applying Bayes theorem, for a posterior that the customer is young, we get:

$$P(Young \mid C = 0, F = 1, S = 1, B = 0) = \frac{P(C = 0, F = 1, S = 1, B = 0 \mid Young)P(Young)}{P(C = 0, F = 1, S = 1, B = 0 \mid Young) + P(C = 0, F = 1, S = 1, B = 0 \mid Old)}$$

$$= \frac{\frac{1}{2} \times 1 \times 1 \times 1 \times \frac{1}{3}}{\frac{1}{2} \times 1 \times 1 \times 1 + \frac{1}{4} \times \frac{1}{4} \times \frac{1}{4} \times \frac{1}{4}} = \frac{128}{387}$$

Similarly, for the posterior that the customer is old:

$$P(Old \mid C = 0, F = 1, S = 1, B = 0) = \frac{P(C = 0, F = 1, S = 1, B = 0 \mid Old)P(Old)}{P(C = 0, F = 1, S = 1, B = 0 \mid Young) + P(C = 0, F = 1, S = 1, B = 0 \mid Old)}$$

$$= \frac{\frac{1}{4} \times \frac{1}{4} \times \frac{1}{4} \times \frac{1}{4} \times \frac{2}{3}}{\frac{1}{2} \times 1 \times 1 \times 1 + \frac{1}{4} \times \frac{1}{4} \times \frac{1}{4} \times \frac{1}{4}} = \frac{2}{387}$$

So, from these values, we see that the ratios of the posterior probabilities $\frac{P(Young \mid C=0, F=1, S=1, B=0)}{P(Old \mid C=0, F=1, S=1, B=0)} > 1$, which shows that the new customer is younger than 60.

1.2 The Federalist Papers [15pts] **[P]**

The Federalist Papers (https://en.wikipedia.org/wiki/The_Federalist_Papers) were a series of essays written in 1787–1788 meant to persuade the citizens of the State of New York to ratify the Constitution and which were published anonymously under the pseudonym "Publius". In later years the authors were revealed as Alexander Hamilton, John Jay, and James Madison. However, there is some disagreement as to who wrote which essays. Hamilton wrote a list of which essays he had authored only days before being killed in a duel with then Vice President Aaron Burr. Madison wrote his own list many years later, which is in conflict with Hamilton's list on 12 of the essays. Since by this point the two (who were once close friends) had become bitter rivals, historians have long been unsure as to the reliability of both lists. We will try to settle this dispute using a simple Naive Bayes classifier.

The code which is provided loads the documents and builds a "bag of words" representation (https://en.wikipedia.org/wiki/Bag-of-words_model) of each document. Your task is to complete the missing portions of the code and to determine your best guess as to who wrote each of the 12 disputed essays. (Hint: H and M are the labels that stand for Hamilton and Madison, while the label D stands for disputed for the papers we are trying to label in our data. Our job here is to define whether D essays belong to H or M using Naive Bayes. Note that the label D for disputed, is completely unrelated to the feature dimension D which is an integer).

In [2]:
```
import numpy as np
import json
from sklearn.feature_extraction import text

class NaiveBayes(object):

    def __init__(self):
        # Load Documents
        x = open('fedpapers_split.txt').read()
        papers = json.loads(x)

        # split Documents
        papersH = papers[0] # papers by Hamilton
        papersM = papers[1] # papers by Madison
        papersD = papers[2] # disputed papers

        # Number of Documents for H, M and D
        nH = len(papersH)
        nM = len(papersM)
        nD = len(papersD)

        '''To ignore certain common words in English that might skew your model, we add them to the stop words
        list below. You may want to experiment by choosing your own list of stop words, but be sure to keep
        'HAMILTON' and 'MADISON' in this list at a minimum, as their names appear in the text of the papers
        and leaving them in could lead to unpredictable results '''

        stop_words = text.ENGLISH_STOP_WORDS.union({'HAMILTON','MADISON'})
        #stop_words = {'HAMILTON','MADISON'}
        # Form bag of words model using words used at least 10 times
        vectorizer = text.CountVectorizer(stop_words=stop_words,min_df=10)
        X = vectorizer.fit_transform(papersH+papersM+papersD).toarray()

        '''To visualize the full list of words remaining after filtering out stop words and words used less
        than min_df times uncomment the following line'''
        #print(vectorizer.vocabulary_)

        # split word counts into separate matrices
        self.XH, self.XM, self.XD = X[:nH,:], X[nH:nH+nM,:], X[nH+nM:,:]


    def _likelihood_ratio(self, XH, XM): # [5pts]
        '''
        Args:
            XH: nH x D where nH is the number of documents that we have for Hamilton,
                while D is the number of features (we use the word count as the feature)
            XM: nM x D where nM is the number of documents that we have for Madison,
                while D is the number of features (we use the word count as the feature)
        Return:
            fratio: 1 x D vector of the likelihood ratio of different words (Hamilton/Madison)
        '''
        D = XH.shape[1]
        sum_H = XH.sum(axis=0)
        sum_M = XM.sum(axis=0)

        prob_H = (sum_H+1)/(sum_H.sum()+D)
        prob_M = (sum_M+1)/(sum_M.sum()+D)
        fratio = np.divide(prob_H,prob_M).reshape(1,-1)
        return fratio

    def _priors_ratio(self, XH, XM): # [5pts]
        '''
        Args:
            XH: nH x D where nH is the number of documents that we have for Hamilton,
                while D is the number of features (we use the word count as the feature)
            XM: nM x D where nM is the number of documents that we have for Madison,
                while D is the number of features (we use the word count as the feature)
        Return:
            pr: prior ratio of (Hamilton/Madison)
        '''
        pr = XH.sum()/XM.sum()
        return pr

    def classify_disputed(self, fratio, pratio, XD): # [5pts]
        '''
        Args:
            fratio: 1 x D vector of ratio of likelihoods of different words
            pratio: 1 x 1 number
            XD: 12 x D bag of words representation of the 12 disputed documents (D = 1307 which are the number of features for ea
ch document)
        Return:
             1 x 12 list, each entry is H to indicate Hamilton or M to indicate Madison for the corrsponding document
        '''
        h_or_m = []
        for i in range(len(XD)):
            lr_pow = np.array([np.power(a,b) for a,b in zip(fratio,XD[i])])
            lr_pow = np.prod(lr_pow)
            likelihood_ratio = lr_pow*pratio
            if likelihood_ratio>0.5:
                h_or_m.append('H')
            else:
                h_or_m.append('M')
        return h_or_m
```

Processing math: 100%

```
In [3]: if __name__ == '__main__':
            NB = NaiveBayes()
            fratio = NB._likelihood_ratio(NB.XH, NB.XM)
            pratio = NB._priors_ratio(NB.XH, NB.XM)
            resolved = NB.classify_disputed(fratio, pratio, NB.XD)
            print(resolved)
```

```
['H', 'H', 'H', 'H', 'H', 'H', 'H', 'H', 'H', 'H', 'H', 'H']

C:\Users\Prathik\Anaconda3\lib\site-packages\sklearn\feature_extraction\text.py:300: UserWarning: Your stop_words may be inconsi
stent with your preprocessing. Tokenizing the stop words generated tokens ['hamilton', 'madison'] not in stop_words.
  'stop_words.' % sorted(inconsistent))
```

2. Image compression with PCA [30 pts]

Load images data and plot

```
In [4]: # Load Image
        image = plt.imread("hw3_img.jpg")/255.
        #plot image
        fig = plt.figure(figsize=(10,10))
        plt.imshow(image)
```

```
Out[4]: <matplotlib.image.AxesImage at 0x16d13fd2fc8>
```

```
In [5]: def rgb2gray(rgb):
            return np.dot(rgb[...,:3], [0.299, 0.587, 0.114])

        fig = plt.figure(figsize=(10, 10))
        # plot several images
        plt.imshow(rgb2gray(image), cmap=plt.cm.bone)
```

```
Out[5]: <matplotlib.image.AxesImage at 0x16d12efe148>
```

Processing math: 100%

2.1 Image compression [20pts] **[P]**

The SVD allows us to compress an image by throwing away the least important information. The greater the singular values -> the greater the variance -> most information from the corresponding singular vector. SVD each matrix and get rid of the small singular values to compress the image. The loss of inforamtion is negligible as the difference is very difficult to be spotted. Principal Component Analysis (https://en.wikipedia.org/wiki/Principal_component_analysis) (PCA) follows the same process to elimate the small variance eigenvalues and their vectors. With PCA, we center the data first by subtracting the mean. Each singular value tells us how much of the variance of a matrix (e.g. image) is captured in each component. For example, the variance captured by the first component is

$$\frac{\sigma_1}{\sum_{i=1}^{n} \sigma_i}$$

where σ_i is the i^{th} singular value. You need to finish the following functions to do SVD and then reconstruct the image by components.

Processing math: 100%

In [6]:
```python
from matplotlib import pyplot as plt
import numpy as np

class ImgCompression(object):
    def __init__(self):
        pass

    def svd(self, X): # [5pts]
        """
        Do SVD. You could use numpy SVD.
        Your function should be able to handle black and white
        images (N x D arrays) as well as color images (N x D x 3 arrays)
        In the image compression, we assume that each colum of the image is a feature. Image is the matrix X.
        Args:
            X: N x D array corresponding to an image (N x D x 3 if color image)
        Return:
            U: N x N (N x N x 3, for color images)
            S: min(N, D) x 1 (min(N, D) x 3, for color images)
            V: D x D (D x D x 3, for color images)
        """
        N,D = X.shape[0],X.shape[1]
        if X.ndim == 3:
            U = np.zeros((N,N,3))
            S = np.zeros((min(N,D),3))
            V = np.zeros((D,D,3))
            for i in range(3):
                U_temp,S_temp,V_temp = np.linalg.svd(X[:,:,i],compute_uv=True, full_matrices=True,hermitian=False)
                U[:,:,i] = U_temp
                S[:,i] = S_temp
                V[:,:,i] = V_temp
        else:
            U,S,V = np.linalg.svd(X,compute_uv=True,full_matrices=True, hermitian=False)
        return U,S,V

    def rebuild_svd(self, U, S, V, k): # [5pts]
        """
        Rebuild SVD by k componments.
        Args:
            U: N x N (N x N x 3, for color images)
            S: min(N, D) x 1 (min(N, D) x 3, for color images)
            V: D x D (D x D x 3, for color images)
            k: int corresponding to number of components
        Return:
            Xrebuild: N x D array of reconstructed image (N x D x 3 if color image)

        Hint: numpy.matmul may be helpful for reconstructing color images
        """

        N,D = U.shape[0],V.shape[0]


        if U.ndim == 3:
            Xrebuild = np.zeros((N,D,3))
            for i in range(3):
                U_temp = U[:,0:k,i]
                S_temp = S[:,i]
                S_temp = np.diag(S_temp[0:k])
                V_temp = V[0:k,:,i]
                Xrebuild_temp = U_temp@S_temp@V_temp
                Xrebuild[:,:,i] = Xrebuild_temp
        else:
            U_new = U[:,0:k]
            S_new = np.diag(S[0:k])
            V_new = V[0:k,:]
            Xrebuild = U_new@S_new@V_new

        return Xrebuild


    def compression_ratio(self, X, k): # [5pts]
        """
        Compute compression of an image: (num stored values in compressed)/(num stored values in original)
        Args:
          X: N x D array corresponding to an image (N x D x 3 if color image)
          k: int corresponding to number of components
        Return:
          compression_ratio: float of proportion of storage used by compressed image
        """
        N,D = X.shape[0],X.shape[1]
        compression_ratio = k/min(N,D)
        return compression_ratio


    def recovered_variance_proportion(self, S, k): # [5pts]
        """
        Compute the proportion of the variance in the original matrix recovered by a rank-k approximation

        Args:
         S: min(N, D) x 1 (min(N, D) x 3 for color images) of singular values for the image
         k: int, rank of approximation
        Return:
         recovered_var: int (array of 3 ints for color image) corresponding to proportion of recovered variance
        """
```
Processing math: 100%

```
        if S.ndim == 1:
            recovered_var = 0
            denom = np.sum(S**2)
            for i in range(k):
                recovered_var += ((S[i]**2)/denom)

        elif S.shape[1] == 3:
            recovered_var = []
            for col in range(S.shape[1]):
                var_temp = 0
                denom = np.sum(S[:,col]**2)
                for i in range(k):
                    var_temp += (S[i,col]**2)/denom
                recovered_var.append(var_temp)

        return recovered_var
```

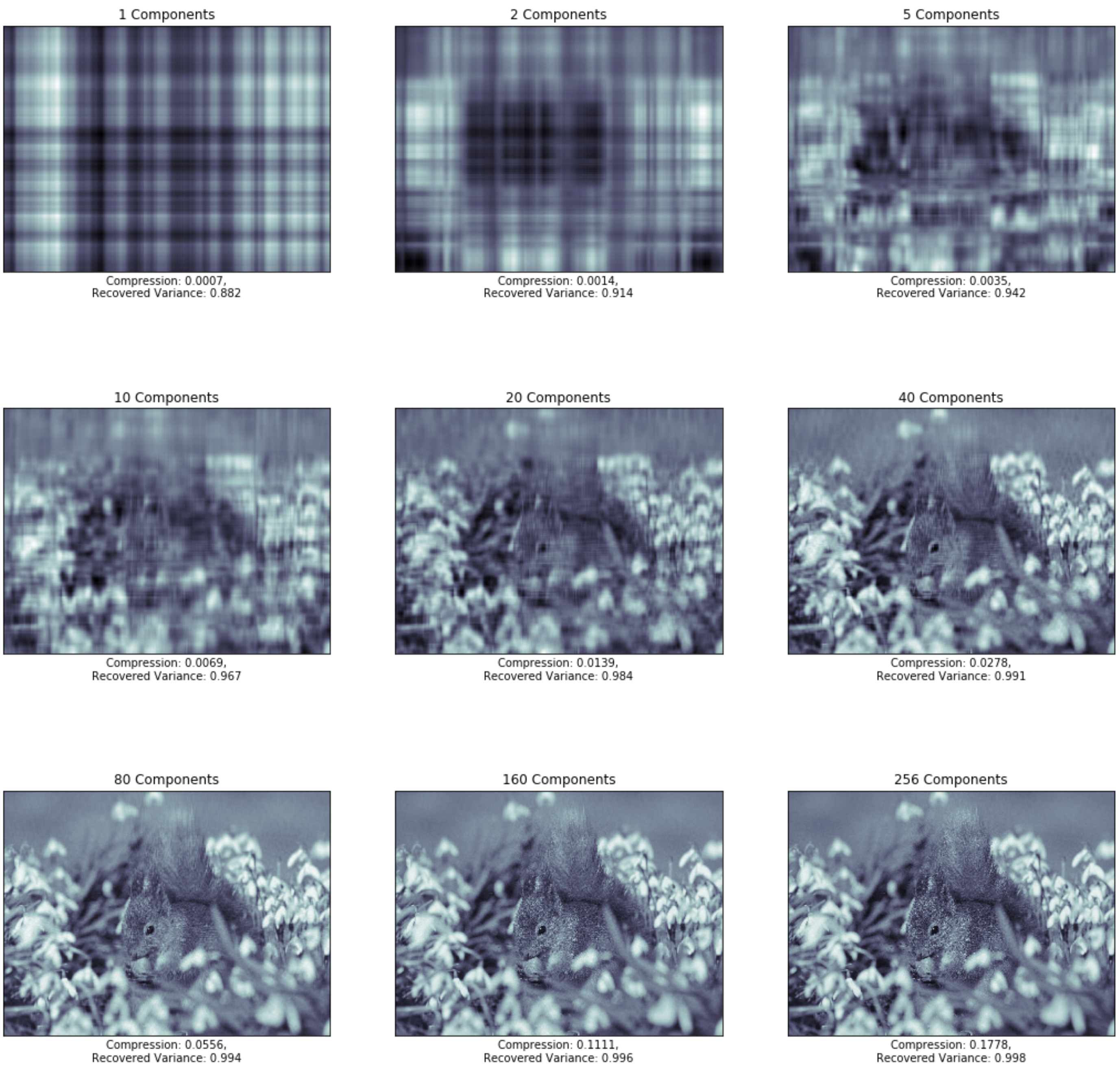
2.2 Black and white [5 pts] **[W]**

Use your implementation to generate a set of images compressed to different degrees. Include the images in your non-programming submission to the assignment.

In [7]:
```python
#helper do not need to change
imcompression = ImgCompression()
bw_image = rgb2gray(image)
U, S, V = imcompression.svd(bw_image)
component_num = [1,2,5,10,20,40,80,160,256]

fig = plt.figure(figsize=(18, 18))

# plot several images
i=0
for k in component_num:
    img_rebuild = imcompression.rebuild_svd(U, S, V, k)
    c = np.around(imcompression.compression_ratio(bw_image, k), 4)
    r = np.around(imcompression.recovered_variance_proportion(S, k), 3)
    ax = fig.add_subplot(3, 3, i + 1, xticks=[], yticks=[])
    ax.imshow(img_rebuild, cmap=plt.cm.bone)
    ax.set_title(f"{k} Components")
    ax.set_xlabel(f"Compression: {c},\nRecovered Variance: {r}")
    i = i+1
```



2.3 Color image [5 pts] **[W]**

Use your implementation to generate a set of images compressed to different degrees. Include the images in your non-programming submission to the assignment.

In [8]:

```python
#helper do not need to change
imcompression = ImgCompression()
U, S, V = imcompression.svd(image)
component_num = [1,2,5,10,20,40,80,160,256]

fig = plt.figure(figsize=(18, 18))

# plot several images
i=0
for k in component_num:
    img_rebuild = imcompression.rebuild_svd(U, S, V, k)
    c = np.around(imcompression.compression_ratio(image, k), 4)
    r = np.around(imcompression.recovered_variance_proportion(S, k), 3)
    ax = fig.add_subplot(3, 3, i + 1, xticks=[], yticks=[])
    ax.imshow(img_rebuild)
    ax.set_title(f"{k} Components")
    ax.set_xlabel(f"Compression: {np.around(c,4)},\nRecovered Variance:  R: {r[0]}  G: {r[1]}  B: {r[2]}")
    i = i+1
```

```
Clipping input data to the valid range for imshow with RGB data ([0..1] for floats or [0..255] for integers).
Clipping input data to the valid range for imshow with RGB data ([0..1] for floats or [0..255] for integers).
Clipping input data to the valid range for imshow with RGB data ([0..1] for floats or [0..255] for integers).
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Clipping input data to the valid range for imshow with RGB data ([0..1] for floats or [0..255] for integers).
```
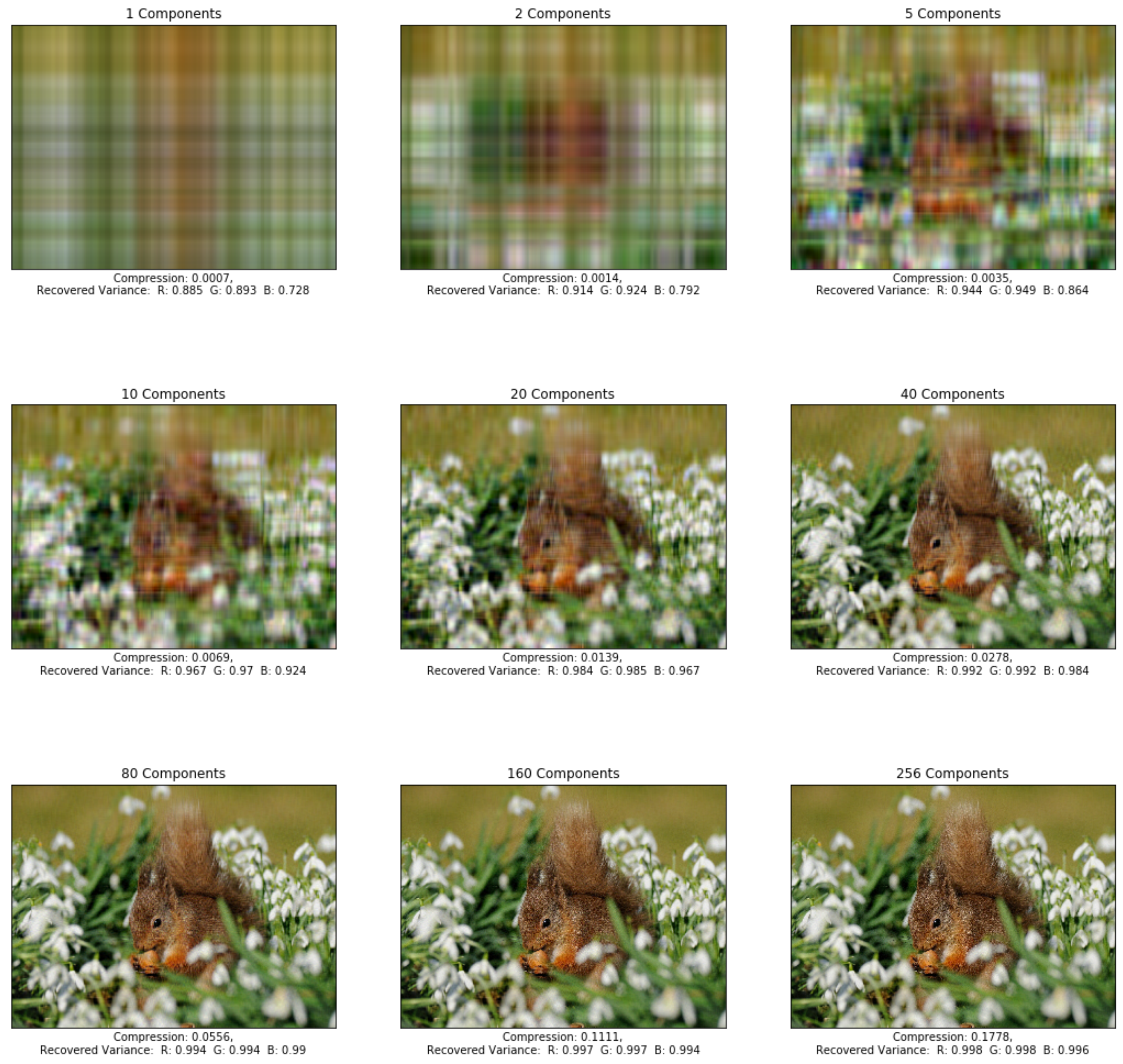


1 Components
Compression: 0.0007,
Recovered Variance: R: 0.885 G: 0.893 B: 0.728
2 Components
Compression: 0.0014,
Recovered Variance: R: 0.914 G: 0.924 B: 0.792
5 Components
Compression: 0.0035,
Recovered Variance: R: 0.944 G: 0.949 B: 0.864
10 Components
Compression: 0.0069,
Recovered Variance: R: 0.967 G: 0.97 B: 0.924
20 Components
Compression: 0.0139,
Recovered Variance: R: 0.984 G: 0.985 B: 0.967
40 Components
Compression: 0.0278,
Recovered Variance: R: 0.992 G: 0.992 B: 0.984
80 Components
Compression: 0.0556,
Recovered Variance: R: 0.994 G: 0.994 B: 0.99
160 Components
Compression: 0.1111,
Recovered Variance: R: 0.997 G: 0.997 B: 0.994
256 Components
Compression: 0.1778,
Recovered Variance: R: 0.998 G: 0.998 B: 0.996

3 Polynomial regression and regularization [Undergrad: 55 pts + 20 Bonus pts | Grad: 75pts]

3.1 Regression and regularization implementations **[P]**

We have three methods to fit linear and ridge regression models: 1) close form; 2) gradient descent (GD); 3) Stochastic gradient descent (SGD). For undergraduate students, you are required to implement the closed form for linear regression and for ridge regression, the others 4 methods are bonus parts. For graduate students, you are required to implement all of them. We use the term weight in the following code. Weights and parameters (θ) have the same meaning here. We used parameters (θ) in the lecture slides.

Processing math: 100%

```
In [1]: import numpy as np
        class Regression(object):
            def __init__(self):
                pass

            def rmse(self, pred, label): # [5pts]
                '''
                This is the root mean square error.
                Args:
                    pred: numpy array of length N x 1, the prediction of labels
                    label: numpy array of length N x 1, the ground truth of labels
                Return:
                    a float value
                '''
                rmse = np.sqrt(((pred-label)**2).mean())
                return rmse

            def construct_polynomial_feats(self, x, degree): # [5pts]
                """
                Args:
                    x: numpy array of length N, the 1-D observations
                    degree: the max polynomial degree
                Return:
                    feat: numpy array of shape Nx(degree+1), remember to include
                    the bias term. feat is in the format of:
                    [[1.0, x1, x1^2, x1^3, ....,],
                     [1.0, x2, x2^2, x2^3, ....,],
                     ......
                    ]
                """
                x = x.reshape(-1,1)
                x_rep = np.repeat(x,degree+1,axis=1)
                deg_arr = np.arange(degree+1)
                feat = np.power(x_rep,deg_arr)
                return feat


            def predict(self, xtest, weight): # [5pts]
                """
                Args:
                    xtest: NxD numpy array, where N is number
                           of instances and D is the dimensionality of each
                           instance
                    weight: Dx1 numpy array, the weights of linear regression model
                Return:
                    prediction: Nx1 numpy array, the predicted labels
                """
                prediction = xtest@weight
                return prediction

            # =================
            # LINEAR REGRESSION
            # Hints: in the fit function, use close form solution of the linear regression to get weights.
            # For inverse, you can use numpy linear algebra function
            # For the predict, you need to use linear combination of data points and their weights (y = theta0*1+theta1*X1+...)

            def linear_fit_closed(self, xtrain, ytrain): # [5pts]
                """
                Args:
                    xtrain: N x D numpy array, where N is number of instances and D is the dimensionality of each instance
                    ytrain: N x 1 numpy array, the true labels
                Return:
                    weight: Dx1 numpy array, the weights of linear regression model
                """
                weight = np.linalg.inv(xtrain.T@xtrain)@xtrain.T@ytrain
                return weight

            def linear_fit_GD(self, xtrain, ytrain, epochs=5, learning_rate=0.001): # [5pts]
                """
                Args:
                    xtrain: NxD numpy array, where N is number
                            of instances and D is the dimensionality of each
                            instance
                    ytrain: Nx1 numpy array, the true labels
                Return:
                    weight: Dx1 numpy array, the weights of linear regression model
                """
                N,D = xtrain.shape
                weight = np.zeros((D,1))
                for i in range(epochs):
                    pred = xtrain.dot(weight)
                    weight += (learning_rate/N)*(xtrain.T).dot((ytrain-pred))

                return weight

            def linear_fit_SGD(self, xtrain, ytrain, epochs=1000, learning_rate=0.001): # [5pts]
                """
                Args:
                    xtrain: NxD numpy array, where N is number
                            of instances and D is the dimensionality of each
                            instance
                    ytrain: Nx1 numpy array, the true labels
                Return:
```
Processing math: 100%

```
            weight: Dx1 numpy array, the weights of linear regression model
        """
        N,D = xtrain.shape
        weight = np.zeros((D,1))
        it=0
        while it<=epochs:
            for i in range(N):
                pred = xtrain[i].dot(weight)
                weight += (learning_rate*(xtrain[i])*(ytrain[i]-pred)[0]).reshape(-1,1)
            it += 1

        return weight
    # =================
    # RIDGE REGRESSION

    def ridge_fit_closed(self, xtrain, ytrain, c_lambda): # [5pts]
        """
        Args:
            xtrain: N x D numpy array, where N is number of instances and D is the dimensionality of each instance
            ytrain: N x 1 numpy array, the true labels
            c_lambda: floating number
        Return:
            weight: Dx1 numpy array, the weights of ridge regression model
        """
        N,D = xtrain.shape
        weights = np.linalg.inv(xtrain.T@xtrain+c_lambda*np.identity(D))@xtrain.T@ytrain
        return weights


    def ridge_fit_GD(self, xtrain, ytrain, c_lambda, epochs=500, learning_rate=1e-7): # [5pts]
        """
        Args:
            xtrain: NxD numpy array, where N is number
                    of instances and D is the dimensionality of each
                    instance
            ytrain: Nx1 numpy array, the true labels
            c_lambda: floating number
        Return:
            weight: Dx1 numpy array, the weights of linear regression model
        """
        N,D = xtrain.shape
        weight = np.zeros((D,1))

        for i in range(epochs):
            pred = xtrain.dot(weight)
            weight += (learning_rate/N)*((xtrain.T).dot((ytrain-pred))+c_lambda)

        return weight


    def ridge_fit_SGD(self, xtrain, ytrain, c_lambda, epochs=100, learning_rate=0.001): # [5pts]
        """
        Args:
            xtrain: NxD numpy array, where N is number
                    of instances and D is the dimensionality of each
                    instance
            ytrain: Nx1 numpy array, the true labels
        Return:
            weight: Dx1 numpy array, the weights of linear regression model
        """
        N,D = xtrain.shape
        weight = np.zeros((D,1))
        it=0
        while it<=epochs:
            for i in range(N):
                pred = xtrain[i].dot(weight)
                weight += (learning_rate*((xtrain[i])*(ytrain[i]-pred)[0])).reshape(-1,1)
            it += 1
            weight += learning_rate*(c_lambda)
        return weight


    def ridge_cross_validation(self, X, y, kfold=10, c_lambda=100): # [8 pts]
        """
        Args:
            X: NxD numpy array, where N is number
                    of instances and D is the dimensionality of each
                    instance
            y: Nx1 numpy array, the true labels
            kfold: integer, size of the fold for the data split
            c_lambda: floating number
        Return:
            mean_error: the mean of the RMSE for each fold
        """
        N,D = X.shape
        X_folds = np.array_split(X,kfold,axis=0)
        y_folds = np.array_split(y,kfold,axis=0)
        rmse_vals = []

        for i in range(kfold):
            Xtrain = [x for ind,x in enumerate(X_folds) if ind != i]
            Xtrain = np.vstack(Xtrain)
            Xtest = [x for ind,x in enumerate(X_folds) if ind == i]
            Xtest = np.vstack(Xtest)
```

Processing math: 100%

```
            ytrain = [y for ind,y in enumerate(y_folds) if ind != i]
            ytrain = np.vstack(ytrain)
            ytest = y_folds[i]

            weights = self.ridge_fit_closed(Xtrain,ytrain,c_lambda)
            pred = self.predict(Xtest,weights)

            rmse_res = self.rmse(pred,ytest)
            rmse_vals.append(rmse_res)
        mean_rmse = np.mean(rmse_vals)
        return mean_rmse
```

3.2 About RMSE [5pts] **[W]**

Do you know whether this RMSE is good or not? If you don't know, we could normalize our labels between 0 and 1. After normalization, what does it mean when RMSE = 1?

Hint: think of the way that you can enforce your RMSE = 1. Note that you can not change the actual labels to make RMSE = 1.

Analysis:

The RMSE can be expressed as :

$$\sqrt{\frac{(y_{pred} - y_{act})^2}{N_{obs}}}$$

where y_{pred}, y_{act} and N_{obs} are the predicted target, actual value and number of observations. Setting the above expression to 1, we get:

$$(y_{pred} - y_{act})^2 = N_{obs}^2$$

The above condition is definitely achieved when the error between each predicted point and observed point is 1 (i.e. if the actual label is 0.5, predicting either -0.5 or 1.5). In the classification case (either 0 or 1 as possible outputs) an RMSE of 1 indicates complete misclassification; in the regression setting, an RMSE of 1 for normalized data is quite poor performance.

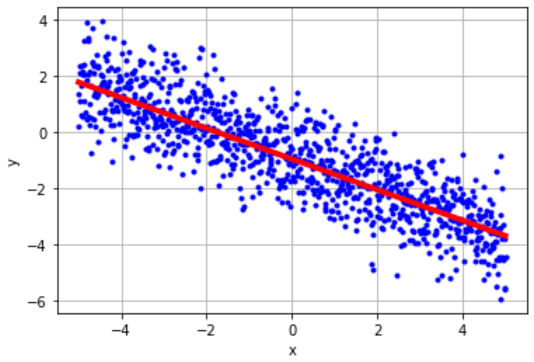
3.3 Testing: general functions and linear regression [5 pts] **[W]**

Let's first construct a dataset for polynomial regression.

In this case, we construct the polynomial features up to degree 5, where the groundtruth function is just a linear function (i.e., only require polynomial features up to degree 1).

In [10]:
```
#helper do not need to change
def plot_curve(x, y, curve_type='.', color='b', lw=2):
    plt.plot(x, y, curve_type, color=color, linewidth=lw)
    plt.xlabel('x')
    plt.ylabel('y')
    plt.grid(True)
```

In [11]:
```
#helper, do not need to change
POLY_DEGREE = 5
NUM_OBS = 1000

rng = np.random.RandomState(seed=4)

true_weight = -rng.rand(POLY_DEGREE + 1, 1)
true_weight[2:, :] = 0
x_all = np.linspace(-5, 5, NUM_OBS)
reg = Regression()
x_all_feat = reg.construct_polynomial_feats(x_all, POLY_DEGREE)
y_all = np.dot(x_all_feat, true_weight) + rng.randn(x_all_feat.shape[0], 1) # in the second term, we add noise to data
# Note that here we try to produce y_all as our training data
plot_curve(x_all, y_all) # Data with noise that we are going to predict
plot_curve(x_all, np.dot(x_all_feat, true_weight), curve_type='-', color='r', lw=4) # the groundtruth information

indices = rng.permutation(NUM_OBS)
```

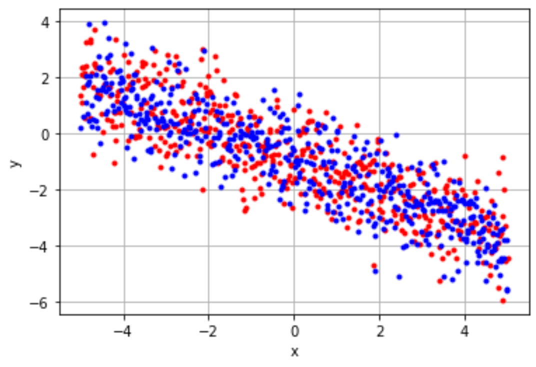


Processing math: 100%

In the figure above, the red curve is the true fuction we want to learn, while the blue dots are the noisy observations. The observations are generated by $Y = X\theta + \sigma$, where σ~N(0,1) are i.i.d. generated noise.

Now let's split the data into two parts, namely the training set and test set. The red dots are for training, while the blue dots are for testing.

```
In [12]: train_indices = indices[:NUM_OBS//2]
         test_indices = indices[NUM_OBS//2:]

         plot_curve(x_all[train_indices], y_all[train_indices], color='r')
         plot_curve(x_all[test_indices], y_all[test_indices], color='b')
```



Now let's first train using the entire training set, and see how we performs on the test set and how the learned function look like.

```
In [13]: #helper, do not need to change
         weight = reg.linear_fit_closed(x_all_feat[train_indices], y_all[train_indices])
         y_test_pred = reg.predict(x_all_feat[test_indices], weight)
         test_rmse = reg.rmse(y_test_pred, y_all[test_indices])
         print('test rmse: %.4f' % test_rmse)

         test rmse: 0.9222
```

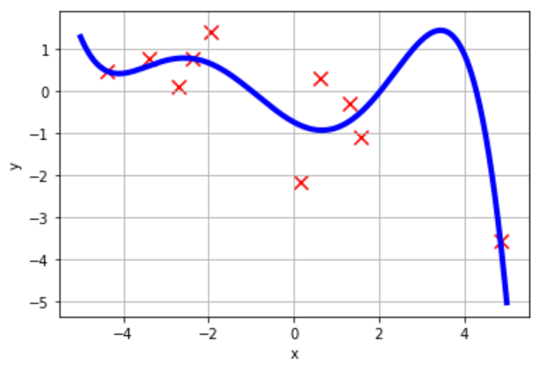
```
In [14]: weight = reg.linear_fit_GD(x_all_feat[train_indices], y_all[train_indices], epochs=5000, learning_rate=1e-7)
         y_test_pred = reg.predict(x_all_feat[test_indices], weight)
         test_rmse = reg.rmse(y_test_pred, y_all[test_indices])
         print('test rmse: %.4f' % test_rmse)

         test rmse: 1.4478
```

And what if we just use the first 10 observations to train?

```
In [15]: sub_train = train_indices[:10]
         weight = reg.linear_fit_closed(x_all_feat[sub_train], y_all[sub_train])
         y_test_pred = reg.predict(x_all_feat[test_indices], weight)
         test_rmse = reg.rmse(y_test_pred, y_all[test_indices])
         print('test rmse: %.4f' % test_rmse)

         test rmse: 2.1910
```

Did you see a worse performance? Let's take a closer look at what we have learned.

```
In [16]: #helper, do not need to change
         y_pred = reg.predict(x_all_feat, weight)
         plot_curve(x_all, y_pred, curve_type='-', color='b', lw=4)
         plt.scatter(x_all[sub_train], y_all[sub_train], s=100, c='r', marker='x')

         y_test_pred = reg.predict(x_all_feat[test_indices], weight)
```



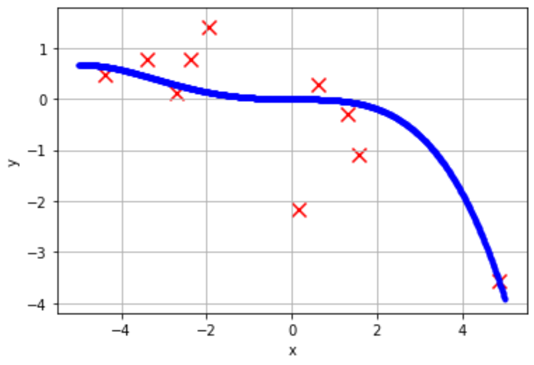
3.4 Testing: ridge regression [5 pts]

Now let's try ridge regression. Similarly, undergraduate students need to implement the closed form, and graduate students need to implement all the three methods. We will call the prediction function from linear regression part.

Again, let's see what we have learned. You only need to run the cell corresponding to your specific implementation.

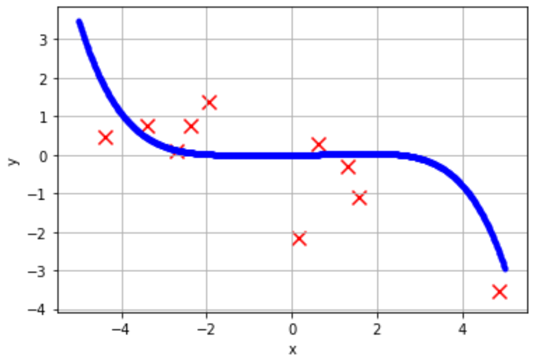
In [17]:
```
sub_train = train_indices[:10]
print(x_all_feat[sub_train].shape)
print(y_all[sub_train].shape)
weight = reg.ridge_fit_closed(x_all_feat[sub_train], y_all[sub_train], c_lambda=1000)

y_pred = reg.predict(x_all_feat, weight)
plot_curve(x_all, y_pred)
plt.scatter(x_all[sub_train], y_all[sub_train], s=100, c='r', marker='x')

y_test_pred = reg.predict(x_all_feat[test_indices], weight)
test_rmse = reg.rmse(y_test_pred, y_all[test_indices])
print('test rmse: %.4f' % test_rmse)
```

```
(10, 6)
(10, 1)
test rmse: 1.4610
```



In [18]:
```
sub_train = train_indices[:10]
weight = reg.ridge_fit_GD(x_all_feat[sub_train], y_all[sub_train], c_lambda=1000, learning_rate=1e-7)

y_pred = reg.predict(x_all_feat, weight)
plot_curve(x_all, y_pred)
plt.scatter(x_all[sub_train], y_all[sub_train], s=100, c='r', marker='x')

y_test_pred = reg.predict(x_all_feat[test_indices], weight)
test_rmse = reg.rmse(y_test_pred, y_all[test_indices])
print('test rmse: %.4f' % test_rmse)
```

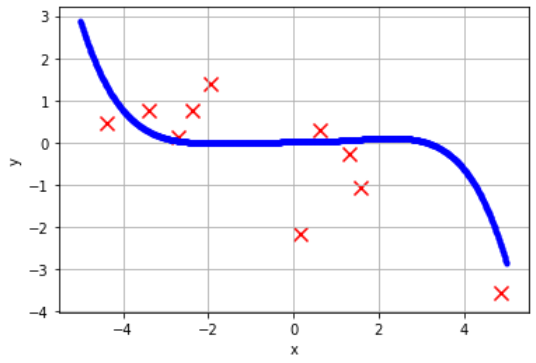
```
test rmse: 1.7635
```



Processing math: 100%

In [19]:
```
sub_train = train_indices[:10]
weight = reg.ridge_fit_SGD(x_all_feat[sub_train], y_all[sub_train], c_lambda=1000, learning_rate=1e-7)

y_pred = reg.predict(x_all_feat, weight)
plot_curve(x_all, y_pred)
plt.scatter(x_all[sub_train], y_all[sub_train], s=100, c='r', marker='x')

y_test_pred = reg.predict(x_all_feat[test_indices], weight)
test_rmse = reg.rmse(y_test_pred, y_all[test_indices])
print('test rmse: %.4f' % test_rmse)
```

```
test rmse: 1.8152
```



3.5 Cross validation [7 pts] **[W]**

Let's use Cross Validation to find the best value for c_lambda in ridge regression.

In [20]:
```
# We provided 6 possible values for lambda, and you will use them in cross validation.
# For cross validation, use 10-fold method and only use it for your training data (you already have the train_indices to get trai
ning data).
# For the training data, split them in 10 folds which means that use 10 percent of training data for test and 90 percent for trai
ning.
# At the end for each lambda, you have caluclated 10 rmse and get the mean value of that.
# That's it. Pick up the lambda with the lowest mean value of rmse.
# Hint: np.concatenate is your friend.
best_lambda = None
best_error = None
kfold = 10
lambda_list = [0, 0.1, 1, 5, 10, 100, 1000]
for lm in lambda_list:
    err = reg.ridge_cross_validation(x_all_feat[train_indices], y_all[train_indices], kfold, lm)
    print('lambda: %.2f' % lm, 'error: %.6f'% err)
    if best_error is None or err < best_error:
        best_error = err
        best_lambda = lm

print('best_lambda: %.2f' % best_lambda)
weight = reg.ridge_fit_closed(x_all_feat[train_indices], y_all[train_indices], c_lambda=10)
y_test_pred = reg.predict(x_all_feat[test_indices], weight)
test_rmse = reg.rmse(y_test_pred, y_all[test_indices])
print('test rmse: %.4f' % test_rmse)
```

```
lambda: 0.00 error: 0.999078
lambda: 0.10 error: 0.999079
lambda: 1.00 error: 0.999098
lambda: 5.00 error: 0.999341
lambda: 10.00 error: 0.999962
lambda: 100.00 error: 1.029726
lambda: 1000.00 error: 1.135153
best_lambda: 0.00
test rmse: 0.9223
```

4 Understanding PCA [20 pts] **[W]**

In this problem, we will investigate how PCA can be used to improve features for regression and classification tasks and how the data itself affects the behavior of PCA. Implement PCA in the below cell. Note that you will not submit your code for this problem to the autograder.

4.1 Intrinsic Dimensionality [10 pts] **[W]**

Assume a dataset is composed of N datapoints, each of which has D features with D < N. The *dimension* of our data would be D. It is possible, however, that many of these dimensions contain redundant information. The *intrinsic dimensionality* is the number of dimensions we need to reconstruct our data with high fidelity. For our purposes, we will define the intrinsic dimension as the number of principal components needed to reconstruct 99% of the variation within our data.

We define a set of features as linearly independent if we cannot construct one out of a linear combination of the others. The number of linearly independent features is the number of nonzero principal components (where we define 0 is anything less than 10^{-11} due to floating point error). Zero principal components mean that we can not find any weights to linearly combine features in order to create an indenpendent feature. Thus, our algorithm will assign 0 to these weights.

Processing math: 100%

In [21]:
```python
def pca(X):
    """
    Decompose dataset into principal components.
    You may use your SVD function from the previous part in your implementation.

    Args:
        X: N x D array corresponding to a dataset, in which N is the number of points and D is the number of features
    Return:
        U: N x N
        S: min(N, D) x 1
        V: D x D
    """
    X = X.astype(float)
    X = (X-X.mean(axis=0))#/(np.std(X,axis=0))

    U,S,V = np.linalg.svd(X,compute_uv=True,full_matrices=True, hermitian=False)
    S = S.reshape(-1,1)

    max_abs_cols = np.argmax(np.abs(U), axis=0)
    signs = np.sign(U[max_abs_cols, range(U.shape[1])])
    U *= signs

    return U,S,V

def intrinsic_dimension(S, recovered_variance=.99):
    """
    Find the number of principal components necessary to recover given proportion of variance

    Args:
        S: 1-d array corresponding to the singular values of a dataset

        recovered_variance: float in [0,1].  Minimum amount of variance
            to recover from given principal components
    Return:
        dim: int, the number of principal components necessary to recover
            the given proportion of the variance
    """
    recvar = 0.0
    denom = (S**2).sum()
    for dim in range(len(S)):
        recvar += (S[dim]**2)/denom
        if recvar>=recovered_variance:
            break
    return dim+1


def num_linearly_ind_features(S, eps=1e-11):
    """
    Find the number of linearly independent features in dataset

    Args:
        S: 1-d array corresponding to the singular values of a dataset
    Return:
        dim: int, the number of linearly independent dimensions in our data
    """
    dim = np.count_nonzero(S)
    return int(dim)

def apply_PCA(X, retained_variance=0.99):
    """
    Apply the functions you just implemented
    Args:
        X: N x D array corresponding to a dataset, in which N is the number of points and D is the number of features
        retained variance: floating number
    Return:
        (X_new, num_linearly_ind_features, intrinsic_dimension): The X projection on the new feature space, the number of linearl
y independent dimensions in our data, the intrinsic dimension
    """
    N,D = X.shape
    U,S,V = pca(X)

    S_square = np.diag(np.append(S,np.zeros(abs(D-N))))

    X_new = (U@S_square)[:,0:D]
    linearly_ind_features = num_linearly_ind_features(S.ravel())
    intrinsic_dim = intrinsic_dimension(S)
    return (X_new, linearly_ind_features, intrinsic_dim)
```

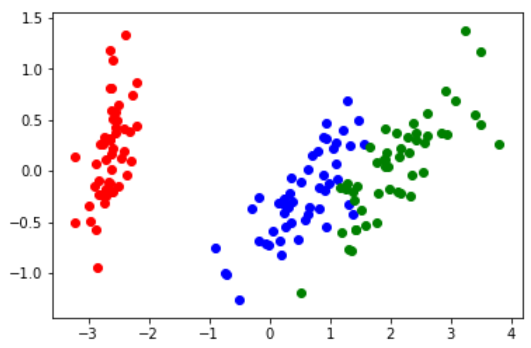
PCA is used to transform multivariate data tables into smaller sets so as to observe the hidden trends and variations in the data. Here you will visualize two datasets (iris and wine) using PCA. Use the above implementation of PCA and reduce the datasets such that they contain only two features. Make 2-D scatter plots of the data points using these features. Make sure to differentiate the data points according to their true labels. The datasets have already been loaded for you. In addition, return the retained variance obtained from the reduced features.

Processing math: 100%

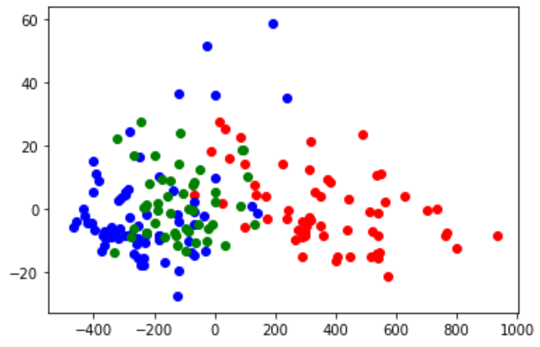
```
In [22]: def visualize(X,y):
             """
             Args:
             xtrain: NxD numpy array, where N is number
                   of instances and D is the dimensionality of each
                   instance
             ytrain: numpy array (N,), the true labels

             Return:
             retained variance: scalar

             Plot:
             scatter plot with the datapoints projected onto new feature space
             """
             (X_new, linearly_ind_features, intrinsic_dim) = apply_PCA(X)

             U,S,V = pca(X)
             retained_variance = (S[0]**2+S[1]**2)/((S**2).sum())

             reduced_pts = X_new[:,0:2]

             labels = []
             zero_labels = np.argwhere(y==0).ravel()
             one_labels = np.argwhere(y==1).ravel()
             two_labels = np.argwhere(y==2).ravel()

             labels.append(zero_labels)
             labels.append(one_labels)
             labels.append(two_labels)
             cols = ["r", "b", "g"]
             for i in range(3):
                 col_x = reduced_pts[:,0][labels[i]]
                 col_y = reduced_pts[:,1][labels[i]]
                 plt.scatter(col_x,col_y,color=cols[i])
             plt.show()
             return retained_variance[0]
```

```
In [23]: # use PCA for visualization of iris and wine data
         data=load_iris(return_X_y=True)
         X=data[0]
         y=data[1]
         print(y.shape)
         retained_variance_for_iris=visualize(X,y)
         print("Retained variance for iris dataset ",retained_variance_for_iris)

         data=load_wine(return_X_y=True)
         X=data[0]
         y=data[1]
         retained_variance_for_wine=visualize(X,y)
         print("Retained variance for wine dataset ",retained_variance_for_wine)
```

```
(150,)
```



```
Retained variance for iris dataset  0.977685206318795
```



```
Retained variance for wine dataset  0.9998271461166034
```

Processing math: 100%

Now you will use PCA on an actual real-world dataset. Implement feature reduction on the dataset using PCA with 99% retained variance. Use it to obtain the reduced features. On the reduced dataset, use linear regression and calculate the rmse values on test data. Your are encouraged to experiment with hyperparameters like the learning rate, number of epochs and regularization strength. Compare these results with those obtained by implementing regression on the unreduced dataset.

In [24]:
```
# helper
def apply_regression(X_train,y_train,X_test):
    weight = reg.ridge_fit_closed(X_train, y_train, c_lambda=1600)
    y_pred = reg.predict(X_test, weight)
    return y_pred
```

In [25]:
```
#load the dataset
data=np.load("data.npy",allow_pickle=True)
# separate the data
X=data[:,:-1]
y=data[:,-1]
X_PCA, ind_features, intrinsic_dimensions = apply_PCA(X)
print("data shape with PCA ",X_PCA.shape)
print("Number of independent features ",ind_features)
print("Number of intrinsic components ",intrinsic_dimensions)

#get training and testing data
X_train=X_PCA[:int(0.8*len(data)),:]
y_train=y[:int(0.8*len(data))].reshape(-1,1)
X_test=X_PCA[int(0.8*len(data)):]
y_test=y[int(0.8*len(data)):].reshape(-1,1)

# use Ridge Regression for getting predicted labels
y_pred=apply_regression(X_train,y_train,X_test)

#calculate RMSE
rmse_score = reg.rmse(y_pred, y_test)
print("rmse score with PCA",rmse_score)
```

```
data shape with PCA  (1460, 34)
Number of independent features  34
Number of intrinsic components  3
rmse score with PCA 306374.2910736947
```

In [26]:
```
# Ridge regression without PCA
X_train=X[:int(0.8*len(data)),:]
y_train=y[:int(0.8*len(data))].reshape(-1,1)
X_test=X[int(0.8*len(data)):]
y_test=y[int(0.8*len(data)):].reshape(-1,1)

#use Ridge Regression for getting predicted labels
y_pred=apply_regression(X_train,y_train,X_test)

#calculate RMSE
rmse_score = reg.rmse(y_pred, y_test)
print("rmse score without PCA",rmse_score)
```

```
rmse score without PCA 52357.77579653398
```

4.2 Feature Scaling [10 pts] **[W]**

Principal component analysis is not agnostic to the scale of your features. Measuring a feature with different units can change your principal components.

For this problem, randomly choose one column in each of the above datasets and multiply it by 1000. For each of the datasets, answer the following:

1. How does this change the distribution of variance among the first 10 components?
2. How does this change the first principal component of the data?
3. How does this affect the number of linearly independent components and intrinsic dimensionality? Why?

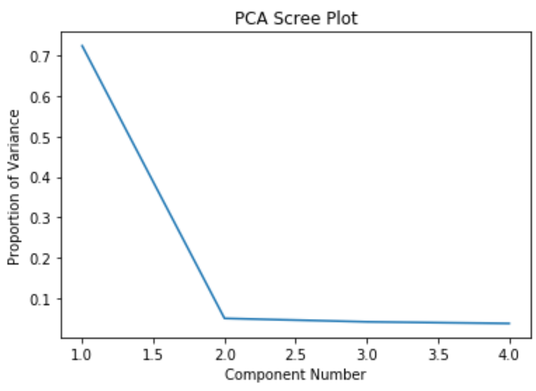
It may be helpful to plot the variance captured by each component in a scree plot (see function below) and to make a bar plot of the absolute value of each feature in the first principal component. Hint: Exploring the imported datasets (i.e. Boston, Diabetes, Digits, etc.) may help you understand the answers to these questions.

In [27]:
```
# helper fuctions
def randomly_perturb_data(data, multiplier=1000):
    """
    Multiply a random column in data by multiplier

    Inputs:
        data: N*D numpy array of features
        multiplier: multiplier by which to perturb a random column in data

    Returns:
        perturbed_data: Data with random column multiplied by multiplier
    """
    #np.random.seed(2)
    i = np.random.randint(data.shape[1])
    copy = data.copy()
    copy[:,i] *= multiplier
    return copy


def scree_plot(S, n_components=10):
    """
    Plot proportion of variance contained in each individual component
    """
    plt.plot(range(1, n_components+1), (S/S.sum())[:n_components])
    plt.ylabel("Proportion of Variance")
    plt.xlabel("Component Number")
    plt.title("PCA Scree Plot")
    plt.show()

def plot_component_vector(V):
    v = V[:,0]
    print(np.abs(v))
    plt.bar(range(1, len(v)+1), np.abs(v))
    plt.show()
```

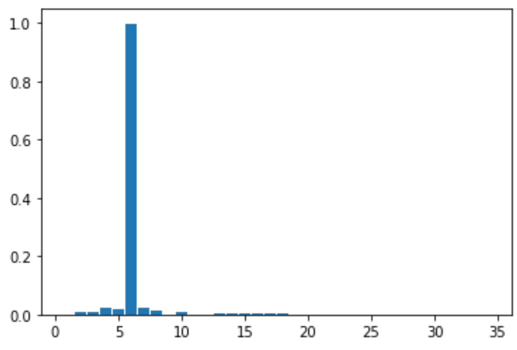
In [28]:
```
data=np.load("data.npy",allow_pickle=True)
# separate the data
X=data[:,:-1]
y=data[:,-1]
X_pert = randomly_perturb_data(X)
```

Processing math: 100%

```
In [29]: #Case 1: Without perturbation
         U,S,V = pca(X)
         scree_plot(S, n_components=4)
         plot_component_vector(V)
         X_new, linearly_ind_features, intrinsic_dim = apply_PCA(X,retained_variance=1)
         print('Number of linearly independent features: ',linearly_ind_features)
         print('Intrinsic dimension: ',intrinsic_dim)
```



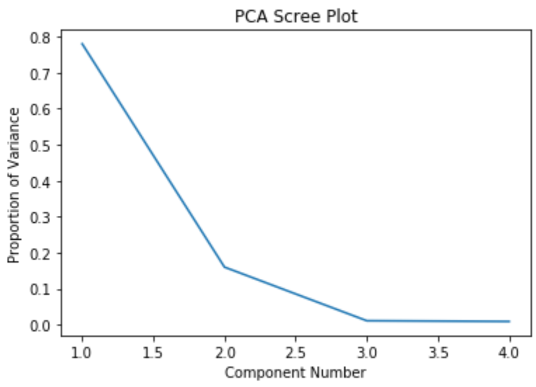
```
[1.40465845e-03 1.10465105e-02 6.88715734e-03 2.16798677e-02
 2.00849163e-02 9.98960322e-01 2.46262124e-02 1.58356753e-02
 8.02559688e-04 9.31934661e-03 1.34870514e-04 1.14593439e-03
 4.98460054e-03 3.11296953e-03 5.02551664e-03 3.53569711e-03
 3.51585468e-03 1.62193124e-03 2.30485919e-04 1.38918439e-04
 3.18259935e-05 8.58251909e-05 7.29957407e-05 6.89228982e-05
 6.05818068e-06 5.60913737e-06 1.46215507e-05 1.05754902e-05
 1.71470438e-05 7.61101851e-06 7.68549251e-06 2.08697411e-05
 0.00000000e+00 0.00000000e+00]
```



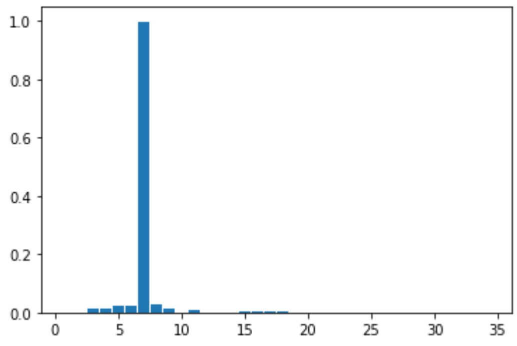
```
Number of linearly independent features:  34
Intrinsic dimension:  3
```

Processing math: 100%

In [30]:
```
#Case 2: With perturbation
U_pert,S_pert,V_pert = pca(X_pert)
scree_plot(S_pert, n_components=4)
plot_component_vector(V_pert)
X_new, linearly_ind_features, intrinsic_dim = apply_PCA(X_pert,retained_variance=1)
print('Number of linearly independent features: ',linearly_ind_features)
print('Intrinsic dimension: ',intrinsic_dim)
```



```
[3.83602648e-04 1.39526812e-03 1.28531154e-02 1.50344562e-02
 2.28149477e-02 2.13101397e-02 9.98738856e-01 2.81990294e-02
 1.45101164e-02 3.83258937e-04 9.80132406e-03 6.88586745e-04
 2.77597530e-04 4.96130196e-04 4.96247861e-03 3.26655971e-03
 3.50629869e-03 1.51451850e-03 2.42528147e-04 1.38941455e-04
 3.18288963e-05 8.58224991e-05 7.29963119e-05 6.89240215e-05
 6.05785688e-06 5.60890997e-06 1.46215327e-05 1.05754303e-05
 1.71471500e-05 7.61104030e-06 7.68549258e-06 2.08697194e-05
 0.00000000e+00 0.00000000e+00]
```



```
Number of linearly independent features:  34
Intrinsic dimension:  2
```

Analysis

Based on the above plots, it becomes clear that perturbing a random column (i.e. multiplying by 1000) indeed affects the PCA representation of it. Specifically,

1. The distribution of variance becomes more heavily skewed toward the first principle component (and observes a sharper decline) in the case of the perturbed data. This can be explained due to the much larger magnitude of a single column (which is thus presumed by PCA to contain more "information" or variance, even though it is just on a larger scale).
2. The magnitude of the first principle component also drastically decreases.
3. As expected, the number of linearly independent dimensions stays the same, since multiplying a column by a constant number does not alter the rank of a matrix. However, the number of intrinsic dimensions is reduced to just 1 on perturbation, because almost all the variance is captured in just the first principle component (again, because of the extraordinarily large magnitude of a single component).

5 Manifold learning [Bonus for everyone][30 pts]

While PCA is wonderful tool for dimensionality reduction it does not work very well when dealing with non-linear relationships between features. Manifold learning is a class of algorithms that can be used to reduce dimensions in complex high-dimensional datasets. While a number of methods have been proposed to perform this type of operation, we will focus on Isomap. Isomap has been shown to be sensitive to data noise amongst other issues, however it has been shown to perform reasonably well for real world data. The algorithm consists of two main steps: first computing a manifold distance matrix, followed by classical mutidimensional scaling. You will be creating your implementation of Isomap. In order to do so, you must read the original paper "A Global Geometric Framework for Nonlinear Dimensionality Reduction" (http://web.mit.edu/cocosci/Papers/sci_reprint.pdf) by Tenenbaum et al. (2000), which outlines the method. You are also encouraged to read this general survey of manifold learning (https://cseweb.ucsd.edu/~lcayton/resexam.pdf) by Cayton (2005), where the original algorithm is further explained in a more detailed yet simplified fashion.

5.1 Implementation [23 pts] **[P]**

Processing math: 100%

In [31]:
```python
import numpy as np
from scipy.sparse import csr_matrix
from scipy.sparse.csgraph import floyd_warshall

class Isomap(object):
    def __init__(self): # No need to implement
        pass

    def pairwise_dist(self, x, y): # [3 pts]
        """
        Args:
            x: N x D numpy array
            y: M x D numpy array
        Return:
                dist: N x M array, where dist2[i, j] is the euclidean distance between
                x[i, :] and y[j, :]
        """
        dist = np.linalg.norm(x[:,None]-y,axis=2)
        return dist

    def manifold_distance_matrix(self, x, K): # [10 pts]
        """
        Args:
            x: N x D numpy array
        Return:
            dist_matrix: N x N numpy array, where dist_matrix[i, j] is the euclidean distance between points if j is in the neigh
borhood N(i)
            or comp_adj = shortest path distance if j is not in the neighborhood N(i).
        Hint: After creating your k-nearest weighted neighbors adjacency matrix, you can convert it to a sparse graph
        object csr_matrix (https://docs.scipy.org/doc/scipy/reference/generated/scipy.sparse.csr_matrix.html) and utilize
        the pre-built Floyd-Warshall algorithm (https://docs.scipy.org/doc/scipy/reference/generated/scipy.sparse.csgraph.floyd_w
arshall.html)
        to compute the manifold distance matrix.
        """

        N = x.shape[0]
        dist_matrix = np.ones((N, N))*np.inf
        for i in range(N):
            dis = np.linalg.norm(x - np.tile(x[i],(len(x),1)),axis=1)
            order = np.argsort(dis,axis=-1)
            dis = np.sort(dis)
            dist = dis[1:K + 1]
            order = order[1:K + 1]
            dist_matrix[i, order] = dist
            dist_matrix[order, i] = dist

        np.fill_diagonal(dist_matrix,0)
        dist_matrix = csr_matrix(dist_matrix)
        dist_matrix = floyd_warshall(dist_matrix)
        return dist_matrix

    def multidimensional_scaling(self, dist_matrix, d): # [10 pts]
        """
        Args:
            dist_matrix: N x N numpy array, the manifold distance matrix
            d: integer, size of the new reduced feature space
        Return:
            S: N x d numpy array, X embedding into new feature space.
        """
        N = len(dist_matrix)
        S = np.zeros((N,d))
        eVal,eVect = np.linalg.eig(dist_matrix)
        idx = eVal.argsort()[::-1]
        eVal = eVal[idx]
        eVect = eVect[:,idx]

        eVect = eVect[:,0:d]
        eVal = np.diag(eVal[0:d])

        S = eVect@np.sqrt(eVal)
        return S

    # you do not need to change this
    def __call__(self, data, K, d):
        # get the manifold distance matrix
        W = self.manifold_distance_matrix(data, K)
        # compute the multidimensional scaling embedding
        emb_X = self.multidimensional_scaling(W, d)
        return emb_X
```

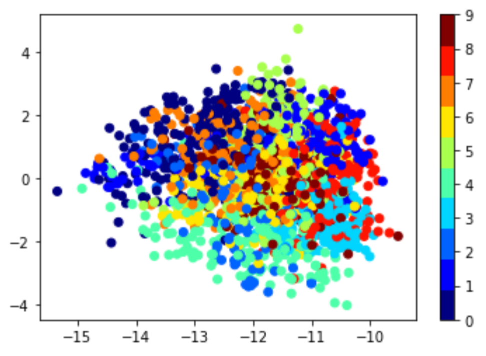
5.2 Examples for different datasets [7pts] **[W]**

Apply your implementation of Isomap for some of the datasets (e.g. MNIST and Iris). Discuss how the new embedding compares to PCA.

Processing math: 100%

```
In [32]: # example MNIST data
         mnist = load_digits()
         proj = Isomap()(mnist.data, 10, 2)
         plt.scatter(proj[:, 0], proj[:, 1], c=mnist.target, cmap=plt.cm.get_cmap('jet', 10))
         plt.colorbar(ticks=range(10))
```

```
Out[32]: <matplotlib.colorbar.Colorbar at 0x16d2031cbc8>
```



Processing math: 100%