Objective: To develop a mathematical understanding of PCA

Test data

Non-linear Iterative Partial Least-Squares (NIPALS) algorithm

Steps to compute PCA using NIPALS algorithm

- Step 1: Initialize an arbitrary column vector \mathbf{t}_a either randomly or by just copying any column of X.
- Step 2: Take very column of \mathbf{X} , $\mathbf{X_k}$ and regress it onto the \mathbf{t}_a vector and store the regression coefficients as \mathbf{p}_{ka} . (Note: This simply means performing an ordinary least squares regression (y=mx) with $x=t_a$ and $y=X_k$ with $m=(\mathbf{x^Tx})^{-1}\mathbf{x^Ty}$). In the current notation we get

$$p_{ka} = rac{\mathbf{t_a^T} \mathbf{X}_k}{\mathbf{t_a^T} \mathbf{t_a}}$$

Repeat it for each of the columns of X to get the entire vector \mathbf{p}_k . This is shown in the illustration above where each column from X is regressed, one at a time, on \mathbf{t}_a , to calculate the loading entry, p_{ka}

In practice we don't do this one column at time; we can regress all columns in X in go:

$$\mathbf{p_a^T} = \frac{1}{\mathbf{t_a^T t_a}}.\,\mathbf{t_a^T X_a}$$

where $\mathbf{t_a}$ is an N imes 1 column vector, and \mathbf{X}_a us an N imes K matrix.

• The loading vector $\mathbf{p_a^T}$ won't have unit length (magnitude) yet. So we simply rescale it to have magnitude of 1.0:

$$\mathbf{p_a^T} = rac{\mathbf{p_a^T}}{\sqrt{\mathbf{p_a^T}\mathbf{p_a}}}$$

• Step 4: Regress every row in X onto this normalized loadings vector. As illustrated below, in our linear regression the rows in X are our y-variable each time, while the loadings vector is our x-variable. The regression coefficient becomes the score value for that i^{th} row:

$$p_{i,a} = rac{\mathbf{x}_i^T \mathbf{p}_a}{\mathbf{p}_a^T \mathbf{p}_a}$$

where x_i^T is a $K \times 1$ column vector. We can combine these N separate least-squares models and calculate them in one go to get the entire vector,

$$\mathbf{t}_a^T = rac{1}{\mathbf{p}_a^T \mathbf{p}_a} \mathbf{X} \mathbf{p}_a^T$$

where p_a is a $K \times 1$ column vector.

- Step 5: Continue looping over steps 2,3,4 until the change in vector t_a is below a chosen tolerance
- Step 6: On convergence, the score vector and the loading vectors, \mathbf{t}_a and \mathbf{p}_a are stored as the a^{th} column in matrix \mathbf{T} and \mathbf{P} . We then deflate the \mathbf{X} matrix. This crucial step removes the variability captured in this component (t_a and p_a) from \mathbf{X} :

$$E_a = X_a - t_a p_a^T \ X_{a+1} = E_a$$

For the first component, X_a is just the preprocessed raw data. So we can see that the second component is actually calculated on the residuals E_1 , obtained after extracting the first component. This is called deflation, and nicely shows why each component is orthogonal to the others. Each subsequent component is only seeing variation remaining after removing all the others; there is no possibility that two components can explain the same type of variability. After deflation we go back to step 1 and repeat the entire process for the next component.

IMPLEMENTATION IN PYTHON

```
In [28]:
          def PCA(X,no_components):
              tol = 0.0000001
              it=1000
              obsCount, varCount = X.shape
              Xa = X - np.mean(X, axis = 0)
              \#Xh = X-np.tile(np.mean(X,axis=0).reshape(-1,1).T, obsCount).reshape(4,3)
              T = np.zeros((obsCount,no_components))
              P = np.zeros((varCount,no_components))
              pcvar = np.zeros((varCount,1))
              varTotal = np.sum(np.var(Xa,axis=0,ddof=1))
              currVar = varTotal
              nr=0
              for h in range(no_components):
                   th = Xa[:,0].reshape(-1,1)
                  ende = False
                  while ende != True:
                       nr = nr + 1
                       ph = np.dot(Xa.T,th)/np.dot(th.T,th)
                       ph = ph /np.linalg.norm(ph)
                       thnew = np.dot(Xa,ph)/np.dot(ph.T,ph)
                       prec = np.dot((thnew-th).T,(thnew-th))
                       th = thnew
                       if prec <= (tol*tol):</pre>
                           ende = True
                       elif it <=nr:</pre>
                           ende = True
                           print("Iternation stops without convergence")
                   Ea = Xa - np.dot(th,ph.T)
```

```
Xa = Ea
T[:,h] = th.flatten()
P[:,h] = ph.flatten()
oldVar = currVar
currVar = np.sum(np.var(Xa,axis=0,ddof=1))
pcvar[h] = (oldVar - currVar) / varTotal
nr = 0
return T,P,pcvar
```

Advantages of the NIPALS algorithm

- The NIPALS algorithm computes one component at a time. The first component computed is equivalent to the t1 and p1 vectors that would have been found from an eigenvalue or singular value decomposition.
- The algorithm can handle missing data in X.
- The algorithm always converges, but the convergence can sometimes be slow.
- It is also known as the Power algorithm to calculate eigenvectors and eigenvalues.
- It works well for very large data sets.
- It is used by most software packages, especially those that handle missing data.
- Of interest: it is well known that Google used this algorithm for the early versions of their search engine, called PageRank148.

```
no_components=3
In [14]:
            T,P,pcvar = PCA(X,no_components)
            print("T (Scores)")
            print(T)
            print(" ")
            print("P (Loadings)")
            print(P)
            print(np.sqrt(pcvar)/np.sum(np.sqrt(pcvar)))
           T (Scores)
           [[-4.25324997e+03 -8.41288672e-01 8.37859036e-03]
            [ 2.97275001e+03 -1.25977272e-01 -1.82476780e-01]
[ 3.62475003e+03 -1.56843494e-01 1.65224286e-01]
[-2.34425007e+03 1.12410944e+00 8.87390330e-03]]
           P (Loadings)
           [[ 1.21901390e-05 5.66460728e-01 8.24088735e-01]
            [ 9.99999997e-01 5.32639787e-05 -5.14047689e-05]
             [ 7.30130279e-05 -8.24088733e-01 5.66460726e-01]]
           [[9.99753412e-01]
            [2.10083377e-04]
            [3.65048880e-05]]
```

SVD

```
In [15]: from numpy.linalg import svd
U, S, PTrans = svd(X, full_matrices=False)
Sigma = np.diag(S)
T=np.dot(U,Sigma)
P=PTrans.T

print("T (Scores)")
print(T)
print(" ")
print(" ")
print("P (Loadings)")
print(P)
```

SKLEARN PCA

```
In [16]:
         from sklearn.decomposition import PCA
          pca = PCA()
          T=pca.fit_transform(X)
          Prans=pca.components_ #eigen vectors.T
          latent = pca.explained variance
          explained = pca.explained_variance_ratio_
          P=PTrans.T
          S=pca.singular_values_
          Sigma=np.diag(S)
          print("T (Scores)")
          print(T)
          print(" ")
          print("P (Loadings)")
          print(P)
          print("Sigma (Variance)")
          print(S)
          #print(pca.singular_values_/np.sqrt(3))
         T (Scores)
         [[ 4.25324997e+03 -8.41288672e-01 -8.37858943e-03]
          [-2.97275001e+03 -1.25977271e-01 1.82476780e-01]
          [-3.62475003e+03 -1.56843494e-01 -1.65224286e-01]
          [ 2.34425007e+03 1.12410944e+00 -8.87390454e-03]]
         P (Loadings)
         [[ 1.21901390e-05 -5.66460727e-01 -8.24088736e-01]
          [ 9.9999997e-01 -5.32639789e-05 5.14047691e-05]
          [ 7.30130279e-05  8.24088734e-01 -5.66460725e-01]]
         Sigma (Variance)
         [6.74994067e+03 1.41840009e+00 2.46466604e-01]
In [17]: | pca.explained_variance_ratio_
Out[17]: array([9.99999955e-01, 4.41567976e-08, 1.33326424e-09])
          explained_variance_2 = (S ** 2) / 4
In [18]:
          explained variance ratio 2 = (explained variance 2 / explained variance 2.sum())
          print(explained_variance_ratio_2)
```

[9.99999955e-01 4.41567976e-08 1.33326424e-09]

Eigenvalue decomposition approach

Recall that the latent variable directions (the loading vectors) were oriented so that the variance of the scores in that direction were maximal. We can cast this as an optimization problem. For

the first component:

$$max(\phi) = \mathbf{t_1^T} \mathbf{t_1} = \mathbf{p_1^T} \mathbf{X^T} \mathbf{X} \mathbf{p_1}$$

such that

$$\mathbf{p_1^T}\mathbf{p_1} = 1$$

•

This is equivalent to

$$max(\phi) = \mathbf{p_1^TX^TXp_1} - \lambda(\mathbf{p_1^Tp_1} - 1)$$

because we can move the constraint into the objective function with a Lagrange multiplier, λ . The maximum value must occur when the partial derivatives with respect to $\mathbf{p_1}$,

our search variable, are zero:

$$\frac{\partial \phi}{\partial p_1} = \frac{\partial (\mathbf{p}_1^T \mathbf{X}^T \mathbf{X} \mathbf{p}_1 - \lambda(\mathbf{p}_1^T \mathbf{p}_1 - 1))}{\partial \mathbf{p}_1} = 0$$
$$2\mathbf{X}^T \mathbf{X} \mathbf{p}_1 - 2\lambda_1 \mathbf{p}_1 = 0$$
$$(\mathbf{X}^T \mathbf{X} - \lambda_1 \mathbf{I}) \mathbf{p}_1 = 0$$
$$\mathbf{X}^T \mathbf{X} \mathbf{p}_1 = \lambda_1 \mathbf{p}_1$$

which is just the eigenvalue equation, indicating that $\mathbf{p_1}$ is the eigenvector of $\mathbf{X^TX}$ and λ_1 is the eigenvalue. One can show that $\lambda_1 = \mathbf{t_1^Tt_1}$, which is proportional to the variance of the first component. In a similar manner we can calculate the second eigenvalue, but this time we add the additional constraint that $\mathbf{p_1} \perp \mathbf{p_2}$. Writing out this objective function and taking partial derivatives leads to showing that

$$\mathbf{X^TXp_2} = \lambda_2\mathbf{p_2}$$

From this we learn that:

- The loadings are the eigenvectors of $\mathbf{X}^T\mathbf{X}$.
- Sorting the eigenvalues in order from largest to smallest gives the order of the corresponding eigenvectors, the loadings.
- We know from the theory of eigenvalues that if there are distinct eigenvalues, then their eigenvectors are linearly independent (orthogonal).
- We also know the eigenvalues of $\mathbf{X}^T\mathbf{X}$ must be real values and positive; this matches with the interpretation that the eigenvalues are proportional to the variance of each score vector.
- Also, the sum of the eigenvalues must add up to sum of the diagonal entries of X^TX, which represents of the total variance of the X matrix, if all eigenvectors are extracted. So plotting the eigenvalues is equivalent to showing the proportion of variance explained in X by each component. This is not necessarily a good way to judge the number of components to use, but it is a rough guide: use a Pareto plot of the eigenvalues (though in the context of eigenvalue problems, this plot is called a scree plot).

```
In [19]: | cov = np.cov(X, rowvar = False)
          evals , P = LA.eigh(cov)
          idx = np.argsort(evals)[::-1]
          P = P[:,idx]
          evals = evals[idx]
          T = np.dot(X, P)
          Sigma=LA.norm(T,axis=0)
          print("T (Scores)")
          print(T)
          print("P (Loadings)")
          print(P)
          print("Sigma (Variance)")
          print(Sigma)
         T (Scores)
         [[ 4.25324997e+03 8.41288672e-01 8.37858943e-03]
          [-2.97275001e+03 1.25977271e-01 -1.82476780e-01]
          [-3.62475003e+03 1.56843494e-01 1.65224286e-01]
          [ 2.34425007e+03 -1.12410944e+00 8.87390454e-03]]
         P (Loadings)
         [[-1.21901390e-05 -5.66460727e-01 8.24088736e-01]
          [-9.99999997e-01 -5.32639789e-05 -5.14047691e-05]
          [-7.30130279e-05 8.24088734e-01 5.66460725e-01]]
         Sigma (Variance)
         [6.74994067e+03 1.41840009e+00 2.46466604e-01]
```

Task 1: Test if the loading vectors are orthogonal and orthonormal or not

```
In [20]: dot1 = np.dot(P[:,0], P[:,1])
    dot2 = np.dot(P[:,1], P[:,2])
    dot3 = np.dot(P[:,0], P[:,1])
    print(dot1)

    dot4 = P.T.dot(P)
    print(dot4)

-4.472333961502706e-19
    [[ 1.00000000e+00 -4.48550678e-19 -3.82279445e-19]
        [-4.48550678e-19    1.000000000e+00    2.10601467e-16]
        [-3.82279445e-19    2.10601467e-16    1.000000000e+00]]

Orthonormal
```

Task 2: Test if the scores vectors are orthogonal and orthonormal or not

```
In [30]: dotT = T.T.dot(T)
    print(dotT)

[[ 4.55616990e+07 -1.95286340e-11 -1.55750968e-11]
    [-1.95286340e-11 2.01185881e+00 4.06619183e-15]
    [-1.55750968e-11 4.06619183e-15 6.07457869e-02]]
```

Task 3: Add more columns to the original data matrix by:

- Make some of the columns to be the linear combination of others
- Duplicate some columns

Orthogonal, not orthonormal.

Add noise as some columns

Then apply PCA to the dataset and report your findings here

```
In [29]:
          noise = np.random.normal(scale = 1, size = (X.shape[0],1))
          X_{alt} = np.hstack([X, X[:,2][:,None], 2*X[:,0][:,None] - X[:,1][:,None], noise])
          X_alt = X_alt - np.mean(X_alt, axis=0)
          print(np.mean(X_alt, axis=0))
          T_alt, P_alt, var_alt = PCA(X_alt, 6)
          print(np.diag(T_alt.T.dot(T_alt)))
          print("Length of P-s",np.diag(P_alt.T.dot(P_alt)))
          print("P",P_alt.T.dot(P_alt))
         [2.77555756e-17 0.000000000e+00 0.00000000e+00 0.00000000e+00
          1.13686838e-13 5.55111512e-17]
         [9.11211784e+07 4.77474771e+00 9.47991363e-01 1.33303002e-25
          1.20403253e-27 1.46941337e-31]
         Length of P-s [1. 1. 1. 1. 1.]
         P [[ 1.00000000e+00 -1.07542143e-13 -3.60930266e-14 -8.55433489e-01
            5.17912270e-01 -8.69564978e-05]
          [-1.07542143e-13 1.00000000e+00 6.66633950e-19 5.91024167e-05
            7.82195217e-05 9.52692294e-01]
          [-3.60930266e-14 6.66633950e-19 1.00000000e+00 -1.18996428e-05
           -9.28560522e-04 7.73849921e-02]
          [-8.55433489e-01 5.91024167e-05 -1.18996428e-05 1.00000000e+00
            1.50858562e-16 -5.22843266e-14]
          [ 5.17912270e-01 7.82195217e-05 -9.28560522e-04 1.50858562e-16
            1.00000000e+00 2.76166024e-15]
          [-8.69564978e-05 9.52692294e-01 7.73849921e-02 -5.22843266e-14
            2.76166024e-15 1.00000000e+00]]
```

No longer orthogonal. Assume that when adding dependent columns, x-basis is no longer orthogonal, which means that the P-space is also no longer orthogonal.

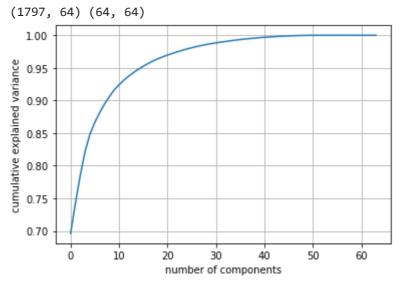
Objective: Learn to do clustering and noise reduction in data using PCA

```
In [1]:
         import matplotlib.pyplot as plt
         import numpy as np
         from numpy.linalg import svd
         from sklearn.datasets import load_digits
         digits = load_digits()
         digits.data.shape
Out[1]: (1797, 64)
        PCA using SVD
In [2]:
        def pca(X):
             U, S, PTrans = svd(X, full_matrices=False)
             Sigma = np.diag(S)
             T=np.dot(U,Sigma)
             P=PTrans.T
             return T, Sigma, P #Score, Variace, Loadings
In [3]:
        def plot_digits(data):
             fig, axes = plt.subplots(4, 10, figsize=(10, 4),
                                      subplot_kw={'xticks':[], 'yticks':[]},
                                      gridspec_kw=dict(hspace=0.1, wspace=0.1))
             for i, ax in enumerate(axes.flat):
                 ax.imshow(data[i].reshape(8, 8),
                           cmap='binary', interpolation='nearest',
                           clim=(0, 16))
In [4]:
        # Find out the original dimension of the data
         X=digits.data
         y=digits.target
         print("Shape of X",X.shape)
         print("Shape of y", y.shape)
        Shape of X (1797, 64)
        Shape of y (1797,)
         #Visualize the original data
In [5]:
         plot_digits(X)
```

Task 1: Dimensionality reduction: Conduct PCA on the the matrix

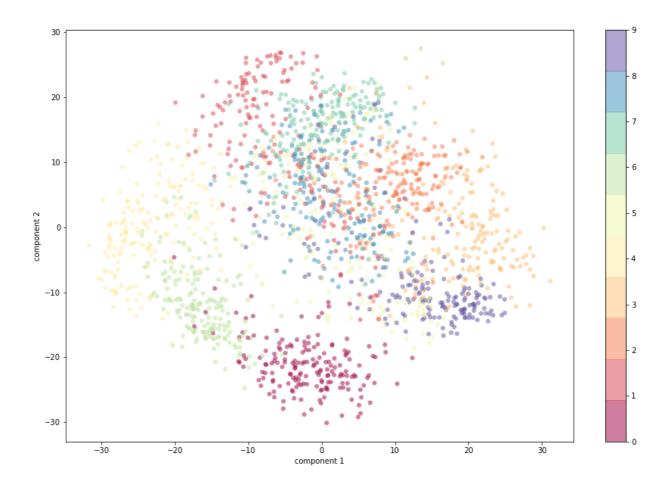
\boldsymbol{X} to find out the dimension required to capture 80% of the variance

```
T, sigma, P = pca(X)
In [6]:
         print(T.shape, P.shape)
         def variance_keeper(T, P, sigma, variance_limit):
             sigmas = []
             sum_sigma = np.trace(sigma)
             for i in range(len(np.diag(sigma))):
                 if (sum(sigmas)/sum_sigma > variance_limit):
                     break
                 else:
                      sigmas.append(sigma[i,i])
             return(T[:,0:len(sigmas)], P[:,0:len(sigmas)], np.array(sigmas), len(sigmas))
         SS = np.diag(sigma)
         explained variance = (SS ** 2)/4
         explained_variance_ratio = (explained_variance / explained_variance.sum())
         plt.plot(np.cumsum(explained_variance_ratio))
         plt.grid()
         plt.xlabel('number of components')
         plt.ylabel('cumulative explained variance');
```



We need about 3/4 components to cover 80% of the variance

Task 2: Clustering: Project the original data matrix X on the first two PCs and draw the scalar plot



Task 3: Denoising: Remove noise from the noisy data

```
In [33]: # Adding noise to the original data
X=digits.data
y=digits.target
np.random.seed(42)
noisy = np.random.normal(X, 4)
plot_digits(noisy)
```

Tips:

- Decompose the noisy data using PCA
- Reconstruct the data using just a few dominant components. For eg. check the variance plot

Since the nature of the noise is more or less similar across all the digits, they are not the fearues with enough variance to discriminate between the digits.

```
In [79]: T, sigma, P = pca(noisy)
```

```
print(T.shape)

n_comp = 12

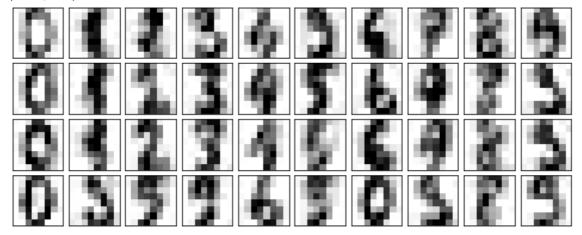
T_new = T[:,0:n_comp]
P_new = P[:,0:n_comp]

print(T_new.shape)

#T_new, P_new, sigmas, n = variance_keeper(T, P, sigma, 0.4)
#print(n)

X_denoised = T_new.dot(P_new.T)
plot_digits(X_denoised)
```

(1797, 64) (1797, 12)



Task 4: Study the impact of normalization of the dataset before conducting PCA. Discuss if it is critical to normalize this particular data compared to the dataset in other notebooks

```
In [95]: X_norm = X - np.mean(X,axis = 0)
    #X_norm = noisy - np.mean(noisy,axis = 0)
    T, sigma, P = pca(X_norm)
    print(X_norm.shape)

    print(np.max(X))

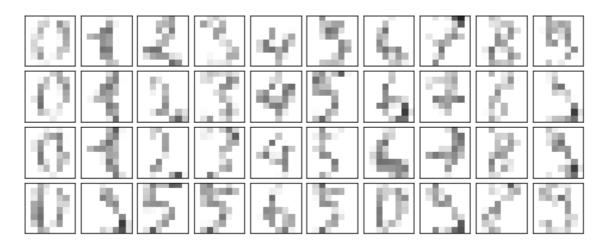
    n_comp = 64

    T_new = T[:,0:n_comp]
    P_new = P[:,0:n_comp]
    print(T_new.shape)

    X_denoised = T_new.dot(P_new.T)
    plot_digits(X_denoised)

(1797, 64)
```

(1797, 64) 16.0 (1797, 64)



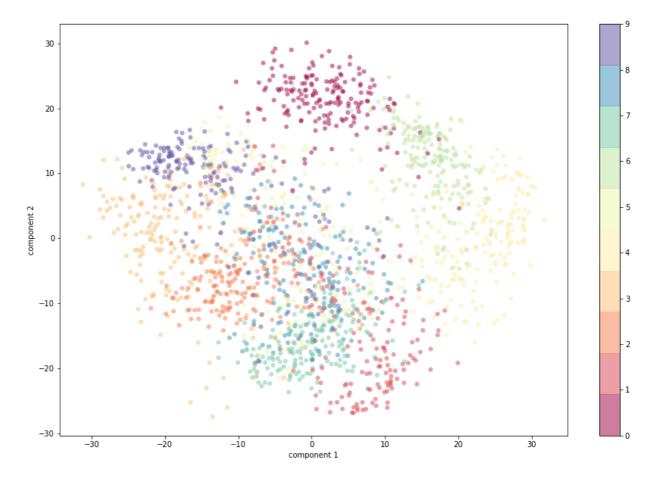
It is not necessary to normalize the data in this task. Here, the data lives in the area $\in [0,16]$, thus shifting the data values so that the mean is about 0, makes no sense. This will only result in the loss of much data. However, it may be usefull to normalize the postion of the digits in each image. I.e. shifting the pixel position so that the center position of the digit in each image lay in the center of the image.

All the above excercise can be done using the SKLEAR library as follows

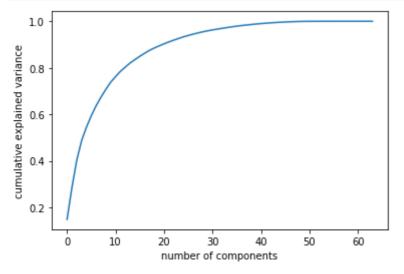
```
In [6]: from sklearn.decomposition import PCA X=digits.data y=digits.target

In [7]: pca = PCA(2) # project from 64 to 2 dimensions projected = pca.fit_transform(digits.data) print(digits.data.shape) print(projected.shape) plot_digits(digits.data)

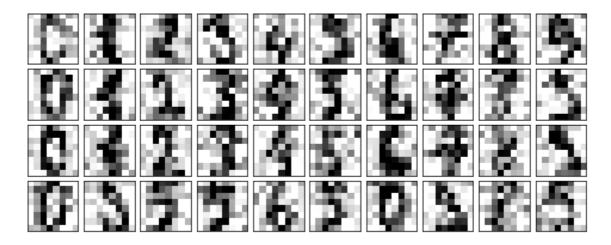
(1797, 64) (1797, 2)
```



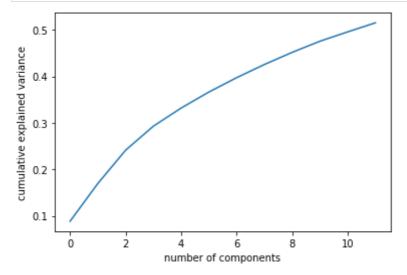
```
In [9]: pca = PCA().fit(digits.data)
   plt.plot(np.cumsum(pca.explained_variance_ratio_))
   plt.xlabel('number of components')
   plt.ylabel('cumulative explained variance');
```



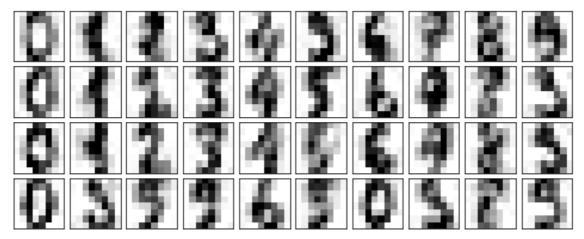
```
In [10]: np.random.seed(42)
    noisy = np.random.normal(digits.data, 4)
    plot_digits(noisy)
```



```
In [11]: pca = PCA(0.50).fit(noisy) # 50% of the variance amounts to 12 principal components.
    pca.n_components_
    plt.plot(np.cumsum(pca.explained_variance_ratio_))
    plt.xlabel('number of components')
    plt.ylabel('cumulative explained variance');
```



In [12]: components = pca.transform(noisy)
 filtered = pca.inverse_transform(components)
 plot_digits(filtered)



Objective: To understand the importance of scaling on PCA

```
In [8]: from sklearn.decomposition import PCA
from sklearn import preprocessing
from sklearn import metrics
import numpy as np
import matplotlib.pyplot as plt
from sklearn.datasets import load_wine
```

Task 0: Write the function to compute the pca using Eigenvector approach

```
In [9]: from numpy.linalg import svd
    def pca(X):
        U, S, P_trans = svd(X, full_matrices = False)
        Sigma = np.diag(S)
        T = np.dot(U,Sigma)
        P = P_trans.T
        return T, Sigma, P #Score, Variace, Loadings
In [10]: features, target = load_wine(return_X_y=True)
    X=features
```

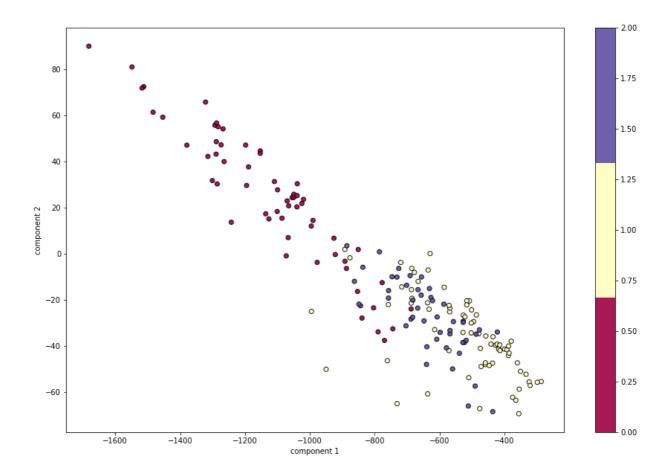
Three different ways of scaling

y=target

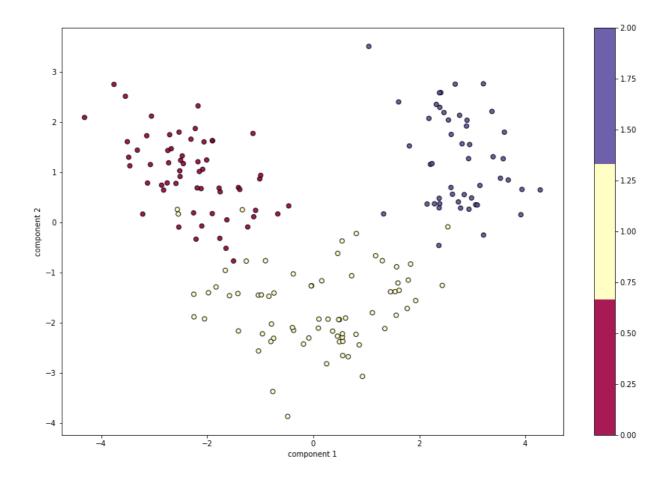
(178, 13)

- Scaling by removing the mean and divising by the standard deviation #standard_scaling=preprocessing.StandardScaler() #X_standard=standard_scaling.fit_transform(X)
- Scaling to min and maximum values of each feature #minmax_scaling=preprocessing.MinMaxScaler() #X_minmax=minmax_scaling.fit_transform(X)
- Scaling by diving by the maximum absolute values of each features #max_abs_scaler=preprocessing.MaxAbsScaler() #X maxabs=max abs scaler.fit transform(X)

Task 1: Create the scores plot without any scaling

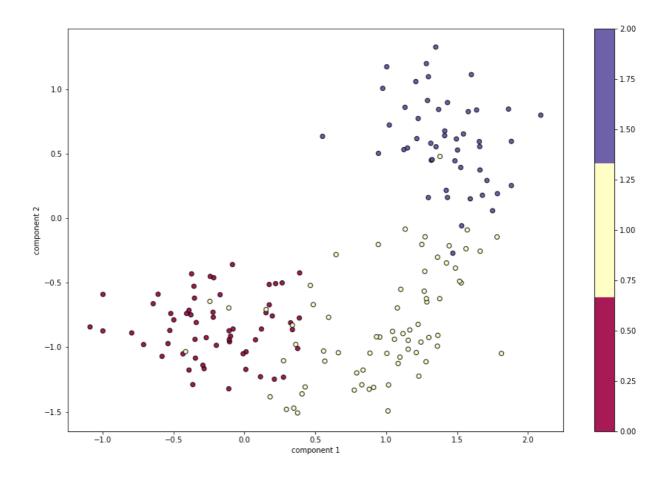


Task 2: Create the scores plot with standard scaling

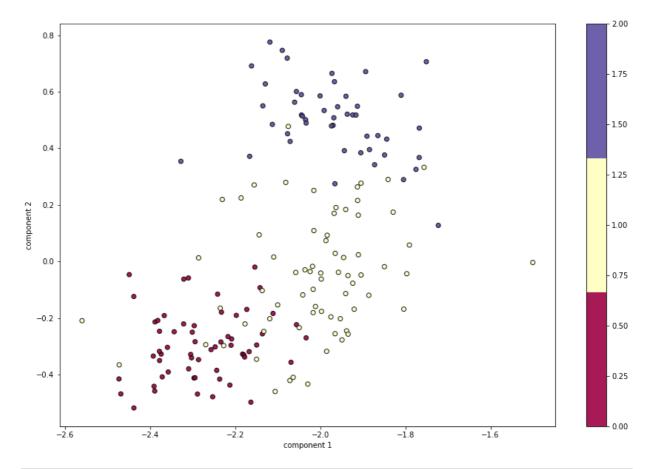


Task 3: Create the scores plot with min max scaling

1680.0



Task 4: Create the scores plot with max abs scaling



In []: