Objective: To understand the importance of scaling on PCA

```
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 pcausing Eigenvector approach

```
In [82]:
          from numpy.linalg import svd
          import numpy.linalq as la
          def pca(X):
              """PCA with eigenvector approach"""
              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)
              return T, Sigma, P # Score, Variance, Loadings
          def pca svd(X):
              """PCA with SVD approach"""
              U, S, PT = svd(X, full matrices=False)
              Sigma = np.diag(S)
              T = np.dot(U, Sigma)
              return T, Sigma, PT.T
```

```
In [77]:
    X, y = load_wine(return_X_y=True)

# Standard scaler
    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 feature
    max_abs_scaler = preprocessing.MaxAbsScaler()
    X_maxabs = max_abs_scaler.fit_transform(X)
```

Three different ways of scaling

Scaling by removing the mean and divising by the standard deviation

```
#standard_scaling=preprocessing.StandardScaler()
#X standard=standard scaling.fit transform(X)
```

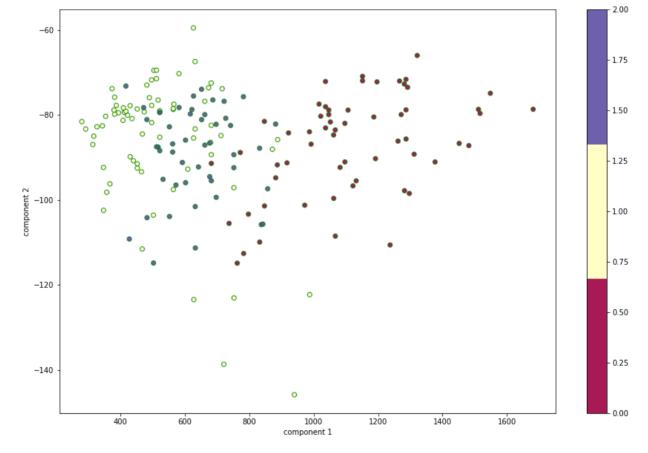
- Scaling to min and maximum values of each feature
 - #minmax_scaling=preprocessing.MinMaxScaler()
 #X minmax=minmax scaling.fit transform(X)
- Scaling by diving by the maximum absolute values of each features

```
#max_abs_scaler=preprocessing.MaxAbsScaler()
#X maxabs=max abs scaler.fit transform(X)
```

Task 1: Create the scores plot without any scaling

```
In [78]:
    T, S, P = pca(X)

plt.figure(figsize=(15,10))
plt.scatter(
        T[:, 0], T[:, 1],
        c=y, edgecolor='green', alpha=0.9,
        cmap=plt.cm.get_cmap('Spectral', 3)
)
plt.xlabel('component 1')
plt.ylabel('component 2')
plt.colorbar();
```

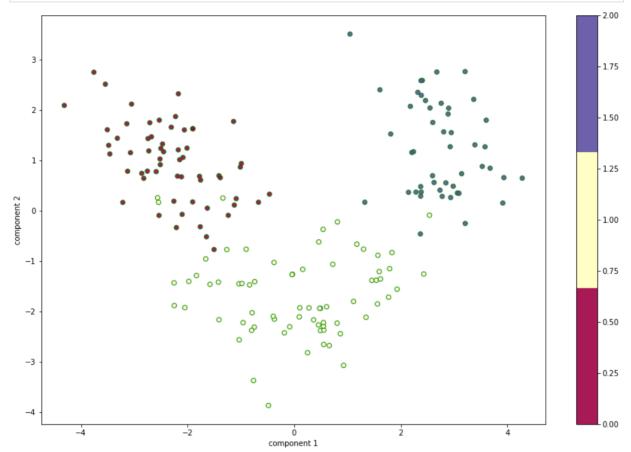


Task 2: Create the scores plot without any standard scaling

With standard scaling?

```
In [79]:
T, S, P = pca(X_standard)
plt.figure(figsize=(15,10))
```

```
plt.scatter(
    T[:, 0], T[:, 1],
    c=y, edgecolor='green', alpha=0.9,
    cmap=plt.cm.get_cmap('Spectral', 3)
)
plt.xlabel('component 1')
plt.ylabel('component 2')
plt.colorbar();
```



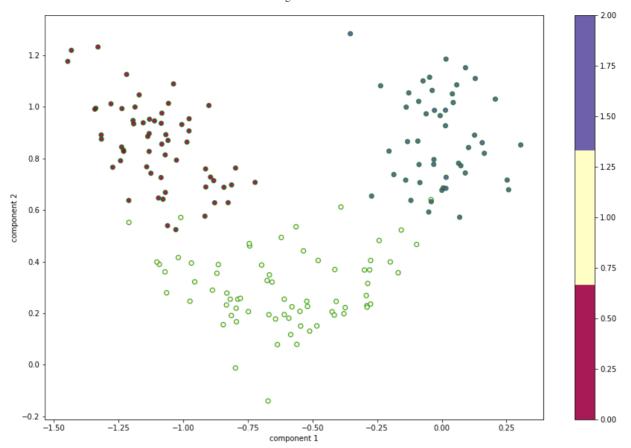
Task 3: Create the scores plot without any min max scaling

With minmax scaling?

```
In [80]:
    T, S, P = pca(X_minmax)

plt.figure(figsize=(15,10))
plt.scatter(
    T[:, 0], T[:, 1],
    c=y, edgecolor='green', alpha=0.9,
    cmap=plt.cm.get_cmap('Spectral', 3)
)

plt.xlabel('component 1')
plt.ylabel('component 2')
plt.colorbar();
```



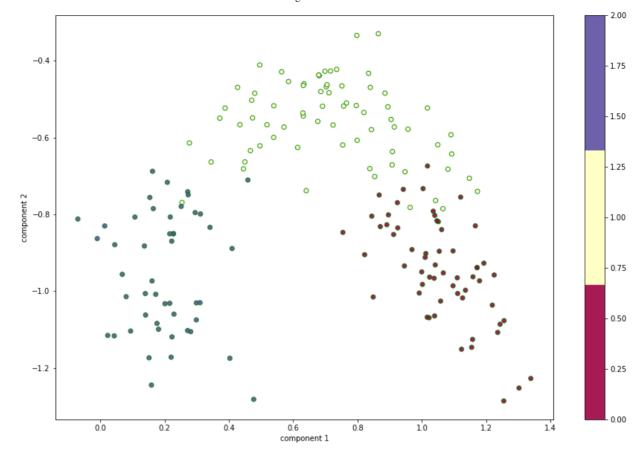
Task 4: Create the scores plot without any max abs scaling scaling

With max abs scaling?

```
In [81]:
    T, S, P = pca(X_maxabs)

plt.figure(figsize=(15,10))
plt.scatter(
    T[:, 0], T[:, 1],
    c=y, edgecolor='green', alpha=0.9,
    cmap=plt.cm.get_cmap('Spectral', 3)
)

plt.xlabel('component 1')
plt.ylabel('component 2')
plt.colorbar();
```



In []:

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

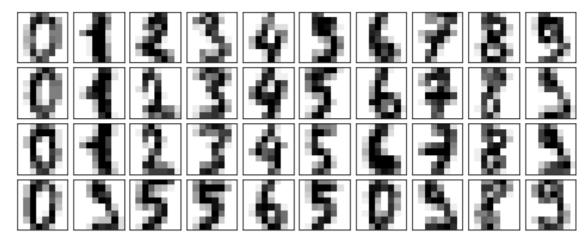
```
import matplotlib.pyplot as plt
import numpy as np
from numpy.linalg import svd
from sklearn.datasets import load_digits

digits = load_digits()
digits.data.shape

Out[2]: (1797, 64)

PCA using SVD
```

```
In [3]:
         def pca(X):
             U, S, PT = svd(X, full_matrices=False)
             Sigma = np.diag(S)
             T = np.dot(U, Sigma)
             return T, Sigma, PT.T # Score, Variance, Loadings
In [4]:
         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 [5]:
        # 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,)
In [6]:
         #Visualize the original data
         plot digits(X)
```

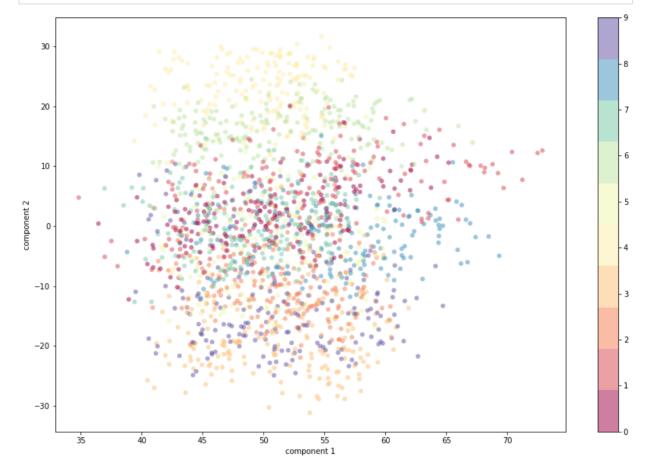


Task 1: Dimensionality reduction: Conduct PCA on the the matrix \$X\$ to find out the dimension required to capture 80% of the variance

```
In [7]:
          import seaborn as sns
          T, S, P = pca(X)
          #plt.plot(sorted(S, reverse=True));
In [8]:
          #SS, _
                 = np.linalg.eig(S)
          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');
           1.00
         cumulative explained variance
           0.95
           0.90
           0.85
           0.80
           0.75
           0.70
                           1000
                                                            4000
                                                 3000
                                      2000
                                number of components
```

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

```
cmap=plt.cm.get_cmap('Spectral', 10))
plt.xlabel('component 1')
plt.ylabel('component 2')
plt.colorbar();
```



Task 3: Denoising: Remove noise from the noisy data

```
In [10]: # 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 [11]:
    T, S, P = pca(noisy)
    n_comps = None
    X_denoised = np.dot(noisy, P)
    plot_digits(X_denoised @ P.T)
```

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

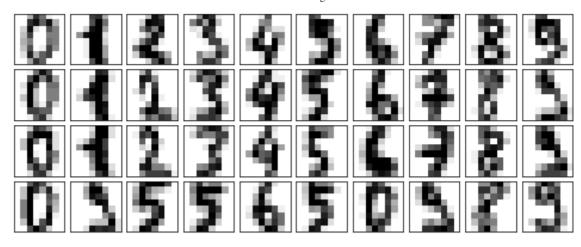
All the above excercise can be done using the SKLEAR library as follows

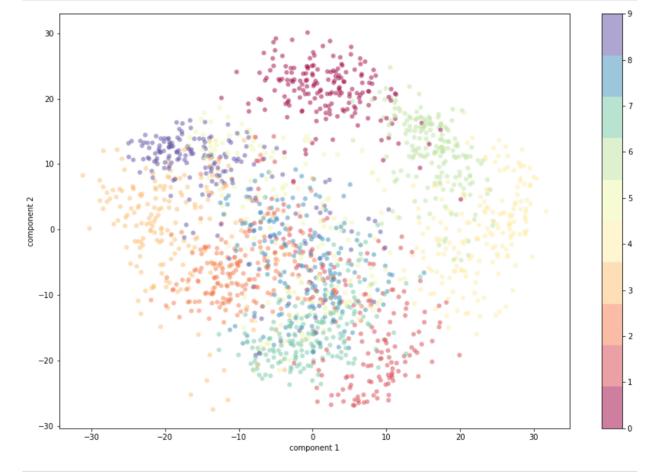
```
In [12]: from sklearn.decomposition import PCA

X = digits.data
y = digits.target

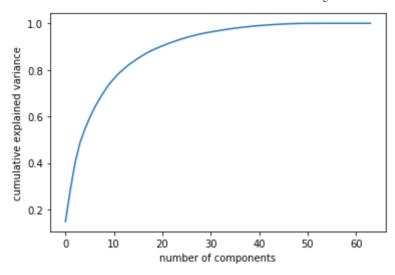
In [13]: pca = PCA(n_components=2) # project from 64 to 2 dimensions
projected = pca.fit_transform(digits.data)
print(digits.data.shape)
print(projected.shape)
plot_digits(digits.data)

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



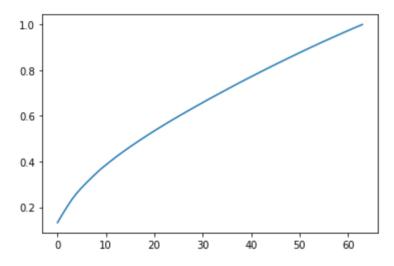


```
pca = PCA().fit(digits.data)
    plt.plot(np.cumsum(pca.explained_variance_ratio_))
    plt.xlabel('number of components')
    plt.ylabel('cumulative explained variance');
```

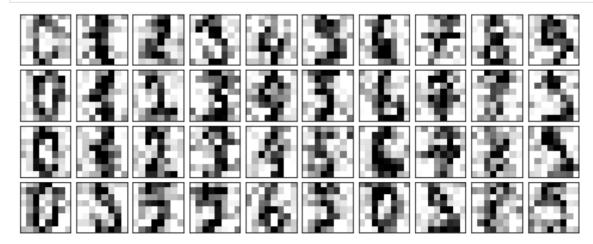


```
In [16]:
    S_diag = np.diag(S)#**2 / 4
    SS = S_diag / np.sum(S_diag)
    plt.plot(np.cumsum(SS))
```

Out[16]: [<matplotlib.lines.Line2D at 0x7fc119270ac0>]



```
np.random.seed(42)
noisy = np.random.normal(digits.data, 4)
plot_digits(noisy)
```

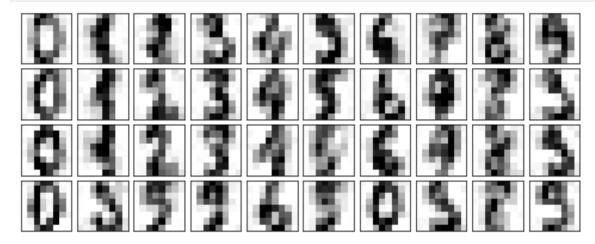


```
pca = PCA(0.50).fit(noisy) # 50% of the variance amounts to 12 principal comp
pca.n_components_
plt.plot(np.cumsum(pca.explained_variance_ratio_))
```

```
plt.xlabel('number of components')
plt.ylabel('cumulative explained variance');
```

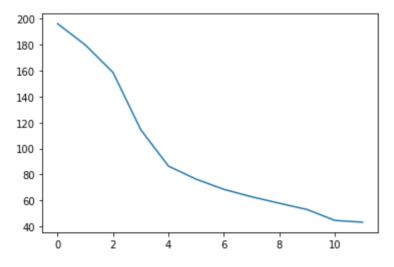
```
0.5 - 0.4 - 0.4 - 0.2 - 0.1 - 0.2 - 0.1 - 0.2 - 0.1 - 0.2 - 0.1 - 0.2 - 0.1 - 0.2 - 0.1 - 0.2 - 0.1 - 0.2 - 0.1 - 0.2 - 0.1 - 0.2 - 0.1 - 0.2 - 0.1 - 0.2 - 0.1 - 0.2 - 0.2 - 0.1 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 -
```

```
In [19]: components = pca.transform(noisy)
    filtered = pca.inverse_transform(components)
    plot_digits(filtered)
```



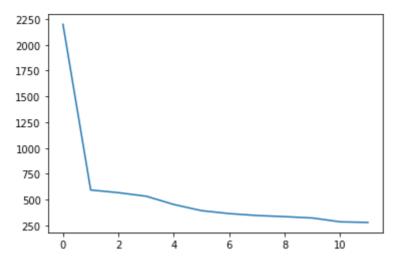
```
In [20]: plt.plot(pca.explained_variance_)
```

Out[20]: [<matplotlib.lines.Line2D at 0x7fc117b2bac0>]



```
In [21]: plt.plot(np.diag(S)[:12])
```

Out[21]: [<matplotlib.lines.Line2D at 0x7fc118a17be0>]



In []:
In []:

Objective: To develop a mathematical understanding of PCA

Test data

```
In [2]: import numpy as np
    from scipy import linalg as LA

X = np.array([
            [0.387,4878, 5.42],
            [0.723,12104,5.25],
            [1,12756,5.52],
            [1,524,6787,3.94],
        ])
X -= np.mean(X, axis=0)
```

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^T}\mathbf{x})^{-1}\mathbf{x^T}\mathbf{y}\$). In the current notation we get \$\$p_{ka}=\frac{\mathbf{t_a^T}\mathbf

Repeat it for each of the columns of X to get the entire vector \mathcal{p}_{k} . This is shown in the illustration above where each column from X is regressed, one at a time, on \mathcal{L}_{a} , to calculate the loading entry, \mathcal{L}_{p}_{k}

In practice we don't do this one column at time; we can regress all columns in \$X\$ in go: $\$\mathrm{p_a^T}=\frac{1}{\mathrm{nathbf\{t_a^T\}}}\$ where $\mathrm{mathbf\{t_a\}}\$ is an \$N \times 1\$ column vector, and $\mathrm{mathbf\{X\}_{a}}\$ us an \$N \times 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}=\frac{\pi^T}{\frac{p_a^T}}\$\$
- 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}=\frac{mathbf\{x\}_{i}^{T}\mathbb{p}_{a}}{\mathbf{p}_{a}^{T}\mathbb{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}=\frac{1} {\mathbb{p}_{a}^{T}\mathbb{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}\$:

```
$E_{a}=X_{a}-t_{a}p_{a}^{T}$
```

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 [3]:
         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.

```
In [4]:
        no components=3
        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]
         [ 9.9999997e-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 [5]:
    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(" ")
```

[7.30130279e-05 -8.24088734e-01 -5.66460725e-01]]

[6.74994067e+03 1.41840009e+00 2.46466604e-01]

SKLEARN PCA

Sigma (Variance)

```
In [6]:
         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]
         [ 9.99999997e-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]
In [7]:
         pca.explained variance ratio
Out[7]: array([9.99999955e-01, 4.41567976e-08, 1.33326424e-09])
In [8]:
         explained variance 2 = (S ** 2) / 4
         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: $\frac{\pi}{p_1^T} \frac{1}{T}\right$ \mathbf{X^T}\mathbf{X^T}\mathbf{Xp_1}\$\$ such that $\frac{\pi}{p_1^T} \frac{1}{T}$

This is equivalent to $\frac{p_1^T} \int \frac{y_1^T}{mathbf\{p_1^T\}} \frac{y_1^T}{mathbf\{p_1^T\}}$

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

our search variable, are zero: $\frac{\pi p_1}= \frac{p_1}= \frac{p_1}= \frac{p_1^T X^T Xp_1}-\lambda(\mathbb{p}_1)}{p_1^T}=0$

 $$\$2\mathbb{X}^T \times p_1$-2\lambda_1\mathbb{E}_0$\$\$(\mathbb{X}^T \times p_1)=0\$\$\$(\mathbb{X}^T \times p_1)=\lambda_1\mathbb{E}_1.$ $\lambda_1\mathbb{E}_1.$ $\lambda_1\mathbb{E}_1.$ $\lambda_1\mathbb{E}_1.$ $\lambda_1\mathbb{E}_1.$ $\lambda_1.$ \lambd

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

From this we learn that:

- The loadings are the eigenvectors of \$\mathbf{X^TX}\$.
- 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^TX}\$ 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 \$\mathbf{X^TX}\$, which represents of the total variance of the \$\mathbf{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 [9]: 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(P)
print("Sigma (Variance)")
print(Sigma)
T (Scores)
[[ 4.25324997e+03     8.41288672e-01     8.37858943e-03]
```

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

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

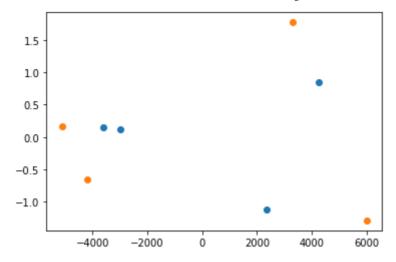
Task 3: Add more columns to the original data matrix by:

- Make some of the columns to be the linear combination of others
- Duplicate some columns
- Add noise as some columns
- Add a few columns of categorical values

Then apply PCA to the dataset and report your findings here

```
In [64]:
          import pandas as pd
          import matplotlib.pyplot as plt
          from sklearn import preprocessing
          X aug = pd.DataFrame(X.copy())
          # Duplicating a couple of columns
          X_aug['1_copy'] = X_aug[1]
          X \text{ aug}['2 \text{ copy'}] = X \text{ aug}[2]
          # Adding Gaussian noise as columns
          X aug['noise 1'] = np.random.normal(0, 1, len(X aug.index))
          X_aug['noise_2'] = np.random.normal(0, 1, len(X aug.index))
          # Adding random categorical columns
          cat dog = lambda x: 'Cat' if x < 0 else 'Dog'
          X aug['cat 1'] = X aug['noise 1'].apply(cat dog)
          X aug['cat 2'] = X aug['noise 2'].apply(cat dog)
          print(X aug)
          # Need to encode string categoricals
          le = preprocessing.LabelEncoder()
          le.fit(X aug['cat 1'])
          X aug['cat 1'] = le.transform(X aug['cat 1'])
          X aug['cat 2'] = le.transform(X aug['cat 2'])
          X aug
                                   2
                                        1 copy
                                                2 сору
                                                         noise 1
                                                                    noise 2 cat 1 cat 2
                           1
         0 -0.5215 -4253.25 0.3875 -4253.25
                                               0.3875 -0.878956 -0.808482
                                                                              Cat
         1 -0.1855 2972.75
                              0.2175 2972.75
                                                0.2175 -1.350578 0.105816
                                                                              Cat
                                                                                     Dog
                             0.4875 3624.75
                                                                   1.428250
                    3624.75
                                               0.4875 0.223769
                                                                              Dog
            0.0915
                                                                                     Dog
            0.6155 -2344.25 -1.0925 -2344.25 -1.0925 -0.762587
                                                                   1.046066
                                                                              Cat
                                                                                     Dog
                 0
                          1
                                  2
                                      1_copy 2_copy
                                                       noise_1
                                                                noise_2 cat_1 cat_2
Out[64]:
          0 -0.5215 -4253.25 0.3875 -4253.25 0.3875 -0.878956 -0.808482
                                                                           0
                                                                                 0
          1 -0.1855
                    2972.75
                             0.2175
                                     2972.75
                                              0.2175 -1.350578
                                                                0.105816
                                                                           0
                                                                                  1
          2
            0.0915
                    3624.75 0.4875
                                     3624.75 0.4875 0.223769
                                                               1.428250
                                                                            1
                                                                                  1
             0.6155 -2344.25 -1.0925 -2344.25 -1.0925 -0.762587
                                                               1.046066
                                                                           0
                                                                                  1
In [65]:
          pca = PCA(n components=2)
          T aug = pca.fit transform(X aug)
          plt.scatter(T[:, 0], T[:, 1], label='Normal')
          plt.scatter(T aug[:, 0], T aug[:, 1], label='Augmented')
```

Out[65]: <matplotlib.collections.PathCollection at 0x7f2dcf31b9d0>



In []: # Slighly different transformed values due to the randomly generated noise co # More explanations / plots