

```
In [1]: import matplotlib.pyplot as plt
import numpy as np
from mpl_toolkits.mplot3d import Axes3D
```

Projection is not always the best approach to dimensionality reduction. For example, consider the famous *Swiss roll* toy dataset

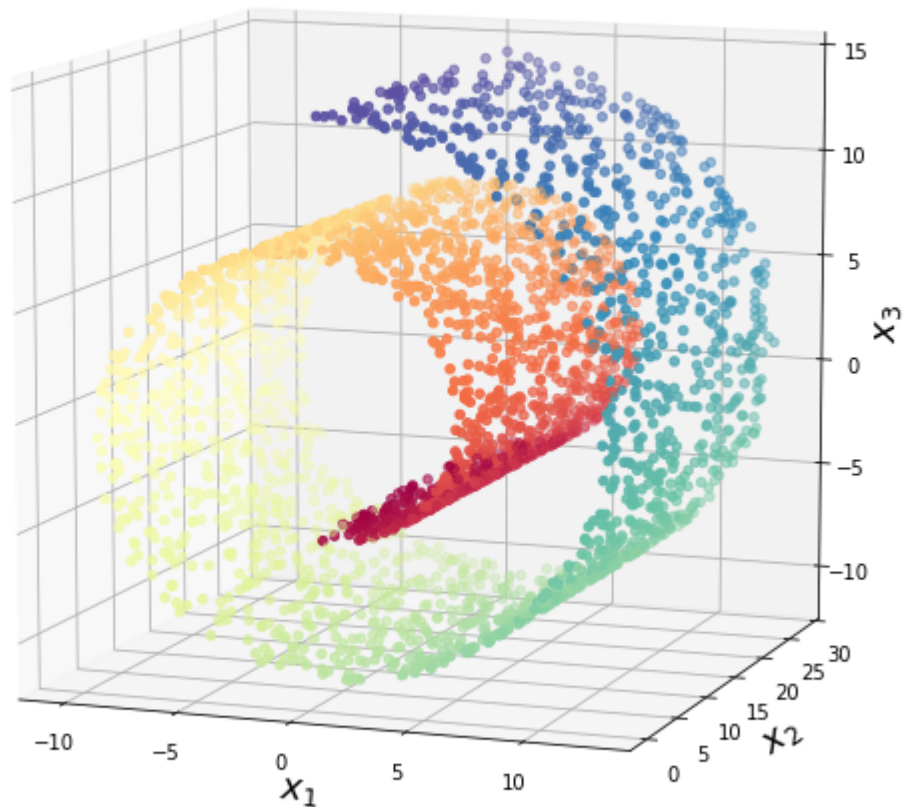
```
In [171]: 'Make a Swiss roll'
m = 3000
t = 1.5 * np.pi * (1 + 2 * np.random.rand(1, m))
x1 = t * np.cos(t)
x2 = 30 * np.random.rand(1, m)
x3 = t * np.sin(t)
X = np.concatenate((x1, x2, x3))
X = X.T
t = np.squeeze(t)

'Plot the Swiss roll'
axes = [-11.5, 14, -2, 30, -12, 15]

fig = plt.figure(figsize=(10,10))
ax = plt.axes(projection='3d')
ax.scatter(X[:, 0], X[:, 1], X[:, 2], c=t, cmap=plt.cm.Spectral)
ax.view_init(10, -70)
ax.set_xlabel("$x_1$", fontsize=18)
ax.set_ylabel("$x_2$", fontsize=18)
ax.set_zlabel("$x_3$", fontsize=18)
ax.set_xlim(axes[0:2])
ax.set_ylim(axes[2:4])
ax.set_zlim(axes[4:6])
plt.title('Swiss roll dataset', fontsize=30)
```

```
Out[171]: Text(0.5, 0.92, 'Swiss roll dataset')
```

Swiss roll dataset



Let's use PCA to project the *Swiss roll* into a two-dimensional subspace

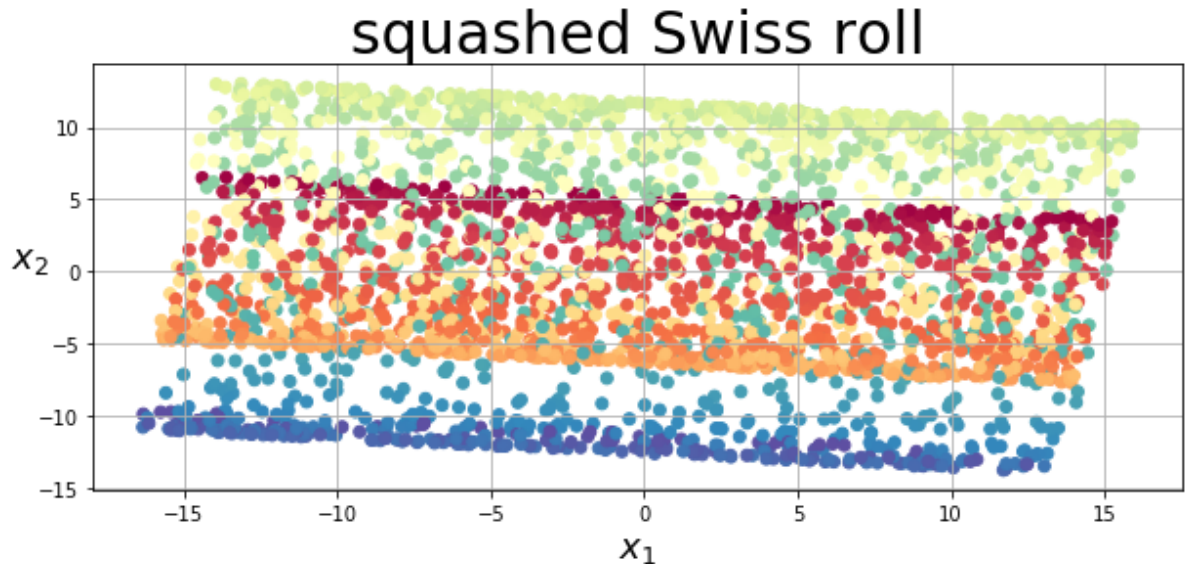
```
In [159]: 'PCA'
# center the dataset
X_centered = X - np.mean(X,axis=0)

# Singular Value Decomposition
u,s,v = np.linalg.svd(X_centered)

# principal components
k = 2
c = v[:, :k]

# projection
X_reduced = X_centered@v[:, :k].T
```

```
In [160]: 'plot PCA projection'
plt.figure(figsize=(10,4))
plt.scatter(X_reduced[:,0],X_reduced[:,1], c=t, cmap=plt.cm.Spectral)
plt.xlabel("$x_1$", fontsize=18)
plt.ylabel("$x_2$", fontsize=18, rotation=0)
plt.title('squashed Swiss roll',fontsize=30)
plt.grid(True)
```



PCA squashes different layers of the Swiss roll together. What we really want is to "unroll" the Swiss roll.

11.3 - Locally Linear Embedding (LLE)

The Swiss roll is an example of a two-dimensional **manifold** embedded in a three-dimensional space. Key property of a manifold: locally, a manifold looks flat. **Locally linear embedding (LLE)** is a clever scheme that exploits this property for unrolling twisted manifolds.

Here's how LLE works:

11.3.1 - Locally Linear Embedding Step by Step

Step 1: First, for each dataset point, the algorithm identifies its k closest neighbors (in the preceding code $k = 10$).

```
In [161]: n_neighbors = 10
m,n = X.shape
# compute all pairwise distances
distance = np.zeros((m,m))
for i in range(m):
    for j in range(m):
        distance[i,j] = np.linalg.norm(X[i]-X[j])
# find local neighborhoods for each point
index = np.argsort(distance,axis=1)
neighborhoods = index[:,1:n_neighbors+1]
```

The above code is slow. A better approach uses scipy distance function

```
In [172]: 'faster alternative'
from scipy.spatial import distance
n_neighbors = 10
m,n = X.shape
# compute all pairwise distances
distances = distance.squareform(distance.pdist(X))
# Find local neighborhoods for each point
index = np.argsort(distances,axis=1)
neighborhoods = index[:,1:n_neighbors+1]
```

For example, the closest neighbors of $X[0]$

```
In [163]: X[0]
```

```
Out[163]: array([ 9.66042746, 16.7876403 ,  9.17960572])
```

are

```
In [164]: X[neighborhoods[0]]
```

```
Out[164]: array([[ 9.56448165, 16.29019057,  9.29570298],
 [10.1177305 , 16.77678891,  8.58641792],
 [ 9.67484816, 17.71733307,  9.16192259],
 [ 9.9906982 , 17.84091668,  8.7582643 ],
 [ 8.75364487, 17.07569776, 10.1812902 ],
 [ 9.10501346, 17.89979871,  9.8170381 ],
 [10.57234096, 17.02986477,  7.91895413],
 [10.68979475, 16.56540252,  7.73115584],
 [10.26008042, 15.28963198,  8.38669504],
 [ 9.49973637, 18.63829849,  9.37255747]])
```

Step 2: Second, the algorithm tries to reconstruct each point as a **linear combination** of its k closest neighbors. More specifically, if we denote by $\bar{x}_1, \bar{x}_2, \dots, \bar{x}_k$ the k closest neighbors of x_i , the algorithm finds the weights w_{ij} that minimize

$$\|x_i - \sum_{j=1}^k w_{ij} \bar{x}_j\|_2^2 + \lambda \sum_{j=1}^k w_{ij}^2$$

subject to the condition

$$\sum_{j=1}^k w_{ij} = 1.$$

The regularization term $\lambda \sum_{j=1}^k w_{ij}^2$ is there to prevent overfitting issues, and the condition $\sum_{j=1}^k w_{ij} = 1$ is imposed to make the algorithm invariant to translations of the dataset.

Using the matrix and the (row) vector

$$\bar{X}_i = \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \\ \vdots \\ \bar{x}_k \end{bmatrix} \quad \text{and} \quad w = [w_{i1} \quad w_{i2} \quad \dots \quad w_{ik}],$$

the problem of finding the weights becomes:

$$\begin{aligned} &\text{minimize } \|x_i - w\bar{X}_i\|_2^2 + \lambda \|w\|_2^2 \\ &\text{subject to } \sum_{j=1}^k w_{ij} = 1 \end{aligned}$$

This is a constrained optimization problem, and its solution can be computed in closed form (hooray for linear algebra!!); see the problem at the end of the Jupyter Notebook.

First, we form the matrix

$$Z_i = \begin{bmatrix} \bar{x}_1 - x_i \\ \bar{x}_2 - x_i \\ \vdots \\ \bar{x}_k - x_i \end{bmatrix}.$$

Second, we compute the matrix

$$C_i = Z_i Z_i^T + \lambda I_k.$$

Third, we solve the linear system

$$C_i w^T = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}$$

for the vector w .

Finally, we normalize w so that its entries add up to 1.

```
In [174]: lam = 1e-3 # regularization parameter
W = np.zeros((m,m)) # store the weights in this matrix
for i in range(m):
    Z = X[neighborhoods[i]]-X[i] # form matrix Z
    C = Z@Z.T # compute matrix C
    C = C + lam*np.identity(n_neighbors)*np.linalg.norm(Z) # add the regularization term
    w = np.linalg.solve(C,np.ones(n_neighbors)) # solve the linear system
    W[i,neighborhoods[i]] = w/np.sum(w) # normalize w
```

After this step, the weight matrix W (containing the weights w_{ij}) encodes the local linear relationships between the dataset points.

Step 3: The goal of the LLE algorithm is to preserve the local linear structure of the high-dimensional space as accurately as possible in a low-dimensional space. Hence, the matrix W is kept fixed and embedded coordinates y_i are sought by minimizing the following function

$$\sum_{i=1}^m \|y_i - \sum_{j=1}^m w_{ij} y_j\|_2^2.$$

Using the matrix

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix},$$

the problem of finding the embedded coordinates y_i becomes

$$\text{minimize } \sum_{i=1}^m \|\text{row } i \text{ of } (I_m - W)Y\|_2^2$$

This optimization problem also has a closed-form solution. To solve it, first we form the matrix

$$M = (I_m - W)^T(I_m - W).$$

If we are embedding the dataset into a space of dimension d , then the columns of Y are the eigenvectors of M associated with the d smallest nonzero eigenvalues.

```
In [175]: d = 2
from scipy.sparse.linalg import eigsh # function for finding eigenvalues and e
         igenvectors of symmetric matrices

#M = (np.identity(m)-W).T@(np.identity(m)-W)
M = np.identity(m)-W.T-W+W.T@W
evalues,evector = eigsh(M,
                        k=d+1,
                        sigma = 0, # compute the eigenvectors with the smalle
st eigenvalues
                        maxiter = 100,
                        tol = 1e-06)
index = np.argsort(evalues) # sort eigenvalues
reduced_X = np.real(evector[:,index[1:d+1]]) # drop the eigenvector with eige
nvalue equal to 0
```

The resulting 2D dataset is shown in the figure below. As you can see, the Swiss roll is completely unrolled, and the distances between points are locally preserved.

In [176]: 'plot the Swiss roll and the unrolled Swiss roll'

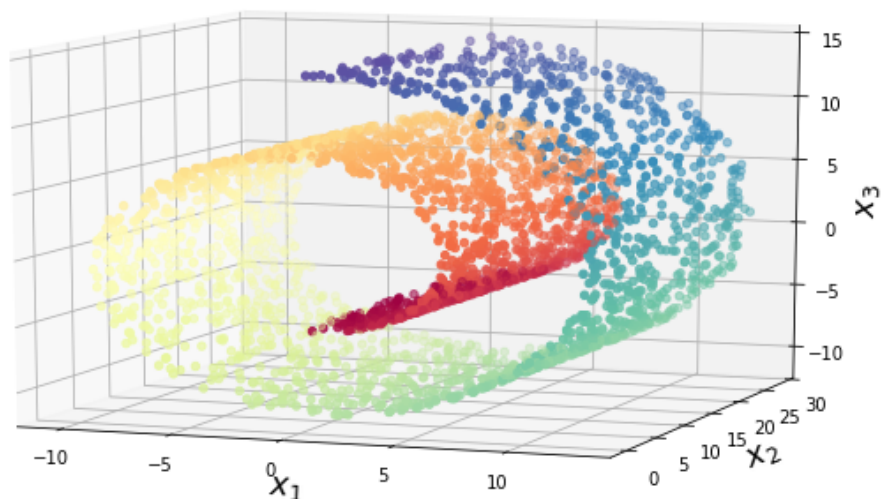
```
fig = plt.figure(figsize=(11, 15))

# Swiss roll
ax = plt.subplot(2,1,1, projection='3d')
axes = [-11.5, 14, -2, 30, -12, 15]
ax.scatter(X[:, 0], X[:, 1], X[:, 2], c=t, cmap=plt.cm.Spectral)
ax.view_init(10, -70)
ax.set_xlabel("$x_1$", fontsize=18)
ax.set_ylabel("$x_2$", fontsize=18)
ax.set_zlabel("$x_3$", fontsize=18)
ax.set_xlim(axes[0:2])
ax.set_ylim(axes[2:4])
ax.set_zlim(axes[4:6])
plt.title('Swiss roll', fontsize=20)

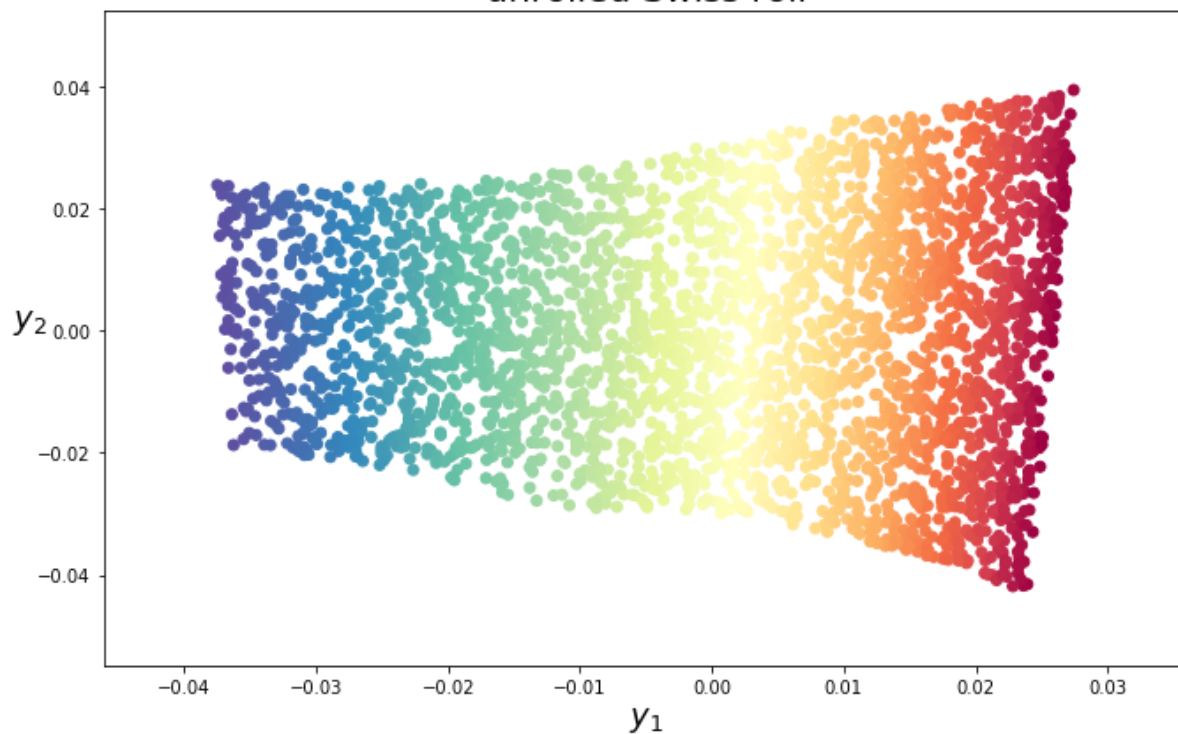
# unrolled Swiss roll
plt.subplot(2,1,2)
plt.scatter(reduced_X[:,0], reduced_X[:,1], c=t, cmap=plt.cm.Spectral)
plt.xlabel("$y_1$", fontsize=18)
plt.ylabel("$y_2$", fontsize=18, rotation=0)
plt.title('unrolled Swiss roll', fontsize=20)
```

```
Out[176]: Text(0.5, 1.0, 'unrolled Swiss roll')
```

Swiss roll



unrolled Swiss roll



Amazing, isn't it?

11.3.1 Locally Linear Embedding Implementation

```

In [2]: def lle(X,d=2,n_neighbors=5):
    from scipy.spatial import distance
    from scipy.sparse.linalg import eigsh
    from scipy.linalg import solve

    m,n = X.shape
    'step 1: compute pairwise distances and find neighbors'
    print('step 1: computing pairwise distances')
    distances = distance.squareform(distance.pdist(X))
    index = np.argsort(distances,axis=1)
    neighbors = index[:,1:n_neighbors+1]

    'step 2: solve for reconstruction weights'
    print('step 2: computing weights')
    if n_neighbors>m:
        lam = 1e-3
    else:
        lam = 0
    reg = 1e-3
    W = np.zeros((m,m))
    for i in range(m):
        Z = X[neighbors[i]]-X[i]
        C = Z@Z.T
        C = C + reg*np.identity(n_neighbors)*np.linalg.norm(Z)
        w = solve(C,np.ones(n_neighbors),sym_pos=True)
        W[i,neighbors[i]] = w/np.sum(w)

    'step 3: compute embedding from eigenvectors of the matrix (I-W)^T*(I-W)'
    print('step 3: computing new points')
    M = np.identity(m)-W.T-W+W.T@W
    tol = 1e-05
    max_iter=100
    evals,evecs = eigsh(M,
                        k=d+1,
                        sigma = 0,
                        maxiter = max_iter,
                        tol = tol)
    index = np.argsort(evals)
    reduced_X = np.real(evecs[:,index[1:d+1]])
    return reduced_X

```

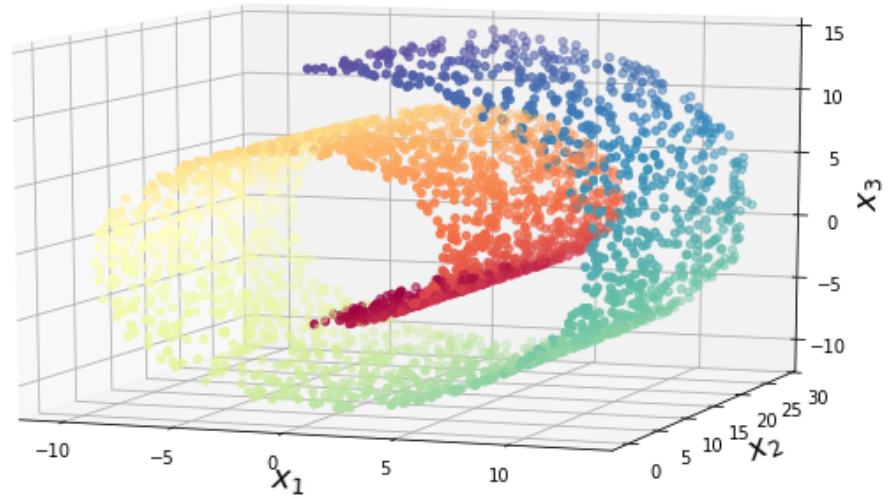
```
In [178]: 'test lle'
reduced_X = lle(X,
                d = 2,
                n_neighbors = 10)
'Plot original and reduced datasets'
fig = plt.figure(figsize=(11, 15))
# Swiss roll
ax = plt.subplot(2,1,1, projection='3d')
axes = [-11.5, 14, -2, 30, -12, 15]
ax.scatter(X[:, 0], X[:, 1], X[:, 2], c=t, cmap=plt.cm.Spectral)
ax.view_init(10, -70)
ax.set_xlabel("$x_1$", fontsize=18)
ax.set_ylabel("$x_2$", fontsize=18)
ax.set_zlabel("$x_3$", fontsize=18)
ax.set_xlim(axes[0:2])
ax.set_ylim(axes[2:4])
ax.set_zlim(axes[4:6])
plt.title('Swiss roll', fontsize=20)

# unrolled Swiss roll
plt.subplot(2,1,2)
plt.scatter(reduced_X[:,0], reduced_X[:,1], c=t, cmap=plt.cm.Spectral)
plt.xlabel("$y_1$", fontsize=18)
plt.ylabel("$y_2$", fontsize=18, rotation=0)
plt.title('unrolled Swiss roll', fontsize=20)
```

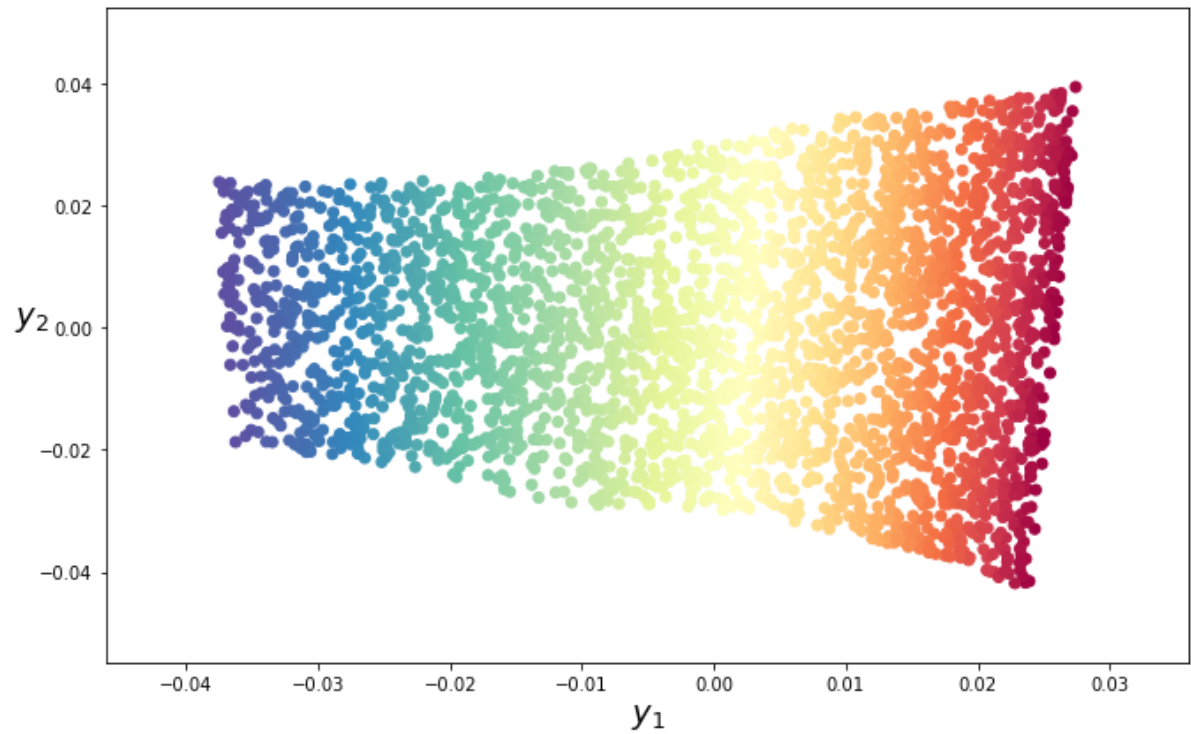
step 1: computing pairwise distances
step 2: computing weights
step 3: computing new points

Out[178]: Text(0.5, 1.0, 'unrolled Swiss roll')

Swiss roll



unrolled Swiss roll



```

In [179]: def lle_sparse(X,d=2,n_neighbors=5):
    'Use this version if the dataset is big'
    from scipy.spatial import distance
    from scipy.sparse import eye
    from scipy.sparse.linalg import eigsh
    from scipy.linalg import solve
    from sklearn.utils import check_random_state

    m,n = X.shape
    'step 1: compute pairwise distances and find neighbors'
    print('step 1: computing pairwise distances')
    distances = distance.squareform(distance.pdist(X))

    index = np.argsort(distances,axis=1)
    neighbors = index[:,1:n_neighbors+1]

    'step 2: solve for reconstruction weights'
    print('step 2: computing weights')
    reg = 1e-3
    W = np.zeros((m,n_neighbors))
    for i in range(m):
        Z = X[neighbors[i]]-X[i]
        C = Z@Z.T
        C = C + reg*np.identity(n_neighbors)*np.linalg.norm(Z) #np.trace(C)
        w = solve(C,np.ones(n_neighbors),sym_pos=True)
        W[i] = w/np.sum(w)

    'step 3: compute embedding from eigenvectors of the matrix (I-W)^T*(I-W)'
    print('step 3: computing new points')
    'form matrix M'
    M = eye(m,format='lil') # sparse matrix
    for i in range(m):
        j = neighbors[i]
        M[i,j] = M[i,j] - W[i]
    M = (M.T * M).tocsr()
    'get eigenvectors'
    random_state = check_random_state(None)
    v0 = random_state.uniform(-1, 1, M.shape[0])
    tol = 1e-06
    max_iter = 100
    evalues,evectors = eigsh(M,
                            k=d+1,
                            sigma = 0,
                            maxiter = max_iter,
                            tol = tol,
                            v0 = v0)
    reduced_X = np.real(evectors[:,1:])*np.sqrt(m)
    return reduced_X

```

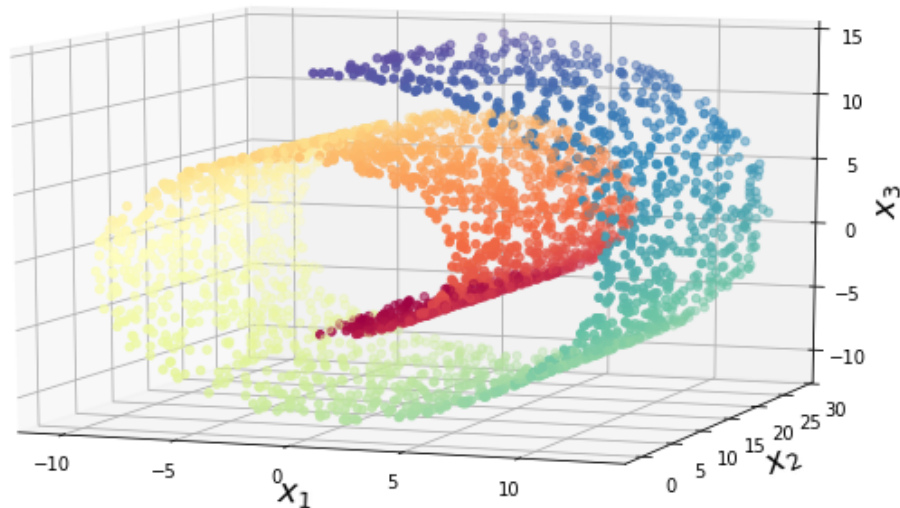
```
In [180]: 'test lle_sparse function'
reduced_X = lle_sparse(X,
                      d = 2,
                      n_neighbors = 10)
'Plot original and reduced datasets'
fig = plt.figure(figsize=(11, 15))
# Swiss roll
ax = plt.subplot(2,1,1, projection='3d')
axes = [-11.5, 14, -2, 30, -12, 15]
ax.scatter(X[:, 0], X[:, 1], X[:, 2], c=t, cmap=plt.cm.Spectral)
ax.view_init(10, -70)
ax.set_xlabel("$x_1$", fontsize=18)
ax.set_ylabel("$x_2$", fontsize=18)
ax.set_zlabel("$x_3$", fontsize=18)
ax.set_xlim(axes[0:2])
ax.set_ylim(axes[2:4])
ax.set_zlim(axes[4:6])
plt.title('Swiss roll', fontsize=20)

# unrolled Swiss roll
plt.subplot(2,1,2)
plt.scatter(reduced_X[:,0], reduced_X[:,1], c=t, cmap=plt.cm.Spectral)
plt.xlabel("$y_1$", fontsize=18)
plt.ylabel("$y_2$", fontsize=18, rotation=0)
plt.title('unrolled Swiss roll', fontsize=20)
```

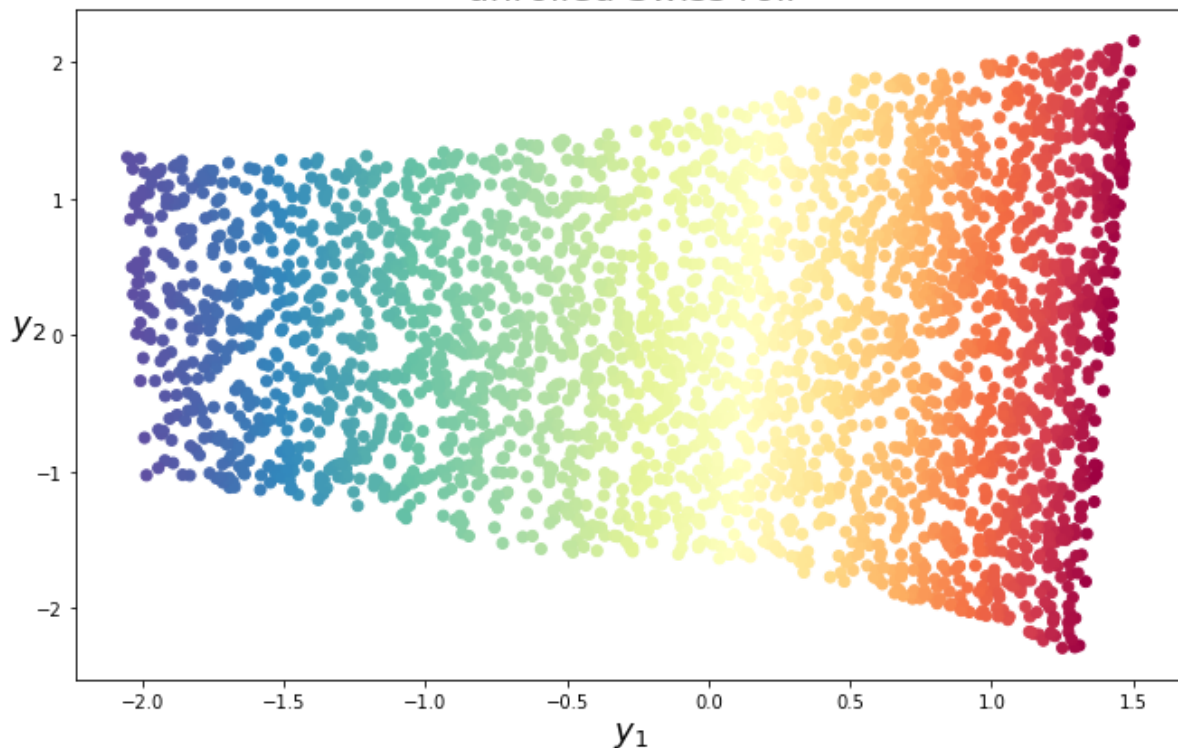
step 1: computing pairwise distances
step 2: computing weights
step 3: computing new points

Out[180]: Text(0.5, 1.0, 'unrolled Swiss roll')

Swiss roll



unrolled Swiss roll



11.3.3 Examples

Example 1: a Spiral

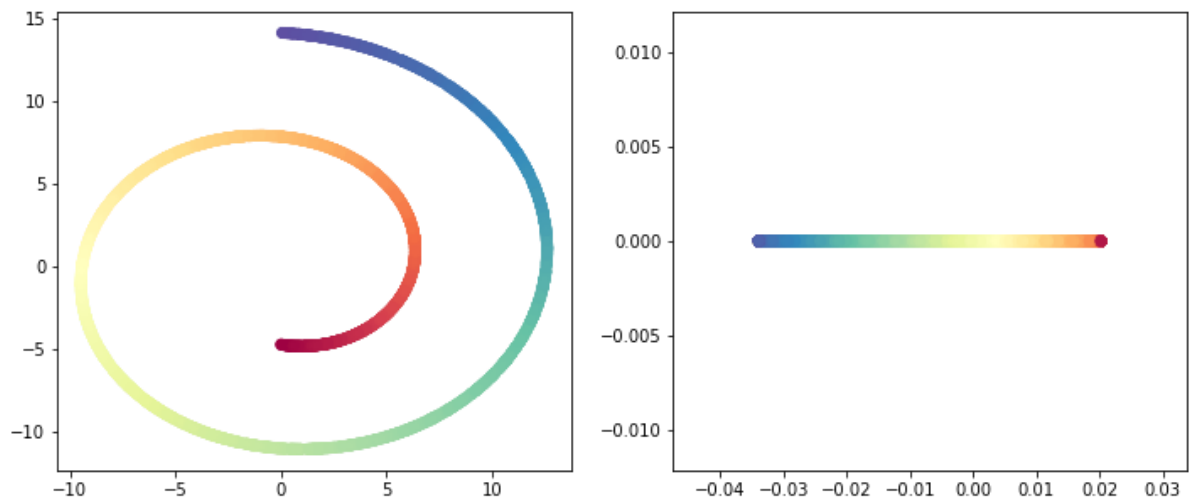
```
In [12]: 'Make a spiral'
m = 3000
t = 1.5 * np.pi * (1 + 2 * np.random.rand(1, m))
x = t * np.cos(t)
y = t * np.sin(t)
X = np.concatenate((x, y))
X = X.T
t = np.squeeze(t)

'Unroll the spiral'
reduced_X = lle(X,
                d = 1,
                n_neighbors = 10)
```

step 1: computing pairwise distances
 step 2: computing weights
 step 3: computing new points

```
In [14]: plt.figure(figsize=(12,5))
'Plot the spiral'
plt.subplot(1,2,1)
plt.scatter(X[:,0],X[:,1],c=t,cmap = plt.cm.Spectral)
'Plot the unrolled spiral'
plt.subplot(1,2,2)
plt.scatter(reduced_X,np.zeros(len(reduced_X)), c=t, cmap=plt.cm.Spectral)
```

Out[14]: <matplotlib.collections.PathCollection at 0x23499b8ec88>

**Example 2: a Sphere with a Hole**

```
In [50]: 'Make a sphere with a hole'
m = 3000
r = 1
phi = 2 * np.pi * np.random.rand(1, m)
t = np.pi/4 + (np.pi-np.pi/4) * np.random.rand(1, m)
x = r*np.sin(t)*np.cos(phi)
y = r*np.sin(t)*np.sin(phi)
z = r*np.cos(t)
X = np.concatenate((x, y,z))
X = X.T
t = np.squeeze(t)

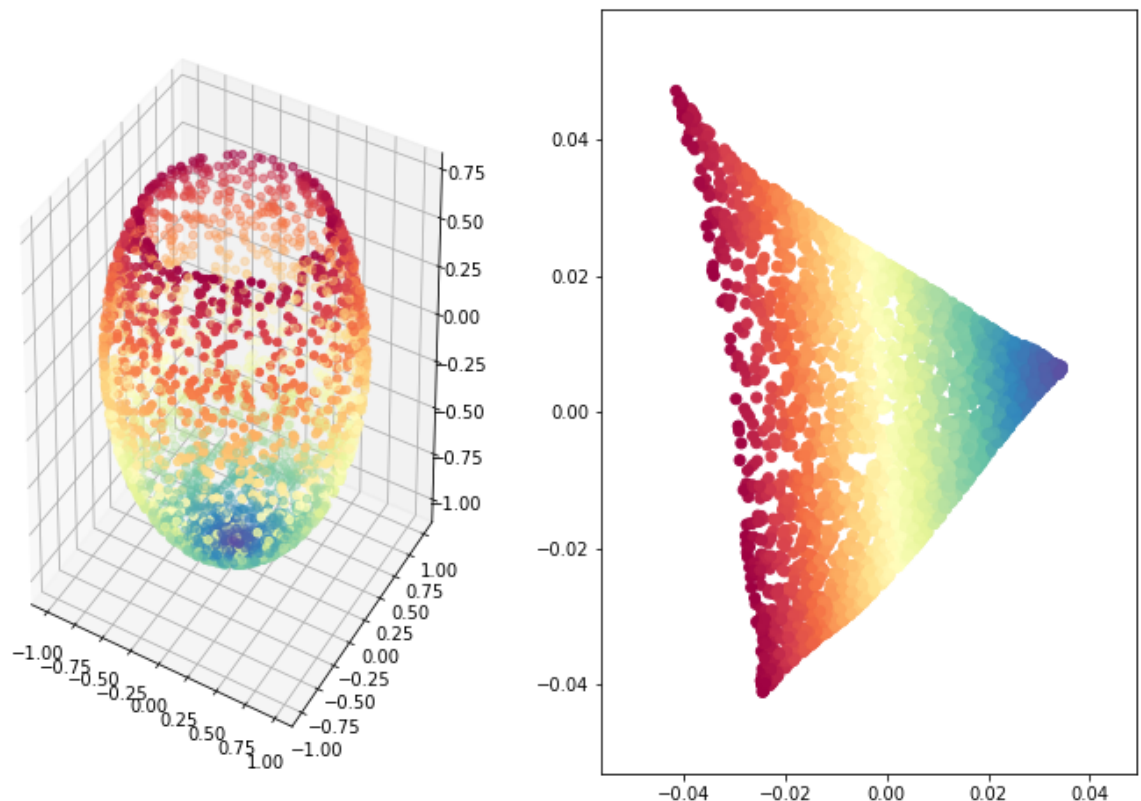
'Unroll the sphere'
reduced_X = lle(X,
                d = 2,
                n_neighbors = 10)
```

step 1: computing pairwise distances
 step 2: computing weights
 step 3: computing new points

```
In [51]: plt.figure(figsize=(12,8))
ax = plt.subplot(1,2,1, projection='3d')
ax.scatter(X[:, 0], X[:, 1], X[:, 2], c=t, cmap=plt.cm.Spectral)

plt.subplot(1,2,2)
plt.scatter(reduced_X[:,0],reduced_X[:,1],c=t,cmap=plt.cm.Spectral)
```

Out[51]: <matplotlib.collections.PathCollection at 0x23497a61908>



Example 3: a Sphere

```
In [54]: 'Make a sphere'
m = 3000
r = 1
phi = 2 * np.pi * np.random.rand(1, m)
t = np.pi * np.random.rand(1, m)
x = r*np.sin(t)*np.cos(phi)
y = r*np.sin(t)*np.sin(phi)
z = r*np.cos(t)
X = np.concatenate((x, y,z))
X = X.T
t = np.squeeze(t)

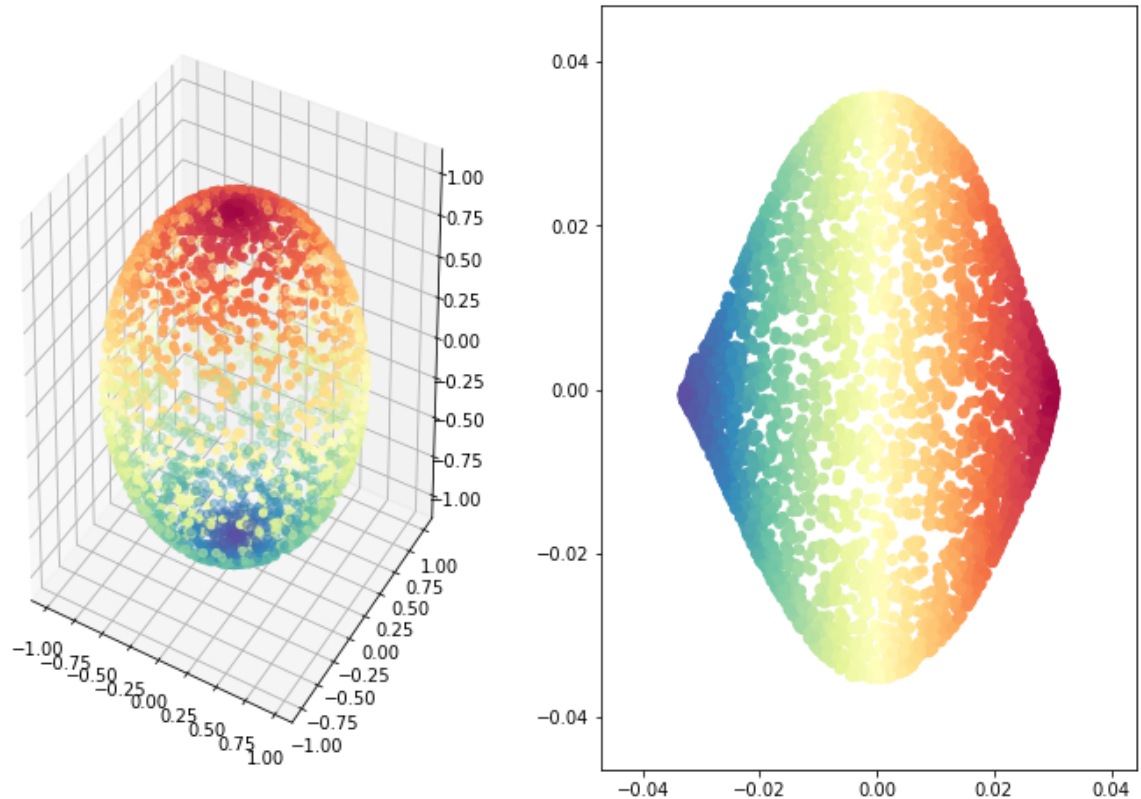
'Unroll the sphere'
reduced_X = lle(X,
                d = 2,
                n_neighbors = 15)
```

step 1: computing pairwise distances
step 2: computing weights
step 3: computing new points

```
In [55]: plt.figure(figsize=(12,8))
ax = plt.subplot(1,2,1, projection='3d')
ax.scatter(X[:, 0], X[:, 1], X[:, 2], c=t, cmap=plt.cm.Spectral)

plt.subplot(1,2,2)
plt.scatter(reduced_X[:,0],reduced_X[:,1],c=t,cmap=plt.cm.Spectral)
```

Out[55]: <matplotlib.collections.PathCollection at 0x234997f4f08>



Example 4: Visualizing 3's and 5's

```
In [168]: 'Load the MNist dataset'
from sklearn.datasets import fetch_openml
mnist = fetch_openml('mnist_784',version=1)
X,y=mnist['data'],mnist['target']
X = X[:5000]
y = y[:5000]
```

```
In [169]: y = y.astype(np.uint8)
```

We'll focus on digits 3 and 5, which are often misclassified

```
In [125]: y35 = y[np.logical_or(y == 3, y == 5)]  
          X35 = X[np.logical_or(y == 3, y == 5)]  
          len(y35)
```

```
Out[125]: 927
```

Now let's use LLE to reduce dimensionality down to 2D so we can plot the dataset:

```
In [126]: reduced_X = lle(X35,  
                           d = 2,  
                           n_neighbors = 15)
```

step 1: computing pairwise distances
step 2: computing weights
step 3: computing new points

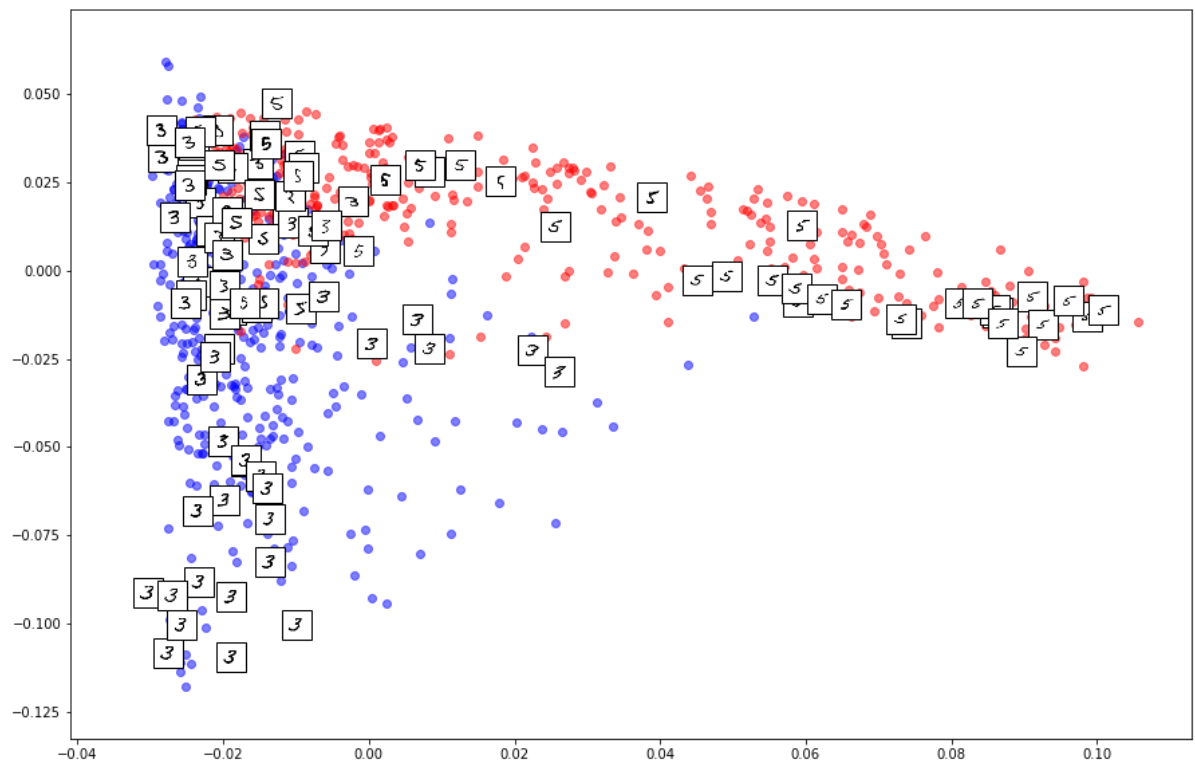
Now let's use Matplotlib's scatter() function to plot a scatterplot, using a different color for each digit.

```

In [127]: colors = ['blue','red']
          digits = [3,5]
          plt.figure(figsize=(15,10))
          for i in range(2):
              plt.scatter(reduced_X[y35==digits[i],0],reduced_X[y35==digits[i],1],color=
              colors[i], alpha = 0.5)
          ax = plt.gcf().gca() # get current axes in current figure

          'Plot scaled-down versions of some of digit images'
          from matplotlib.offsetbox import AnnotationBbox, OffsetImage
          n_digits = 100
          for i in range(n_digits):
              image = X35[i].reshape(28, 28)
              image_coord = reduced_X[i]
              imagebox = AnnotationBbox(OffsetImage(image, zoom=.5, cmap="binary"), image_coord)
              ax.add_artist(imagebox)

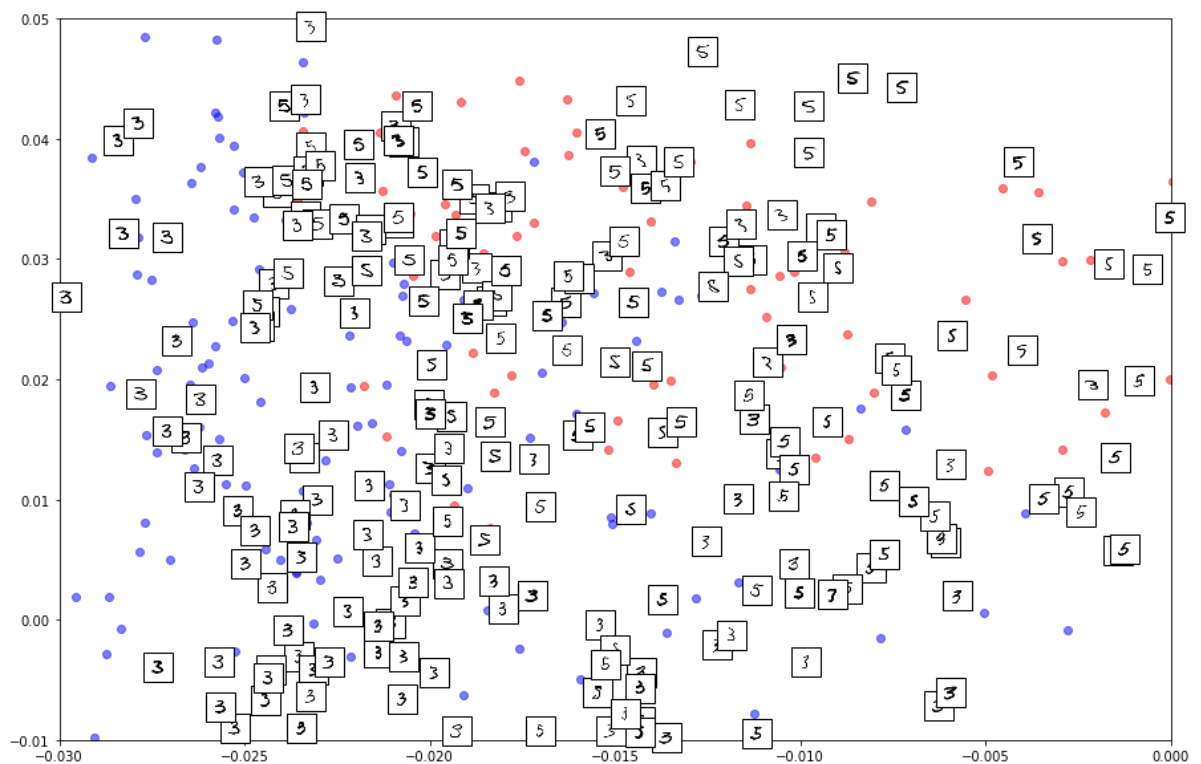
```



Isn't this just beautiful? :) This plot tells us which 3's are easily distinguishable from 5's, and it also tells us which 3's are often hard to distinguish from 5's.

Let's focus on the region where 3's and 5's seem to overlap a lot.

```
In [131]: colors = ['blue','red']
digits = [3,5]
plt.figure(figsize=(15,10))
for i in range(2):
    plt.scatter(reduced_X[y35==digits[i],0],reduced_X[y35==digits[i],1],color=
colors[i], alpha = 0.5)
ax = plt.gcf().gca() # get current axes in current figure
from matplotlib.offsetbox import AnnotationBbox, OffsetImage
n_digits = 500
for i in range(n_digits):
    image = X35[i].reshape(28, 28)
    image_coord = reduced_X[i]
    imagebox = AnnotationBbox(OffsetImage(image, zoom=.5, cmap="binary"), image_coord)
    ax.add_artist(imagebox)
    ax.axis([-0.03,0.00,-0.01,0.05]) # zoom in
```



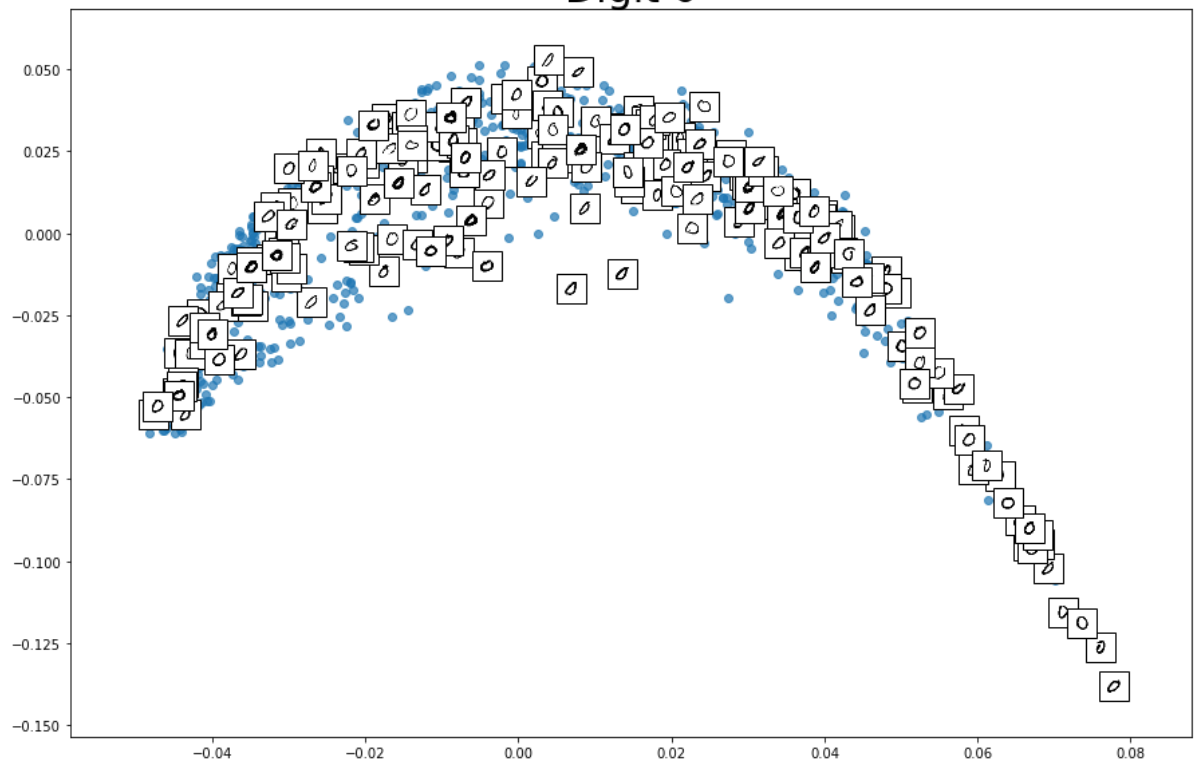
Example 5: Visualizing all the Digits

```
In [ ]: 'Load the MNIST dataset'
from sklearn.datasets import fetch_openml
mnist = fetch_openml('mnist_784',version=1)
X,y=mnist['data'],mnist['target']
X = X[:10000]
y = y[:10000]
```

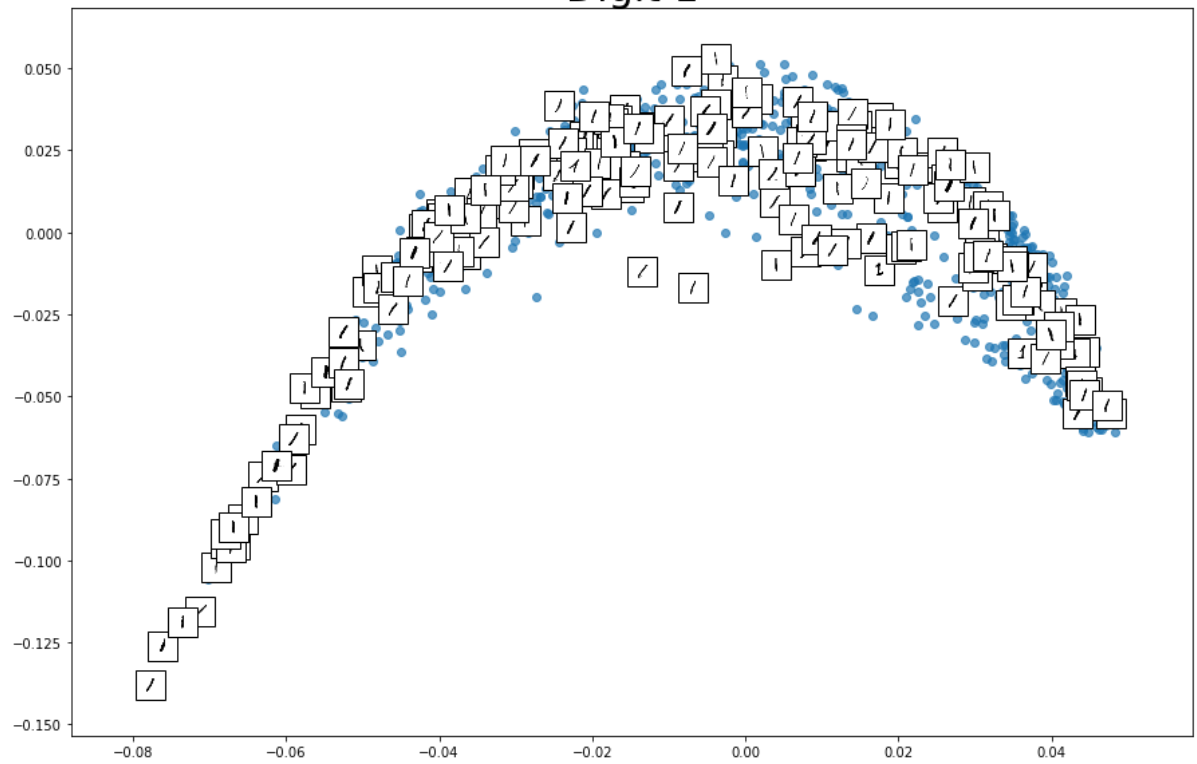
```
In [181]: for i in range(10):
            Xi = X[y==i]
            reduced_X = lle(X2,
                            d = 2,
                            n_neighbors = 15)
            plt.figure(figsize=(15,10))
            plt.scatter(reduced_X[:,0],reduced_X[:,1], alpha = 0.7)
            plt.title('Digit ' +str(i), fontsize=30)

            ax = plt.gcf().gca() # get current axes in current figure
            n_digits = 200
            for i in range(n_digits):
                image = Xi[i].reshape(28, 28)
                image_coord = reduced_X[i]
                imagebox = AnnotationBbox(OffsetImage(image, zoom=.5, cmap="binary"),
                image_coord)
                ax.add_artist(imagebox)
```

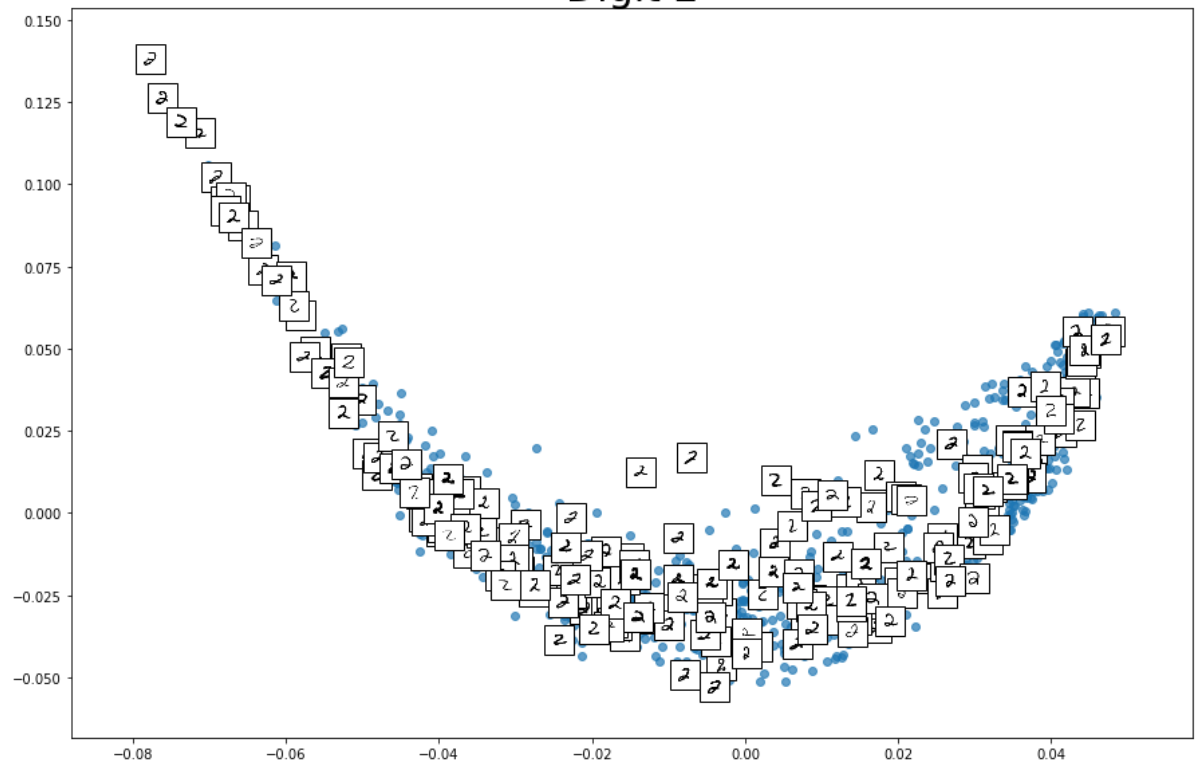

Digit 0



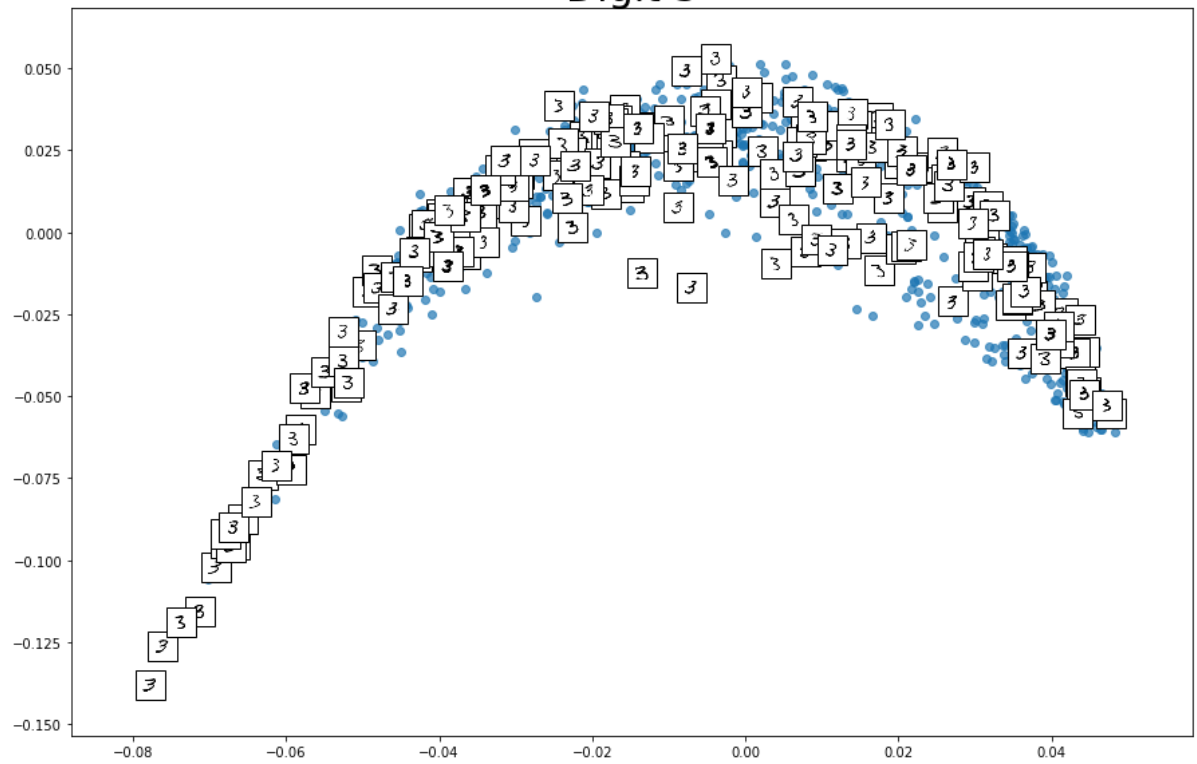
Digit 1



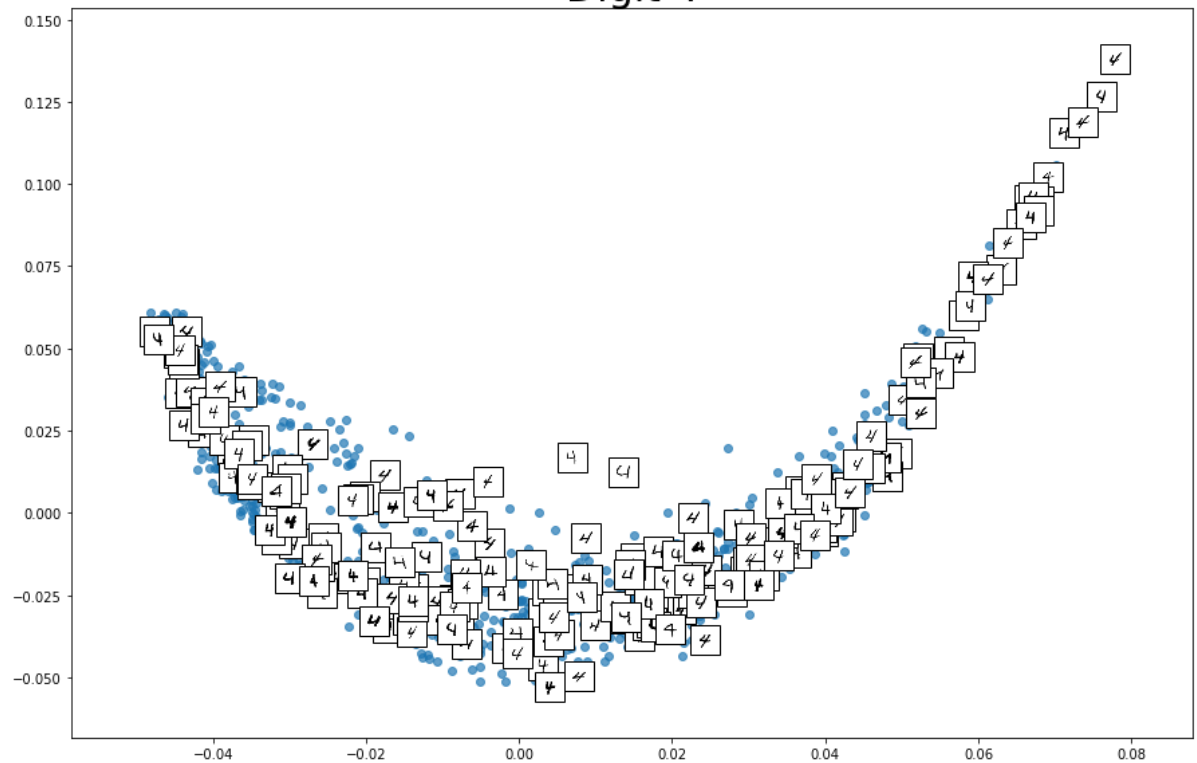
Digit 2



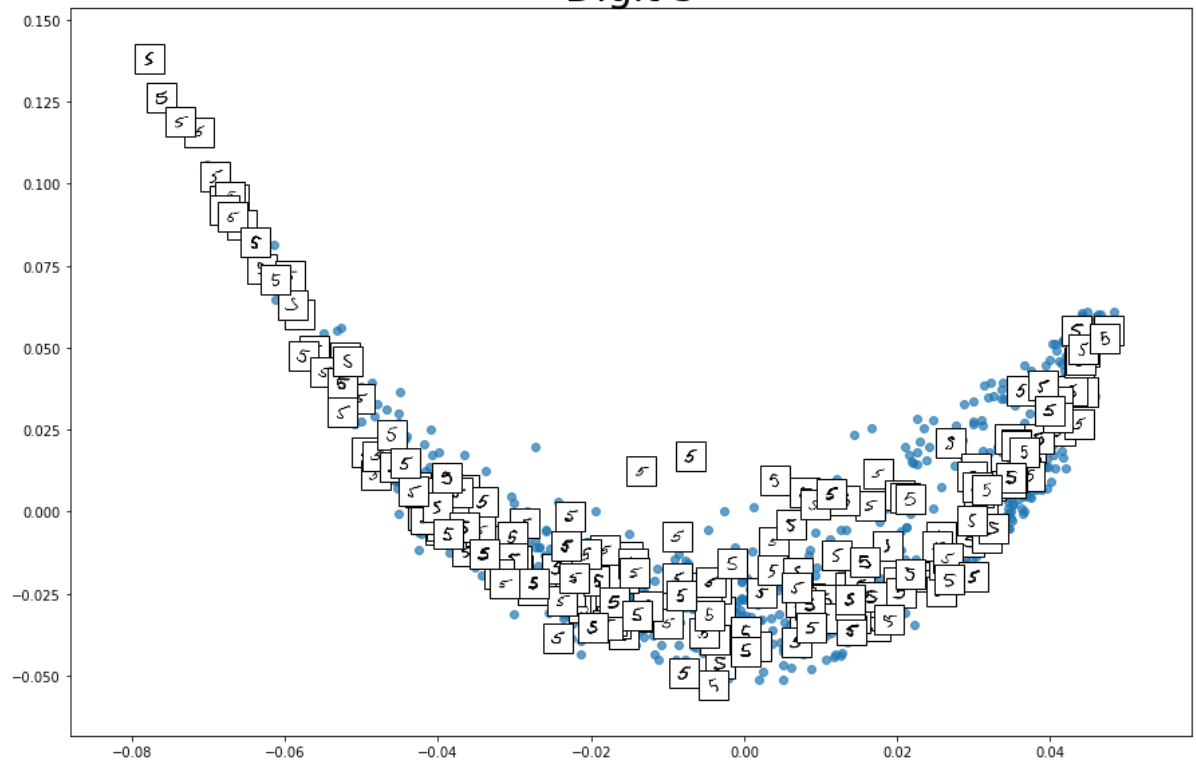
Digit 3



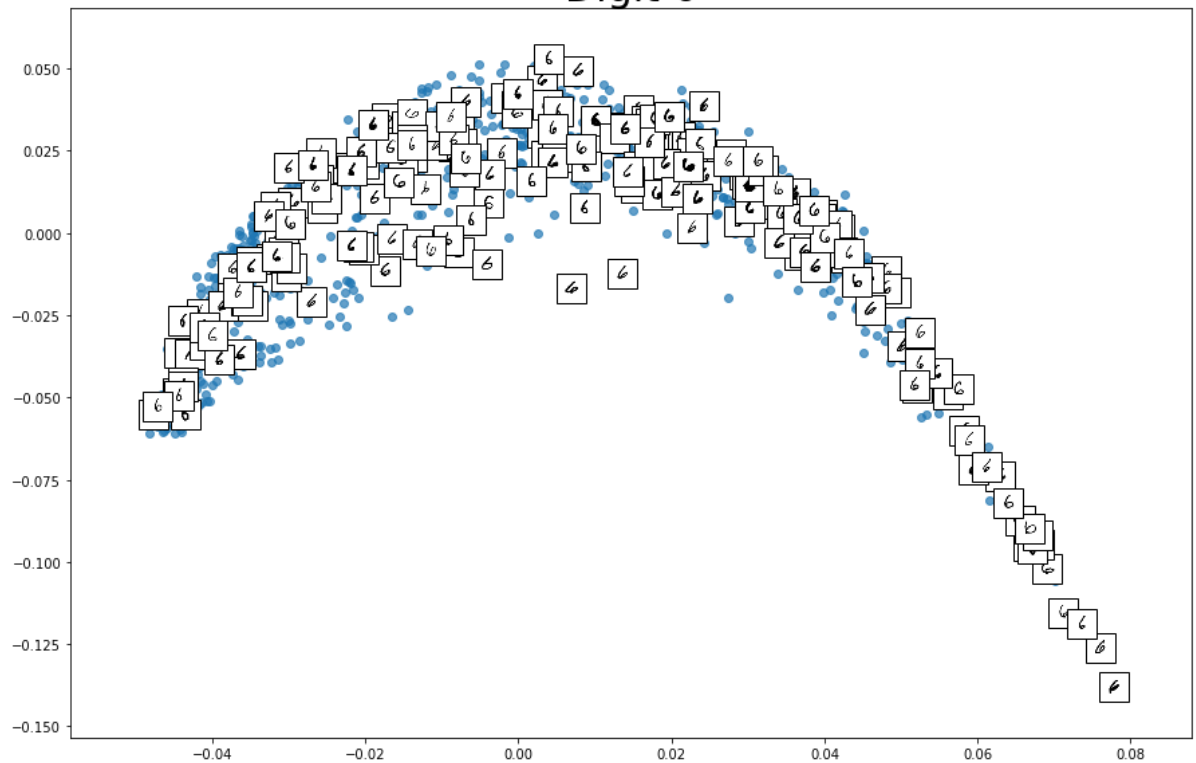
Digit 4



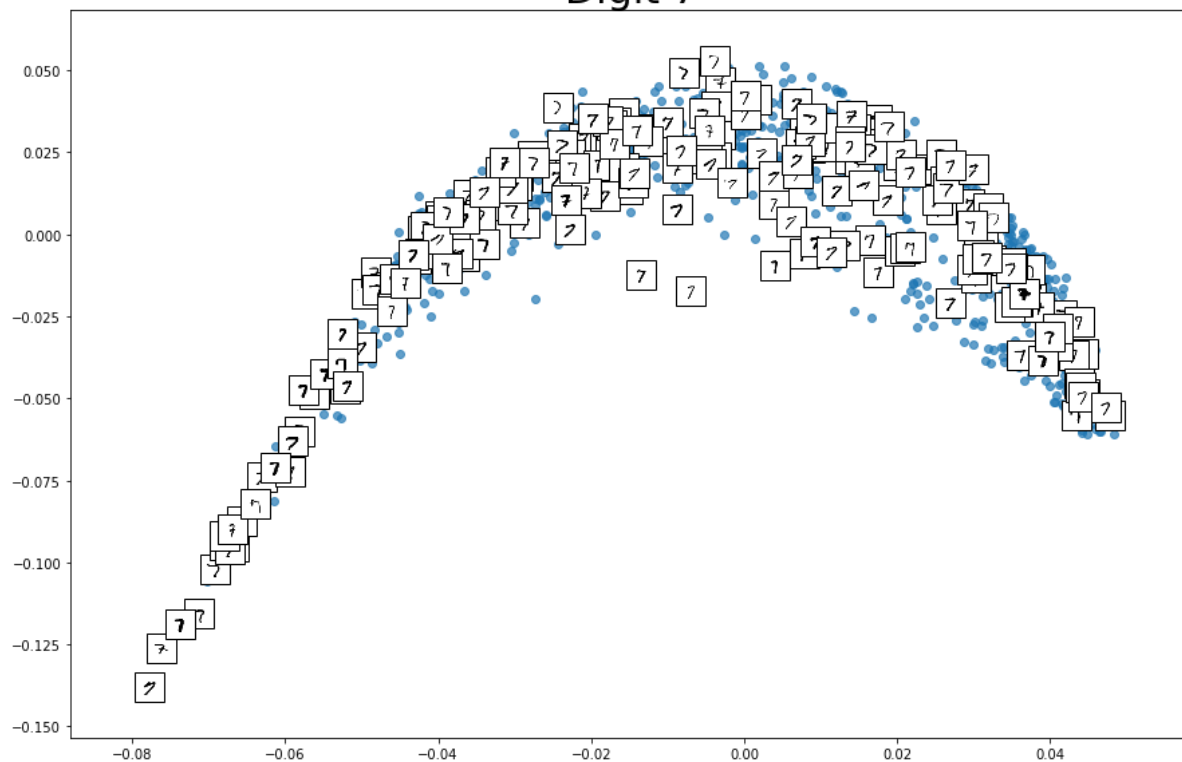
Digit 5



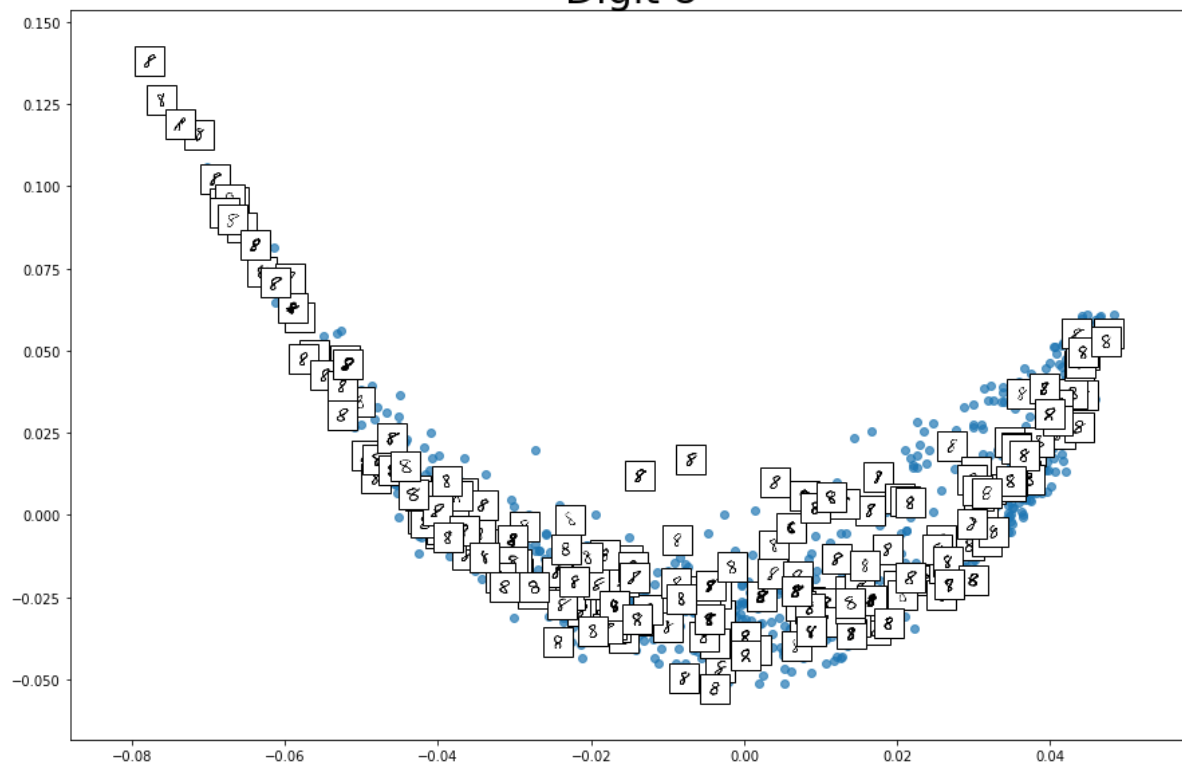
Digit 6

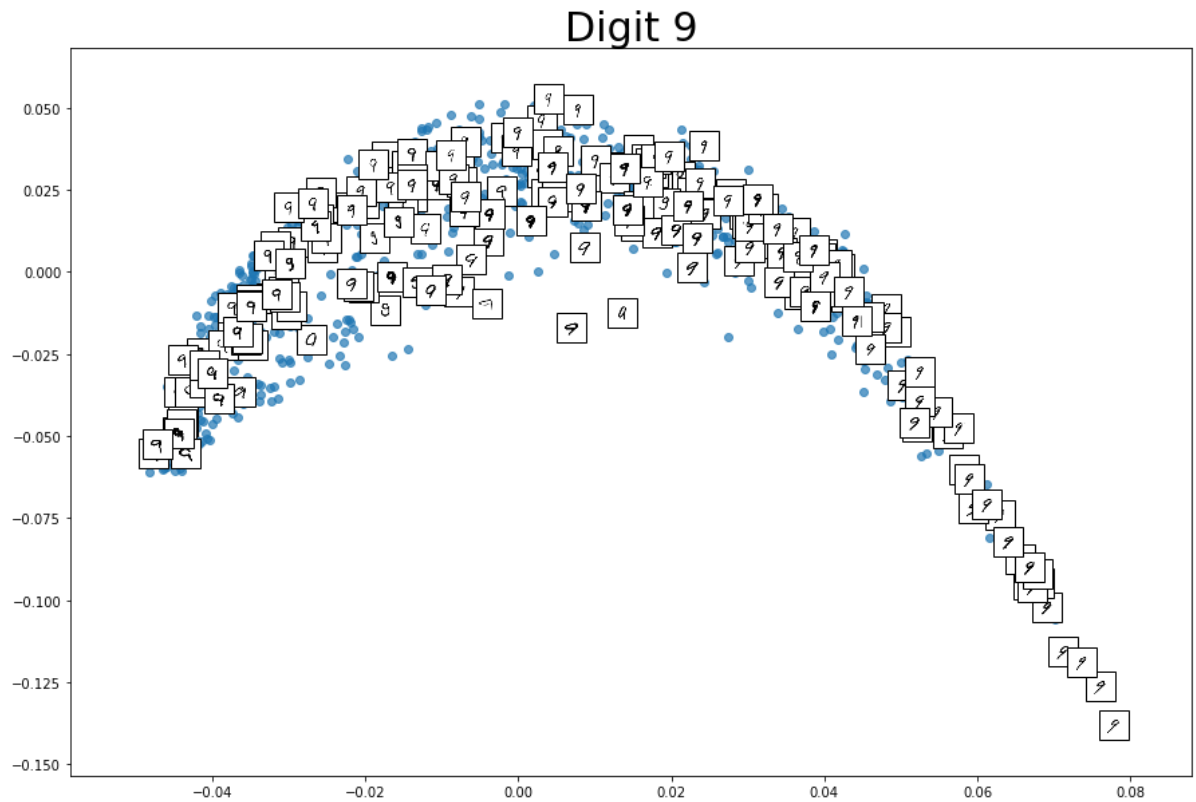


Digit 7



Digit 8





obj74 from coil-100

11.3.4 Problems

Problem 1 (for M562 students and brave M462 students): Let A be an $m \times n$ matrix (with $m > n$), and let b be an m component vector. Consider the following constrained optimization problem:

$$\begin{aligned} \min_x & \|Ax - b\|_2^2 \\ \text{subject to} & \sum_{j=1}^n x_j = 1 \end{aligned}$$

(a) Suppose $\sum_{j=1}^n x_j = 1$ and define the $m \times n$ matrix $B = [b \ b \ \dots \ b]$, show $\|Ax - b\|_2^2 = x^T(A - B)^T(A - B)x$.

(b) Using Lagrange multipliers, solve the constrained optimization problem.