

certain relationships within the data. In the case of MDS, the quantity preserved is the distance between every pair of points.

## Nonlinear Embeddings: Where MDS Fails

Our discussion so far has considered *linear* embeddings, which essentially consist of rotations, translations, and scalings of data into higher-dimensional spaces. Where MDS breaks down is when the embedding is nonlinear—that is, when it goes beyond this simple set of operations. Consider the following embedding, which takes the input and contorts it into an “S” shape in three dimensions:

```
In[12]: def make_hello_s_curve(X):  
        t = (X[:, 0] - 2) * 0.75 * np.pi  
        x = np.sin(t)  
        y = X[:, 1]  
        z = np.sign(t) * (np.cos(t) - 1)  
        return np.vstack((x, y, z)).T
```

```
XS = make_hello_s_curve(X)
```

This is again three-dimensional data, but we can see that the embedding is much more complicated (Figure 5-100):

```
In[13]: from mpl_toolkits import mplot3d  
ax = plt.axes(projection='3d')  
ax.scatter3D(XS[:, 0], XS[:, 1], XS[:, 2],  
             **colorize);
```

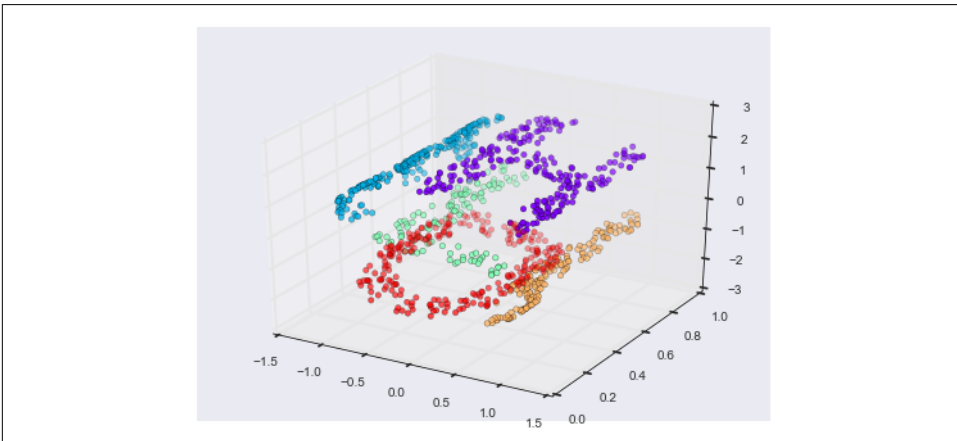


Figure 5-100. Data embedded nonlinearly into three dimensions

The fundamental relationships between the data points are still there, but this time the data has been transformed in a nonlinear way: it has been wrapped up into the shape of an “S.”

If we try a simple MDS algorithm on this data, it is not able to “unwrap” this nonlinear embedding, and we lose track of the fundamental relationships in the embedded manifold (Figure 5-101):

```
In[14]: from sklearn.manifold import MDS
model = MDS(n_components=2, random_state=2)
outS = model.fit_transform(XS)
plt.scatter(outS[:, 0], outS[:, 1], **colorize)
plt.axis('equal');
```

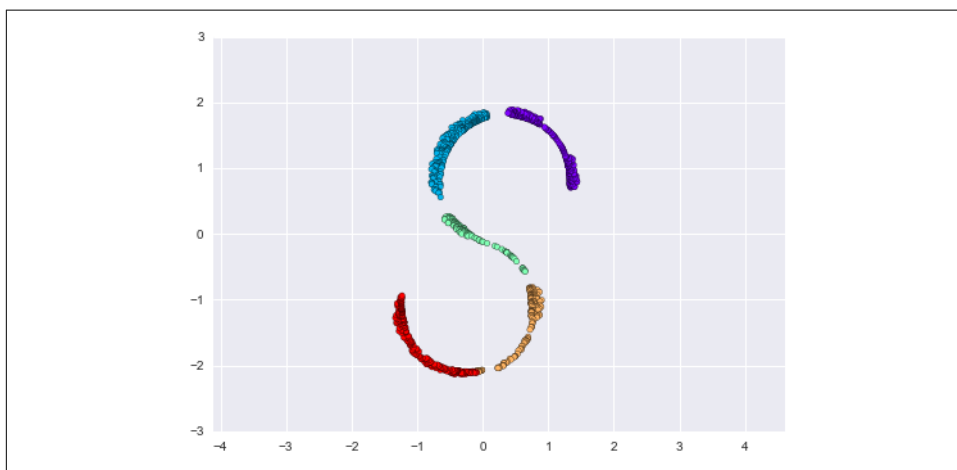


Figure 5-101. The MDS algorithm applied to the nonlinear data; it fails to recover the underlying structure

The best two-dimensional *linear* embedding does not unwrap the S-curve, but instead throws out the original y-axis.

## Nonlinear Manifolds: Locally Linear Embedding

How can we move forward here? Stepping back, we can see that the source of the problem is that MDS tries to preserve distances between faraway points when constructing the embedding. But what if we instead modified the algorithm such that it only preserves distances between nearby points? The resulting embedding would be closer to what we want.

Visually, we can think of it as illustrated in Figure 5-102.