solution09

November 10, 2020

Exercise Sheet 9 **Embedding: Self Organizing Maps (SOMs) and Locally Linear Embedding (LLE)**

The results are strongly affected by the choise of σ and ϵ and the annealing regimes…

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

exp = np.exp
argmin = np.argmin
dist = np.linalg.norm
```

9.1: 1d Self-Organizing Map for 2d data

(a)

[2]:
```
# Generate p = 1000 data points that are uniformly distributed
# inside the rectangle that is x from [0, 2]x[0, 1]
toy_p = 1000 # higher number for better presentation
toy_d = 2
Toy = np.vstack((uniform(low=0, high=2, size=toy_p),
               uniform(low=0, high=1, size=toy_p)))
# toy shape = (2, 1000)
```

(b)

[3]:
```
# Implement a one-dimensional Self-Organizing Map
# (Kohonen network, online algorithm for SOMs)
# using a Gaussian neighborhood function

def h_pq(a, b, s):
    return exp(-(dist(a-b)**2)/(2*(s**2)))

def online_SOM(x_array, w_array, n_M, n_dim,
               sigma, epsilon, s_annealing, e_annealing, n_epoch):
    x_array = np.copy(x_array)
    w_array = np.copy(w_array)
    if np.shape(x_array)[1] < np.shape(x_array)[0]:
```

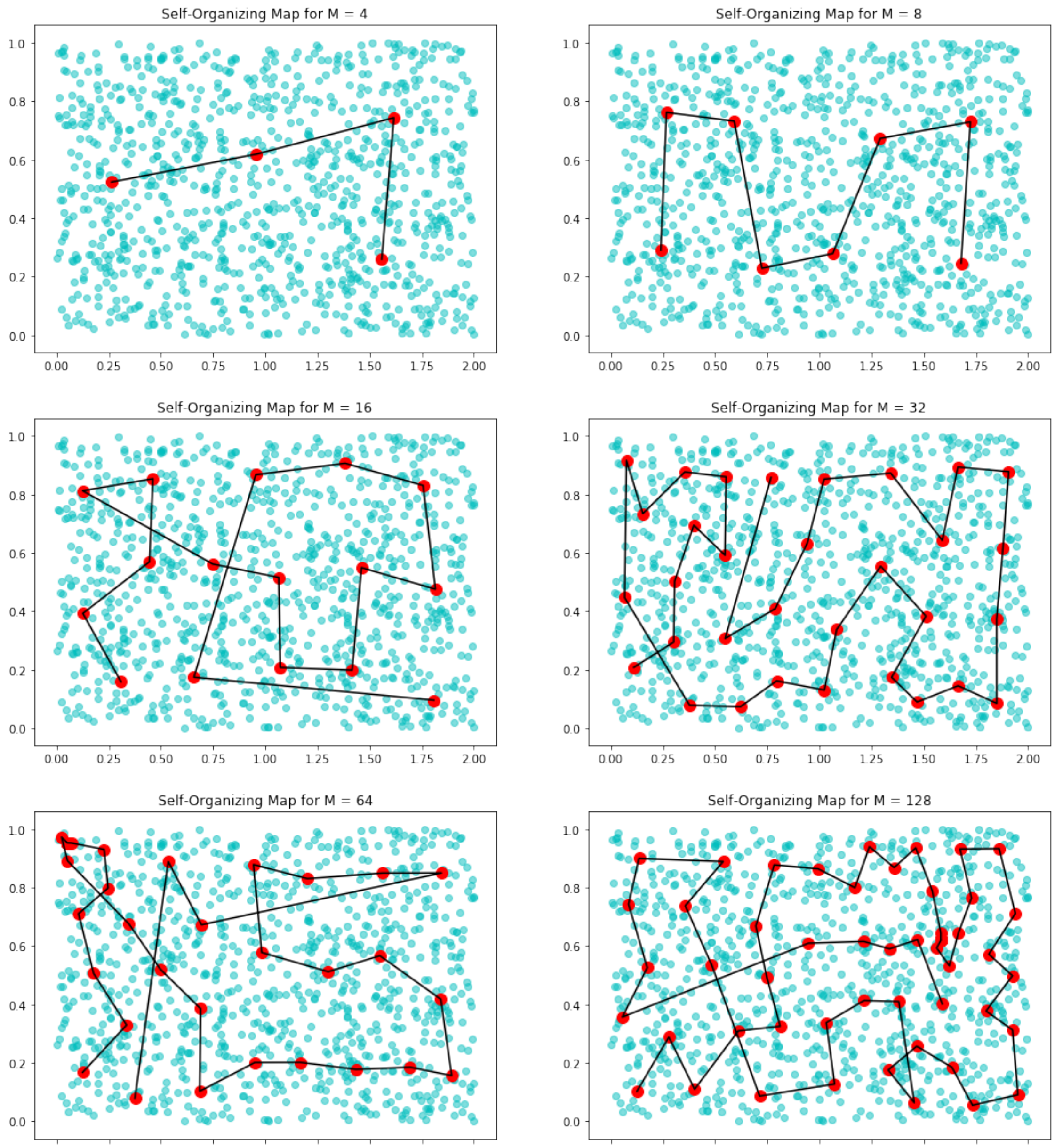
```
        x_array = x_array.T

    # shuffling x_array
    np.random.shuffle(x_array.T)

    n_x = np.shape(x_array)[1]
    x_dim = np.shape(x_array)[0]

    w_progress = np.zeros(shape=(n_x*n_epoch, x_dim, n_M))

    for i_e in range(n_epoch):
        for i_x in range(n_x):
            x = x_array[:, i_x].reshape((x_dim, 1))

#             if i_x + (i_e*n_x) > n_x/4:
            if i_e >= 1:
                epsilon *= e_annealing
            sigma *= s_annealing
            if epsilon < 1e-4:
                print('min epsilon reached for m=', n_M)
                return w_array, w_progress

            # recording the process
            w_progress[i_x + (i_e*n_x)] = w_array

            # the actual algorithm
            i_p = argmin(dist((x-w_array), axis=0))
            w_p = w_array[:, i_p].reshape((x_dim, 1))
            for i_q in range(n_M):
                w_q = w_array[:, i_q].reshape((x_dim, 1))
                d_w_q = epsilon * h_pq(w_p, w_q, sigma) * (x - w_q)
                w_array[:, i_q] = (d_w_q + w_q).reshape(x_dim)
    print(sigma, epsilon)
    return w_array, w_progress
```

[4]:
```
M_list = [4, 8, 16, 32, 64, 128]

m_len = len(M_list)
plt.figure(figsize=(16, 6*int(m_len/2)))
for i_m, m in enumerate(M_list):
    print('doing it for M =', m)

    # initializing the weights
    toy_mean = Toy.mean(axis=1).reshape((toy_d, 1))
    w_array = toy_mean + uniform(low=-0.25, high=0.25, size=(toy_d, m)) # random
#     w_array = np.array([np.zeros(m)+0.5, np.linspace(0, 2, m)]) # informed
```

```
    weights, recordings = online_SOM(Toy, w_array, m, 1, 0.5, 0.9, 0.998, 0.
↪9996, 6)

    # plotting
    plt.subplot(int(m_len/2), 2, i_m+1)
    plt.title('Self-Organizing Map for M = {0}'.format(m))
    plt.scatter(Toy[0], Toy[1], color='c',alpha=0.5)
    # plt.plot(recordings[:, 0, :], recordings[:, 1, :])
    plt.scatter(weights[0], weights[1], s=100, c='r')

#     link_list = []
#     for i_k in range(m):
#         dist_array = dist((weights[:, i_k].reshape((2,1))-weights), axis=0)
#         for n_k in range(1, m):
#             i_k_n = dist_array.argsort()[n_k]
#             if link_list.count(i_k_n) < 2 and link_list.count(i_k) < 2:
#                 link_list.append(i_k)
#                 link_list.append(i_k_n)
#                 k_array = np.array([i_k, i_k_n])
#                 plt.plot(weights[0, k_array], weights[1, k_array], color='k')

    # or
#     plot_array = dist((weights[:, 0].reshape((2,1))-weights), axis=0).
↪argsort()
#     plt.plot(weights[0, plot_array], weights[1, plot_array], color='k')

    # or
    i_k_int = dist((np.zeros((2,1))-weights), axis=0).argsort()[0]
    link_list = [i_k_int]
    for i_link in range(m):
        for i_k_n in dist((weights[:, link_list[-1]].reshape((2,1))-weights),
                          axis=0).argsort()[0:]:
            if i_k_n not in link_list:
                link_list.append(i_k_n)
                break
    k_array = np.array(link_list)
    plt.plot(weights[0, k_array], weights[1, k_array], color='k')

plt.show()
```

```
doing it for M = 4
3.035412572112661e-06 0.12175303096296591
doing it for M = 8
3.035412572112661e-06 0.12175303096296591
doing it for M = 16
3.035412572112661e-06 0.12175303096296591
doing it for M = 32
```

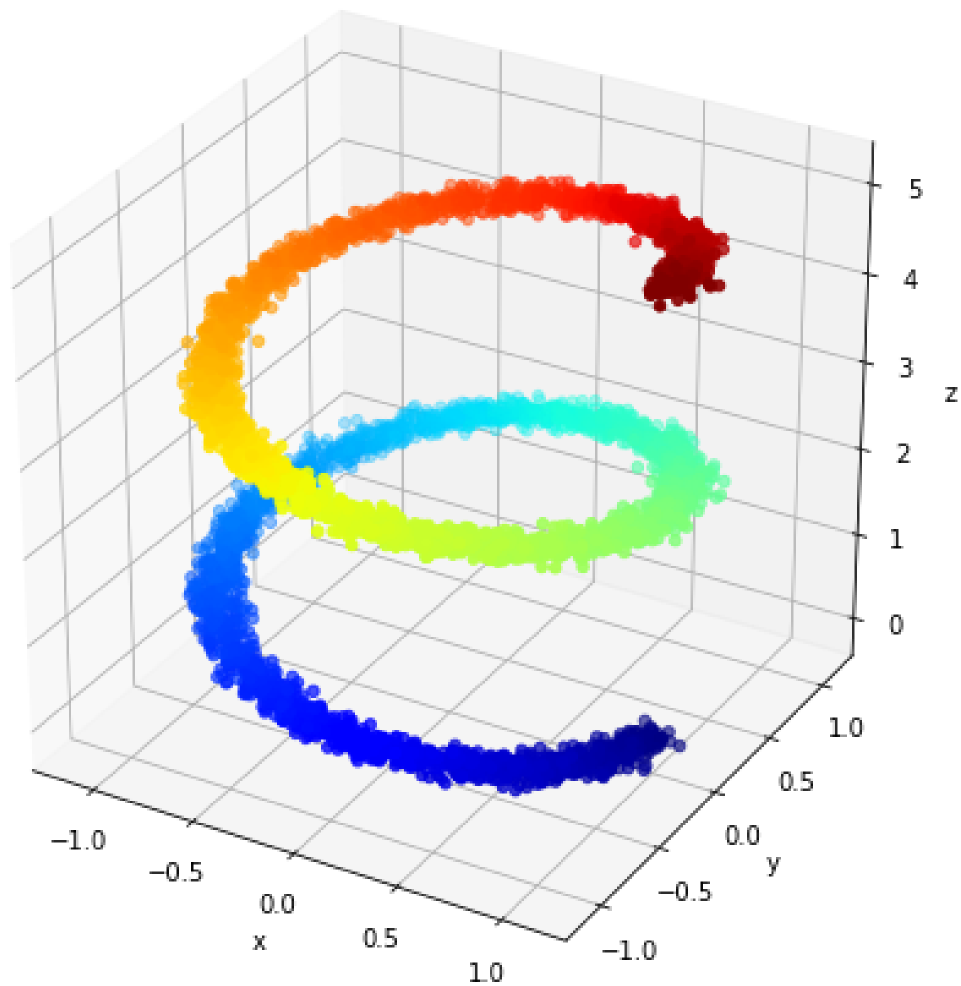
```
3.035412572112661e-06 0.12175303096296591
doing it for M = 64
3.035412572112661e-06 0.12175303096296591
doing it for M = 128
3.035412572112661e-06 0.12175303096296591
```



9.2: 1d Self-Organizing Maps for 3d data

[5]:
```
# Download and visualize the data contained in the file spiral.csv.
# It contains data described by three coordinates x,y,z.
```

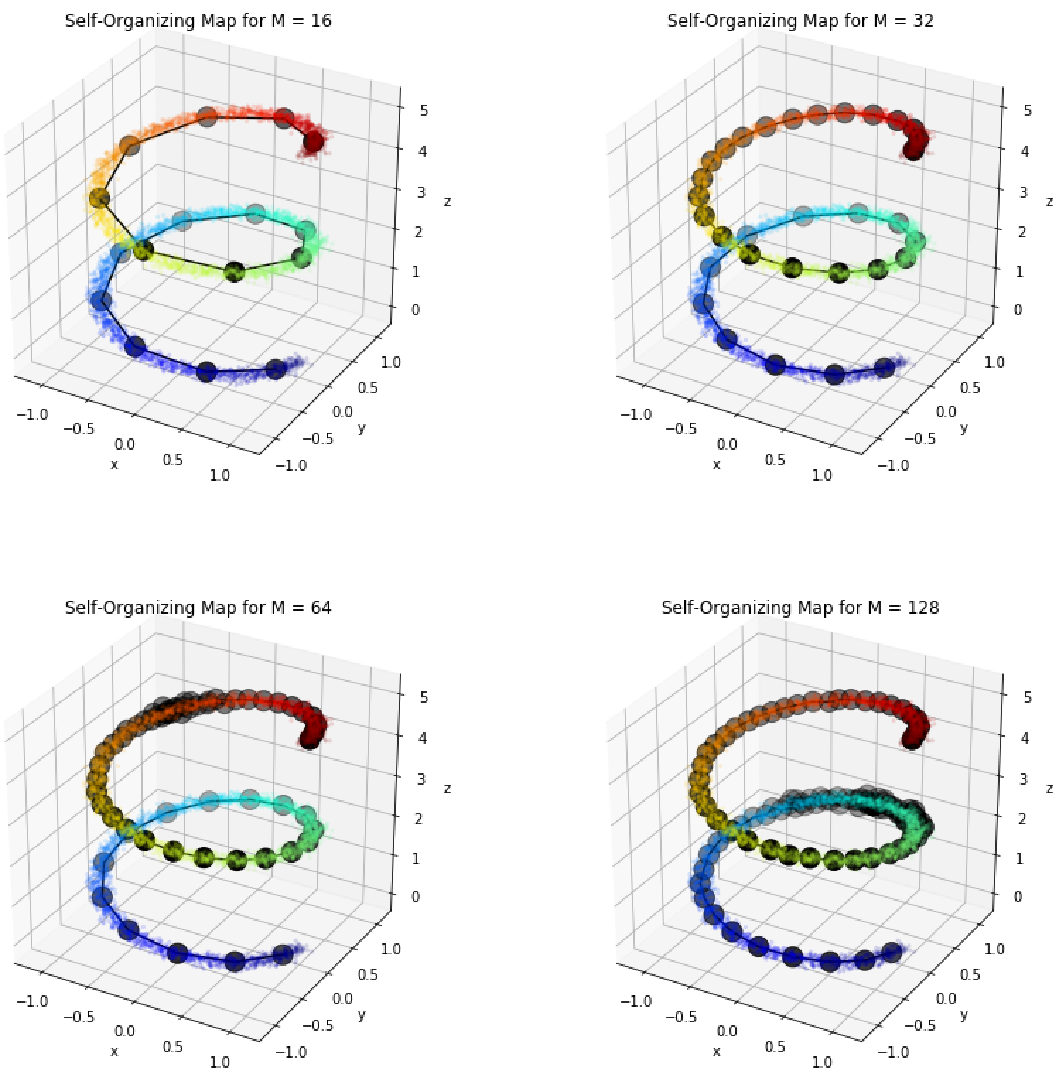
```
spiral = np.genfromtxt('spiral.csv', delimiter=',',
                       skip_header=1, usecols = (1, 2, 3)).T
# spiral.shape = (3, 5000)
spiral_d = len(spiral) # dimension
spiral_p = spiral.shape[1] # samples

fig = plt.figure(figsize=(8, 8))
ax = fig.add_subplot(111, projection='3d')
ax.scatter(spiral[0], spiral[1], spiral[2],
           c=np.arange(len(spiral[2])), cmap='jet')
ax.set_xlabel('x')
ax.set_ylabel('y')
ax.set_zlabel('z')
plt.show()
```



There is a obvious and significant order in the spiral data between the data points.

[6]:
```
M_list = [16, 32, 64, 128]

m_len = len(M_list)
fig = plt.figure(figsize=(14, 7*int(m_len/2)))
for i_m, m in enumerate(M_list):
    print('doing it for M =', m)
    # initializing the weights
    w_array = np.array([np.zeros(m), np.zeros(m), np.linspace(0, 5, m,␣
↪endpoint=True)])
    weights, recordings = online_SOM(spiral, w_array, m, 1, 0.7, 0.9, 0.998, 0.
↪9996, 6)

    # plotting
    ax = fig.add_subplot(int(m_len/2), 2, i_m+1, projection='3d')
    ax.set_title('Self-Organizing Map for M = {0}'.format(m))
    ax.scatter(spiral[0], spiral[1], spiral[2],
               c=np.arange(len(spiral[2])), cmap='jet' ,alpha=0.1, s=5)
#     ax.plot(recordings[:, 0, :], recordings[:, 1, :], recordings[:, 2, :])
    ax.scatter(weights[0], weights[1], weights[2],
               s=200, c='k', edgecolor='k', marker='o')

    weights_z_arg_sorted = weights[2, :].argsort()
    sorted_weights = weights[:, weights_z_arg_sorted]
    ax.plot(sorted_weights[0], sorted_weights[1], sorted_weights[2], color='k')
    ax.set_xlabel('x')
    ax.set_ylabel('y')
    ax.set_zlabel('z')
plt.show()
```

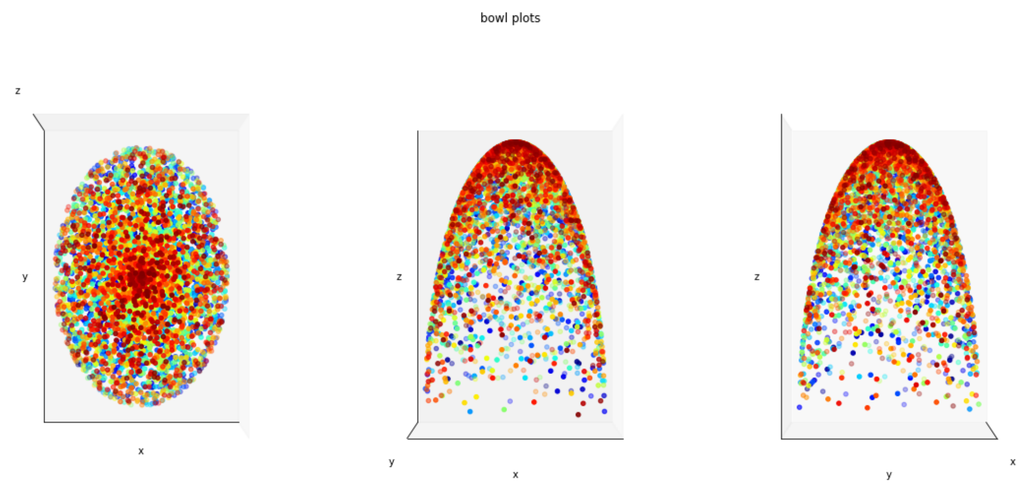
```
doing it for M = 16
min epsilon reached for m= 16
doing it for M = 32
min epsilon reached for m= 32
doing it for M = 64
min epsilon reached for m= 64
doing it for M = 128
min epsilon reached for m= 128
```



9.3: 2d Self-Organizing Maps for 3d data

[7]:
```python
# Visualize the 3d-data in the file bowl.csv.
bowl = np.genfromtxt('bowl.csv', delimiter=',',
                     skip_header=1, usecols = (1, 2, 3)).T
# bowl.shape = (3, 5000)
fig = plt.figure(figsize=(16, 8))
for i_sub, angle in enumerate([[90, 90], [0, 90], [0, 0]]):
    plt.suptitle('bowl plots')
    ax = fig.add_subplot(1, 3, i_sub+1, projection='3d')
    ax.scatter(bowl[0], bowl[1], bowl[2],
               c=np.arange(len(spiral[2])), cmap='jet')
    ax.view_init(elev=angle[0], azim=angle[1])
    ax.set_xlabel('x')
```

```
    ax.set_ylabel('y')
    ax.set_zlabel('z')
    ax.set_xticks([])
    ax.set_yticks([])
    ax.set_zticks([])
plt.tight_layout()
plt.show()
```

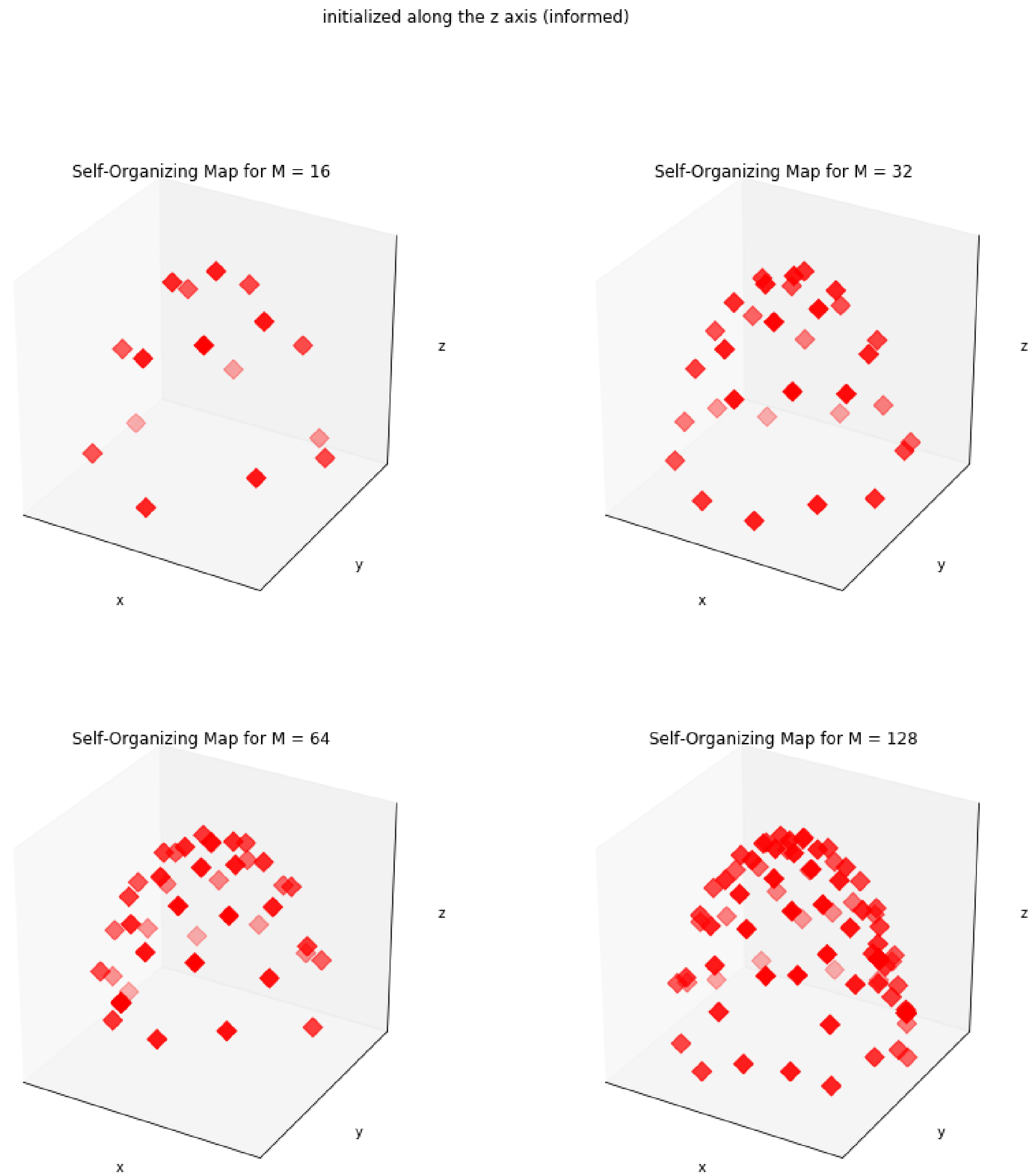


There is no visible order in the data.

[8]:
```
M_list = [16, 32, 64, 128]

m_len = len(M_list)
fig = plt.figure(figsize=(14, 7*int(m_len/2)))
plt.suptitle('initialized along the z axis (informed)')
for i_m, m in enumerate(M_list):
    print('doing it for M =', m)
    # initializing the weights
    aux_array = np.linspace(0, 1, m, endpoint=True)
    w_array = np.array([aux_array, aux_array, aux_array])
    weights, recordings = online_SOM(bowl, w_array, m, 1, 0.7, 0.9, 0.998, 0.
 ↪9996, 6)

    # plotting
    ax = fig.add_subplot(int(m_len/2), 2, i_m+1, projection='3d')
    ax.set_title('Self-Organizing Map for M = {0}'.format(m))
    ax.scatter(weights[0], weights[1], weights[2], s=100, c='r', marker='D')

    ax.set_xlabel('x')
```

```python
    ax.set_ylabel('y')
    ax.set_zlabel('z')
    ax.set_xticks([])
    ax.set_yticks([])
    ax.set_zticks([])
plt.show()
```

```
doing it for M = 16
min epsilon reached for m= 16
doing it for M = 32
min epsilon reached for m= 32
doing it for M = 64
min epsilon reached for m= 64
doing it for M = 128
min epsilon reached for m= 128
```

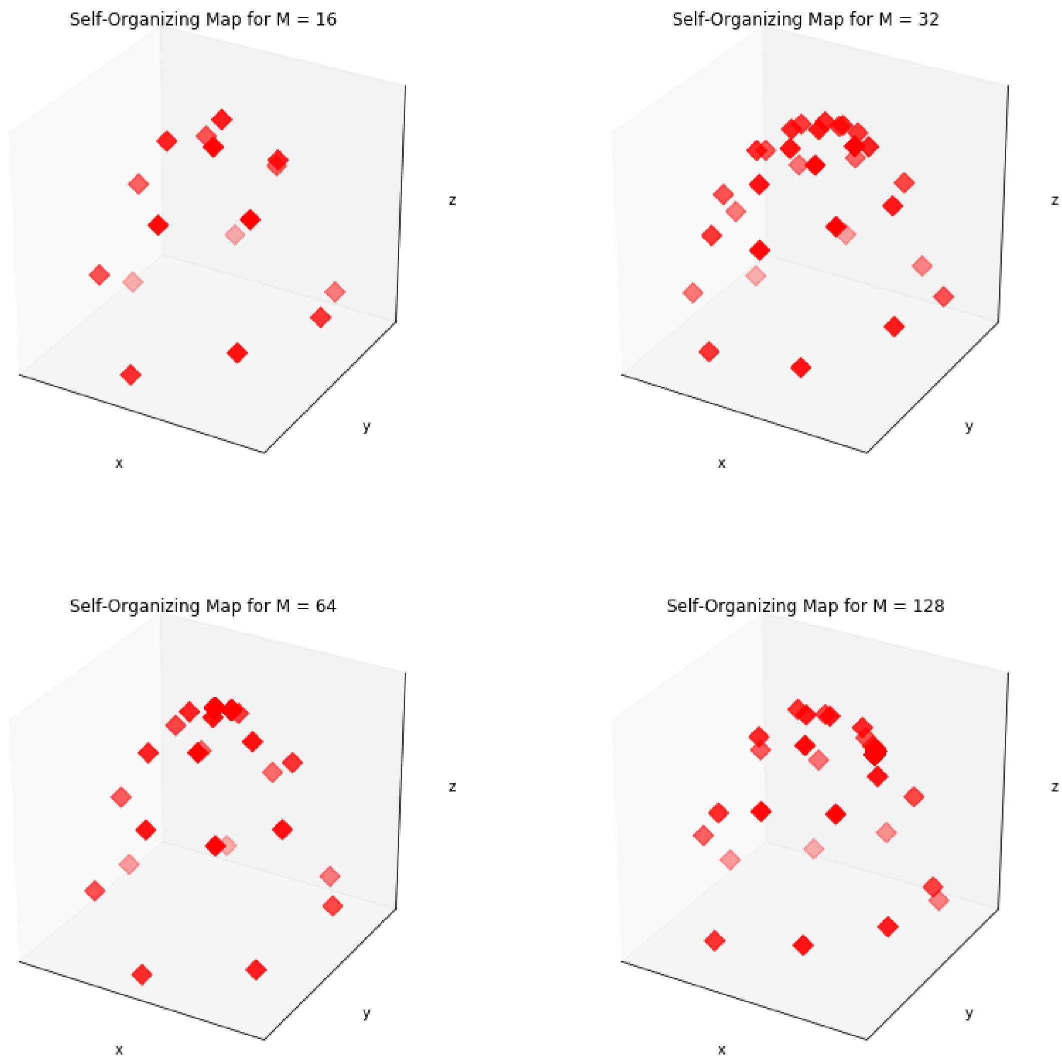



```
[9]: M_list = [16, 32, 64, 128]

     m_len = len(M_list)
     fig = plt.figure(figsize=(14, 7*int(m_len/2)))
     plt.suptitle('initialized randomly around the mean')
     for i_m, m in enumerate(M_list):
         print('doing it for M =', m)
         # initializing the weights
         bowl_mean = bowl.mean(axis=1).reshape((3, 1))
```

```
    w_array = bowl_mean + uniform(low=-0.25, high=0.25, size=(3, m))
    weights, recordings = online_SOM(bowl, w_array, m, 1, 1, 1, 0.9999, 0.9999,␣
 ↪10)

    # plotting
    ax = fig.add_subplot(int(m_len/2), 2, i_m+1, projection='3d')
    ax.set_title('Self-Organizing Map for M = {0}'.format(m))
    ax.scatter(weights[0], weights[1], weights[2], s=100, c='r', marker='D')

    ax.set_xlabel('x')
    ax.set_ylabel('y')
    ax.set_zlabel('z')
    ax.set_xticks([])
    ax.set_yticks([])
    ax.set_zticks([])
plt.show()
```

```
doing it for M = 16
0.0067362626106031364 0.011106497128591908
doing it for M = 32
0.0067362626106031364 0.011106497128591908
doing it for M = 64
0.0067362626106031364 0.011106497128591908
doing it for M = 128
0.0067362626106031364 0.011106497128591908
```

initialized randomly around the mean

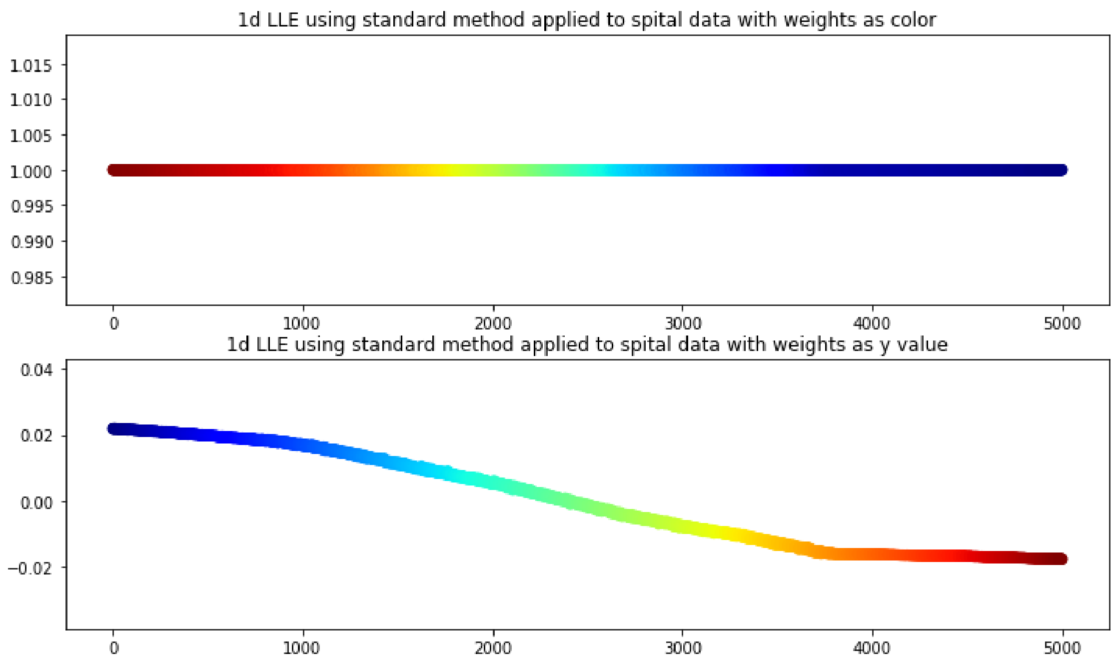


9.4: Locally Linear Embedding

[10]:
```python
# Find an off-the-shelf implementation for Locally Linear Embedding (e.g. Scikit-Learn).
from sklearn import manifold, datasets
```

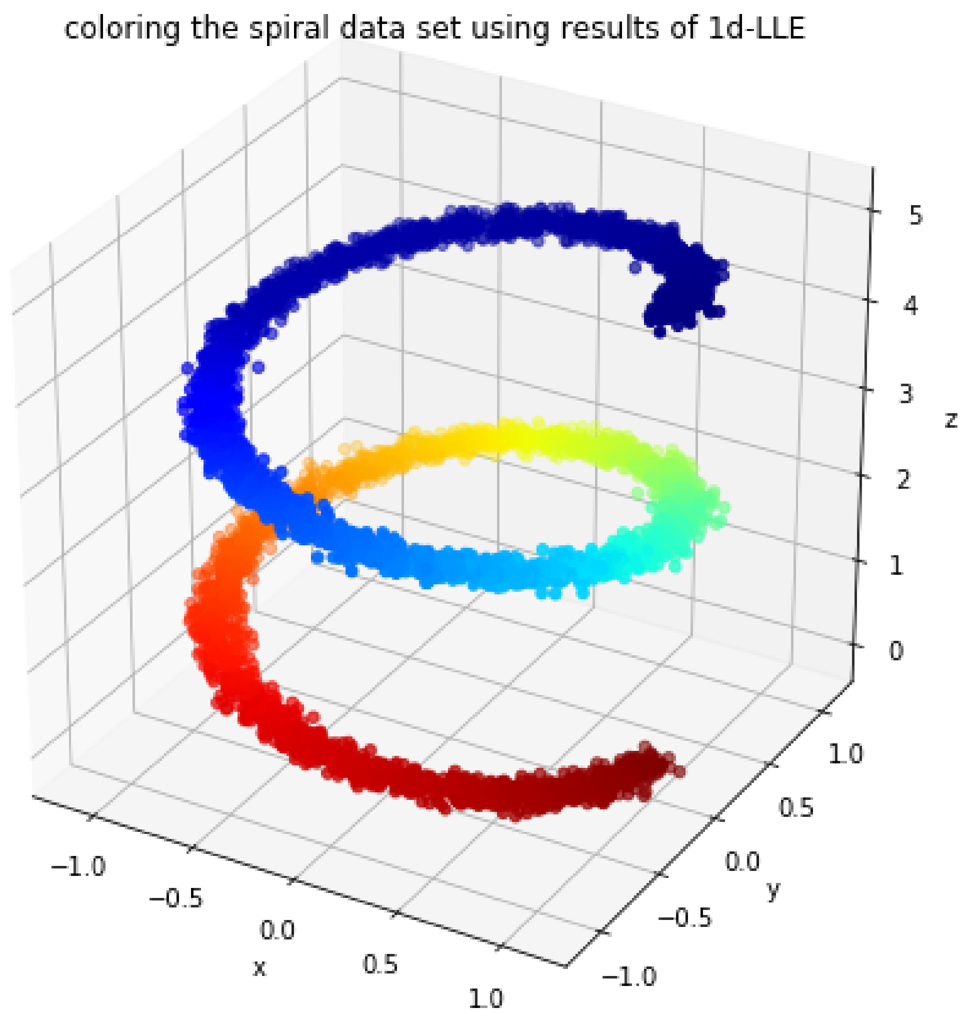
[11]:
```python
k_n = 10 # number of neighbors
n_dim = 1 # output dimension

LLE_method = manifold.LocallyLinearEmbedding(k_n, n_dim, method='standard')
```

```
spiral_1d = LLE_method.fit_transform(spiral.T).T
plt.figure(figsize=(12, 7))
plt.subplot(2, 1, 1)
plt.title('{0}d LLE using standard method applied to spital data with weights␣
 ↪as color'.format(n_dim, 'standard'))
plt.scatter(np.arange(5000), np.ones(5000), c=spiral_1d[0,:], cmap='jet')
plt.subplot(2, 1, 2)
plt.title('{0}d LLE using standard method applied to spital data with weights␣
 ↪as y value'.format(n_dim, 'standard'))
plt.scatter(np.arange(5000), spiral_1d[0,:], c=np.arange(5000), cmap='jet')
plt.show()
```

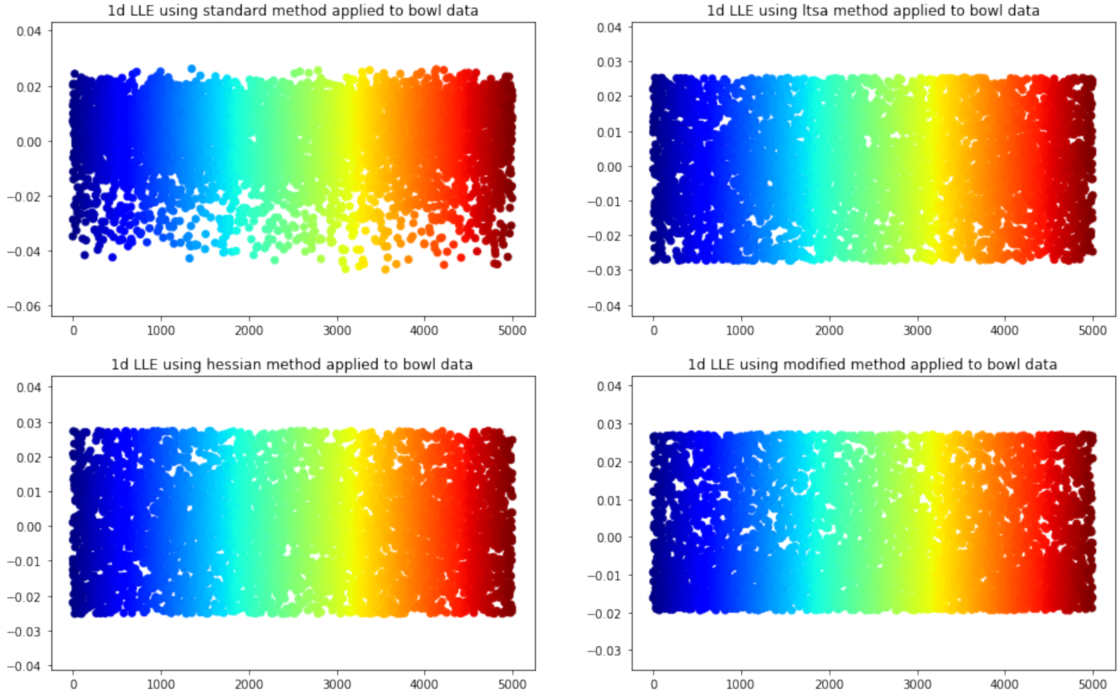


[12]:

```
# using the results of the LLE for coloring:
fig = plt.figure(figsize=(8, 8))
ax = fig.add_subplot(111, projection='3d')
ax.scatter(spiral[0], spiral[1], spiral[2],
           c=spiral_1d[0,:], cmap='jet')
ax.set_xlabel('x')
ax.set_ylabel('y')
ax.set_zlabel('z')
plt.title('coloring the spiral data set using results of 1d-LLE' )
plt.show()
```

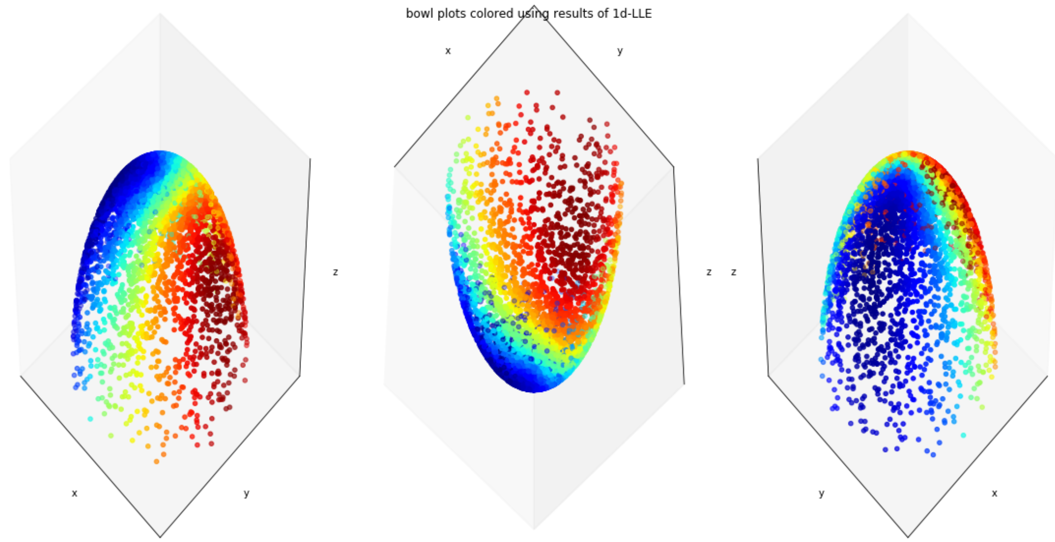


[13]:
```
k_n = 10 # number of neighbors
n_dim = 1 # output dimension

plt.figure(figsize=(16, 10))
for isp, method in enumerate(['standard', 'ltsa', 'hessian', 'modified']):
    plt.subplot(2, 2, isp+1)
    LLE_method = manifold.LocallyLinearEmbedding(k_n, n_dim, method=method)
    bowl_1d = LLE_method.fit_transform(bowl.T).T
    plt.scatter(np.arange(5000), bowl_1d[0,:], c=np.arange(5000), cmap='jet')
    plt.title('{0}d LLE using {1} method applied to bowl data'.format(n_dim,␣
 ↪method))
plt.show()
```

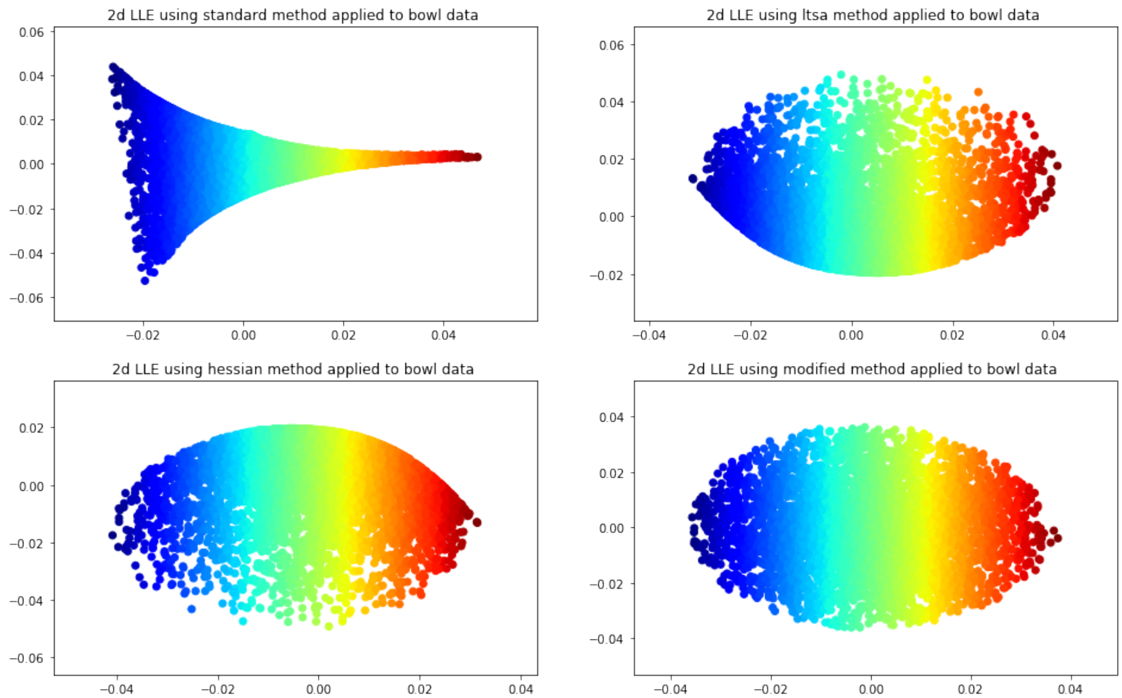


[14]:

```
# using the results of the LLE for coloring the bowl:

fig = plt.figure(figsize=(16, 8))
for i_sub, angle in enumerate([[45, 135], [135, 45], [45, 45]]):
    plt.suptitle('bowl plots colored using results of 1d-LLE')
    ax = fig.add_subplot(1, 3, i_sub+1, projection='3d')
    ax.scatter(bowl[0], bowl[1], bowl[2],
               c=bowl_1d[0,:], cmap='jet')
    ax.view_init(elev=angle[0], azim=angle[1])
    ax.set_xlabel('x')
    ax.set_ylabel('y')
    ax.set_zlabel('z')
    ax.set_xticks([])
    ax.set_yticks([])
    ax.set_zticks([])
plt.tight_layout()
plt.show()
```




```
[15]: # M = 2 embedding dimensions for the bowl data
k_n = 10 # number of neighbors
n_dim = 2 # output dimension

plt.figure(figsize=(16, 10))
for isp, method in enumerate(['standard', 'ltsa', 'hessian', 'modified']):
    plt.subplot(2, 2, isp+1)
    LLE_method = manifold.LocallyLinearEmbedding(k_n, n_dim, method=method)
    bowl_2d = LLE_method.fit_transform(bowl.T).T
    plt.scatter(bowl_2d[0,:], bowl_2d[1,:], c=bowl_2d[0,:], cmap='jet')
    plt.title('{0}d LLE using {1} method applied to bowl data '.format(n_dim,␣
↪method))
plt.show()
```


2d LLE using standard method applied to bowl data
2d LLE using ltsa method applied to bowl data
2d LLE using hessian method applied to bowl data
2d LLE using modified method applied to bowl data

[ ]: