# 02 manifold learning lle

September 29, 2021

## 1 Manifold Learning with Local Linear Embedding

Several techniques approximate a lower dimensional manifold. One example is locally-linear embedding (LLE) that was developed in 2000 by Sam Roweis and Lawrence Saul.

This notebook demonstrates how LLE 'unrolls' the swiss roll, and how it performs on other data.

For each data point, LLE identifies a given number of nearest neighbors and computes weights that represent each point as a linear combination of its neighbors. It finds a lower-dimensional embedding by linearly projecting each neighborhood on global internal coordinates on the lower-dimensional manifold and can be thought of as a sequence of PCA applications.

### 1.1 Imports & Settings

```
[1]: %matplotlib inline
     from pathlib import Path
     from os.path import join
     import numpy as np
     from numpy.random import choice, uniform, randn
     import pandas as pd
     from sklearn.datasets import make_swiss_roll, make_s_curve
     from sklearn.manifold import locally_linear_embedding
     from sklearn.decomposition import PCA
     import seaborn as sns
     import matplotlib.pyplot as plt
     from matplotlib import cm
     from matplotlib.ticker import FuncFormatter
     import ipyvolume as ipv
     import ipyvolume.pylab as p3
     from ipywidgets import HBox
     from plotly.offline import init_notebook_mode, iplot
     import plotly.graph_objs as go
     import colorlover as cl
```

```
[2]: sns.set_style('white')

[3]: DATA_PATH = Path('..', '..', 'data')

[4]: init_notebook_mode(connected=True)
    ipv_cmap = sns.color_palette("Paired", n_colors=10)
```

### 1.2 A Simple Linear Manifold: Ellipse in 3D

#### 1.2.1 PCA: Linear Dimensionality Reduction finds some manifolds

PCA is able to recover the 2D manifold.

```
[7]: pca = PCA(n_components=2)
ellipse2d = pca.fit_transform(ellipse3d)
```

```
[8]: znorm = z - z.min()
znorm /= znorm.ptp()
color = cm.viridis(znorm)

xs, ys, zs = get_2d_projection(ellipse3d, pca)
```

```
p3.figure(width=600, height=600)
p3.plot_wireframe(xs, ys, zs, color="black")
p3.scatter(x, y, z, marker='sphere', color=color[:,0:3], size=1)
p3.view(azimuth=45, elevation=75)
p3.show()
```

VBox(children=(Figure(camera=PerspectiveCamera(fov=45.0, position=(0. →3660254037844386, 1.9318516525781366, 0.3...

#### 1.3 Swiss Roll

```
[9]: n_samples = 10000
palette = sns.color_palette('viridis', n_colors=n_samples)
zeros = np.zeros(n_samples) + .5
```

Create 2D version by sorting datapoints by value and plotting using x, y coordinates only

```
[11]: p3.figure()
    p3.scatter(np.sort(swiss_val), y, zeros, marker='sphere', color=palette, size=1)
    p3.xlim(swiss_val.min(), swiss_val.max())
    fig = p3.gcc()
```

The left box shows the 3D version, the right box shows the 2D manifold that is home to the swiss roll.

```
[12]: HBox([
          ipv.quickscatter(x, y, z, size=1, color=palette, marker='sphere'),
          fig
])
```

HBox(children=(VBox(children=(Figure(camera=PerspectiveCamera(fov=45.0, →position=(0.0, 0.0, 2.0), quaternion=(...

### 1.3.1 Linear cuts along the axes

Linear methods will have a hard time.

```
[13]: p3.figure(width=400, height=400)
    p3.scatter(zeros, y, z, marker='sphere', color=palette, size=1)
    p3.view(azimuth=15, elevation=45)
    fig1 = p3.gcc()
```

```
[14]: p3.figure(width=400, height=400)
      p3.scatter(x, zeros, z, marker='sphere', color=palette, size=1)
      p3.view(azimuth=15, elevation=45)
      fig2 = p3.gcc()
[15]: p3.figure(width=400, height=400)
      p3.scatter(x, y, zeros, marker='sphere', color=palette, size=1)
      p3.view(azimuth=15, elevation=45)
      fig3 = p3.gcc()
[16]: HBox([
          fig1, fig2, fig3]
     HBox(children=(VBox(children=(Figure(camera=PerspectiveCamera(fov=45.0,
      →position=(0.36602540378443865, 1.41421...
     1.3.2 Can PCA find the Swiss Roll Manifold?
[17]: pca = PCA(n_components=2)
      swiss_2d = pca.fit_transform(swiss_3d)
[18]: p3.figure(width=400, height=400)
      xs, ys, zs = get_2d_projection(swiss_3d, pca)
      p3.plot_wireframe(xs, ys, zs, color='black')
      p3.scatter(*swiss_3d.T, marker='sphere', color=palette, size=1)
      p3.view(azimuth=15, elevation=45)
      fig1 = p3.gcc()
[19]: p3.figure(width=400, height=400)
      min_2d, max_2d = swiss_2d[:, :2].min(0), swiss_2d[:, :2].max(0)
      x2d, y2d = np.meshgrid(np.linspace(min_2d[0], max_2d[0], 100),
                           np.linspace(min_2d[1], max_2d[1], 100))
      p3.plot_wireframe(x2d, y2d, np.zeros(shape=(100, 100)) + .5, color='black'),
```

PCA is unable to capture the manifold structure and instead squashes the swiss roll sideways:

```
[20]: HBox([
fig1, fig2]
)
```

p3.scatter(\*np.c\_[swiss\_2d, np.zeros(n\_samples) + .5].T, marker='sphere', color=palette, size=1)

p3.view(azimuth=45, elevation=45)

fig2 = p3.gcc()

```
HBox(children=(VBox(children=(Figure(camera=PerspectiveCamera(fov=45.0, → position=(0.36602540378443865, 1.41421...
```

#### 1.3.3 Manifold learning can make a classification task linear

We'll compare two cases with very different spatial location of the classes.

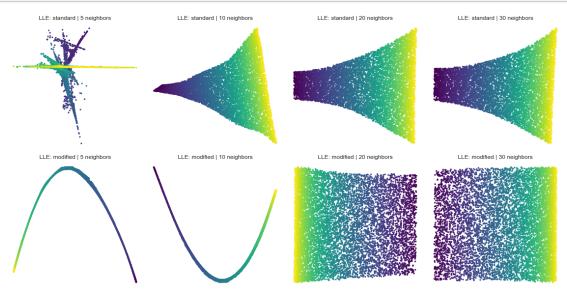
```
[21]: cpos, cneg = 'red', 'blue'
[22]: pos_class = swiss_3d[:, 0] > 4
      X pos = swiss 3d[pos class, :]
      X_neg = swiss_3d[~pos_class, :]
[23]: p3.figure(width=400, height=400)
      p3.scatter(*X_pos.T, marker='sphere', color=cpos, size=1)
      p3.scatter(*X_neg.T, marker='sphere', color=cneg, size=1)
      p3.view(azimuth=15, elevation=45)
      fig1 = p3.gcc()
[24]: p3.figure(width=400, height=400)
      p3.scatter(np.sort(swiss_val)[pos_class],
                 X pos[:, 1],
                 zeros, marker='sphere',
                 color=cpos,
                 size=1)
      p3.scatter(np.sort(swiss_val)[~pos_class],
                 X_neg[:, 1],
                 zeros, marker='sphere',
                 color=cneg, size=1)
      p3.view(azimuth=15, elevation=45)
      fig2 = p3.gcc()
[25]: HBox([fig1, fig2])
     HBox(children=(VBox(children=(Figure(camera=PerspectiveCamera(fov=45.0,
      →position=(0.36602540378443865, 1.41421...
[26]: pos_class = 2 * (np.sort(swiss_val) - 4) > swiss_3d[:, 1]
      X_pos = swiss_3d[pos_class]
      X_neg = swiss_3d[~pos_class]
[27]: p3.figure(width=600, height=400)
      p3.scatter(*X_pos.T, marker='sphere', color=cpos, size=1)
      p3.scatter(*X_neg.T, marker='sphere', color=cneg, size=1)
      p3.view(azimuth=15, elevation=45)
      fig1 = p3.gcc()
```

In this case, the classes are linearly separable given their manifold.

```
[29]: HBox([fig1, fig2])
```

HBox(children=(VBox(children=(Figure(camera=PerspectiveCamera(fov=45.0, → position=(0.36602540378443865, 1.41421...

### 1.3.4 Local-Linear Embedding learns the Swill Roll manifold



#### 1.4 S-Curve

```
[31]: scurve_3d, scurve_val = make_s_curve(
    n_samples=n_samples, noise=.05, random_state=42)
scurve_3d = scurve_3d[scurve_val.argsort()[::-1]]
scurve_3d[:, 1] *= 10
```

#### 1.4.1 Can PCA identify the S-Curve Manifold?

```
[32]: pca = PCA(n_components=2)
scurve_2d = pca.fit_transform(scurve_3d)
```

```
p3.figure(width=500, height=500)
xs, ys, zs = get_2d_projection(scurve_3d, pca)
p3.plot_wireframe(xs, ys, zs, color='black')
p3.scatter(*scurve_3d.T, marker='sphere', color=palette, size=1)
p3.view(azimuth=15, elevation=45)
fig1 = p3.gcc()
```

```
[35]: HBox([
fig1, fig2]
)
```

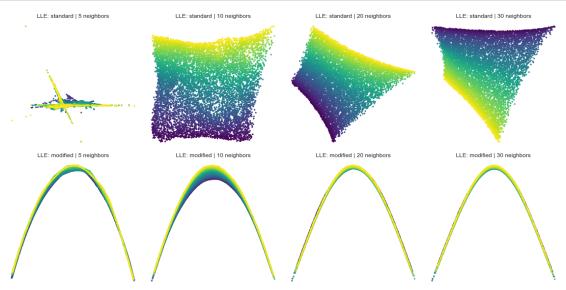
HBox(children=(VBox(children=(Figure(camera=PerspectiveCamera(fov=45.0, → position=(0.36602540378443865, 1.41421...

### 1.4.2 Local-Linear Embedding

```
[36]: fig, axes = plt.subplots(nrows=2, ncols=4, figsize=(16, 8))
for row, method in enumerate(['standard', 'modified']):
    for col, n_neighbors in enumerate([5, 10, 20, 30]):
        embedded, err = locally_linear_embedding(scurve_3d,
```

```
n_neighbors=n_neighbors,
n_components=2,
method=method,
random_state=42)

axes[row, col].scatter(*embedded.T, c=palette, s=5)
axes[row, col].set_title(f'LLE: {method} | {n_neighbors} neighbors')
axes[row, col].set_axis_off()
fig.tight_layout()
```



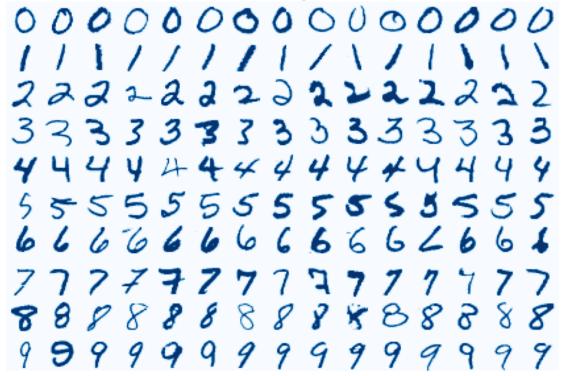
## 1.5 Handwritten Digits - MNIST Data

## 1.5.1 Load Data

```
for row, label in enumerate(digits):
    label_idx = np.argwhere(mnist_label == label).squeeze()
    sample_indices = choice(label_idx, size=n_samples, replace=False)
    i = row * h
    for col, sample_idx in enumerate(sample_indices):
        j = col * w
        sample = mnist_data[sample_idx].reshape(h, w)
        mnist_sample[i:i+h, j:j + w] = sample

ax.imshow(mnist_sample, cmap='Blues')
ax.set_title('MNIST Images', fontsize=16)
plt.axis('off')
fig.tight_layout()
```

MNIST Images

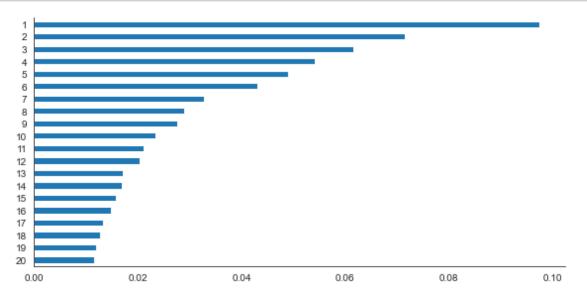


#### 1.5.2 PCA

### Explained Variance

```
[41]: n_components = 20
mnist_pca = PCA(n_components=n_components)
mnist_pca.fit(mnist_data)
```

[41]: PCA(n\_components=20)

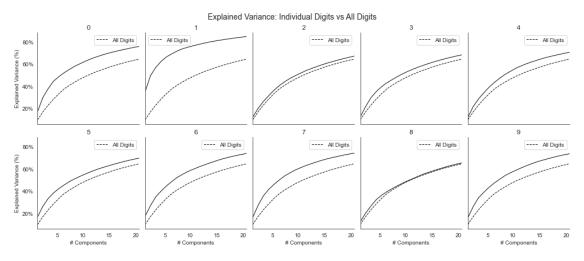


```
[43]: n_components = 20
pca = PCA(n_components=n_components)
explained_var = pd.DataFrame(index=list(range(1, n_components + 1)))
for digit in digits:
    digit_data = mnist_data[mnist_label == digit]
    pca.fit(digit_data)
    explained_var[digit] = pca.explained_variance_ratio_
```

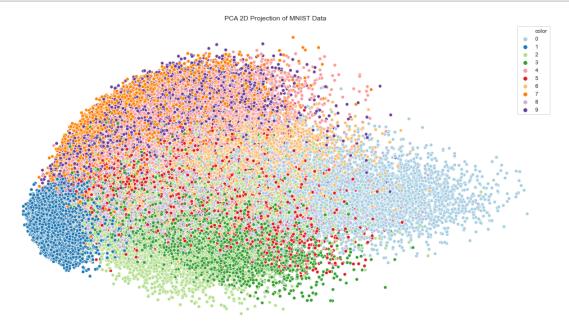
The below plot illustrates how much more variance PCA is able to capture for individual digits.

```
c='k',
    ls='--',
    label='All Digits',
    legend=True)
ax.set_xlabel('# Components')
ax.set_ylabel('Explained Variance (%)')
ax.yaxis.set_major_formatter(FuncFormatter(lambda y, _: '{:.0%}'.format(y)))

plt.gcf().suptitle('Explained Variance: Individual Digits vs All Digits',
    fontsize=14)
sns.despine()
plt.tight_layout()
plt.subplots_adjust(top=.9)
```



[0 1 2 3 4 5 6 7 8 9]



### 1.5.3 Local Linear Embedding

The following locally\_linear\_embedding on mnist.data takes fairly long to run, hence we are providing pre-computed results so you can explore the visualizations regardless of your hardware setup.

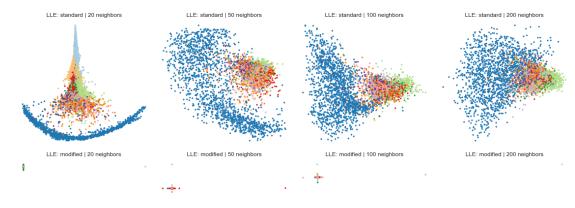
```
[50]: # commented out to avoid long run time
# lle, err = locally_linear_embedding(X=mnist.data, n_components=2, □
→ n_neighbors=20, method='standard')
```

```
[51]: mnist_path = Path('data', 'mnist')
mnist_lle_path = mnist_path / 'lle'
```

```
[52]: mnist_labels = np.load(mnist_path / 'labels.npy')
color = [sns.color_palette('Paired', 10)[int(i)] for i in mnist_labels]
```

```
fig, axes = plt.subplots(nrows=2, ncols=4, figsize=(16, 8))

for row, method in enumerate(['standard', 'modified']):
    for col, n_neighbors in enumerate([20, 50, 100, 200]):
        x, y = np.load(mnist_lle_path / method / f'{n_neighbors}.npy').T
        axes[row, col].scatter(x, y, c=color, s=5)
        axes[row, col].set_title(f'LLE: {method} | {n_neighbors} neighbors')
        axes[row, col].set_axis_off()
    fig.tight_layout()
```



#### Plotly Visualization

```
size=5,
                color=color,
                autocolorscale=True,
                showscale=False,
                opacity=.9,
                colorbar=go.scattergl.marker.ColorBar(
                    title='Class'
                ),
                line=dict(width=1))),
    ],
    layout=dict(title=title,
                width=1200,
                font=dict(color='white'),
                xaxis=dict(
                    title=x,
                    hoverformat='.1f',
                    showgrid=False),
                yaxis=dict(title=y,
                           hoverformat='.1f',
                            showgrid=False),
                paper_bgcolor='rgba(0,0,0,0)',
                plot_bgcolor='rgba(0,0,0,0)'
                ))
iplot(fig, show_link=False)
```

```
[55]: method = 'standard'
n_neigbhors = 100
embedding = np.load(mnist_lle_path / method / f'{n_neigbhors}.npy')
color = [plotly_cmap[int(i)] for i in mnist_labels]
plotly_scatter(embedding, mnist_labels, color=color, title='Local Linear_

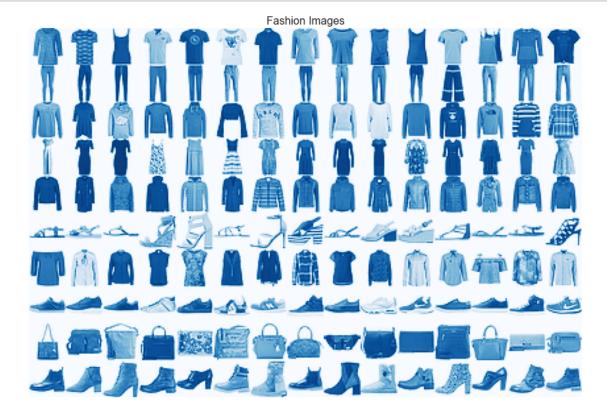
→Embedding (Standard) | 100 Neighbors')
```

### 1.6 Fashion MNIST Data

### 1.6.1 Load Data

#### 1.6.2 Visualize Data

```
[59]: h = w = int(np.sqrt(fashion_data.shape[1])) # 28 x 28 pixels
      n_samples = 15
[60]: fig, ax = plt.subplots(figsize=(18, 8))
      fashion_sample = np.empty(shape=(h * len(classes),
                                       w * n_samples))
      for row, label in enumerate(classes):
          label_idx = np.argwhere(fashion_label == label).squeeze()
          sample_indices = choice(label_idx, size=n_samples, replace=False)
          i = row * h
          for col, sample_idx in enumerate(sample_indices):
              j = col * w
              sample = fashion_data[sample_idx].reshape(h, w)
              fashion_sample[i:i+h, j:j + w] = sample
      ax.imshow(fashion_sample, cmap='Blues')
      ax.set_title('Fashion Images', fontsize=16)
      plt.axis('off')
      fig.tight_layout()
```

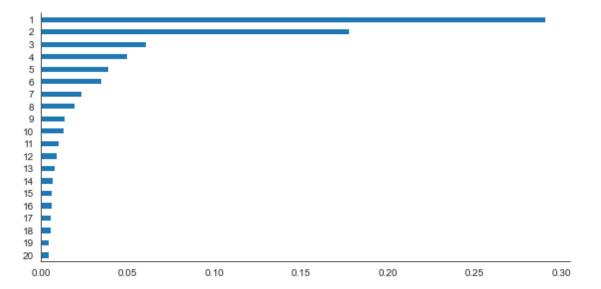


#### 1.6.3 PCA

```
[61]: n_components = 20
mnist_pca = PCA(n_components=n_components)
mnist_pca.fit(fashion_data)
```

[61]: PCA(n\_components=20)

### **Explained Variance**

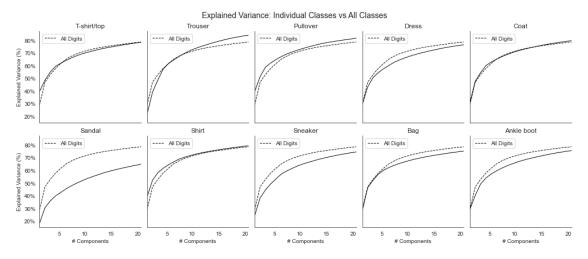


```
[63]: n_components = 20
pca = PCA(n_components=n_components)
explained_var = pd.DataFrame(index=list(range(1, n_components + 1)))
for label in classes:
    class_data = fashion_data[fashion_label == label]
    pca.fit(class_data)
    explained_var[label] = pca.explained_variance_ratio_
```

The below plot illustrates how much more variance PCA is able to capture for individual digits.

```
[64]: axes = explained_var.cumsum().plot(subplots=True, layout=(2, 5), figsize=(14, 6), rot=0,
```

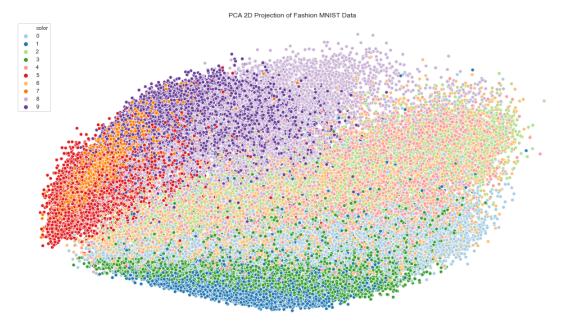
```
lw=1,
                                    sharey=True,
                                    xlim=(1, 20),
                                    color='k',
                                    title=named_classes,
                                    legend=False)
for ax in axes.flatten():
    ev.cumsum().plot(ax=ax,
                     lw=1,
                      c='k',
                     ls='--',
                      label='All Digits',
                     legend=True)
    ax.set_xlabel('# Components')
    ax.set_ylabel('Explained Variance (%)')
    ax.yaxis.set_major_formatter(FuncFormatter(lambda y, _: '{:.0%}'.format(y)))
plt.gcf().suptitle('Explained Variance: Individual Classes vs All Classes', u
\rightarrowfontsize=14)
sns.despine()
plt.tight_layout()
plt.subplots_adjust(top=.9)
```



```
[65]: fashion_pca = PCA(n_components=2)
fashion_pca_2d = fashion_pca.fit_transform(fashion_data)
```

```
[66]: fashion_pca_df = pd.DataFrame(fashion_pca_2d, columns=['x', 'y']).

→assign(color=fashion_label)
```



```
[68]: pca = PCA(n_components=3)
  fashion_3d = pca.fit_transform(fashion_data)
  pd.Series(pca.explained_variance_ratio_)

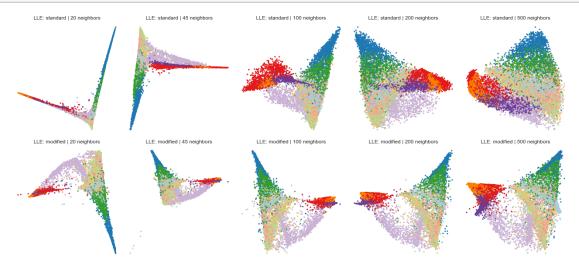
[68]: 0      0.290565
      1      0.177385
      2      0.060176
      dtype: float64
```

```
[69]: ipv_color = [ipv_cmap[int(t)] for t in fashion_label]
ipv.quickscatter(*fashion_3d.T, size=.5, color=ipv_color, marker='sphere')
```

VBox(children=(Figure(camera=PerspectiveCamera(fov=45.0, position=(0.0, 0.0, 2.  $\rightarrow$ 0), quaternion=(0.0, 0.0, 0.0, ...

### 1.6.4 Local Linear Embedding

### 2D Projection



### Plotly Visualization