Week_9_Dimensionality_Reduction

May 6, 2024

1 PCA

Let's start with several figures to explain the concepts of PCA and Manifold Learning. Below is the code to generate these figures

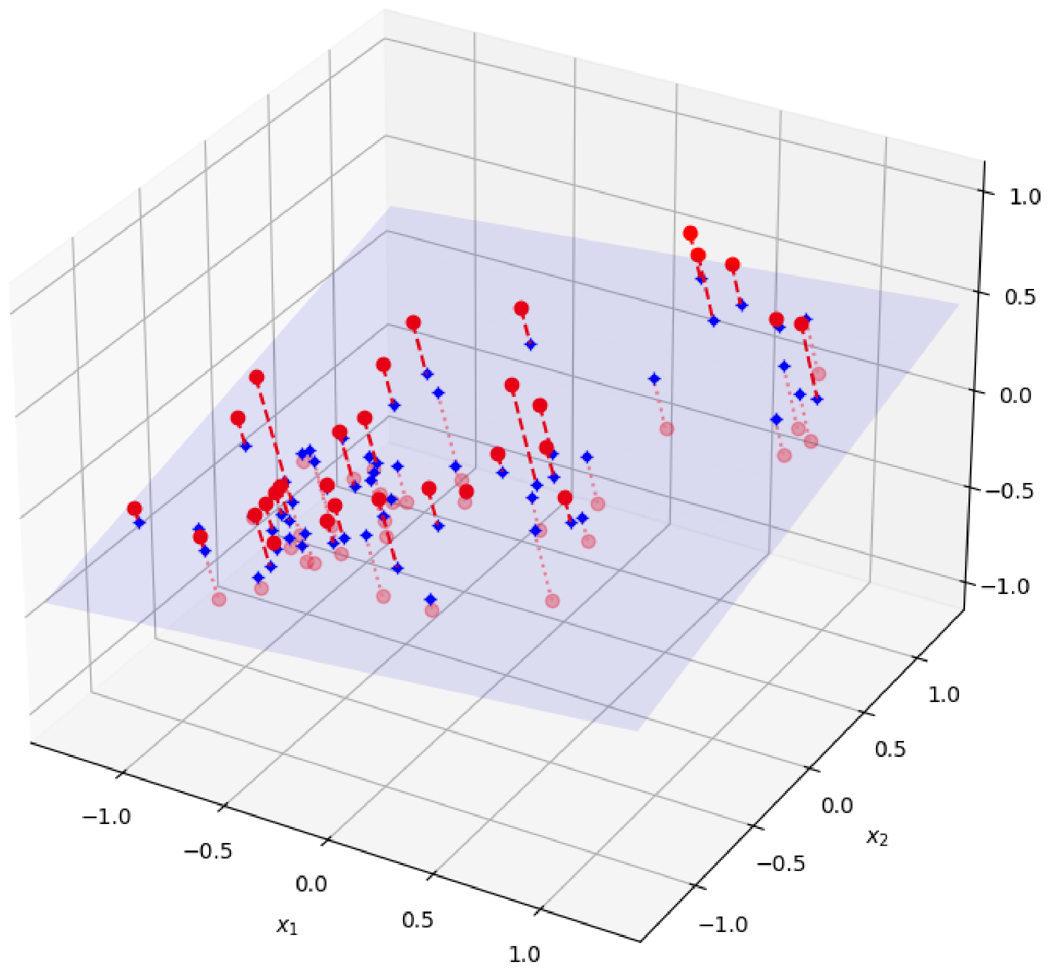
Let's generate a small 3D dataset. It's an oval shape, rotated in 3D space, with points distributed unevenly, and with quite a lot of noise:

[1]:
```python
# extra code

import numpy as np
from scipy.spatial.transform import Rotation

m = 60
X = np.zeros((m, 3))  # initialize 3D dataset
np.random.seed(42)
angles = (np.random.rand(m) ** 3 + 0.5) * 2 * np.pi  # uneven distribution
X[:, 0], X[:, 1] = np.cos(angles), np.sin(angles) * 0.5  # oval
X += 0.28 * np.random.randn(m, 3)  # add more noise
X = Rotation.from_rotvec([np.pi / 29, -np.pi / 20, np.pi / 4]).apply(X)
X += [0.2, 0, 0.2]  # shift a bit
```

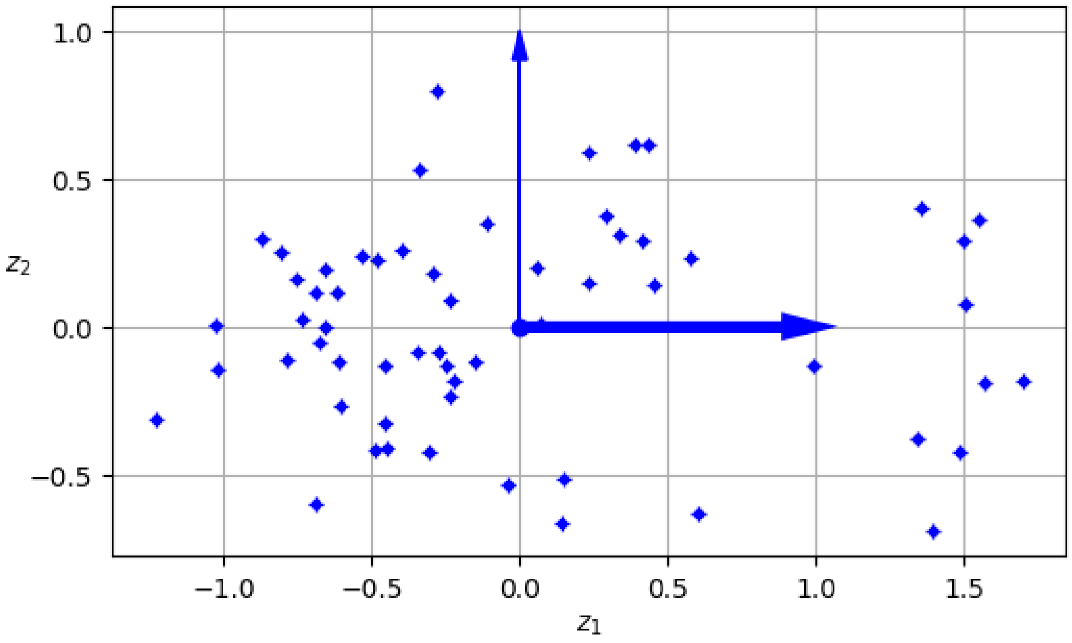
Plot the 3D dataset, with the projection plane.

[2]:
```python
# extra code - this cell generates figure below

import matplotlib.pyplot as plt
from sklearn.decomposition import PCA

pca = PCA(n_components=2)
X2D = pca.fit_transform(X)  # dataset reduced to 2D
X3D_inv = pca.inverse_transform(X2D)  # 3D position of the projected samples
X_centered = X - X.mean(axis=0)
U, s, Vt = np.linalg.svd(X_centered)

axes = [-1.4, 1.4, -1.4, 1.4, -1.1, 1.1]
x1, x2 = np.meshgrid(np.linspace(axes[0], axes[1], 10),
                     np.linspace(axes[2], axes[3], 10))
w1, w2 = np.linalg.solve(Vt[:2, :2], Vt[:2, 2])  # projection plane coefs
```

```python
z = w1 * (x1 - pca.mean_[0]) + w2 * (x2 - pca.mean_[1]) - pca.mean_[2]  # plane
X3D_above = X[X[:, 2] >= X3D_inv[:, 2]]  # samples above plane
X3D_below = X[X[:, 2] < X3D_inv[:, 2]]  # samples below plane

fig = plt.figure(figsize=(9, 9))
ax = fig.add_subplot(111, projection="3d")

# plot samples and projection lines below plane first
ax.plot(X3D_below[:, 0], X3D_below[:, 1], X3D_below[:, 2], "ro", alpha=0.3)
for i in range(m):
    if X[i, 2] < X3D_inv[i, 2]:
        ax.plot([X[i][0], X3D_inv[i][0]],
                [X[i][1], X3D_inv[i][1]],
                [X[i][2], X3D_inv[i][2]], ":", color="#F88")

ax.plot_surface(x1, x2, z, alpha=0.1, color="b")  # projection plane
ax.plot(X3D_inv[:, 0], X3D_inv[:, 1], X3D_inv[:, 2], "b+")  # projected samples
ax.plot(X3D_inv[:, 0], X3D_inv[:, 1], X3D_inv[:, 2], "b.")

# now plot projection lines and samples above plane
for i in range(m):
    if X[i, 2] >= X3D_inv[i, 2]:
        ax.plot([X[i][0], X3D_inv[i][0]],
                [X[i][1], X3D_inv[i][1]],
                [X[i][2], X3D_inv[i][2]], "r--")

ax.plot(X3D_above[:, 0], X3D_above[:, 1], X3D_above[:, 2], "ro")

def set_xyz_axes(ax, axes):
    ax.xaxis.set_rotate_label(False)
    ax.yaxis.set_rotate_label(False)
    ax.zaxis.set_rotate_label(False)
    ax.set_xlabel("$x_1$", labelpad=8, rotation=0)
    ax.set_ylabel("$x_2$", labelpad=8, rotation=0)
    ax.set_zlabel("$x_3$", labelpad=8, rotation=0)
    ax.set_xlim(axes[0:2])
    ax.set_ylim(axes[2:4])
    ax.set_zlim(axes[4:6])

set_xyz_axes(ax, axes)
ax.set_zticks([-1, -0.5, 0, 0.5, 1])

plt.show()
```

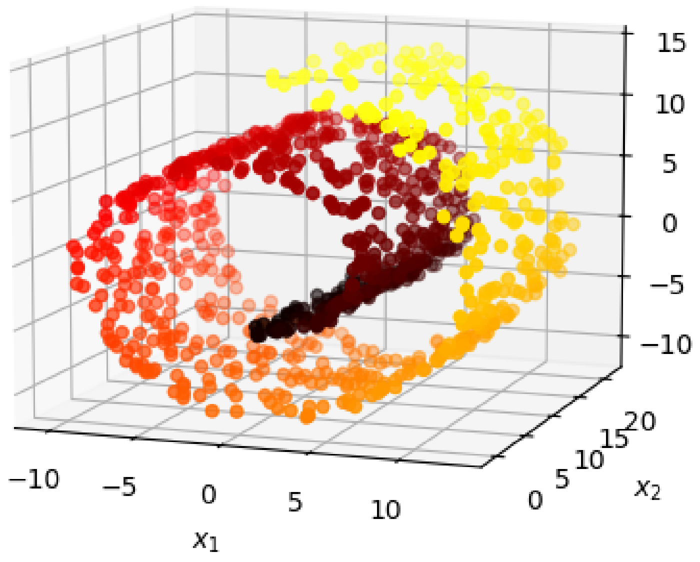


[3]:
```
# extra code – this cell generates figure below

fig = plt.figure()
ax = fig.add_subplot(1, 1, 1, aspect='equal')
ax.plot(X2D[:, 0], X2D[:, 1], "b+")
ax.plot(X2D[:, 0], X2D[:, 1], "b.")
ax.plot([0], [0], "bo")
ax.arrow(0, 0, 1, 0, head_width=0.05, length_includes_head=True,
         head_length=0.1, fc='b', ec='b', linewidth=4)
ax.arrow(0, 0, 0, 1, head_width=0.05, length_includes_head=True,
         head_length=0.1, fc='b', ec='b', linewidth=1)
ax.set_xlabel("$z_1$")
ax.set_yticks([-0.5, 0, 0.5, 1])
ax.set_ylabel("$z_2$", rotation=0)
ax.set_axisbelow(True)
ax.grid(True)
```

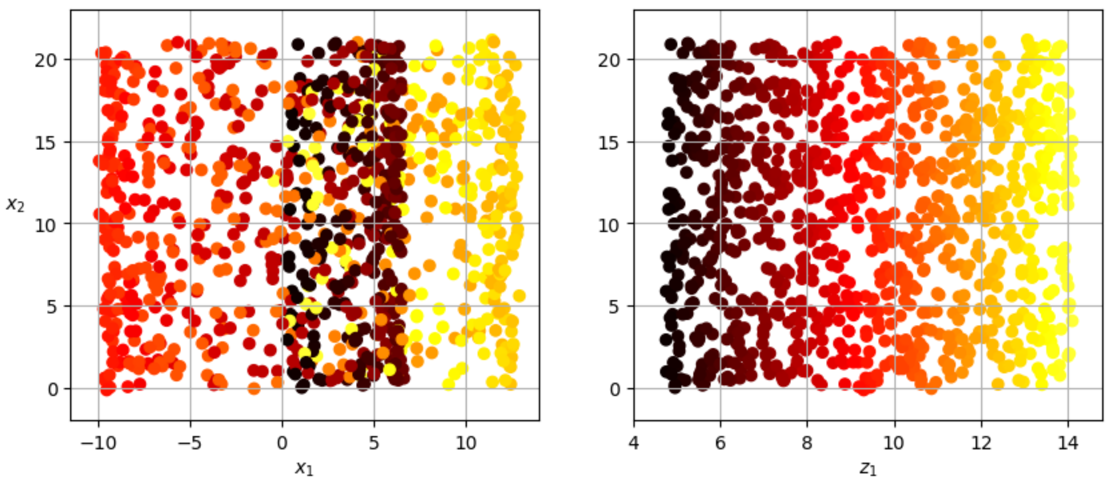


[4]:
```
from sklearn.datasets import make_swiss_roll

X_swiss, t = make_swiss_roll(n_samples=1000, noise=0.2, random_state=42)
```

[5]:
```
# extra code – this cell generates figure below

from matplotlib.colors import ListedColormap

darker_hot = ListedColormap(plt.cm.hot(np.linspace(0, 0.8, 256)))

axes = [-11.5, 14, -2, 23, -12, 15]

fig = plt.figure(figsize=(6, 5))
ax = fig.add_subplot(111, projection='3d')

ax.scatter(X_swiss[:, 0], X_swiss[:, 1], X_swiss[:, 2], c=t, cmap=darker_hot)
ax.view_init(10, -70)
set_xyz_axes(ax, axes)
plt.show()
```

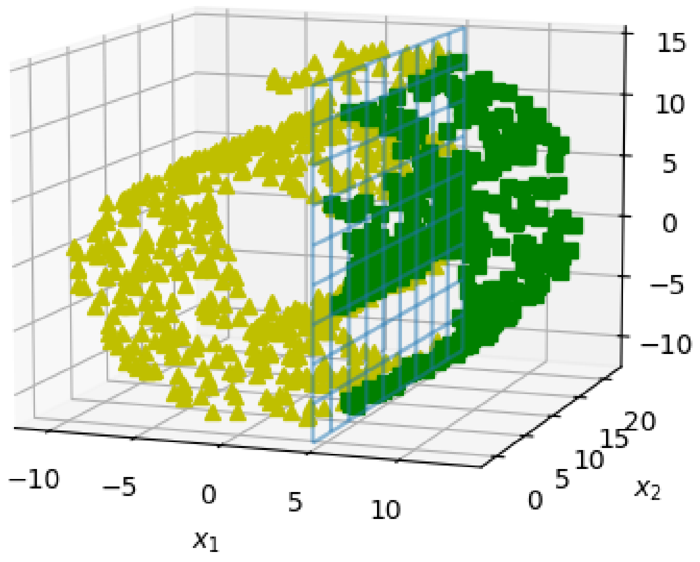


[6]:
```
# extra code – this cell generates figure below

plt.figure(figsize=(10, 4))

plt.subplot(121)
plt.scatter(X_swiss[:, 0], X_swiss[:, 1], c=t, cmap=darker_hot)
plt.axis(axes[:4])
plt.xlabel("$x_1$")
plt.ylabel("$x_2$", labelpad=10, rotation=0)
plt.grid(True)

plt.subplot(122)
plt.scatter(t, X_swiss[:, 1], c=t, cmap=darker_hot)
plt.axis([4, 14.8, axes[2], axes[3]])
plt.xlabel("$z_1$")
plt.grid(True)

plt.show()
```

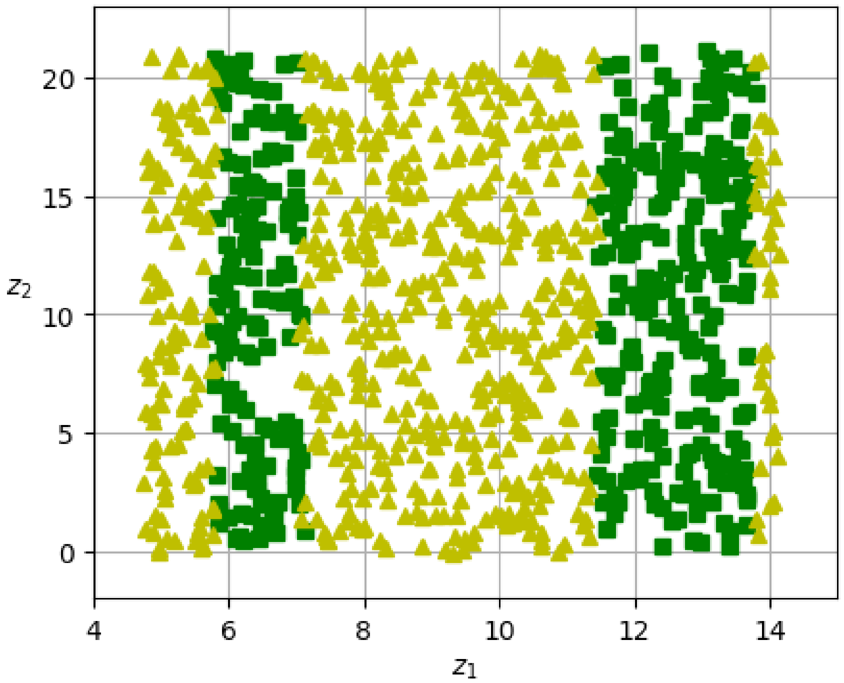


[7]:
```
# extra code - this cell generates figure below

axes = [-11.5, 14, -2, 23, -12, 15]
x2s = np.linspace(axes[2], axes[3], 10)
x3s = np.linspace(axes[4], axes[5], 10)
x2, x3 = np.meshgrid(x2s, x3s)

positive_class = X_swiss[:, 0] > 5
X_pos = X_swiss[positive_class]
X_neg = X_swiss[~positive_class]

fig = plt.figure(figsize=(6, 5))
ax = plt.subplot(1, 1, 1, projection='3d')
ax.view_init(10, -70)
ax.plot(X_neg[:, 0], X_neg[:, 1], X_neg[:, 2], "y^")
ax.plot_wireframe(5, x2, x3, alpha=0.5)
ax.plot(X_pos[:, 0], X_pos[:, 1], X_pos[:, 2], "gs")
set_xyz_axes(ax, axes)
plt.show()

fig = plt.figure(figsize=(5, 4))
ax = plt.subplot(1, 1, 1)
ax.plot(t[positive_class], X_swiss[positive_class, 1], "gs")
ax.plot(t[~positive_class], X_swiss[~positive_class, 1], "y^")
ax.axis([4, 15, axes[2], axes[3]])
ax.set_xlabel("$z_1$")
ax.set_ylabel("$z_2$", rotation=0, labelpad=8)
ax.grid(True)
plt.show()
```

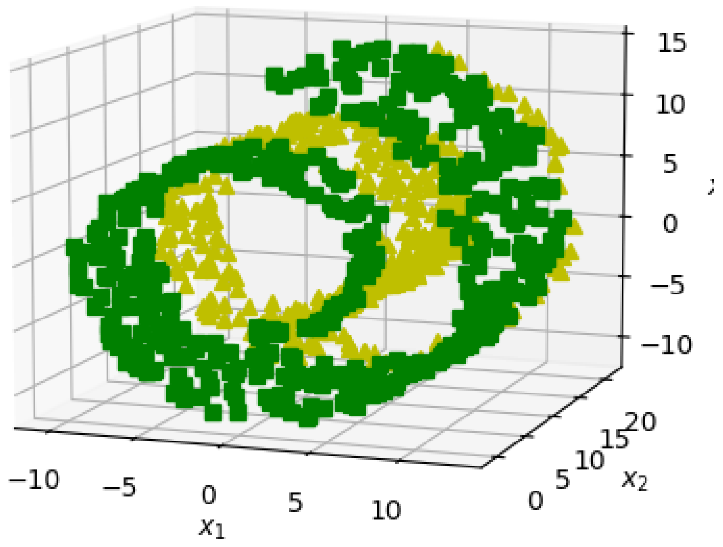
```python
positive_class = 2 * (t[:] - 4) > X_swiss[:, 1]
X_pos = X_swiss[positive_class]
X_neg = X_swiss[~positive_class]

fig = plt.figure(figsize=(6, 5))
ax = plt.subplot(1, 1, 1, projection='3d')
ax.view_init(10, -70)
ax.plot(X_neg[:, 0], X_neg[:, 1], X_neg[:, 2], "y^")
ax.plot(X_pos[:, 0], X_pos[:, 1], X_pos[:, 2], "gs")
ax.xaxis.set_rotate_label(False)
ax.yaxis.set_rotate_label(False)
ax.zaxis.set_rotate_label(False)
ax.set_xlabel("$x_1$", rotation=0)
ax.set_ylabel("$x_2$", rotation=0)
ax.set_zlabel("$x_3$", rotation=0)
ax.set_xlim(axes[0:2])
ax.set_ylim(axes[2:4])
ax.set_zlim(axes[4:6])

plt.show()

fig = plt.figure(figsize=(5, 4))
ax = plt.subplot(1, 1, 1)
ax.plot(t[positive_class], X_swiss[positive_class, 1], "gs")
ax.plot(t[~positive_class], X_swiss[~positive_class, 1], "y^")
ax.plot([4, 15], [0, 22], "b-", linewidth=2)
ax.axis([4, 15, axes[2], axes[3]])
ax.set_xlabel("$z_1$")
ax.set_ylabel("$z_2$", rotation=0, labelpad=8)
ax.grid(True)
plt.show()
```



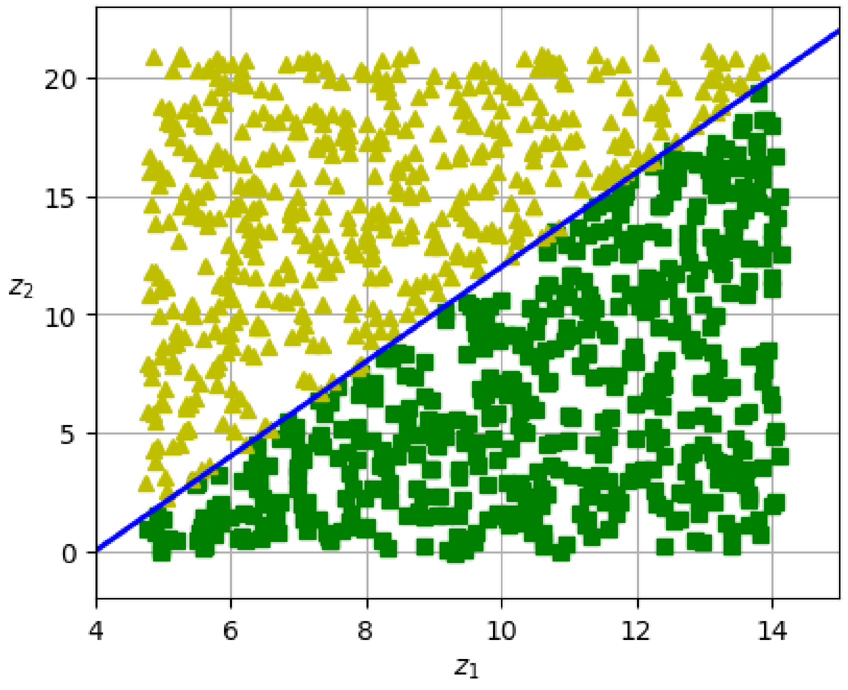
15
10
5
0
−5
−10
−10
−5
0
5
10
x_1
0
5
10
15
20
x_2



20
15
10
5
0
z_2
4
6
8
10
12
14
z_1

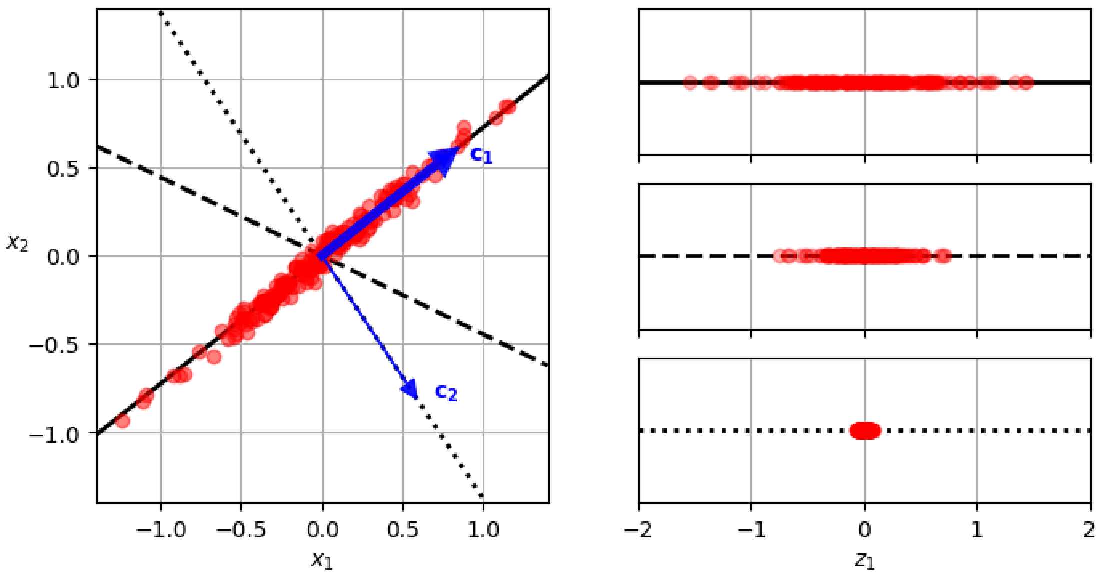


15
10
5
0
−5
−10
−10
−5
0
5
10
x_1
0
5
10
15
20
x_2



20
15
10
5
0
z_2
4
6
8
10
12
14
z_1

[8]:
```python
# extra code - this cell generates figure below

angle = np.pi / 5
stretch = 5
m = 200

np.random.seed(3)
X_line = np.random.randn(m, 2) / 10
X_line = X_line @ np.array([[stretch, 0], [0, 1]])  # stretch
X_line = X_line @ [[np.cos(angle), np.sin(angle)],
                   [np.sin(angle), np.cos(angle)]]  # rotate

u1 = np.array([np.cos(angle), np.sin(angle)])
u2 = np.array([np.cos(angle - 2 * np.pi / 6), np.sin(angle - 2 * np.pi / 6)])
u3 = np.array([np.cos(angle - np.pi / 2), np.sin(angle - np.pi / 2)])

X_proj1 = X_line @ u1.reshape(-1, 1)
X_proj2 = X_line @ u2.reshape(-1, 1)
X_proj3 = X_line @ u3.reshape(-1, 1)

plt.figure(figsize=(8, 4))
plt.subplot2grid((3, 2), (0, 0), rowspan=3)
plt.plot([-1.4, 1.4], [-1.4 * u1[1] / u1[0], 1.4 * u1[1] / u1[0]], "k-",
         linewidth=2)
plt.plot([-1.4, 1.4], [-1.4 * u2[1] / u2[0], 1.4 * u2[1] / u2[0]], "k--",
         linewidth=2)
plt.plot([-1.4, 1.4], [-1.4 * u3[1] / u3[0], 1.4 * u3[1] / u3[0]], "k:",
         linewidth=2)
plt.plot(X_line[:, 0], X_line[:, 1], "ro", alpha=0.5)
plt.arrow(0, 0, u1[0], u1[1], head_width=0.1, linewidth=4, alpha=0.9,
          length_includes_head=True, head_length=0.1, fc="b", ec="b", zorder=10)
plt.arrow(0, 0, u3[0], u3[1], head_width=0.1, linewidth=1, alpha=0.9,
          length_includes_head=True, head_length=0.1, fc="b", ec="b", zorder=10)
plt.text(u1[0] + 0.1, u1[1] - 0.05, r"$\mathbf{c_1}$", color="blue")
plt.text(u3[0] + 0.1, u3[1], r"$\mathbf{c_2}$", color="blue")
plt.xlabel("$x_1$")
plt.ylabel("$x_2$", rotation=0)
plt.axis([-1.4, 1.4, -1.4, 1.4])
plt.grid()

plt.subplot2grid((3, 2), (0, 1))
plt.plot([-2, 2], [0, 0], "k-", linewidth=2)
plt.plot(X_proj1[:, 0], np.zeros(m), "ro", alpha=0.3)
plt.gca().get_yaxis().set_ticks([])
plt.gca().get_xaxis().set_ticklabels([])
plt.axis([-2, 2, -1, 1])
plt.grid()
plt.subplot2grid((3, 2), (1, 1))
plt.plot([-2, 2], [0, 0], "k--", linewidth=2)
plt.plot(X_proj2[:, 0], np.zeros(m), "ro", alpha=0.3)
plt.gca().get_yaxis().set_ticks([])
plt.gca().get_xaxis().set_ticklabels([])
plt.axis([-2, 2, -1, 1])
plt.grid()

plt.subplot2grid((3, 2), (2, 1))
plt.plot([-2, 2], [0, 0], "k:", linewidth=2)
plt.plot(X_proj3[:, 0], np.zeros(m), "ro", alpha=0.3)
plt.gca().get_yaxis().set_ticks([])
plt.axis([-2, 2, -1, 1])
plt.xlabel("$z_1$")
plt.grid()

plt.show()
```



1.1 Principal Components

[9]:
```
import numpy as np

# X = [...]  # the small 3D dataset was created earlier in this notebook
X_centered = X - X.mean(axis=0)
U, s, Vt = np.linalg.svd(X_centered)
c1 = Vt[0]
```

```
c2 = Vt[1]
```

Note: in principle, the SVD factorization algorithm returns three matrices, U, Σ and V, such that X = UΣV , where U is an m × m matrix, Σ is an m × n matrix, and V is an n × n matrix. But the svd() function returns U, s and V instead. s is the vector containing all the values on the main diagonal of the top n rows of Σ. Since Σ is full of zeros elsewhere, your can easily reconstruct it from s, like this:

[10]:
```
# extra code – shows how to construct Σ from s
m, n = X.shape
Σ = np.zeros_like(X_centered)
Σ[:n, :n] = np.diag(s)
assert np.allclose(X_centered, U @ Σ @ Vt)
```

1.2 Projecting Down to d Dimensions

[11]:
```
W2 = Vt[:2].T
X2D = X_centered @ W2
```

1.3 Using Scikit-Learn

Scikit-Learn's PCA class uses SVD to implement PCA, just like we did earlier in thischapter. The following code applies PCA to reduce the dimensionality of the datasetdown to two dimensions (note that it automatically takes care of centering the data):

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

pca = PCA(n_components=2)
X2D = pca.fit_transform(X)
```

[13]:
```
pca.components_
```

[13]:
```
array([[ 0.67857588,  0.70073508,  0.22023881],
       [ 0.72817329, -0.6811147 , -0.07646185]])
```

1.4 Explained Variance Ratio

Another useful piece of information is the explained variance ratio of each principal component, available via the explained_variance_ratio_ variable. The ratioindicates the proportion of the dataset's variance that lies along each principal component. For example, let's look at the explained variance ratios of the first twocomponents of the 3D dataset represented in second figure in this note:

[14]:
```
pca.explained_variance_ratio_
```

[14]:
```
array([0.7578477 , 0.15186921])
```

The first dimension explains about 76% of the variance, while the second explains about 15%.

By projecting down to 2D, we lost about 9% of the variance:

[15]:
```
1 - pca.explained_variance_ratio_.sum()  # extra code
```

[15]:
```
0.09028309326742046
```

1.5 Chosing the Right Number of Dimensions

Instead of arbitrarily choosing the number of dimensions to reduce down to, itis simpler to choose the number of dimensions that add up to a sufficiently largeportion of the variance—say, 95% (An exception to this rule, of course, is if you arereducing dimensionality for data visualization, in which case you will want to reducethe dimensionality down to 2 or 3). The following code loads and splits the MNIST dataset (introduced inWeek 43)and performs PCA without reducing dimensionality, then computes the minimumnumber of dimensions required to preserve 95% of the training set's variance:

[16]:
```
from sklearn.datasets import fetch_openml

mnist = fetch_openml('mnist_784', as_frame=False, parser="auto")
X_train, y_train = mnist.data[:60_000], mnist.target[:60_000]
X_test, y_test = mnist.data[60_000:], mnist.target[60_000:]

pca = PCA()
pca.fit(X_train)
cumsum = np.cumsum(pca.explained_variance_ratio_)
d = np.argmax(cumsum >= 0.95) + 1  # d equals 154
```

Note: I added parser="auto" when calling fetch_openml() to avoid a warning about the fact that the default value for that parameter will change in the future (it's irrelevant in this case).

[17]:
```
d
```

[17]:
```
154
```

You could then set n_components=d and run PCA again, but there's a better option. Instead of specifying the number of principal components you want to preserve, you can set n_components to be a float between 0.0 and 1.0, indicating the ratio of variance you wish to preserve:

[18]:
```
pca = PCA(n_components=0.95)
X_reduced = pca.fit_transform(X_train)
```

The actual number of components is determined during training, and it is stored in the n_components_ attribute:

[19]:
```
pca.n_components_
```

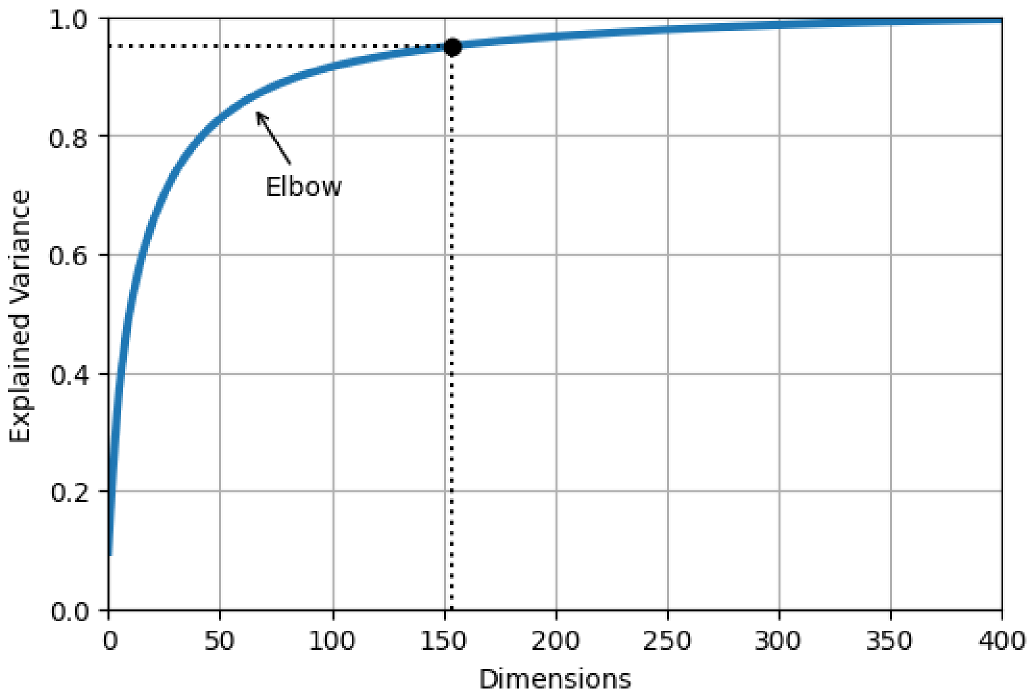
[19]:
```
154
```

[20]:
```
pca.explained_variance_ratio_.sum()  # extra code
```

[20]:
```
0.9501960192613031
```

Yet another option is to plot the explained variance as a function of the number of dimensions (simply plot cumsum; see figure below). There will usually be an elbow in the curve, where the explained variance stops growing fast. In this case, you can see that reducing the dimensionality down to about 100 dimensions wouldn't lose too much explained variance

[21]:
```
# extra code – this cell generates figure below

plt.figure(figsize=(6, 4))
plt.plot(cumsum, linewidth=3)
plt.axis([0, 400, 0, 1])
plt.xlabel("Dimensions")
plt.ylabel("Explained Variance")
plt.plot([d, d], [0, 0.95], "k:")
plt.plot([0, d], [0.95, 0.95], "k:")
plt.plot(d, 0.95, "ko")
plt.annotate("Elbow", xy=(65, 0.85), xytext=(70, 0.7),
             arrowprops=dict(arrowstyle="->"))
plt.grid(True)
plt.show()
```



Lastly, if you are using dimensionality reduction as a preprocessing step for a supervised learning task (e.g., classification), then you can tune the number of dimensions as you would any other hyperparameter (see Week 3). For example, the following code example creates a two-step pipeline, first reducing dimensionality using PCA, then classifying using a random forest. Next, it uses RandomizedSearchCV to find a good combination of hyperparameters for both PCA and the random forest classifier. This example does a quick search, tuning only 2 hyperparameters, training on just 1,000 instances, and running for just 10 iterations, but feel free to do a more thorough search if you have the time:

[22]:
```python
from sklearn.ensemble import RandomForestClassifier
from sklearn.model_selection import RandomizedSearchCV
from sklearn.pipeline import make_pipeline

clf = make_pipeline(PCA(random_state=42),
                    RandomForestClassifier(random_state=42))
param_distrib = {
    "pca__n_components": np.arange(10, 80),
    "randomforestclassifier__n_estimators": np.arange(50, 500)
}
rnd_search = RandomizedSearchCV(clf, param_distrib, n_iter=10, cv=3,
                                random_state=42)
rnd_search.fit(X_train[:1000], y_train[:1000])
```

[22]:
```
RandomizedSearchCV(cv=3,
                   estimator=Pipeline(steps=[('pca', PCA(random_state=42)),
                                             ('randomforestclassifier',
RandomForestClassifier(random_state=42))]),
                   param_distributions={'pca__n_components': array([10, 11, 12,
13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26,
       27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43,
       44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60,
       6…
       414, 415, 416, 417, 418, 419, 420, 421, 422, 423, 424, 425, 426,
       427, 428, 429, 430, 431, 432, 433, 434, 435, 436, 437, 438, 439,
       440, 441, 442, 443, 444, 445, 446, 447, 448, 449, 450, 451, 452,
       453, 454, 455, 456, 457, 458, 459, 460, 461, 462, 463, 464, 465,
       466, 467, 468, 469, 470, 471, 472, 473, 474, 475, 476, 477, 478,
       479, 480, 481, 482, 483, 484, 485, 486, 487, 488, 489, 490, 491,
       492, 493, 494, 495, 496, 497, 498, 499])},
                   random_state=42)
```

Let's look at the best hyperparameters found:

[23]:
```python
print(rnd_search.best_params_)
```

```
{'randomforestclassifier__n_estimators': 465, 'pca__n_components': 23}
```

It's interesting to note how low the optimal number of components is: we reduced a 784-dimensional dataset to just 23 dimensions! This is tied to the fact that we used a random forest, which is a pretty powerful model. If we used a linear model instead, such as an SGDClassifier, the search would find that we need to preserve moredimensions (about 70).

[24]:
```python
from sklearn.linear_model import SGDClassifier
from sklearn.model_selection import GridSearchCV
```

```
clf = make_pipeline(PCA(random_state=42), SGDClassifier())
param_grid = {"pca__n_components": np.arange(10, 80)}
grid_search = GridSearchCV(clf, param_grid, cv=3)
grid_search.fit(X_train[:1000], y_train[:1000])
```

[24]:
```
GridSearchCV(cv=3,
             estimator=Pipeline(steps=[('pca', PCA(random_state=42)),
                                       ('sgdclassifier', SGDClassifier())]),
             param_grid={'pca__n_components': array([10, 11, 12, 13, 14, 15, 16,
17, 18, 19, 20, 21, 22, 23, 24, 25, 26,
       27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43,
       44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60,
       61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77,
       78, 79])})
```

[25]:
```
grid_search.best_params_
```

[25]:
```
{'pca__n_components': 67}
```

1.6 PCA for Compression

After dimensionality reduction, the training set takes up much less space. For exam- ple, after applying PCA to the MNIST dataset while preserving 95% of its variance, we are left with 154 features, instead of the original 784 features. So the dataset is now less than 20% of its original size, and we only lost 5% of its variance! This is a reasonable compression ratio, and it's easy to see how such a size reduction would speed up a classification algorithm tremendously

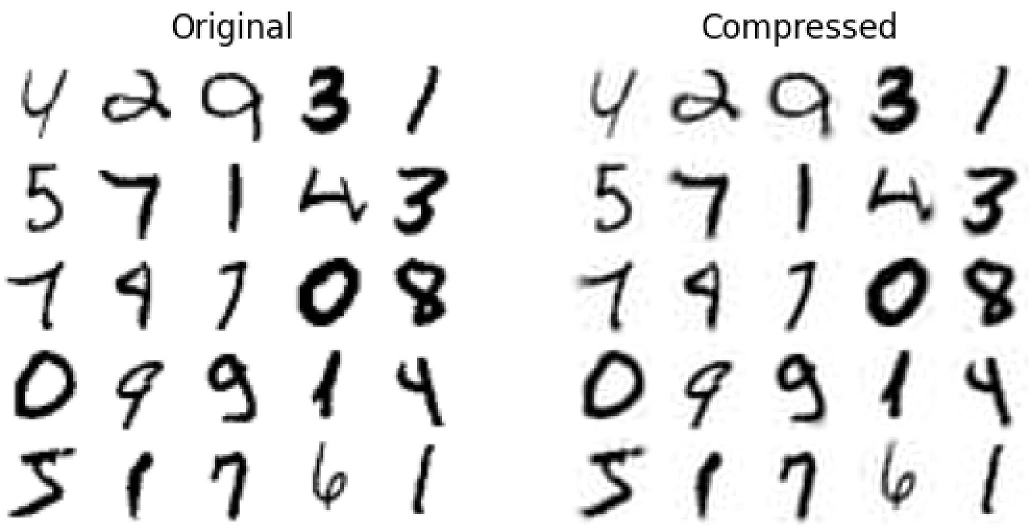
[26]:
```
pca = PCA(0.95)
X_reduced = pca.fit_transform(X_train, y_train)
```

It is also possible to decompress the reduced dataset back to 784 dimensions by applying the inverse transformation of the PCA projection. This won't give you back the original data, since the projection lost a bit of information (within the 5% variance that was dropped), but it will likely be close to the original data. The mean squared distance between the original data and the reconstructed data (compressed and then decompressed) is called the reconstruction error. The inverse_transform() method lets us decompress the reduced MNIST dataset back to 784 dimensions:

[27]:
```
X_recovered = pca.inverse_transform(X_reduced)
```

Figure below shows a few digits from the original training set (on the left), and the corresponding digits after compression and decompression. You can see that there is a slight image quality loss, but the digits are still mostly intact.

[28]:
```
# extra code – this cell generates figure below

plt.figure(figsize=(7, 4))
for idx, X in enumerate((X_train[::2100], X_recovered[::2100])):
    plt.subplot(1, 2, idx + 1)
    plt.title(["Original", "Compressed"][idx])
    for row in range(5):
        for col in range(5):
            plt.imshow(X[row * 5 + col].reshape(28, 28), cmap="binary",
                       vmin=0, vmax=255, extent=(row, row + 1, col, col + 1))
            plt.axis([0, 5, 0, 5])
            plt.axis("off")
```



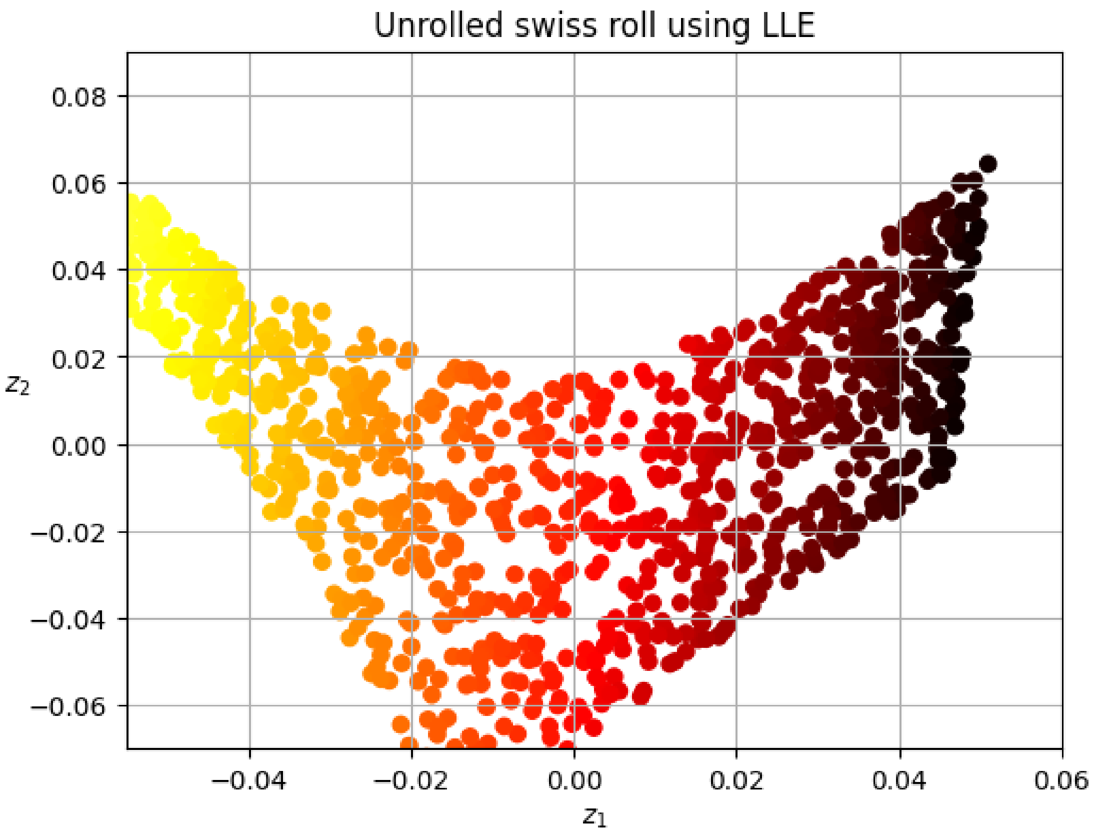
2 LLE

Locally linear embedding (LLE) is a nonlinear dimensionality reduction (NLDR) tech- nique. It is a manifold learning technique that does not rely on projections, unlike PCA and random projection. In a nutshell, LLE works by first measuring how each training instance linearly relates to its nearest neighbors, and then looking for a low-dimensional representation of the training set where these local relationships are best preserved (more details shortly). This approach makes it particularly good at unrolling twisted manifolds, especially when there is not too much noise. The following code makes a Swiss roll, then uses Scikit-Learn's LocallyLinearEmbed ding class to unroll it:

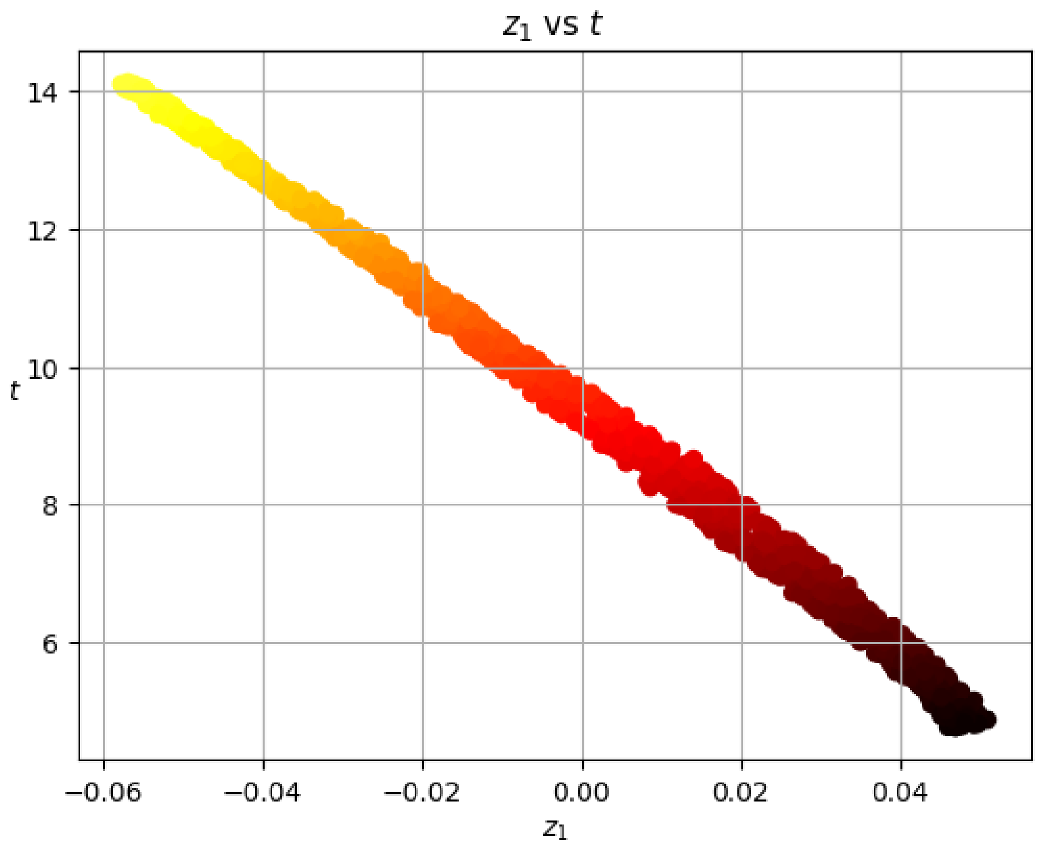
[29]:
```
from sklearn.datasets import make_swiss_roll
from sklearn.manifold import LocallyLinearEmbedding

X_swiss, t = make_swiss_roll(n_samples=1000, noise=0.2, random_state=42)
lle = LocallyLinearEmbedding(n_components=2, n_neighbors=10, random_state=42)
X_unrolled = lle.fit_transform(X_swiss)
```

The variable t is a 1D NumPy array containing the position of each instance along the rolled axis of the Swiss roll. We don't use it in this example, but it can be used as a target for a nonlinear regression task. The resulting 2D dataset is shown in figure below. As you can see, the Swiss roll is completely unrolled, and the distances between instances are locally well preserved. However, distances are not preserved on a larger scale: the unrolled Swiss roll shouldbe a rectangle, not this kind of stretched and twisted band. Nevertheless, LLE did apretty good job of modeling the manifold.

[30]:
```
# extra code – this cell generates figure below

plt.scatter(X_unrolled[:, 0], X_unrolled[:, 1],
            c=t, cmap=darker_hot)
plt.xlabel("$z_1$")
plt.ylabel("$z_2$", rotation=0)
plt.axis([-0.055, 0.060, -0.070, 0.090])
plt.grid(True)

plt.title("Unrolled swiss roll using LLE")
plt.show()
```



[31]:
```
# extra code – shows how well correlated z1 is to t: LLE worked fine
plt.title("$z_1$ vs $t$")
plt.scatter(X_unrolled[:, 0], t, c=t, cmap=darker_hot)
plt.xlabel("$z_1$")
plt.ylabel("$t$", rotation=0)
plt.grid(True)
plt.show()
```



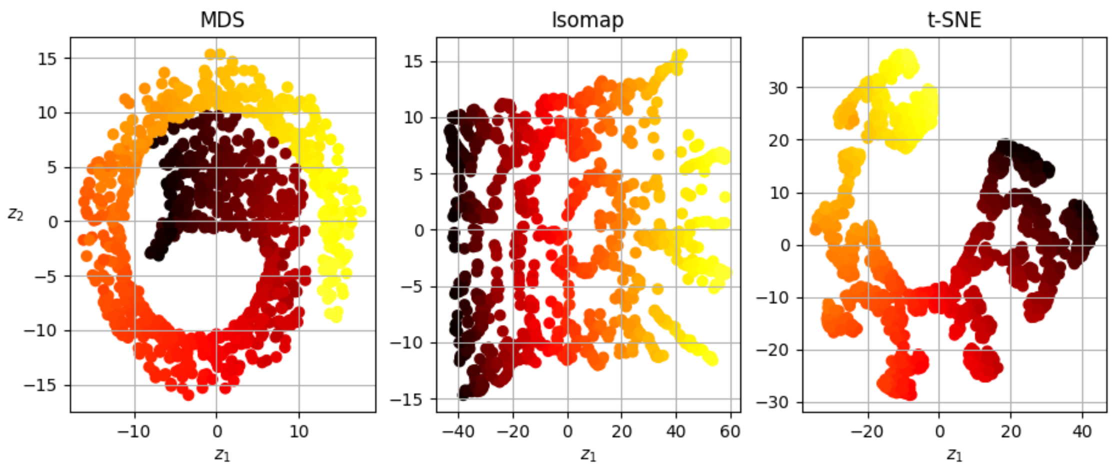
Note: I added normalized_stress=False below to avoid a warning about the fact that the default value for that hyperparameter will change in the future

[32]:
```
from sklearn.manifold import MDS

mds = MDS(n_components=2, normalized_stress=False, random_state=42)
X_reduced_mds = mds.fit_transform(X_swiss)
```

[33]:
```
from sklearn.manifold import Isomap

isomap = Isomap(n_components=2)
X_reduced_isomap = isomap.fit_transform(X_swiss)
```

[34]:
```
from sklearn.manifold import TSNE

tsne = TSNE(n_components=2, init="random", learning_rate="auto",
            random_state=42)
X_reduced_tsne = tsne.fit_transform(X_swiss)
```

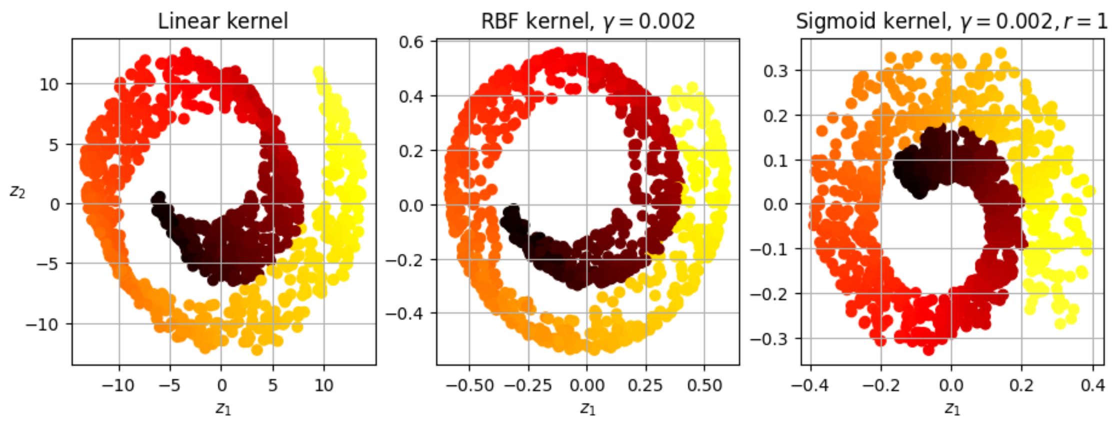
[35]:
```
# extra code - this cell generates figure below

titles = ["MDS", "Isomap", "t-SNE"]

plt.figure(figsize=(11, 4))

for subplot, title, X_reduced in zip((131, 132, 133), titles,
                                     (X_reduced_mds, X_reduced_isomap,␣
 ↪X_reduced_tsne)):
    plt.subplot(subplot)
    plt.title(title)
    plt.scatter(X_reduced[:, 0], X_reduced[:, 1], c=t, cmap=darker_hot)
    plt.xlabel("$z_1$")
    if subplot == 131:
        plt.ylabel("$z_2$", rotation=0)
    plt.grid(True)

plt.show()
```



3 Kernel PCA

[36]:
```
from sklearn.decomposition import KernelPCA

rbf_pca = KernelPCA(n_components=2, kernel="rbf", gamma=0.04, random_state=42)
X_reduced = rbf_pca.fit_transform(X_swiss)
```

[37]:
```
lin_pca = KernelPCA(kernel="linear")
rbf_pca = KernelPCA(kernel="rbf", gamma=0.002)
sig_pca = KernelPCA(kernel="sigmoid", gamma=0.002, coef0=1)

kernel_pcas = ((lin_pca, "Linear kernel"),
               (rbf_pca, rf"RBF kernel, $\gamma={rbf_pca.gamma}$"),
               (sig_pca, rf"Sigmoid kernel, $\gamma={sig_pca.gamma}, r={sig_pca.
 ↪coef0}$"))

plt.figure(figsize=(11, 3.5))
for idx, (kpca, title) in enumerate(kernel_pcas):
    kpca.n_components = 2
    kpca.random_state = 42
    X_reduced = kpca.fit_transform(X_swiss)

    plt.subplot(1, 3, idx + 1)
    plt.title(title)
    plt.scatter(X_reduced[:, 0], X_reduced[:, 1], c=t, cmap=darker_hot)
    plt.xlabel("$z_1$")
    if idx == 0:
        plt.ylabel("$z_2$", rotation=0)
    plt.grid()

plt.show()
```


Linear kernel
RBF kernel, $\gamma = 0.002$
Sigmoid kernel, $\gamma = 0.002, r = 1$
z_2
z_1