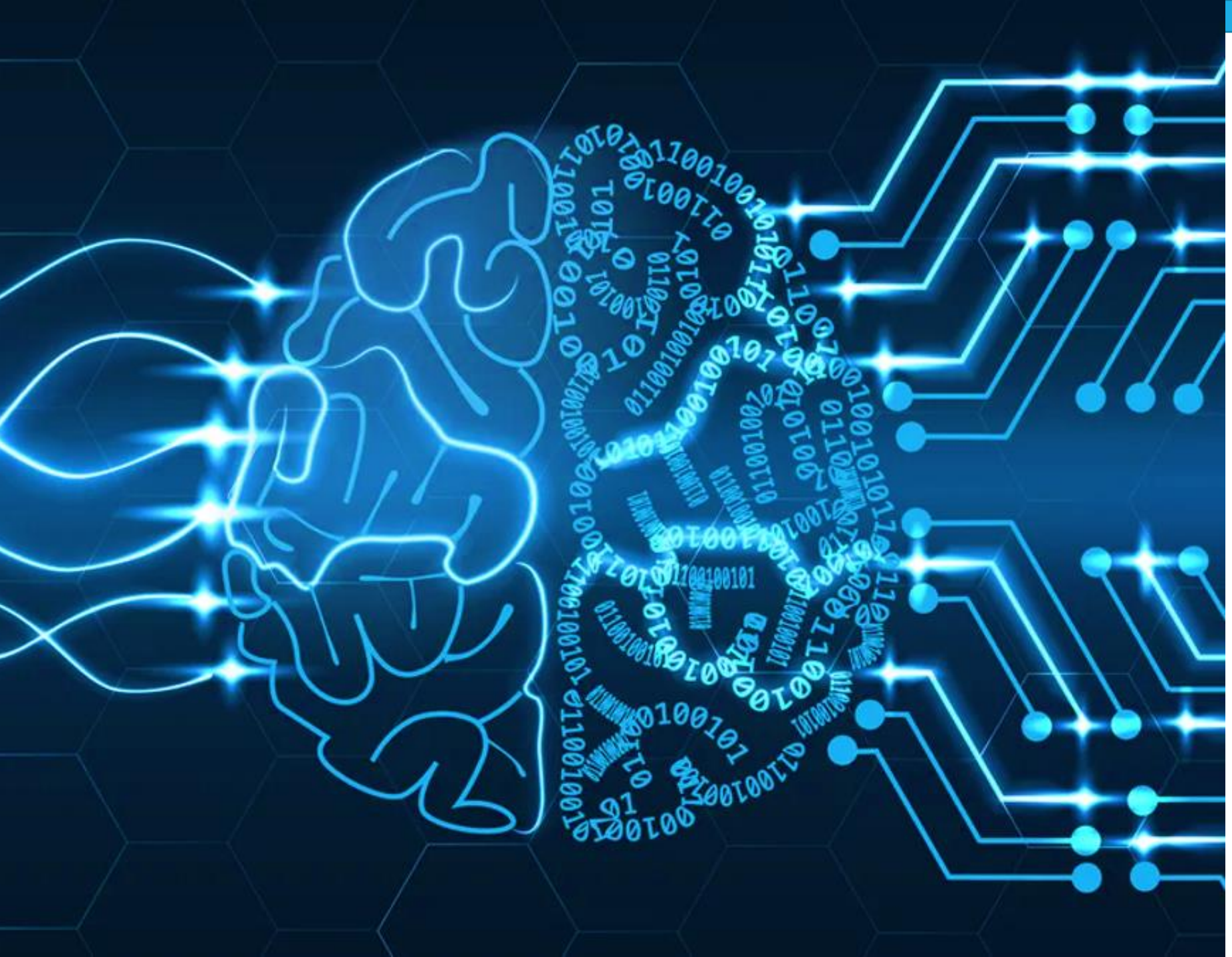

کاهش ابعاد

اردیبهشت ۱۴۰۲

دانشکده مهندسی صنایع

دانشگاه صنعتی شریف

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بسم الله الرحمن الرحیم

Dimensionality Reduction

Many Machine Learning problems involve thousands or even millions of features for each training instance. Not only do all these features make training extremely slow, but they can also make it much harder to find a good solution, as we will see. This problem is often referred to as the curse of dimensionality.

Fortunately, in real-world problems, it is often possible to reduce the number of features considerably, turning an intractable problem into a tractable one. For example, consider the MNIST images (introduced in Chapter 3): the pixels on the image borders are almost always white, so you could completely drop these pixels from the training set without losing much information. Figure 7-6 confirms that these pixels are utterly unimportant for the classification task. Additionally, two neighboring pixels are often highly correlated: if you merge them into a single pixel (e.g., by taking the mean of the two pixel intensities), you will not lose much information.

Warning

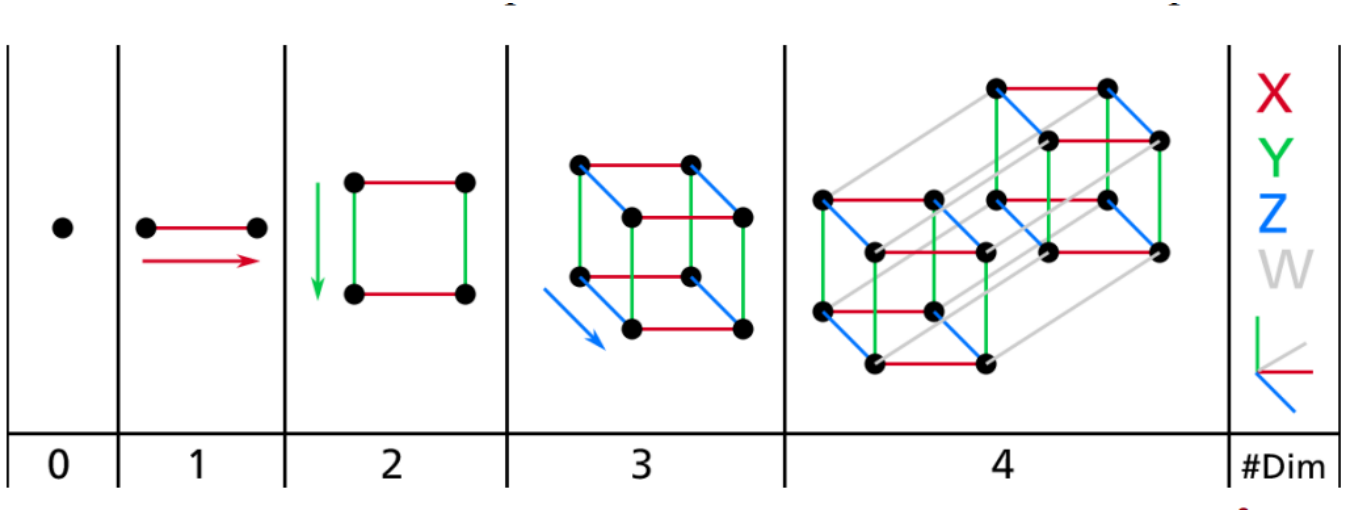
Reducing dimensionality does cause some information loss (just like compressing an image to JPEG can degrade its quality), so even though it will speed up training, it may make your system perform slightly worse. It also makes your pipelines a bit more complex and thus harder to maintain. So, if training is too slow, you should first try to train your system with the original data before considering using dimensionality reduction. In some cases, reducing the dimensionality of the training data may filter out some noise and unnecessary details and thus result in higher performance, but in general it won’t; it will just speed up training.

Dimensionality Reduction

Apart from speeding up training, dimensionality reduction is also extremely useful for data visualization (or $DataViz$). Reducing the number of dimensions down to two (or three) makes it possible to plot a condensed view of a high-dimensional training set on a graph and often gain some important insights by visually detecting patterns, such as clusters. Moreover, $DataViz$ is essential to communicate your conclusions to people who are not data scientists—in particular, decision makers who will use your results.

The Curse of Dimensionality

We are so used to living in three dimensions that our intuition fails us when we try to imagine a high-dimensional space. Even a basic 4D hypercube is incredibly hard to picture in our minds (see Figure bellow), let alone a 200-dimensional ellipsoid bent in a 1,000-dimensional space.

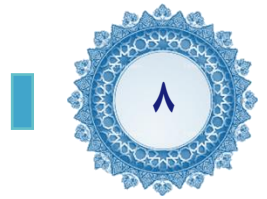


The Curse of Dimensionality

It turns out that many things behave very differently in high-dimensional space. For example, if you pick a random point in a unit square (a 1 × 1 square), it will have only about a 0.4% chance of being located less than 0.001 from a border (in other words, it is very unlikely that a random point will be “extreme” along any dimension). But in a 10,000-dimensional unit hypercube, this probability is greater than 99.999999%. Most points in a high-dimensional hypercube are very close to the border.

The Curse of Dimensionality

Here is a more troublesome difference: if you pick two points randomly in a unit square, the distance between these two points will be, on average, roughly 0.52. If you pick two random points in a unit 3D cube, the average distance will be roughly 0.66. But what about two points picked randomly in a $1{,}000{,}000$-dimensional hypercube? The average distance, believe it or not, will be about 408.25 (roughly $\sqrt{1{,}000{,}000/6}$)! This is counterintuitive: how can two points be so far apart when they both lie within the same unit hypercube? Well, there's just plenty of space in high dimensions. As a result, high-dimensional datasets are at risk of being very sparse: most training instances are likely to be far away from each other. This also means that a new instance will likely be far away from any training instance, making predictions much less reliable than in lower dimensions, since they will be based on much larger extrapolations. In short, the more dimensions the training set has, the greater the risk of overfitting it.



The Curse of Dimensionality

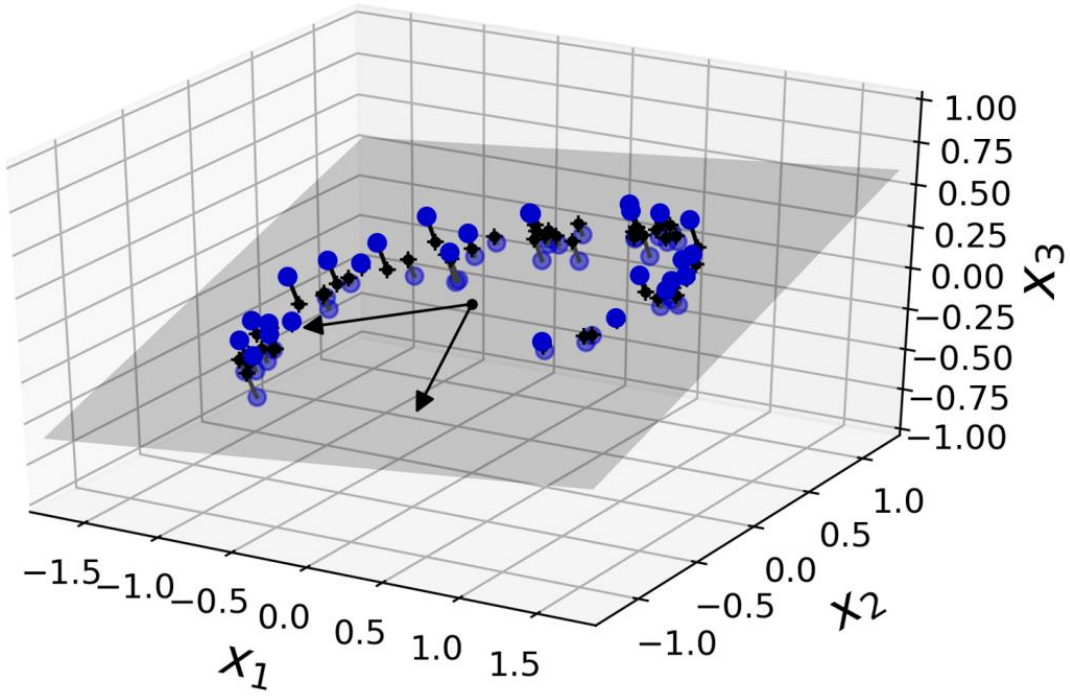
In theory, one solution to the curse of dimensionality could be to increase the size of the training set to reach a sufficient density of training instances. Unfortunately, in practice, the number of training instances required to reach a given density grows exponentially with the number of dimensions. With just 100 features (significantly fewer than in the MNIST problem), you would need more training instances than atoms in the observable universe in order for training instances to be within 0.1 of each other on average, assuming they were spread out uniformly across all dimensions.

Main Approaches for Dimensionality Reduction

Before we dive into specific dimensionality reduction algorithms, let's take a look at the two main approaches to reducing dimensionality:

- Projection
- Manifold Learning

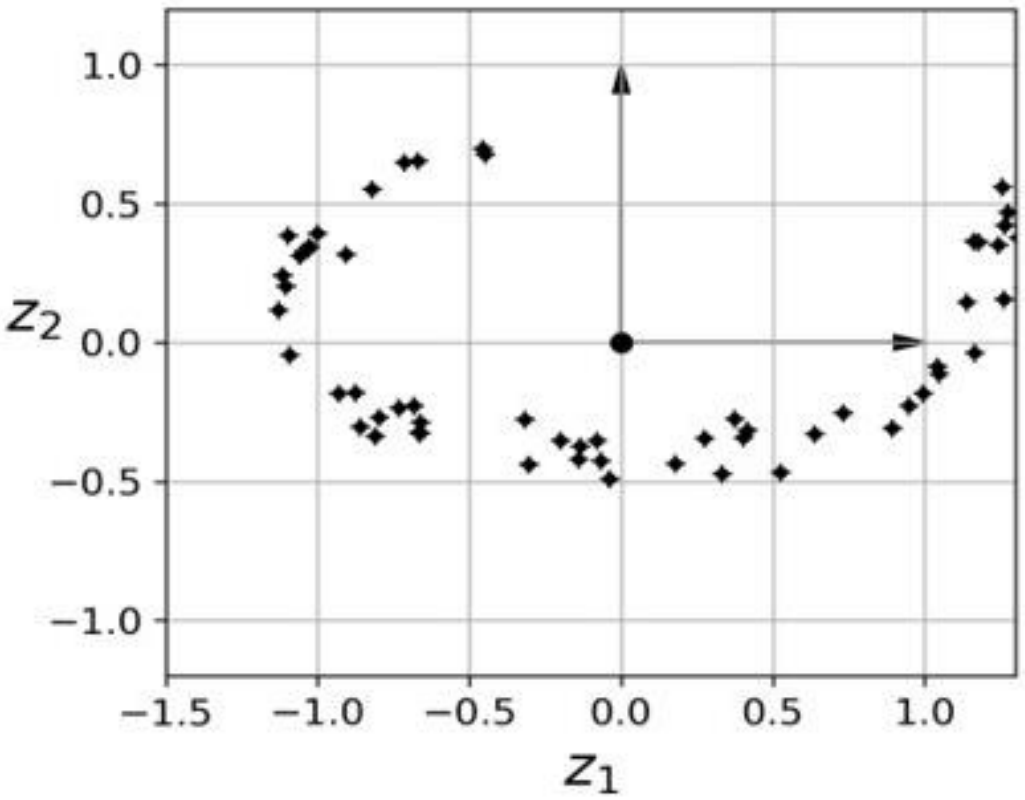
Projection



In most real-world problems, training instances are not spread out uniformly across all dimensions. Many features are almost constant, while others are highly correlated (as discussed earlier for MNIST). As a result, all training instances lie within (or close to) a much lower-dimensional subspace of the high-dimensional space. This sounds very abstract, so let's look at an example. In the figure below, you can see a 3D dataset represented by circles.

Projection

Notice that all training instances lie close to a plane: this is a lower-dimensional (2D) subspace of the high-dimensional (3D) space. If we project every training instance perpendicularly onto this subspace (as represented by the short lines connecting the instances to the plane), we get the new 2D dataset shown in Figure 8-3. Ta-da! We have just reduced the dataset's dimensionality from 3D to 2D. Note that the axes correspond to new features z and z (the coordinates of the projections on the plane).



Projection Challenges

Projection is not always the best approach to dimensionality reduction. In many cases the subspace may twist and turn, such as in the famous Swiss roll toy dataset represented in Figure 8-4.

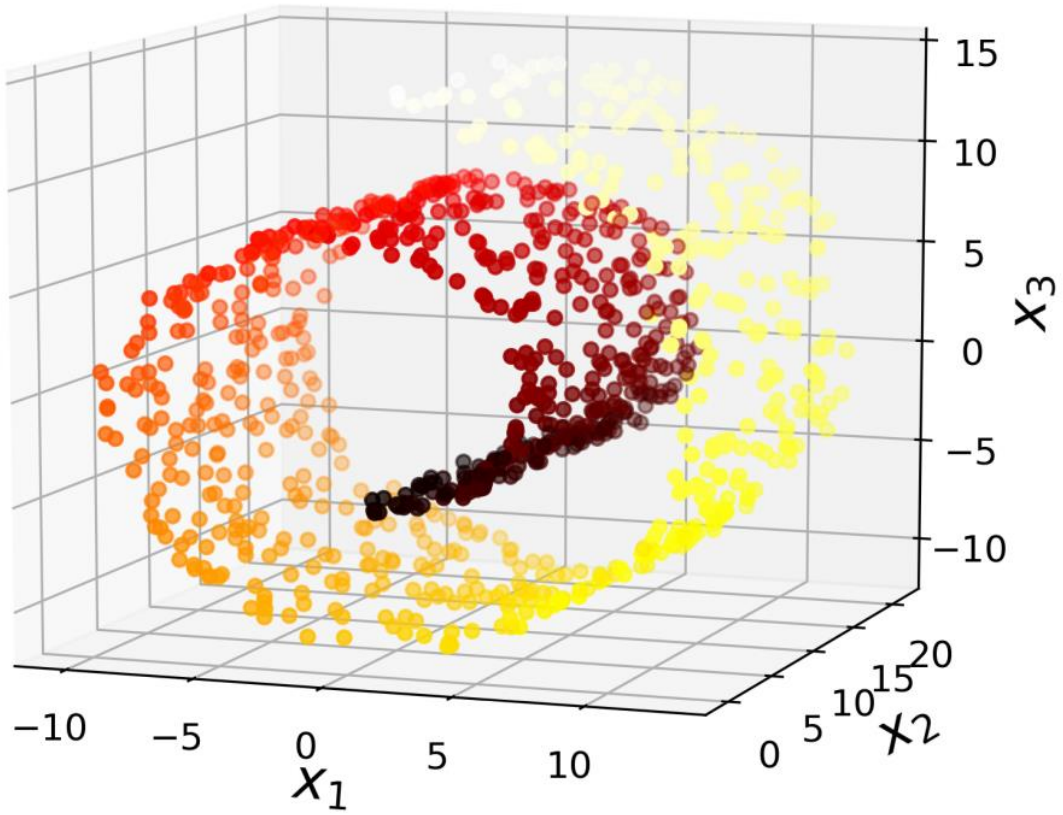


Figure 8-4. Swiss roll dataset

Problems with projection

Simply projecting onto a plane (e.g., by dropping x) would squash different layers of the Swiss roll together, as shown on the left side of Figure 8-5. What you really want is to unroll the Swiss roll to obtain the 2D dataset on the right side of Figure 8-5.

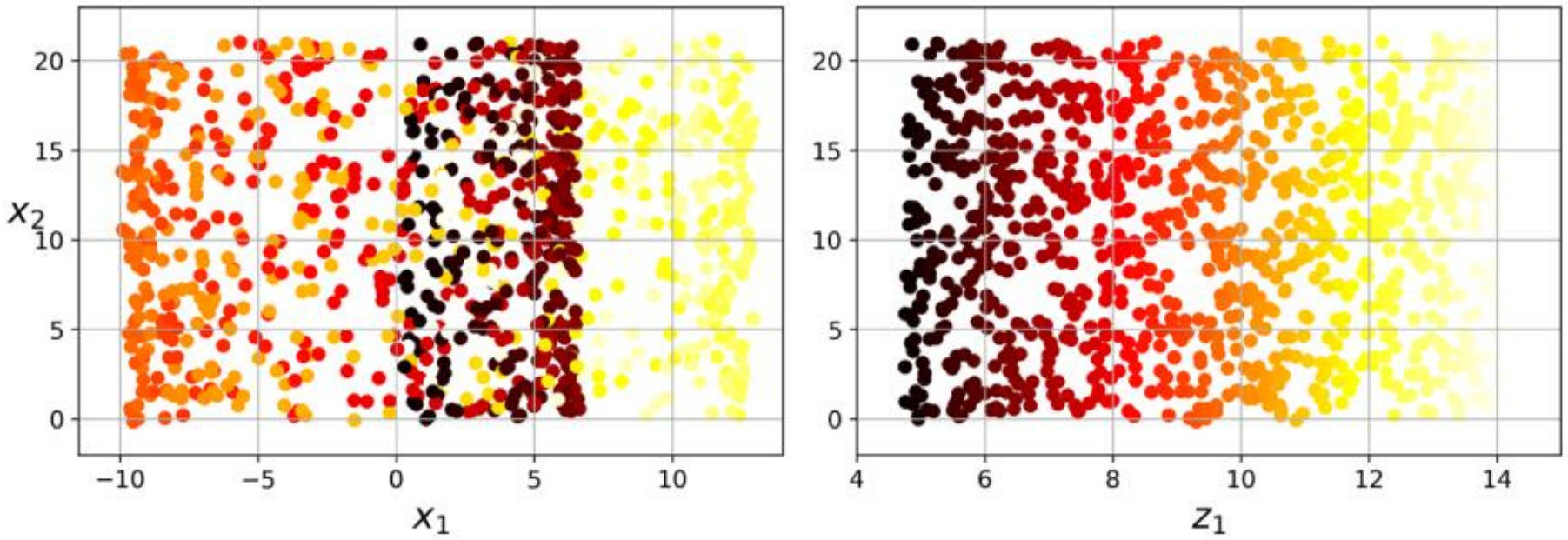


Figure 8-5. Squashing by projecting onto a plane (left) versus unrolling the Swiss roll (right)

Manifold Learning

The Swiss roll is an example of a 2D manifold. Put simply, a 2D manifold is a 2D shape that can be bent and twisted in a higher-dimensional space. More generally, a d-dimensional manifold is a part of an n-dimensional space (where d < n) that locally resembles a d-dimensional hyperplane. In the case of the Swiss roll, d = 2 and n = 3: it locally resembles a 2D plane, but it is rolled in the third dimension. Many dimensionality reduction algorithms work by modeling the manifold on which the training instances lie; this is called Manifold Learning. It relies on the manifold assumption, also called the manifold hypothesis, which holds that most real-world high-dimensional datasets lie close to a much lower-dimensional manifold. This assumption is very often empirically observed.

Manifold Learning

Once again, think about the MNIST dataset: all handwritten digit images have some similarities. They are made of connected lines, the borders are white, and they are more or less centered. If you randomly generated images, only a ridiculously tiny fraction of them would look like handwritten digits. In other words, the degrees of freedom available to you if you try to create a digit image are dramatically lower than the degrees of freedom you would have if you were allowed to generate any image you wanted. These constraints tend to squeeze the dataset into a lower-dimensional manifold.

Manifold Learning

The manifold assumption is often accompanied by another implicit assumption: that the task at hand (e.g., classification or regression) will be simpler if expressed in the lower-dimensional space of the manifold. For example, in the top row of Figure 8-6 the Swiss roll is split into two classes: in the 3D space (on the left), the decision boundary would be fairly complex, but in the 2D unrolled manifold space (on the right), the decision boundary is a straight line.

Manifold learning

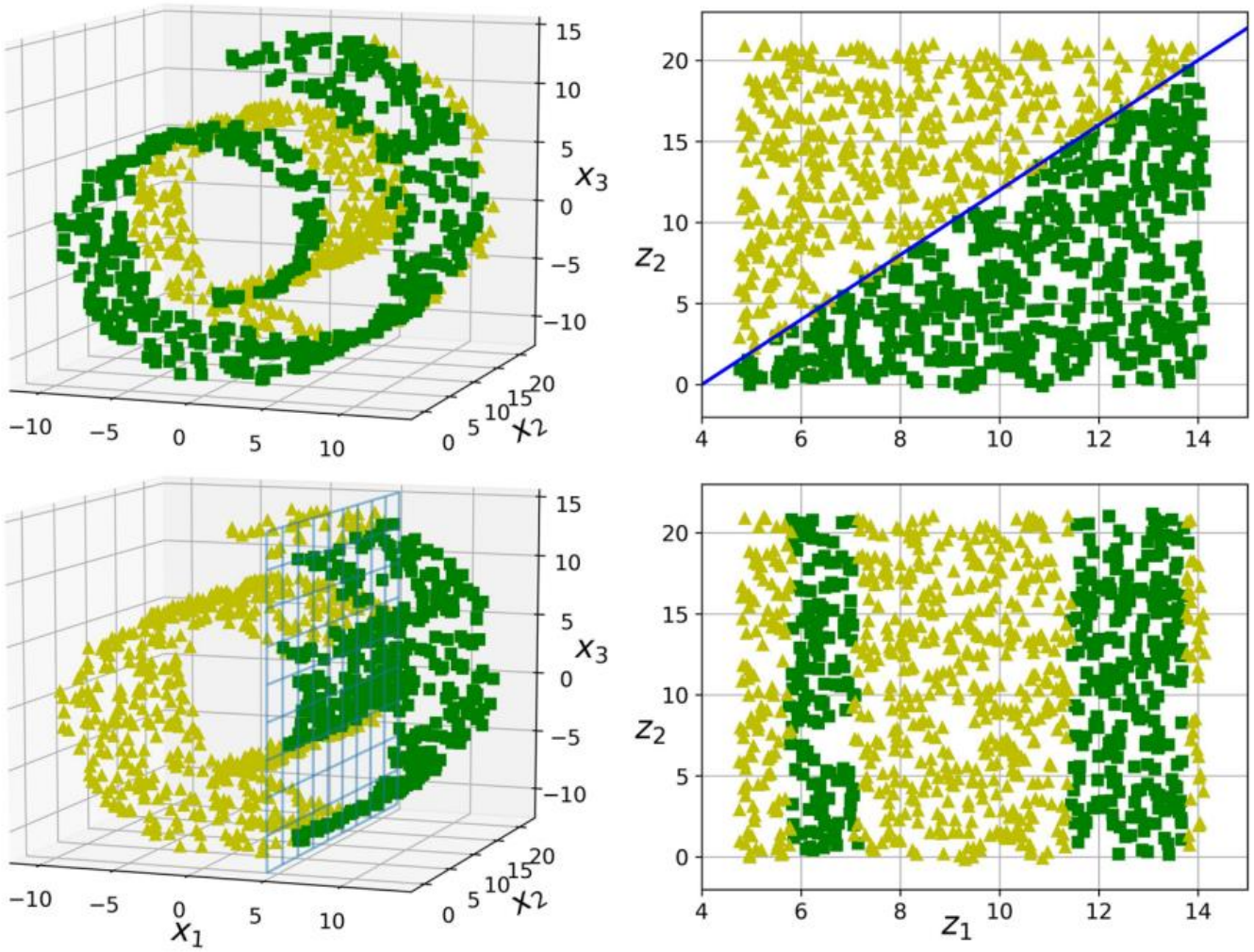


Figure 8-6. The decision boundary may not always be simpler with lower dimensions

However, this implicit assumption does not always hold. For example, in the bottom row of Figure 8-6, the decision boundary is located at $x = 5$. This decision boundary looks very simple in the original 3D space (a vertical plane), but it looks more complex in the unrolled manifold (a collection of four independent line segments)

Manifold Learning

In short, reducing the dimensionality of your training set before training a model will usually speed up training, but it may not always lead to a better or simpler solution; it all depends on the dataset. Hopefully you now have a good sense of what the curse of dimensionality is and how dimensionality reduction algorithms can fight it, especially when the manifold assumption holds. The rest of this chapter will go through some of the most popular algorithms.

PCA

Principal Component Analysis (PCA) is by far the most popular dimensionality reduction algorithm. First it identifies the hyperplane that lies closest to the data, and then it projects the data onto it, just like in Figure 8-2.

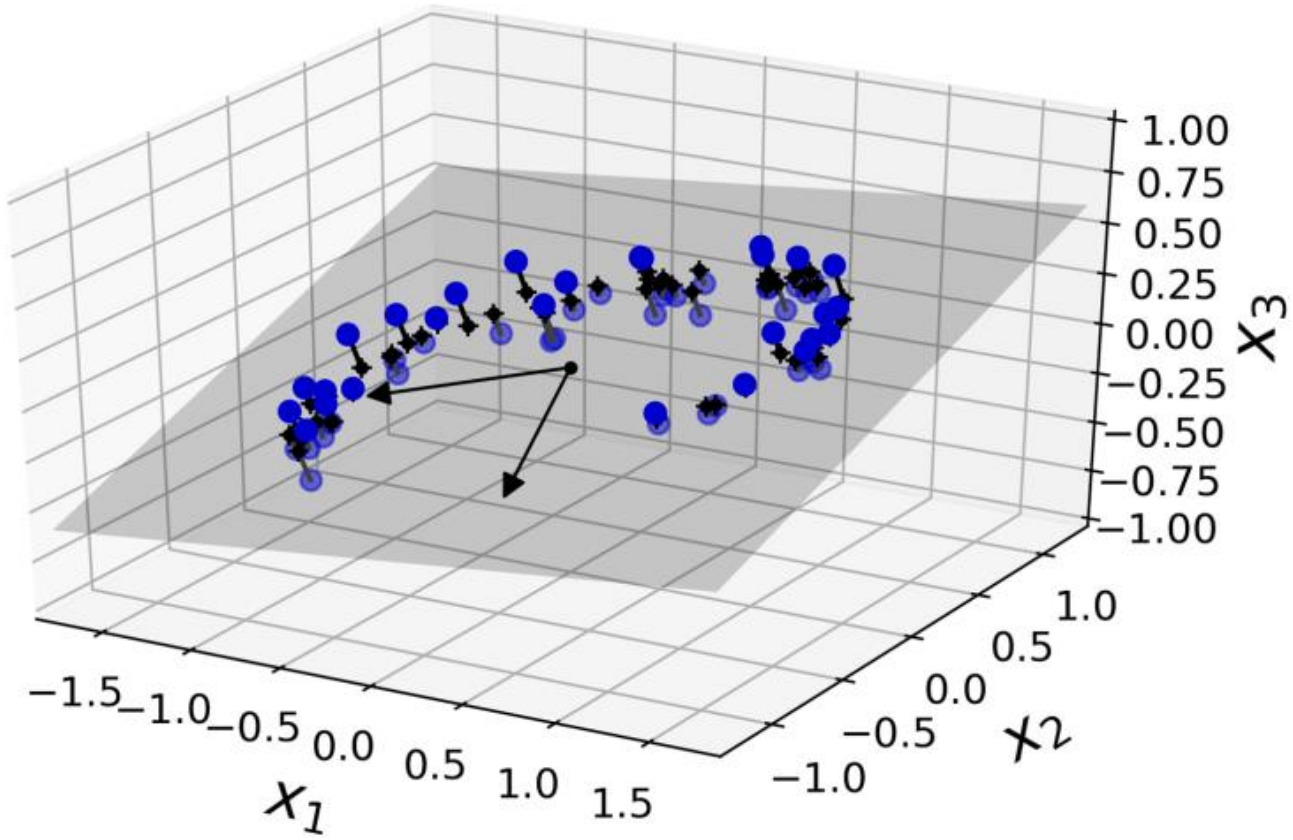


Figure 8-2. A 3D dataset lying close to a 2D subspace

Preserving the Variance

Before you can project the training set onto a lower-dimensional hyperplane, you first need to choose the right hyperplane. For example, a simple 2D dataset is represented on the left in Figure 8-7, along with three different axes (i.e., 1D hyperplanes). On the right is the result of the projection of the dataset onto each of these axes. As you can see, the projection onto the solid line preserves the maximum variance, while the projection onto the dotted line preserves very little variance and the projection onto the dashed line preserves an intermediate amount of variance.

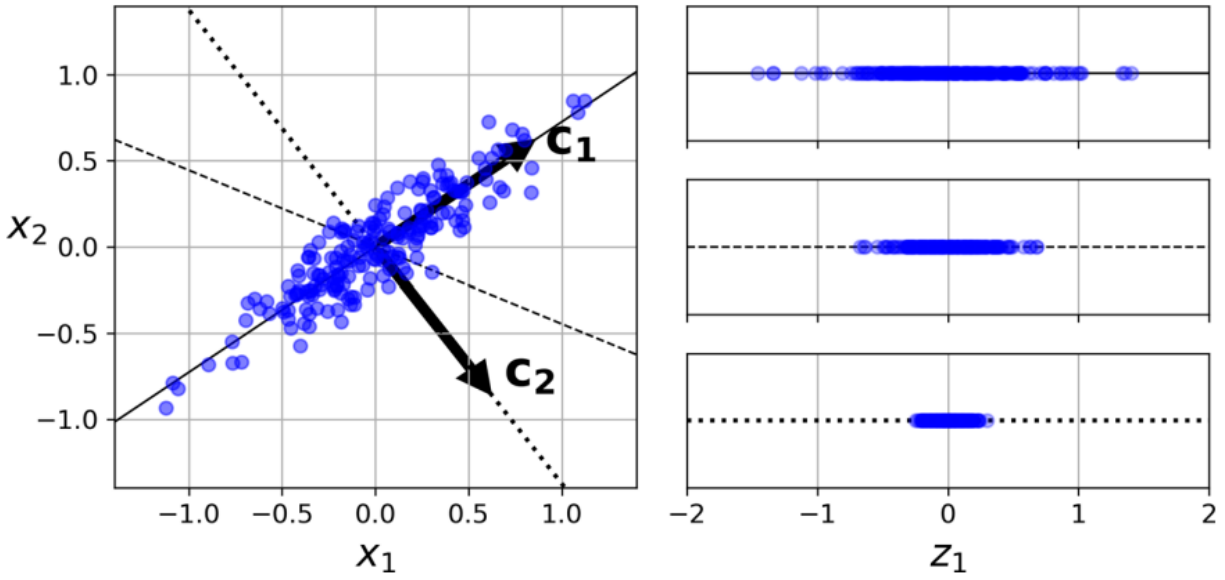


Figure 8-7. Selecting the subspace to project on

Preserving the Variance

It seems reasonable to select the axis that preserves the maximum amount of variance, as it will most likely lose less information than the other projections. Another way to justify this choice is that it is the axis that minimizes the mean squared distance between the original dataset and its projection onto that axis. This is the rather simple idea behind PCA.

Principal Components

PCA identifies the axis that accounts for the largest amount of variance in the training set. In Figure 8-7, it is the solid line. It also finds a second axis, orthogonal to the first one, that accounts for the largest amount of remaining variance. In this 2D example there is no choice: it is the dotted line. If it were a higher-dimensional dataset, PCA would also find a third axis, orthogonal to both previous axes, and a fourth, a fifth, and so on—as many axes as the number of dimensions in the dataset.

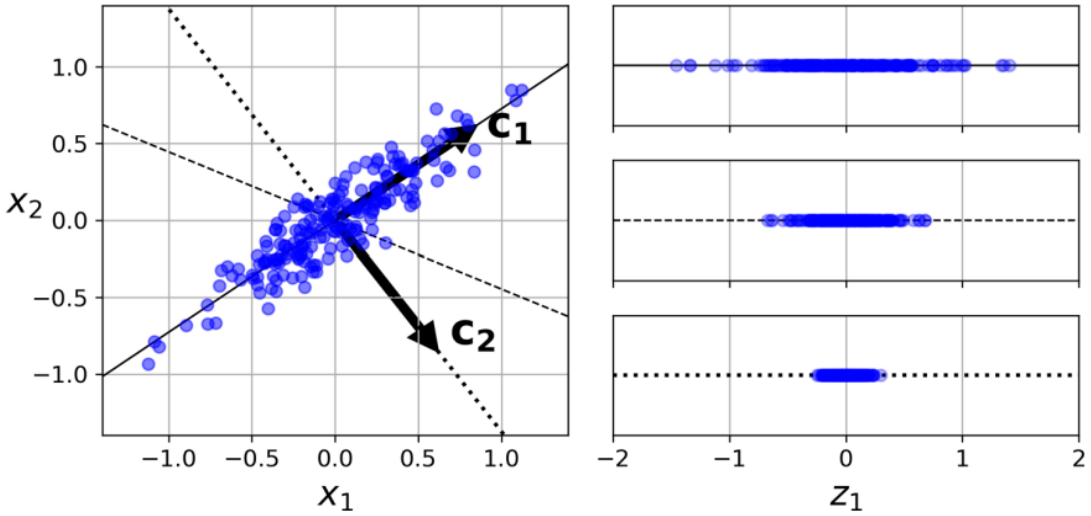


Figure 8-7. Selecting the subspace to project on

Principal Components

The i^{th} axis is called the i^{th} principal component (PC) of the data. In Figure 8-7, the first PC is the axis on which vector c_1 lies, and the second PC is the axis on which vector c_2 lies. In Figure 8-2 the first two PCs are the orthogonal axes on which the two arrows lie, on the plane, and the third PC is the axis orthogonal to that plane.

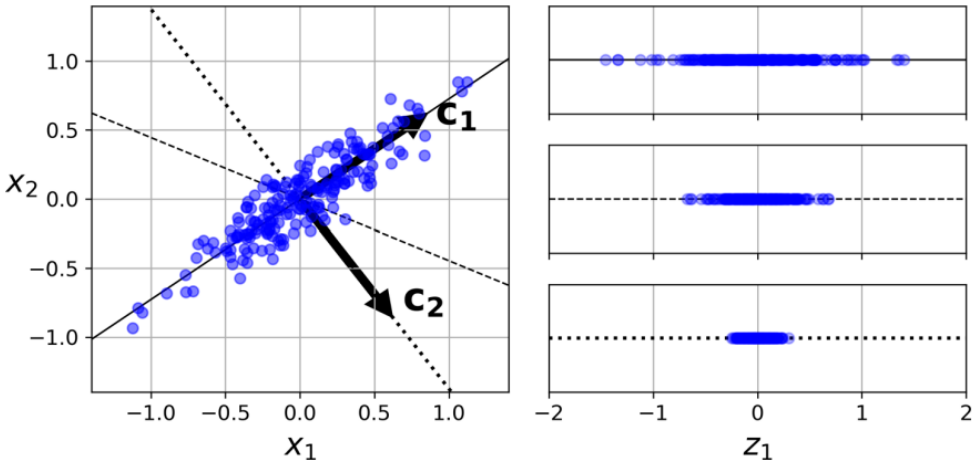


Figure 8-7. Selecting the subspace to project on

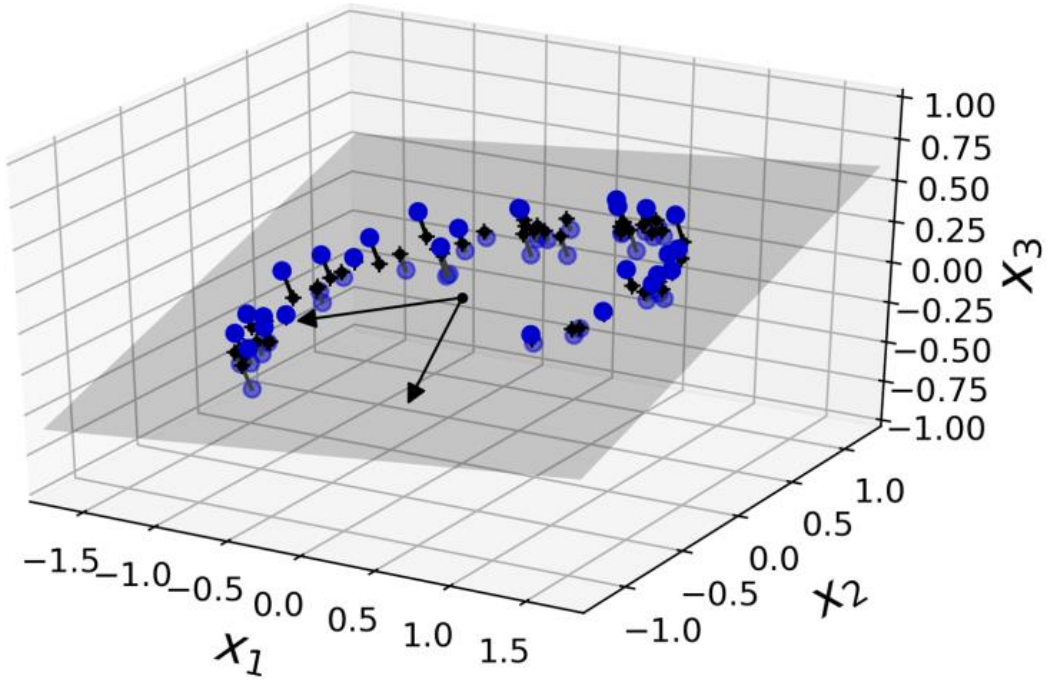


Figure 8-2. A 3D dataset lying close to a 2D subspace

Principal Components

For each principal component, PCA finds a zero-centered unit vector pointing in the direction of the PC. Since two opposing unit vectors lie on the same axis, the direction of the unit vectors returned by PCA is not stable: if you perturb the training set slightly and run PCA again, the unit vectors may point in the opposite direction as the original vectors. However, they will generally still lie on the same axes. In some cases, a pair of unit vectors may even rotate or swap (if the variances along these two axes are close), but the plane they define will generally remain the same.

How to Find Principal Component?

There is a standard matrix factorization technique called Singular Value Decomposition (SVD) that can decompose the training set matrix X into the matrix multiplication of three matrices U Σ V , where V contains the unit vectors that define all the principal components that we are looking for, as shown in Equation 8-1.

Equation 8-1. Principal components matrix

$$\mathbf{V} = \begin{pmatrix} | & | & & | \\ \mathbf{c}_1 & \mathbf{c}_2 & \cdots & \mathbf{c}_n \\ | & | & & | \end{pmatrix}$$

Python code for SVD

The following Python code uses NumPy's **svd()** function to obtain all the principal components of the training set, then extracts the two unit vectors that define the first two PCs:

```
X_centered = X - X.mean(axis=0)
U, s, Vt = np.linalg.svd(X_centered)
c1 = Vt.T[:, 0]
c2 = Vt.T[:, 1]
```

PCA assumes that the dataset is centered around the origin. As we will see, ScikitLearn's PCA classes take care of centering the data for you. If you implement PCA yourself (as in the preceding example), or if you use other libraries, don't forget to center the data first.

Projecting Down to d Dimensions

Once you have identified all the principal components, you can reduce the dimensionality of the dataset down to *d* dimensions by projecting it onto the hyperplane defined by the first *d* principal components. Selecting this hyperplane ensures that the projection will preserve as much variance as possible. For example, in Figure 8-2 the 3D dataset is projected down to the 2D plane defined by the first two principal components, preserving a large part of the dataset's variance. As a result, the 2D projection looks very much like the original 3D dataset.

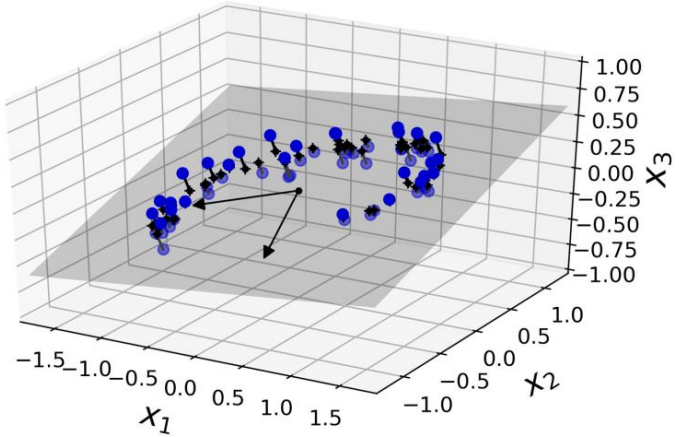


Figure 8-2. A 3D dataset lying close to a 2D subspace

Projecting Down to d Dimensions

To project the training set onto the hyperplane and obtain a reduced dataset X of dimensionality d, compute the matrix multiplication of the training set matrix X by the matrix W , defined as the matrix containing the first d columns of V, as shown in Equation 8-2.

Equation 8-2. Projecting the training set down to d dimensions

$$\mathbf{X}_{d\text{-proj}} = \mathbf{X}\mathbf{W}_d$$

The following Python code projects the training set onto the plane defined by the first two principal components:

```
W2 = Vt.T[:, :2]
X2D = X_centered.dot(W2)
```

PCA Using Scikit-Learn

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

```
from sklearn.decomposition import PCA

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

After fitting the PCA transformer to the dataset, its components_ attribute holds the transpose of W (e.g., the unit vector that defines the first principal component is equal to **pca.components_.T[:, 0]**).

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 ratio indicates 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 two components of the 3D dataset represented in Figure 8-2:

```
>>> pca.explained_variance_ratio_
array([0.84248607, 0.14631839])
```

This output tells you that 84.2% of the dataset's variance lies along the first PC, and 14.6% lies along the second PC. This leaves less than 1.2% for the third PC, so it is reasonable to assume that the third PC probably carries little information.

Choosing the Right Number of Dimensions

Instead of arbitrarily choosing the number of dimensions to reduce down to, it is simpler to choose the number of dimensions that add up to a sufficiently large portion of the variance (e.g., 95%). Unless, of course, you are reducing dimensionality for data visualization—in that case you will want to reduce the dimensionality down to 2 or 3.

The following code performs PCA without reducing dimensionality, then computes the minimum number of dimensions required to preserve 95% of the training set's variance:

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

Choosing the Right Number of Dimensions

You could then set **n_components=d** and run PCA again. But there is a much 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:

```
pca = PCA(n_components=0.95)
X_reduced = pca.fit_transform(X_train)
```

Choosing the Right Number of Dimensions

Yet another option is to plot the explained variance as a function of the number of dimensions (simply plot **cumsum**; see Figure 8-8). 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.

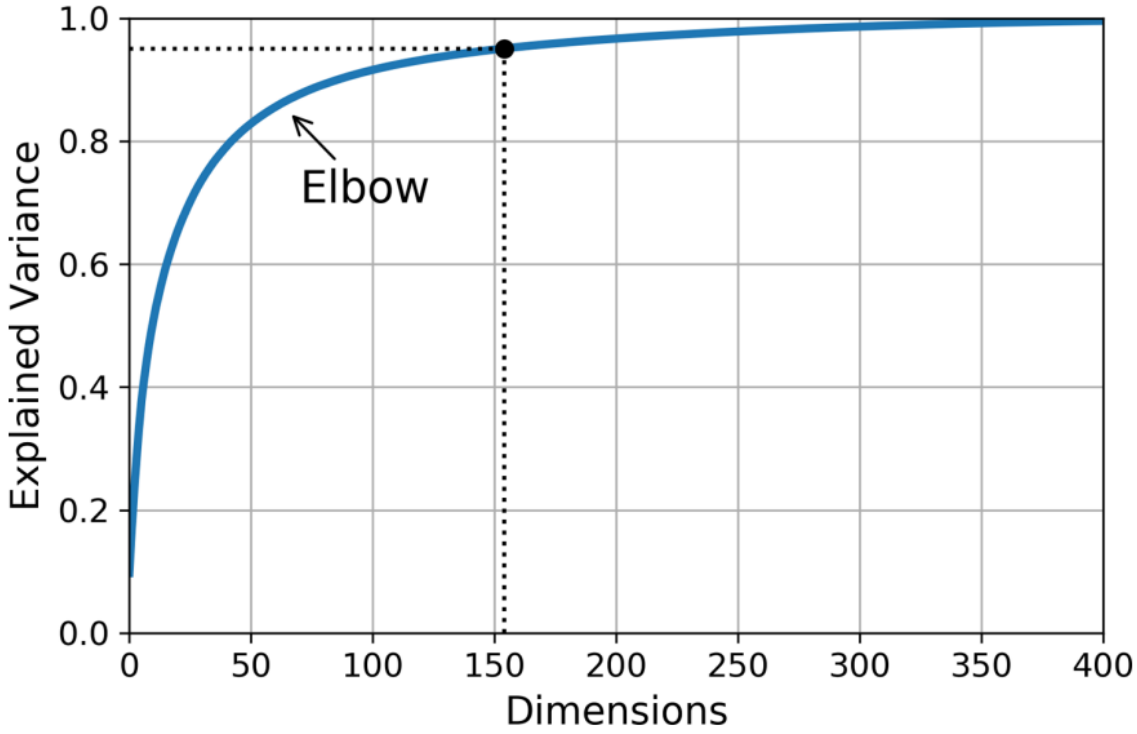


Figure 8-8. Explained variance as a function of the number of dimensions

PCA for Compression

After dimensionality reduction, the training set takes up much less space. As an example, try applying PCA to the MNIST dataset while preserving 95% of its variance. You should find that each instance will have just over 150 features, instead of the original 784 features. So, while most of the variance is preserved, the dataset is now less than 20% of its original size! This is a reasonable compression ratio, and you can see how this size reduction can speed up a classification algorithm (such as an SVM classifier) tremendously.

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.

Decompressing

The following code compresses the MNIST dataset down to 154 dimensions, then uses the **inverse_transform()** method to decompress it back to 784 dimensions:

```
pca = PCA(n_components = 154)
X_reduced = pca.fit_transform(X_train)
X_recovered = pca.inverse_transform(X_reduced)
```

The equation of the inverse transformation is shown in Equation 8-3.

Equation 8-3. PCA inverse transformation, back to the original number of dimensions

$$\mathbf{X}_{\text{recovered}} = \mathbf{X}_{d\text{-proj}}\mathbf{W}_d^{\mathsf{T}}$$

Decompressing

Figure 8-9 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.

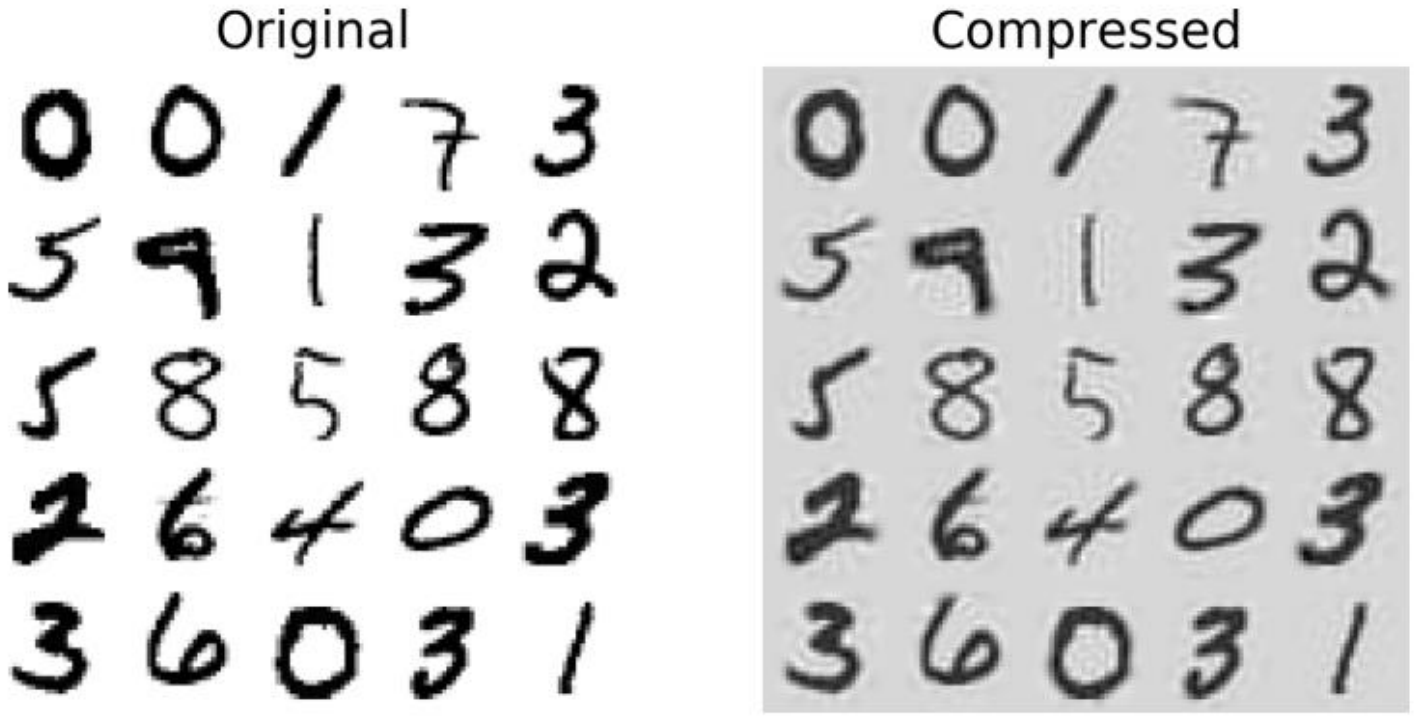


Figure 8-9. MNIST compression that preserves 95% of the variance

Randomized PCA

If you set the svd_solver hyperparameter to "randomized", Scikit-Learn uses a stochastic algorithm called Randomized PCA that quickly finds an approximation of the first d principal components. Its computational complexity is $O(m \times d^2) + O(d^3)$, instead of $O(m \times n^2) + O(n^3)$ for the full SVD approach, so it is dramatically faster than full SVD when d is much smaller than n:

```
rnd_pca = PCA(n_components=154, svd_solver="randomized")
X_reduced = rnd_pca.fit_transform(X_train)
```

By default, svd_solver is actually set to "auto": Scikit-Learn automatically uses the randomized PCA algorithm if m or n is greater than 500 and d is less than 80% of m or n, or else it uses the full SVD approach. If you want to force Scikit-Learn to use full SVD, you can set the **svd_solver** hyperparameter to "full".

Incremental PCA

One problem with the preceding implementations of PCA is that they require the whole training set to fit in memory in order for the algorithm to run. Fortunately, Incremental PCA (IPCA) algorithms have been developed. They allow you to split the training set into mini-batches and feed an IPCA algorithm one mini-batch at a time. This is useful for large training sets and for applying PCA online (i.e., on the fly, as new instances arrive).

Incremental PCA

The following code splits the MNIST dataset into 100 mini-batches (using NumPy's **array_split()** function) and feeds them to Scikit-Learn's IncrementalPCA class to reduce the dimensionality of the MNIST dataset down to 154 dimensions (just like before). Note that you must call the **partial_fit()** method with each mini-batch, rather than the **fit()** method with the whole training set:

```
from sklearn.decomposition import IncrementalPCA

n_batches = 100
inc_pca = IncrementalPCA(n_components=154)
for X_batch in np.array_split(X_train, n_batches):
    inc_pca.partial_fit(X_batch)

X_reduced = inc_pca.transform(X_train)
```

Incremental PCA

Alternatively, you can use NumPy's **memmap** class, which allows you to manipulate a large array stored in a binary file on disk as if it were entirely in memory; the class loads only the data it needs in memory, when it needs it. Since the **IncrementalPCA** class uses only a small part of the array at any given time, the memory usage remains under control. This makes it possible to call the usual **fit()** method, as you can see in the following code:

```
X_mm = np.memmap(filename, dtype="float32", mode="readonly", shape=(m,
n))

batch_size = m // n_batches
inc_pca = IncrementalPCA(n_components=154, batch_size=batch_size)
inc_pca.fit(X_mm)
```

Kernel PCA

In Chapter 5 we discussed the kernel trick, a mathematical technique that implicitly maps instances into a very high-dimensional space (called the feature space), enabling nonlinear classification and regression with Support Vector Machines. Recall that a linear decision boundary in the high-dimensional feature space corresponds to a complex nonlinear decision boundary in the original space.

It turns out that the same trick can be applied to PCA, making it possible to perform complex nonlinear projections for dimensionality reduction. This is called Kernel PCA (kPCA). It is often good at preserving clusters of instances after projection, or sometimes even unrolling datasets that lie close to a twisted manifold.

Kernel PCA

The following code uses Scikit-Learn's **KernelPCA** class to perform **kPCA** with an RBF kernel (see Chapter 5 for more details about the RBF kernel and other kernels):

```
from sklearn.decomposition import KernelPCA

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

Figure 8-10 shows the Swiss roll, reduced to two dimensions using a linear kernel (equivalent to simply using the PCA class), an RBF kernel, and a sigmoid kernel.

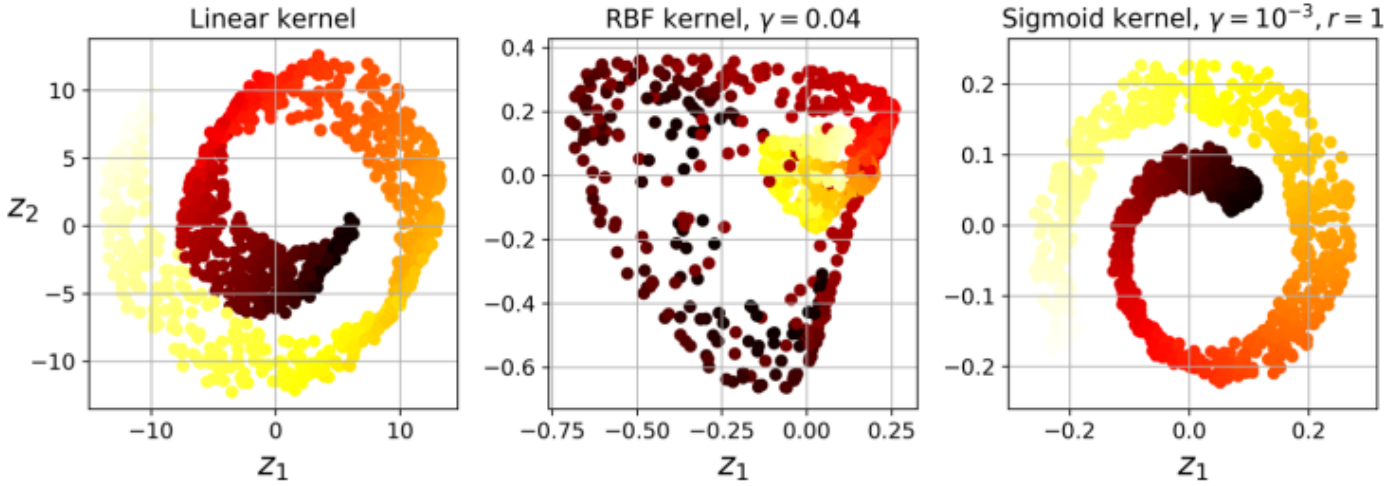


Figure 8-10. Swiss roll reduced to 2D using kPCA with various kernels

Selecting a Kernel and Tuning Hyperparameters

As kPCA is an unsupervised learning algorithm, there is no obvious performance measure to help you select the best kernel and hyperparameter values. That said, dimensionality reduction is often a preparation step for a supervised learning task (e.g., classification), so you can use grid search to select the kernel and hyperparameters that lead to the best performance on that task. The following code creates a two-step pipeline, first reducing dimensionality to two dimensions using kPCA, then applying Logistic Regression for classification. Then it uses **GridSearchCV** to find the best kernel and gamma value for kPCA in order to get the best classification accuracy at the end of the pipeline:

Selecting a Kernel and Tuning Hyperparameters

```
from sklearn.model_selection import GridSearchCV
from sklearn.linear_model import LogisticRegression
from sklearn.pipeline import Pipeline

clf = Pipeline([
        ("kpca", KernelPCA(n_components=2)),
        ("log_reg", LogisticRegression())
    ])

param_grid = [{
        "kpca__gamma": np.linspace(0.03, 0.05, 10),
        "kpca__kernel": ["rbf", "sigmoid"]
    }]

grid_search = GridSearchCV(clf, param_grid, cv=3)
grid_search.fit(X, y)
```

The best kernel and hyperparameters are then available through the best_params_ variable:

```
>>> print(grid_search.best_params_)
{'kpca__gamma': 0.043333333333333335, 'kpca__kernel': 'rbf'}
```

Selecting a Kernel and Tuning Hyperparameters

Another approach, this time entirely unsupervised, is to select the kernel and hyperparameters that yield the lowest reconstruction error. Note that reconstruction is not as easy as with linear PCA. Here's why. Figure 8-11 shows the original Swiss roll 3D dataset (top left) and the resulting 2D dataset after kPCA is applied using an RBF kernel (top right). Thanks to the kernel trick, this transformation is mathematically equivalent to using the feature map ϕ to map the training set to an infinite-dimensional feature space (bottom right), then projecting the transformed training set down to 2D using linear PCA.

Selecting a Kernel and Tuning Hyperparameters

Notice that if we could invert the linear PCA step for a given instance in the reduced space, the reconstructed point would lie in feature space, not in the original space (e.g., like the one represented by an X in the diagram). Since the feature space is infinite-dimensional, we cannot compute the reconstructed point, and therefore we cannot compute the true reconstruction error. Fortunately, it is possible to find a point in the original space that would map close to the reconstructed point. This point is called the reconstruction pre-image. Once you have this pre-image, you can measure its squared distance to the original instance. You can then select the kernel and hyperparameters that minimize this reconstruction pre-image error.

Selecting a Kernel and Tuning Hyperparameters

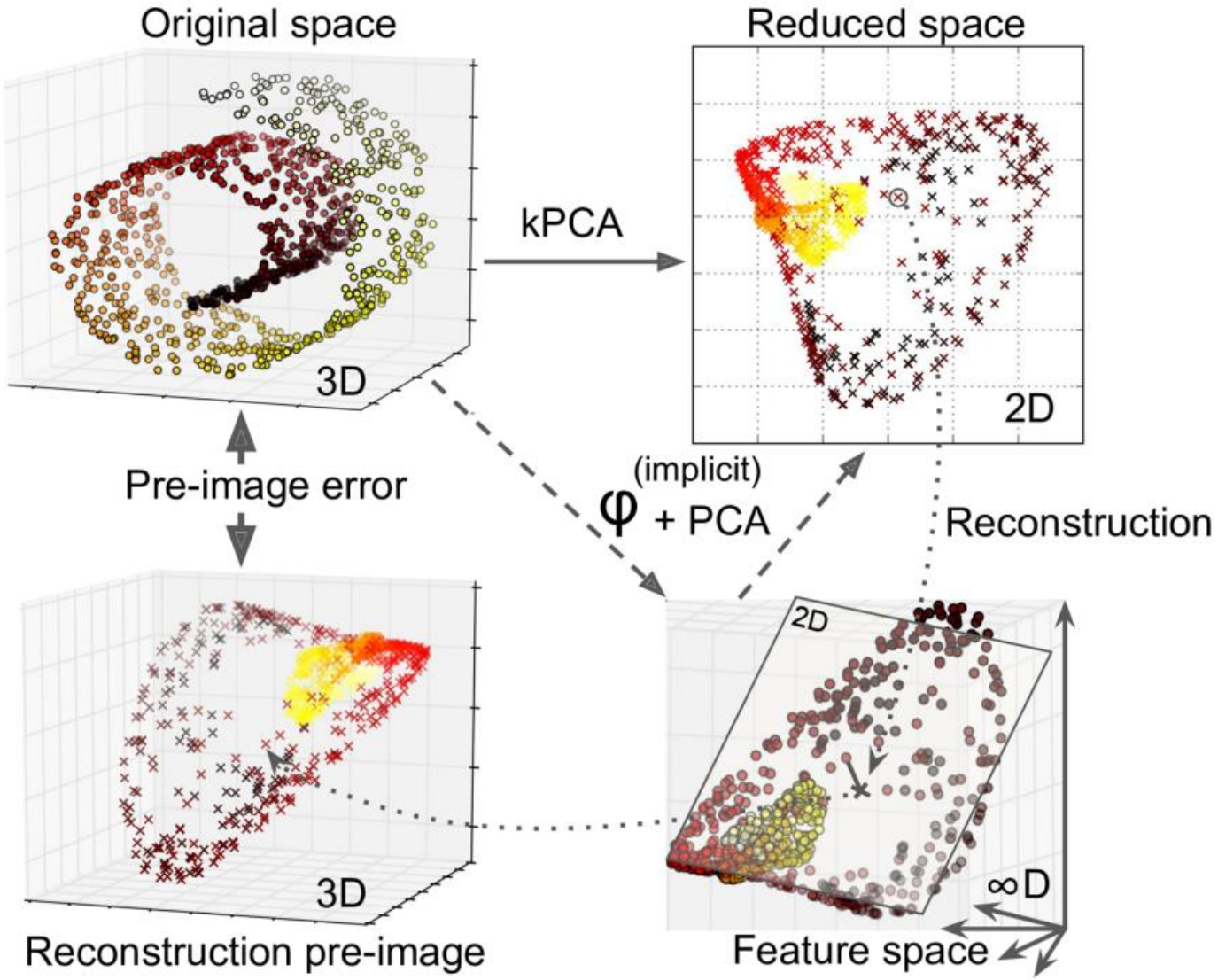


Figure 8-11. Kernel PCA and the reconstruction pre-image error

Selecting a Kernel and Tuning Hyperparameters

You may be wondering how to perform this reconstruction. One solution is to train a supervised regression model, with the projected instances as the training set and the original instances as the targets. Scikit-Learn will do this automatically if you set **fit_inverse_transform=True**, as shown in the following code:

```
rbf_pca = KernelPCA(n_components = 2, kernel="rbf", gamma=0.0433,
                    fit_inverse_transform=True)
X_reduced = rbf_pca.fit_transform(X)
X_preimage = rbf_pca.inverse_transform(X_reduced)
```

You can then compute the reconstruction pre-image error:

```
>>> from sklearn.metrics import mean_squared_error
>>> mean_squared_error(X, X_preimage)
32.786308795766132
```

Now you can use grid search with cross-validation to find the kernel and hyperparameters that minimize this error.

Locally Linear Embedding (LLE)

Locally Linear Embedding (LLE) is another powerful nonlinear dimensionality reduction (NLDR) technique. It is a Manifold Learning technique that does not rely on projections, like the previous algorithms do. In a nutshell, LLE works by first measuring how each training instance linearly relates to its closest neighbors (c.n.), and then looking for a lowdimensional 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.

Locally Linear Embedding (LLE)

The following code uses Scikit-Learn's **LocallyLinearEmbedding** class to unroll the Swiss roll:

```
from sklearn.manifold import LocallyLinearEmbedding

lle = LocallyLinearEmbedding(n_components=2, n_neighbors=10)
X_reduced = lle.fit_transform(X)
```

Locally Linear Embedding (LLE)

The resulting 2D dataset is shown in Figure 8-12. 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 left part of the unrolled Swiss roll is stretched, while the right part is squeezed. Nevertheless, LLE did a pretty good job at modeling the manifold.

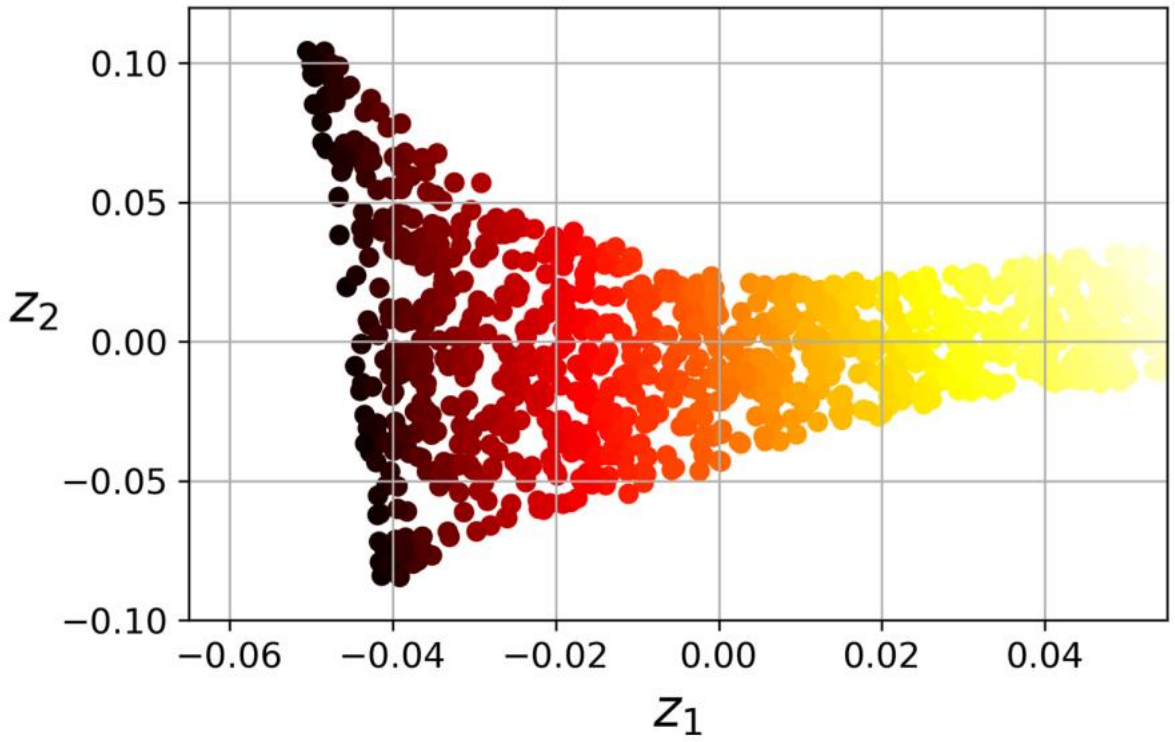


Figure 8-12. Unrolled Swiss roll using LLE

Locally Linear Embedding (LLE)

Here's how LLE works: for each training instance $\boldsymbol{x}^{(i)}$, the algorithm identifies its k closest neighbors (in the preceding code $k = 10$), then tries to reconstruct $\boldsymbol{x}^{(i)}$ as a linear function of these neighbors. More specifically, it finds the weights $w_{i,j}$ such that the squared distance between $\boldsymbol{x}^{(i)}$ and $\sum_{j=1}^{m} w_{i,j}\boldsymbol{x}^{(i)}$ is as small as possible, assuming $w_{i,j} = 0$ if $\boldsymbol{x}^{(j)}$ is not one of the k closest neighbors of $\boldsymbol{x}^{(i)}$. Thus the first step of LLE is the constrained optimization problem described in Equation 8-4, where W is the weight matrix containing all the weights $w_{i,j}$. The second constraint simply normalizes the weights for each training instance $\boldsymbol{x}^{(i)}$.

$$\widehat{\mathbf{W}} = \underset{\mathbf{W}}{\operatorname{argmin}} \sum_{i=1}^{m} \left(\mathbf{x}^{(i)} - \sum_{j=1}^{m} w_{i,j}\mathbf{x}^{(j)} \right)^2$$

$$\text{subject to} \begin{cases} w_{i,j} = 0 & \text{if } \mathbf{x}^{(j)} \text{ is not one of the } k \text{ c.n. of } \mathbf{x}^{(i)} \\ \sum_{j=1}^{m} w_{i,j} = 1 & \text{for } i = 1, 2, \cdots, m \end{cases}$$

Locally Linear Embedding (LLE)

After this step, the weight matrix $\widehat{W}$ (containing the weights $\widehat{w_{i,j}}$) encodes the local linear relationships between the training instances. The second step is to map the training instances into a d-dimensional space (where d < n) while preserving these local relationships as much as possible. If $\boldsymbol{z}^{(i)}$ is the image of $\boldsymbol{x}^{(i)}$ in this d-dimensional space, then we want the squared distance between $\boldsymbol{z}^{(i)}$ and $\sum_{j=1}^{m} \widehat{w_{i,j}} \boldsymbol{z}^{(j)}$ to be as small as possible. This idea leads to the unconstrained optimization problem described in Equation 8-5. It looks very similar to the first step, but instead of keeping the instances fixed and finding the optimal weights, we are doing the reverse: keeping the weights fixed and finding the optimal position of the instances' images in the low-dimensional space. Note that Z is the matrix containing all $\boldsymbol{z}^{(i)}$.

Locally Linear Embedding (LLE)

Equation 8-5. LLE step two: reducing dimensionality while preserving relationships

$$\hat{\mathbf{Z}} = \underset{\mathbf{Z}}{\operatorname{argmin}} \sum_{i=1}^{m} \left(\mathbf{z}^{(i)} - \sum_{j=1}^{m} \hat{w}_{i,j} \mathbf{z}^{(j)} \right)^2$$

Scikit-Learn's LLE implementation has the following computational complexity: $O(m \log(m) n \log(k))$ for finding the k nearest neighbors, $O(mnk^3)$ for optimizing the weights, and $O(dm^2)$ for constructing the lowdimensional representations. Unfortunately, the m in the last term makes this algorithm scale poorly to very large datasets.

Other Dimensionality Reduction Techniques

- Random Projections

  As its name suggests, projects the data to a lower-dimensional space using a random linear projection. This may sound crazy, but it turns out that such a random projection is actually very likely to preserve distances well, as was demonstrated mathematically by William B. Johnson and Joram Lindenstrauss in a famous lemma. The quality of the dimensionality reduction depends on the number of instances and the target dimensionality, but surprisingly not on the initial dimensionality. Check out the documentation for the **sklearn.random_projection** package for more details.

Other Dimensionality Reduction Techniques

- Multidimensional Scaling (MDS)

  Reduces dimensionality while trying to preserve the distances between the instances.

- Isomap

  Creates a graph by connecting each instance to its nearest neighbors, then reduces dimensionality while trying to preserve the *geodesic distances* between the instances.

- t-Distributed Stochastic Neighbor Embedding (t-SNE)

  Reduces dimensionality while trying to keep similar instances close and dissimilar instances apart. It is mostly used for visualization, in particular to visualize clusters of instances in high-dimensional space (e.g., to visualize the MNIST images in 2D).

Other Dimensionality Reduction Techniques

- Linear Discriminant Analysis (LDA)

  Is a classification algorithm, but during training it learns the most discriminative axes between the classes, and these axes can then be used to define a hyperplane onto which to project the data. The benefit of this approach is that the projection will keep classes as far apart as possible, so LDA is a good technique to reduce dimensionality before running another classification algorithm such as an SVM classifier.

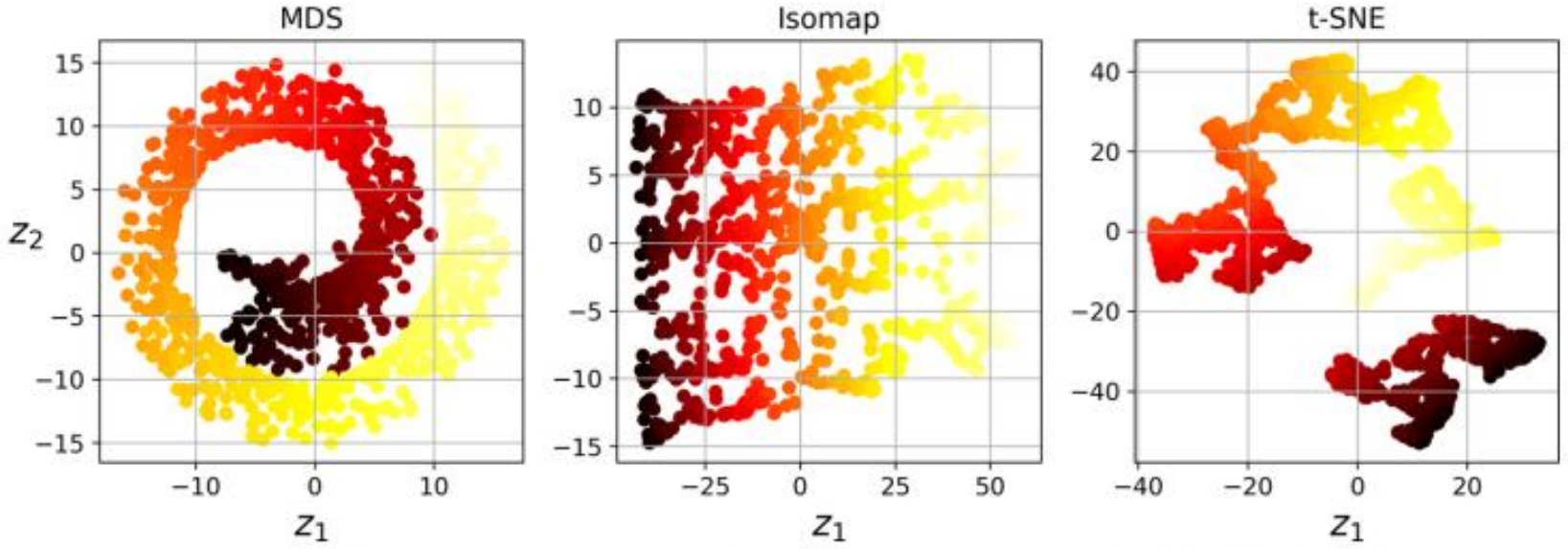


Figure 8-13. Using various techniques to reduce the Swill roll to 2D

Raise Your Hands

- How can you evaluate the performance of a dimensionality reduction algorithm on your dataset?
- Does it make any sense to chain two different dimensionality reduction algorithms?
- Can PCA be used to reduce the dimensionality of a highly nonlinear dataset?

References

- *Gelron, A. (2019). Hands-on machine learning with Scikit-Learn, Keras and TensorFlow: concepts, tools, and techniques to build intelligent systems (2nd ed.). O'Reilly.*