Data Analysis and Machine Learning: Dimensionality Reduction

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Reducing the number of degrees of freedom, overarching view

Many Machine Learning problems involve thousands or even millions of features for each training instance. Not only does this make training extremely slow, it 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.

Here we will discuss some of the most popular dimensionality reduction techniques: the principal component analysis PCA, Kernel PCA, and Locally Linear Embedding (LLE).

Principal Component Analysis

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.

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

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

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

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.

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

PCA and scikit-learn

Scikit-Learn's PCA class implements PCA using SVD decomposition just like we did before. 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, you can access the principal components using the components variable (note that it contains the PCs as horizontal vectors, so, for example, the first principal component is equal to

```
pca.components_.T[:, 0]).
```

Another very useful piece of information is the explained variance ratio of each principal component, available via the *explained_variance_ratio* variable. It indicates the proportion of the dataset's variance that lies along the axis of each principal component. More material to come here.

More on the PCA

Instead of arbitrarily choosing the number of dimensions to reduce down to, it is generally preferable 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 generally want to reduce the dimensionality down to 2 or 3. The following code computes 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)
cumsum = np.cumsum(pca.explained_variance_ratio_)
d = np.argmax(cumsum >= 0.95) + 1
```

You could then set $n\_components = d$ and run PCA again. However, 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)
```

Incremental PCA

One problem with the preceding implementation of PCA is that it requires the whole training set to fit in memory in order for the SVD algorithm to run. Fortunately, Incremental PCA (IPCA) algorithms have been developed: you can split the training set into mini-batches and feed an IPCA algorithm one minibatch at a time. This is useful for large training sets, and also to apply PCA online (i.e., on the fly, as new instances arrive).

Randomized PCA

Scikit-Learn offers yet another option to perform PCA, called Randomized PCA. This is a stochastic algorithm 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 $O(m \times n^2) + O(n^3)$, so it is dramatically faster than the previous algorithms when d is much smaller than n.

Kernel PCA

The kernel trick is 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. For example, the following code uses Scikit-Learn's KernelPCA class to perform kPCA with an

```python
from sklearn.decomposition import KernelPCA
rbf_pca = KernelPCA(n_components = 2, kernel="rbf", gamma=0.04)
X_reduced = rbf_pca.fit_transform(X)
```

LLE

Locally Linear Embedding (LLE) is another very powerful nonlinear dimensionality reduction (NLDR) technique. It is a Manifold Learning technique that does not rely on projections like the previous algorithms. 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 low-dimensional representation of the training set where these local relationships are best preserved (more details shortly).

Other techniques

There are many other dimensionality reduction techniques, several of which are available in Scikit-Learn.

Here are some of the most popular:

- **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).

- Linear Discriminant Analysis (LDA) is actually 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 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 a Support Vector Machine (SVM) classifier discussed in the SVM lectures.