MNIST Dataset

Introduction

In this chapter we will be using the MNIST dataset, which is a set of 70,000 small images of digits handwritten by high school students and employees of the US Census Bureau. Each image is labeled with the digit it represents. This set has been studied so much that it is often called the "hello world" of Machine Learning: whenever people come up with a new classification algorithm, they are curious to see how it will perform on MNIST, and anyone who learns Machine Learning tackles this dataset sooner or later. Scikit-Learn provides many helper functions to download popular datasets. MNIST is one of them.

Keys of mnist dataset

Datasets loaded by Scikit-Learn generally have a similar dictionary structure, including the following:

- A **DESCR** key describing the dataset
- A **data** key containing an array with one row per instance and one column per feature
- A **target** key containing an array with the labels
- **feature_names** giving the description of each feature.

About data

There are 70,000 images, and each image has 784 features. This is because each image is 28×28 pixels, and each feature simply represents one pixel's intensity, from 0 (white) to 255 (black).

Training a Binary Classifier

Let's simplify the problem for now and only try to identify one digit—for example, the number 5. This "5-detector" will be an example of a binary classifier, capable of distinguishing between just two classes, 5 and not-5.

Training by Stochastic Gradient Decent

Now let's pick a classifier and train it. A Stochastic Gradient Descent (SGD) classifier, using Scikit-Learn's SGDClassifier class, has the advantage of being capable of handling very large datasets efficiently. This is in part because SGD deals with training instances independently, one at a time (which also makes SGD well suited for online learning.

Performance Measures

Cross Validation

Let's use the cross_val_score() function to evaluate our SGDClassifier model, using K-fold cross-validation with Seven folds. Remember that K-fold cross-validation means splitting the training set into K folds (in this case, three), then making predictions and evaluating them on each fold using a model trained on the remaining folds. The performance measure value using Cross validation with fold 7 is 95%.

Just like the cross_val_score() function, cross_val_predict() performs K-fold cross-validation, but instead of returning the evaluation scores, it returns the predictions made on each test fold. This means that you get a clean prediction for each instance in the training set ("clean" meaning that the prediction is made by a model that never saw the data during training).

Confusion Matrix

A much better way to evaluate the performance of a classifier is to look at the confusion matrix. The general idea is to count the number of times instances of class A are classified as class B. To get the confusion matrix using the confusion_matrix() function, just pass it the target classes (y_train_5) and the predicted classes (y_train_pred).

Each row in a confusion matrix represents an actual class, while each column represents a predicted class. The first row of this matrix considers non-5 images (the negative class): 53,057 of them were correctly classified as non-5s (they are called true negatives), while the remaining 1,522 were wrongly classified as 5s (false positives). The second row considers the images of 5s (the positive class): 1,325 were wrongly classified as non-5s (false negatives), while the remaining 4,096 were correctly classified as 5s (true positives). A perfect classifier would have only true positives and true negatives, so its confusion matrix would have nonzero values only on its main diagonal.

Precision and Recall

The confusion matrix gives you a lot of information, but sometimes you may prefer a more concise metric. An interesting one to look at is the accuracy of the positive predictions; this is called the precision of the classifier.

A trivial way to have perfect precision is to make one single positive prediction and ensure it is correct (precision = 1/1 = 100%). But this would not be very useful, since the classifier would ignore all but one positive instance. So precision is typically used along with another metric named recall, also called sensitivity or the true positive rate (TPR): this is the ratio of positive instances that are correctly detected by the classifier.

F1 Score

It is often convenient to combine precision and recall into a single metric called the F score, in particular if you need a simple way to compare two classifiers. The F score is the harmonic mean of precision and recall. Whereas the regular mean treats all values equally, the harmonic mean gives much more weight to low values. As a result, the classifier will only get a high F score if both recall and precision are high. To compute the F score, simply call the f1_score() function.

The F score favors classifiers that have similar precision and recall. This is not always what you want: in some contexts, you mostly care about precision, and in other contexts you really care about recall.

Precision/Recall Trade-off

Unfortunately, you can't have it both ways: increasing precision reduces recall, and vice versa. This is called the precision/recall trade-off.

The ROC Curve

The receiver operating characteristic (ROC) curve is another common tool used with binary classifiers. It is very similar to the precision/recall curve, but instead of plotting precision versus recall, the ROC curve plots the true positive rate (another name for recall) against the false positive rate (FPR). The FPR is the ratio of negative instances that are incorrectly classified as positive. It is equal to 1 – the true negative rate (TNR), which is the ratio of negative instances that are correctly classified as negative. The TNR is also called specificity. Hence, the ROC curve plots sensitivity (recall) versus 1 – specificity. To plot the ROC curve, you first use the roc_curve() function to compute the TPR and FPR for various threshold values.

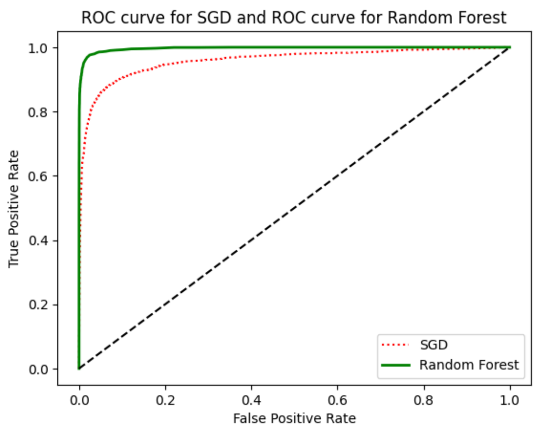
Once again there is a trade-off: the higher the recall (TPR), the more false positives (FPR) the classifier produces. The dotted line represents the ROC curve of a purely random classifier; a good classifier stays as far away from that line as possible (toward the top-left corner).

One way to compare classifiers is to measure the area under the curve (AUC). A perfect classifier will have a ROC AUC equal to 1, whereas a purely random classifier will have a ROC AUC equal to 0.5. Scikit-Learn provides a function to compute the ROC AUC

Roc curve for Randomforest

Let’s now train a RandomForestClassifier and compare its ROC curve and ROC AUC score to those of the SGDClassifier. First, you need to get scores for each instance in the training set. But due to the way it works (see Chapter 7), the RandomForestClassifier class does not have a decision_function() method. Instead, it has a predict_proba() method. Scikit-Learn classifiers generally have one or the other, or both. The predict_proba() method returns an array containing a row per instance and a column per class, each containing the probability that the given instance belongs to the given class (e.g., 70% chance that the image represents a 5).

Comparing ROC curve of SGD and Random Forest



As you can see in above Figure, the RandomForestClassifier ’s ROC curve looks much better than the SGDClassifier ’s: it comes much closer to the top-left corner. As a result, its ROC AUC score is also significantly better.

Multiclass Classification

Whereas binary classifiers distinguish between two classes, multiclass classifiers (also called multinomial classifiers) can distinguish between more than two classes. Some algorithms (such as SGD classifiers, Random Forest classifiers, and naive Bayes classifiers) are capable of handling multiple classes natively. Others (such as Logistic Regression or Support Vector Machine classifiers) are strictly binary classifiers. However, there are various strategies that you can use to perform multiclass classification with multiple binary classifiers.

One way to create a system that can classify the digit images into 10 classes (from 0 to 9) is to train 10 binary classifiers, one for each digit (a 0-detector, a 1-detector, a 2-detector, and so on). Then when you want to classify an image, you get the decision score from each classifier for that image and you select the class whose classifier outputs the highest score. This is called the **one-versus-the-rest (OvR)** strategy (also called one versus-all).

Another strategy is to train a binary classifier for every pair of digits: one to distinguish 0s and 1s, another to distinguish 0s and 2s, another for 1s and 2s, and so on. This is called the **one-versus-one (OvO) strategy**. If there are N classes, you need to train $N \times (N - 1) / 2$ classifiers. The main advantage of OvO is that each classifier only needs to be trained on the part of the training set for the two classes that it must distinguish.

Some algorithms (such as Support Vector Machine classifiers) scale poorly with the size of the training set. For these algorithms OvO is preferred because it is faster to train many classifiers on small training sets than to train few classifiers on large training sets. For most binary classification algorithms, however, OvR is preferred.

Scikit-Learn detects when you try to use a binary classification algorithm for a multiclass classification task, and it automatically runs OvR or OvO, depending on the algorithm.