Multiclass Classification

Whereas binary classifiers distinguish between two classes, *multiclass classifiers* (also called *multinomial classifiers*) can distinguish between more than two classes.

See next page.

Some algorithms (such as Random Forest classifiers or naive Bayes classifiers) are capable of handling multiple classes directly. Others (such as Support Vector Machine classifiers or Linear classifiers) are strictly binary classifiers. However, there are various strategies that you can use to perform multiclass classification using multiple binary classifiers.

For example, 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-all* (OvA) strategy (also called *one-versus-the-rest*).

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. For the MNIST problem, this means training 45 binary classifiers! When you want to classify an image, you have to run the image through all 45 classifiers and see which class wins the most duels. 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, so for these algorithms OvO is preferred since it is faster to train many classifiers on small training sets than training few classifiers on large training sets. For most binary classification algorithms, however, OvA is preferred.

Scikit-Learn detects when you try to use a binary classification algorithm for a multiclass classification task, and it automatically runs OvA (except for SVM classifiers for which it uses OvO). Let's try this with the SGDClassifier:

```
>>> sgd_clf.fit(X_train, y_train) # y_train, not y_train_5
>>> sgd_clf.predict([some_digit])
array([ 5.])
```

That was easy! This code trains the SGDClassifier on the training set using the original target classes from 0 to 9 (y_train), instead of the 5-versus-all target classes (y_train_5). Then it makes a prediction (a correct one in this case). Under the hood, Scikit-Learn actually trained 10 binary classifiers, got their decision scores for the image, and selected the class with the highest score.

To see that this is indeed the case, you can call the decision_function() method. Instead of returning just one score per instance, it now returns 10 scores, one per class:

```
>>> some_digit_scores = sgd_clf.decision_function([some_digit])
>>> some_digit_scores
```

```
array([[-311402.62954431, -363517.28355739, -446449.5306454, -183226.61023518, -414337.15339485, 161855.74572176, -452576.39616343, -471957.14962573, -518542.33997148, -536774.63961222]])
```

The highest score is indeed the one corresponding to class 5:

```
>>> np.argmax(some_digit_scores)
5
>>> sgd_clf.classes_
array([ 0.,  1.,  2.,  3.,  4.,  5.,  6.,  7.,  8.,  9.])
>>> sgd_clf.classes[5]
5.0
```



When a classifier is trained, it stores the list of target classes in its classes_ attribute, ordered by value. In this case, the index of each class in the classes_ array conveniently matches the class itself (e.g., the class at index 5 happens to be class 5), but in general you won't be so lucky.

If you want to force ScikitLearn to use one-versus-one or one-versus-all, you can use the OneVsOneClassifier or OneVsRestClassifier classes. Simply create an instance and pass a binary classifier to its constructor. For example, this code creates a multiclass classifier using the OvO strategy, based on a SGDClassifier:

```
>>> from sklearn.multiclass import OneVsOneClassifier
>>> ovo_clf = OneVsOneClassifier(SGDClassifier(random_state=42))
>>> ovo_clf.fit(X_train, y_train)
>>> ovo_clf.predict([some_digit])
array([ 5.])
>>> len(ovo_clf.estimators_)
45
```

Training a RandomForestClassifier is just as easy:

```
>>> forest_clf.fit(X_train, y_train)
>>> forest_clf.predict([some_digit])
array([ 5.])
```

This time Scikit-Learn did not have to run OvA or OvO because Random Forest classifiers can directly classify instances into multiple classes. You can call predict_proba() to get the list of probabilities that the classifier assigned to each instance for each class:

```
>>> forest_clf.predict_proba([some_digit])
array([[ 0.1,  0. ,  0. ,  0.1,  0. ,  0.8,  0. ,  0. ,  0. ,  0. ]])
```

You can see that the classifier is fairly confident about its prediction: the 0.8 at the 5th index in the array means that the model estimates an 80% probability that the image

represents a 5. It also thinks that the image could instead be a 0 or a 3 (10% chance each).

Now of course you want to evaluate these classifiers. As usual, you want to use cross-validation. Let's evaluate the SGDClassifier's accuracy using the cross_val_score() function:

```
>>> cross_val_score(sgd_clf, X_train, y_train, cv=3, scoring="accuracy")
array([ 0.84063187,  0.84899245,  0.86652998])
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It gets over 84% on all test folds. If you used a random classifier, you would get 10% accuracy, so this is not such a bad score, but you can still do much better. For example, simply scaling the inputs (as discussed in Chapter 2) increases accuracy above 90%:

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>>> from sklearn.preprocessing import StandardScaler
>>> scaler = StandardScaler()
>>> X_train_scaled = scaler.fit_transform(X_train.astype(np.float64))
>>> cross_val_score(sgd_clf, X_train_scaled, y_train, cv=3, scoring="accuracy")
array([ 0.91011798,  0.90874544,  0.906636  ])
```

Error Analysis

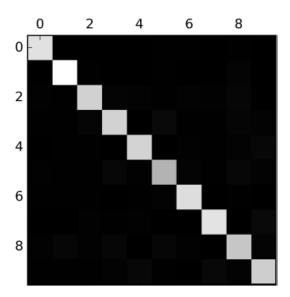
Of course, if this were a real project, you would follow the steps in your Machine Learning project checklist (see Appendix B): exploring data preparation options, trying out multiple models, shortlisting the best ones and fine-tuning their hyperparameters using GridSearchCV, and automating as much as possible, as you did in the previous chapter. Here, we will assume that you have found a promising model and you want to find ways to improve it. One way to do this is to analyze the types of errors it makes.

First, you can look at the confusion matrix. You need to make predictions using the cross_val_predict() function, then call the confusion_matrix() function, just like you did earlier:

```
>>> y_train_pred = cross_val_predict(sgd_clf, X_train_scaled, y_train, cv=3)
>>> conf_mx = confusion_matrix(y_train, y_train_pred)
>>> conf mx
              3, 24,
                       9.
array([[5725,
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                                  49.
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                                            10.
                                                 39.
                                                       4],
                                       5,
     [ 2, 6493, 43,
                      25, 7, 40,
                                            10, 109,
                                                       8],
     [ 51, 41, 5321, 104, 89, 26,
                                       87,
                                            60,
                                                       13],
                                                166,
             46, 141, 5342,
                            1, 231,
     [ 47,
                                            50,
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                                                 45,
                                                       0],
     [ 25,
             24.
                  74,
                      32, 54,
                                 12,
                                      6, 5787,
                                                 15, 236],
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That's a lot of numbers. It's often more convenient to look at an image representation of the confusion matrix, using Matplotlib's matshow() function:

```
plt.matshow(conf_mx, cmap=plt.cm.gray)
plt.show()
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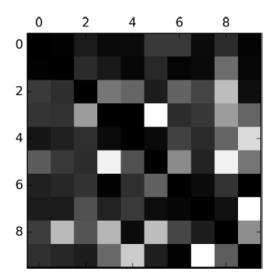
This confusion matrix looks fairly good, since most images are on the main diagonal, which means that they were classified correctly. The 5s look slightly darker than the other digits, which could mean that there are fewer images of 5s in the dataset or that the classifier does not perform as well on 5s as on other digits. In fact, you can verify that both are the case.

Let's focus the plot on the errors. First, you need to divide each value in the confusion matrix by the number of images in the corresponding class, so you can compare error rates instead of absolute number of errors (which would make abundant classes look unfairly bad):

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row_sums = conf_mx.sum(axis=1, keepdims=True)
norm_conf_mx = conf_mx / row_sums
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Now let's fill the diagonal with zeros to keep only the errors, and let's plot the result:

```
np.fill_diagonal(norm_conf_mx, 0)
plt.matshow(norm_conf_mx, cmap=plt.cm.gray)
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Now you can clearly see the kinds of errors the classifier makes. Remember that rows represent actual classes, while columns represent predicted classes. The columns for classes 8 and 9 are quite bright, which tells you that many images get misclassified as 8s or 9s. Similarly, the rows for classes 8 and 9 are also quite bright, telling you that 8s and 9s are often confused with other digits. Conversely, some rows are pretty dark, such as row 1: this means that most 1s are classified correctly (a few are confused with 8s, but that's about it). Notice that the errors are not perfectly symmetrical; for example, there are more 5s misclassified as 8s than the reverse.

Analyzing the confusion matrix can often give you insights on ways to improve your classifier. Looking at this plot, it seems that your efforts should be spent on improving classification of 8s and 9s, as well as fixing the specific 3/5 confusion. For example, you could try to gather more training data for these digits. Or you could engineer new features that would help the classifier—for example, writing an algorithm to count the number of closed loops (e.g., 8 has two, 6 has one, 5 has none). Or you could preprocess the images (e.g., using Scikit-Image, Pillow, or OpenCV) to make some patterns stand out more, such as closed loops.

Analyzing individual errors can also be a good way to gain insights on what your classifier is doing and why it is failing, but it is more difficult and time-consuming. For example, let's plot examples of 3s and 5s:

```
cl_a, cl_b = 3, 5
X_aa = X_train[(y_train == cl_a) & (y_train_pred == cl_a)]
X_ab = X_train[(y_train == cl_a) & (y_train_pred == cl_b)]
X_ba = X_train[(y_train == cl_b) & (y_train_pred == cl_a)]
X_bb = X_train[(y_train == cl_b) & (y_train_pred == cl_b)]
plt.figure(figsize=(8,8))
plt.subplot(221); plot_digits(X_aa[:25], images_per_row=5)
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```

The two 5×5 blocks on the left show digits classified as 3s, and the two 5×5 blocks on the right show images classified as 5s. Some of the digits that the classifier gets wrong (i.e., in the bottom-left and top-right blocks) are so badly written that even a human would have trouble classifying them (e.g., the 5 on the 8th row and 1st column truly looks like a 3). However, most misclassified images seem like obvious errors to us, and it's hard to understand why the classifier made the mistakes it did.³ The reason is that we used a simple SGDClassifier, which is a linear model. All it does is assign a weight per class to each pixel, and when it sees a new image it just sums up the weighted pixel intensities to get a score for each class. So since 3s and 5s differ only by a few pixels, this model will easily confuse them.

The main difference between 3s and 5s is the position of the small line that joins the top line to the bottom arc. If you draw a 3 with the junction slightly shifted to the left, the classifier might classify it as a 5, and vice versa. In other words, this classifier is quite sensitive to image shifting and rotation. So one way to reduce the 3/5 confusion would be to preprocess the images to ensure that they are well centered and not too rotated. This will probably help reduce other errors as well.

Multilabel Classification

Until now each instance has always been assigned to just one class. In some cases you may want your classifier to output multiple classes for each instance. For example, consider a face-recognition classifier: what should it do if it recognizes several people on the same picture? Of course it should attach one label per person it recognizes. Say the classifier has been trained to recognize three faces, Alice, Bob, and Charlie; then when it is shown a picture of Alice and Charlie, it should output [1, 0, 1] (meaning "Alice yes, Bob no, Charlie yes"). Such a classification system that outputs multiple binary labels is called a *multilabel classification* system.

We won't go into face recognition just yet, but let's look at a simpler example, just for illustration purposes:

```
from sklearn.netghbors tmport KNeighborsClassifier

y_train_large = (y_train >= 7)

y_train_odd = (y_train % 2 == 1)

y_multilabel = np.c_[y_train_large, y_train_odd]

knn_clf = KNeighborsClassifier()
knn_clf.fit(X_train, y_multilabel)
```

This code creates a y_multilabel array containing two target labels for each digit image: the first indicates whether or not the digit is large (7, 8, or 9) and the second indicates whether or not it is odd. The next lines create a KNeighborsClassifier instance (which supports multilabel classification, but not all classifiers do) and we train it using the multiple targets array. Now you can make a prediction, and notice that it outputs two labels:

```
>>> knn_clf.predict([some_digit])
array([[False, True]], dtype=bool)
```

And it gets it right! The digit 5 is indeed not large (False) and odd (True).

There are many ways to evaluate a multilabel classifier, and selecting the right metric really depends on your project. For example, one approach is to measure the F_1 score for each individual label (or any other binary classifier metric discussed earlier), then simply compute the average score. This code computes the average F_1 score across all labels:

```
>>> y_train_knn_pred = cross_val_predict(knn_clf, X_train, y_train, cv=3)
>>> f1_score(y_train, y_train_knn_pred, average="macro")
0.96845540180280221
```

This assumes that all labels are equally important, which may not be the case. In particular, if you have many more pictures of Alice than of Bob or Charlie, you may want to give more weight to the classifier's score on pictures of Alice. One simple option is

to give each label a weight equal to its *support* (i.e., the number of instances with that target label). To do this, simply set average="weighted" in the preceding code.⁴

Multioutput Classification

The last type of classification task we are going to discuss here is called *multioutput-multiclass classification* (or simply *multioutput classification*). It is simply a generalization of multilabel classification where each label can be multiclass (i.e., it can have more than two possible values).

To illustrate this, let's build a system that removes noise from images. It will take as input a noisy digit image, and it will (hopefully) output a clean digit image, represented as an array of pixel intensities, just like the MNIST images. Notice that the classifier's output is multilabel (one label per pixel) and each label can have multiple values (pixel intensity ranges from 0 to 255). It is thus an example of a multioutput classification system.



The line between classification and regression is sometimes blurry, such as in this example. Arguably, predicting pixel intensity is more akin to regression than to classification. Moreover, multioutput systems are not limited to classification tasks; you could even have a system that outputs multiple labels per instance, including both class labels and value labels.

Let's start by creating the training and test sets by taking the MNIST images and adding noise to their pixel intensities using NumPy's randint() function. The target images will be the original images:

```
noise = rnd.randint(0, 100, (len(X_train), 784))
noise = rnd.randint(0, 100, (len(X_test), 784))
X_train_mod = X_train + noise
X_test_mod = X_test + noise
y_train_mod = X_train
y_test_mod = X_test
```

Let's take a peek at an image from the test set (yes, we're snooping on the test data, so you should be frowning right now):



On the left is the noisy input image, and on the right is the clean target image. Now let's train the classifier and make it clean this image:

```
knn_clf.fit(X_train_mod, y_train_mod)
clean_digit = knn_clf.predict([X_test_mod[some_index]])
plot_digit(clean_digit)
```



Looks close enough to the target! This concludes our tour of classification. Hopefully you should now know how to select good metrics for classification tasks, pick the appropriate precision/recall tradeoff, compare classifiers, and more generally build good classification systems for a variety of tasks.

- .

```
array([[-311402.62954431, -363517.28355739, -446449.5306454, -183226.61023518, -414337.15339485, 161855.74572176, -452576.39616343, -471957.14962573, -518542.33997148, -536774.63961222]])
```

The highest score is indeed the one corresponding to class 5:

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array([ 0.,  1.,  2.,  3.,  4.,  5.,  6.,  7.,  8.,  9.])
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When a classifier is trained, it stores the list of target classes in its classes_ attribute, ordered by value. In this case, the index of each class in the classes_ array conveniently matches the class itself (e.g., the class at index 5 happens to be class 5), but in general you won't be so lucky.

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Training a RandomForestClassifier is just as easy:

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This time Scikit-Learn did not have to run OvA or OvO because Random Forest classifiers can directly classify instances into multiple classes. You can call predict_proba() to get the list of probabilities that the classifier assigned to each instance for each class:

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You can see that the classifier is fairly confident about its prediction: the 0.8 at the 5th index in the array means that the model estimates an 80% probability that the image

represents a 5. It also thinks that the image could instead be a 0 or a 3 (10% chance each).

Now of course you want to evaluate these classifiers. As usual, you want to use cross-validation. Let's evaluate the SGDClassifier's accuracy using the cross_val_score() function:

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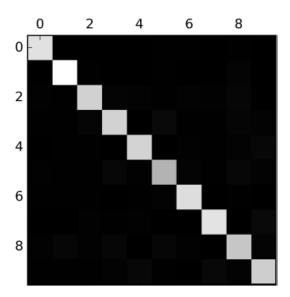
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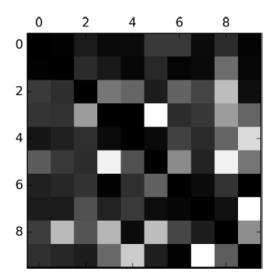
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from sklearn.netghbors tmport KNeighborsClassifier

y_train_large = (y_train >= 7)

y_train_odd = (y_train % 2 == 1)

y_multilabel = np.c_[y_train_large, y_train_odd]

knn_clf = KNeighborsClassifier()
knn_clf.fit(X_train, y_multilabel)
```

This code creates a y_multilabel array containing two target labels for each digit image: the first indicates whether or not the digit is large (7, 8, or 9) and the second indicates whether or not it is odd. The next lines create a KNeighborsClassifier instance (which supports multilabel classification, but not all classifiers do) and we train it using the multiple targets array. Now you can make a prediction, and notice that it outputs two labels:

```
>>> knn_clf.predict([some_digit])
array([[False, True]], dtype=bool)
```

And it gets it right! The digit 5 is indeed not large (False) and odd (True).

There are many ways to evaluate a multilabel classifier, and selecting the right metric really depends on your project. For example, one approach is to measure the F_1 score for each individual label (or any other binary classifier metric discussed earlier), then simply compute the average score. This code computes the average F_1 score across all labels:

```
>>> y_train_knn_pred = cross_val_predict(knn_clf, X_train, y_train, cv=3)
>>> f1_score(y_train, y_train_knn_pred, average="macro")
0.96845540180280221
```

This assumes that all labels are equally important, which may not be the case. In particular, if you have many more pictures of Alice than of Bob or Charlie, you may want to give more weight to the classifier's score on pictures of Alice. One simple option is

to give each label a weight equal to its *support* (i.e., the number of instances with that target label). To do this, simply set average="weighted" in the preceding code.⁴

Multioutput Classification

The last type of classification task we are going to discuss here is called *multioutput-multiclass classification* (or simply *multioutput classification*). It is simply a generalization of multilabel classification where each label can be multiclass (i.e., it can have more than two possible values).

To illustrate this, let's build a system that removes noise from images. It will take as input a noisy digit image, and it will (hopefully) output a clean digit image, represented as an array of pixel intensities, just like the MNIST images. Notice that the classifier's output is multilabel (one label per pixel) and each label can have multiple values (pixel intensity ranges from 0 to 255). It is thus an example of a multioutput classification system.



The line between classification and regression is sometimes blurry, such as in this example. Arguably, predicting pixel intensity is more akin to regression than to classification. Moreover, multioutput systems are not limited to classification tasks; you could even have a system that outputs multiple labels per instance, including both class labels and value labels.

Let's start by creating the training and test sets by taking the MNIST images and adding noise to their pixel intensities using NumPy's randint() function. The target images will be the original images:

```
noise = rnd.randint(0, 100, (len(X_train), 784))
noise = rnd.randint(0, 100, (len(X_test), 784))
X_train_mod = X_train + noise
X_test_mod = X_test + noise
y_train_mod = X_train
y_test_mod = X_test
```

Let's take a peek at an image from the test set (yes, we're snooping on the test data, so you should be frowning right now):



On the left is the noisy input image, and on the right is the clean target image. Now let's train the classifier and make it clean this image:

```
knn_clf.fit(X_train_mod, y_train_mod)
clean_digit = knn_clf.predict([X_test_mod[some_index]])
plot_digit(clean_digit)
```



Looks close enough to the target! This concludes our tour of classification. Hopefully you should now know how to select good metrics for classification tasks, pick the appropriate precision/recall tradeoff, compare classifiers, and more generally build good classification systems for a variety of tasks.

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