4 Evaluation metrics for classification

This chapter covers

- Accuracy as a way of evaluating binary classification models and its limitations
- Determining where our model makes mistakes using a confusion table
- Deriving other metrics like precision and recall from the confusion table
- Using ROC (receiver operating characteristics) and AUC (area under the ROC curve) to further understand the performance of a binary classification model
- Cross-validating a model to make sure it behaves optimally
- Tuning the parameters of a model to achieve the best predictive performance

In this chapter, we continue with the project we started in the previous chapter: churn prediction. We have already downloaded the dataset, performed the initial preprocessing and exploratory data analysis, and trained the model that predicts whether customers will churn. We have also evaluated this model on the validation dataset and concluded that it has 80% accuracy.

The question we postponed until now was whether 80% accuracy is good and what it actually means in terms of the quality of our model. We answer this question in this chapter and discuss other ways of evaluating a

binary classification model: the confusion table, precision and recall, the ROC curve, and AUC.

This chapter provides a lot of complex information, but the evaluation metrics we cover here are essential for doing practical machine learning. Don't worry if you don't immediately understand all the details of the different evaluation metrics: it requires time and practice. Feel free to come back to this chapter to revisit the finer points.

1 Evaluation metrics

We have already built a binary classification model for predicting churning customers. Now we need to be able to determine how good it is.

For this, we use a *metric*—a function that looks at the predictions the model makes and compares them with the actual values. Then, based on the comparison, it calculates how good the model is. This is quite useful: we can use it to compare different models and select the one with the best metric value.

There are different kinds of metrics. In chapter 2, we used RMSE (root mean squared error) to evaluate regression models. However, this metric can be used only for regression models and doesn't work for classification.

For evaluating classification models, we have other more suitable metrics. In this section, we cover the most common evaluation metrics for binary classification, starting with accuracy, which we already saw in chapter 3.

4.1.1 Classification accuracy

As you probably remember, the accuracy of a binary classification model is the percentage of correct predictions it makes (figure 4.1).

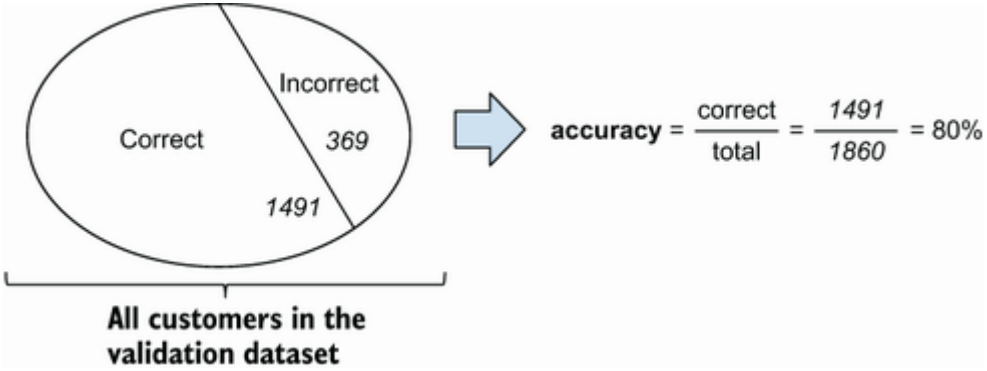


Figure 4.1 The accuracy of a model is the fraction of predictions that turned out to be correct.

This accuracy is the simplest way to evaluate a classifier: by counting the number of cases in which our model turned out to be right, we can learn a lot about the model's behavior and quality.

Computing accuracy on the validation dataset is easy—we simply calculate the fraction of correct predictions:

```
y_pred = model.predict_proba(X_val)[:, 1]    ❶
churn = y_pred >= 0.5                        ❷
(churn == y_val).mean()                      ❸
```

❶ Gets the predictions from the model

❷ Makes "hard" predictions

❸ Computes the accuracy

We first apply the model to the validation set to get the predictions in ❶. These predictions are probabilities, so we cut them at 0.5 in ❷. Finally, we calculate the fraction of predictions that matched reality in ❷.

The result is 0.8016, which means that our model is 80% accurate.

The first thing we should ask ourselves is why we chose 0.5 as the threshold and not any other number. That was an arbitrary choice, but it's actually not difficult to check other thresholds as well: we can just loop over all possible threshold candidates and compute the accuracy for each. Then we can choose the one with the best accuracy score.

Even though it's easy to implement accuracy ourselves, we can use existing implementations as well. The Scikit-learn library offers a variety of metrics, including accuracy and many others that we will use later. You can find these metrics in the metrics package.

We'll continue working on the same notebook that we started in chapter 3. Let's open it and add the `import` statement to import accuracy from Scikit-learn's metrics package:

```
from sklearn.metrics import accuracy_score
```

Now we can loop over different thresholds and check which one gives the best accuracy:

```
thresholds = np.linspace(0, 1, 11)          ❶

for t in thresholds:                        ❷
    churn = y_pred >= t                     ❸
    acc = accuracy_score(y_val, churn)      ❸
    print('%0.2f %0.3f' % (t, acc))         ❹
```

❶ Creates an array with different thresholds: 0.0, 0.1, 0.2, and so on

❷ Loops over each threshold value

❸ Uses the accuracy_score function from Scikit-learn for computing accuracy

❹ Prints the thresholds and the accuracy values to standard output

In this code, we first create an array with thresholds. We use the `linspace` function from NumPy for that: it takes two numbers (0 and 1, in our case) and the number of elements the array should have (11). As a result, we get an array with the numbers 0.0, 0.1, 0.2, ..., 1.0. You can learn more about `linspace` and other NumPy functions in appendix C.

We use these numbers as thresholds: we loop over them, and for each one, we calculate the accuracy. Finally, we print the thresholds and the accuracy scores so we can decide which threshold is the best.

When we execute the code, it prints the following:

```
0.00 0.261
0.10 0.595
0.20 0.690
0.30 0.755
0.40 0.782
0.50 0.802
0.60 0.790
0.70 0.774
0.80 0.742
0.90 0.739
1.00 0.739
```

As we see, using the threshold of 0.5 gives us the best accuracy. Typically, 0.5 is a good threshold value to start with, but we should always try other threshold values to make sure 0.5 is the best choice.

To make it more visual, we can use Matplotlib to create a plot that shows how accuracy changes depending on the threshold. We repeat the same process as previously, but instead of just printing the accuracy scores, we first put the values to a list:

```
thresholds = np.linspace(0, 1, 21)              ❶
accuracies = []                                 ❷
for t in thresholds:
    acc = accuracy_score(y_val, y_pred >= t)    ❸
    accuracies.append(acc)                      ❹
```

❶ Creates different threshold values (this time 21 instead of 11)

❷ Creates an empty list to hold the accuracy values

❸ Calculates the accuracy for a given threshold

❹ Records the accuracy for this threshold

And then we plot these values using Matplotlib:

```
plt.plot(thresholds, accuracies)
```

After executing this line, we should see a plot that shows the relationship between the threshold and the accuracy (figure 4.2). As we already know, the 0.5 threshold is the best in terms of accuracy.

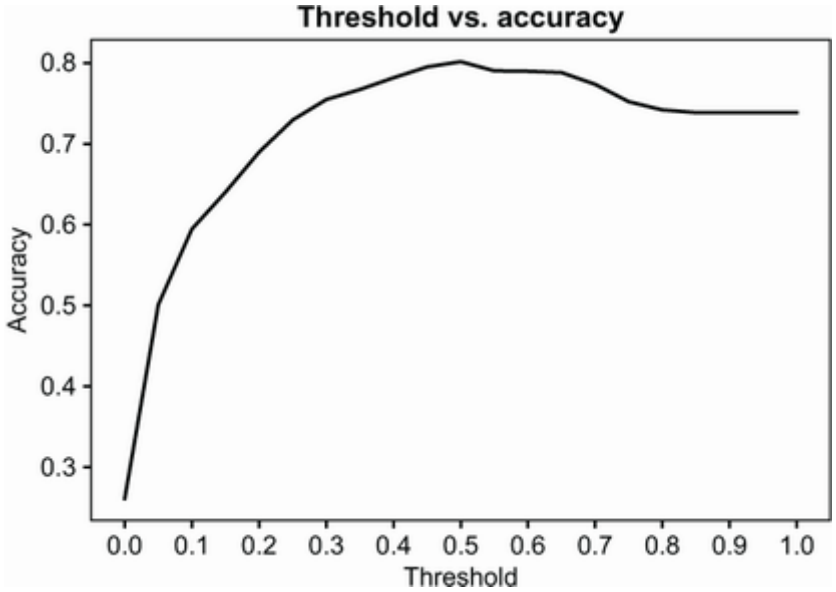


Figure 4.2 Accuracy of our model evaluated at different thresholds. The best accuracy is achieved when cutting the predictions at the 0.5 thresh-

old: if a prediction is higher than 0.5, we predict “churn,” and otherwise, we predict “no churn.”

So, the best threshold is 0.5, and the best accuracy for this model that we can achieve is 80%.

In the previous chapter, we trained a simpler model: we called it model_small. It was based on only three variables: `contract`, `tenure`, and `totalcharges`.

Let’s also check its accuracy. For that, we first make predictions on the validation dataset and then compute the accuracy score:

```
val_dict_small = df_val[small_subset].to_dict(orient='records')   ❶

X_small_val = dv_small.transform(val_dict_small)                  ❶
y_pred_small = model_small.predict_proba(X_small_val)[:, 1]       ❷

churn_small = y_pred_small >= 0.5                                 ❷
accuracy_score(y_val, churn_small)                                ❸
```

❶ Applies one-hot encoding to the validation data

❷ Predicts churn using the small model

❸ Calculates the accuracy of the predictions

When we run this code, we see that the accuracy of the small model is 76%. So, the large model is actually 4% more accurate than the small

model.

However, this still doesn't tell us whether 80% (or 76%) is a good accuracy score.

4.1.2 Dummy baseline

Although it seems like a decent number, to understand whether 80% is actually good, we need to relate it to something—for example, a simple baseline that's easy to understand. One such baseline could be a dummy model that always predicts the same value.

In our example, the dataset is imbalanced, and we don't have many churned users. So, the dummy model can always predict the majority class—"no churn." In other words, this model will always output False, regardless of the features. This is not a super useful model, but we can use it as a baseline and compare it with the other two models.

Let's create this baseline prediction:

```
size_val = len(y_val)                    ❶
baseline = np.repeat(False, size_val)    ❷
```

❶ Gets the number of customers in the validation set

❷ Creates an array with only False elements

To create an array with the baseline predictions, we first need to determine how many elements are in the validation set.

Next, we create an array of dummy predictions—all the elements of this array are False values. We do this using the `repeat` function from NumPy: it takes in an element and repeats it as many times as we ask. For more details about the `repeat` function and other NumPy functions, please refer to appendix C.

Now we can check the accuracy of this baseline prediction using the same code as we used previously:

```
accuracy_score(baseline, y_val)
```

When we run this code, it shows 0.738. This means that the accuracy of the baseline model is around 74% (figure 4.3).

```
size_val = len(y_val)
baseline = np.repeat(False, size_val)
baseline
```

```
array([False, False, False, ..., False, False, False])
```

```
accuracy_score(baseline, y_val)
```

```
0.7387096774193549
```

Figure 4.3 The baseline is a “model” that always predicts the same value for all the customers. The accuracy of this baseline is 74%.

As we see, the small model is only 2% better than the naive baseline, and the large one is 6% better. If we think about all the trouble we have gone through to train this large model, 6% doesn’t seem like a significant improvement over the dummy baseline.

Churn prediction is a complex problem, and maybe this improvement is great. However, that's not evident from the accuracy score alone. According to accuracy, our model is only slightly better than a dummy model that treats all the customers as non-churning and doesn't attempt to keep any of them.

Thus, we need other metrics—other ways of measuring the quality of our model. These metrics are based on the confusion table, the concept that we cover in the next section.

2 Confusion table

Even though accuracy is easy to understand, it's not always the best metric. In fact, it sometimes can be misleading. We've already seen this occur: the accuracy of our model is 80%, and although that seems like a good number, it's just 6% better than the accuracy of a dummy model that always outputs the same prediction of "no churn."

This situation typically happens when we have a class imbalance (more instances of one class than another). We know that this is definitely the case for our problem: 74% of customers did not churn, and only 26% did churn.

For such cases, we need a different way of measuring the quality of our models. We have a few options, and most of them are based on the confusion table: a table that concisely represents every possible outcome for our model's predictions.

4.2.1 Introduction to the confusion table

We know that for a binary classification model, we can have only two possible predictions: True and False. In our case, we can predict that a customer is either going to churn (True) or not (False).

When we apply the model to the entire validation dataset with customers, we split it into two parts (figure 4.4):

- Customers for whom the model predicts “churn”
- Customers for whom the model predicts “no churn”

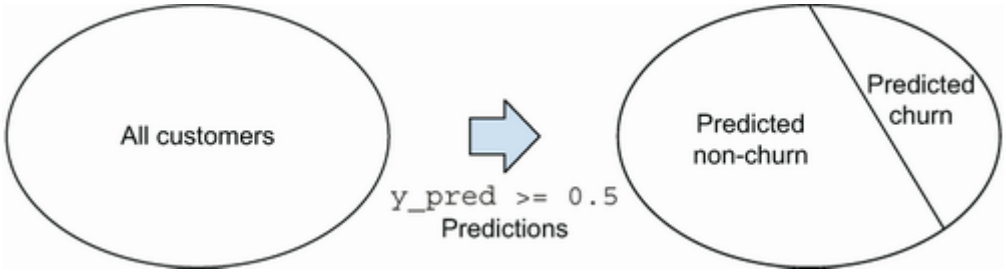


Figure 4.4 Our model splits all the customers in the validation dataset into two groups: customers who we think will churn and customers who will not.

Only two possible correct outcomes can occur: again, True or False. A customer has either actually churned (True) or not (False).

This means that by using the ground truth information—the information about the target variable—we can again split the dataset into two parts (figure 4.5):

- The customers who churned
- The customers who didn't churn

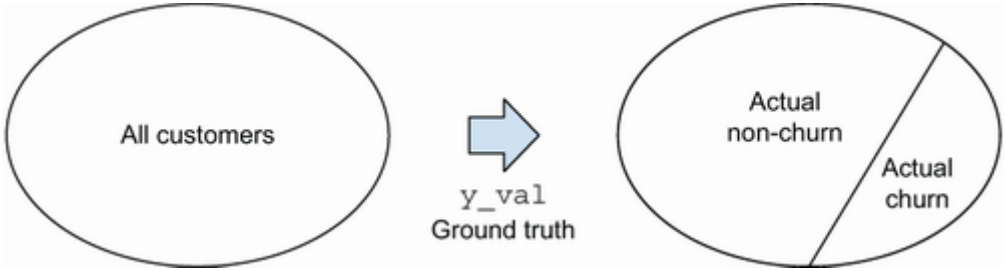


Figure 4.5 Using the ground truth data, we can split the validation dataset into two groups: customers who actually churned and customers who didn't.

When we make a prediction, it will either turn out to be correct or not:

- If we predict "churn," the customer may indeed churn, or they may not.
- If we predict "no churn," it's possible that the customer indeed doesn't churn, but it's also possible that they do churn.

This gives us four possible outcomes (figure 4.6):

- We predict False, and the answer is False.
- We predict False, and the answer is True.
- We predict True, and the answer is False.
- We predict True, and the answer is True.

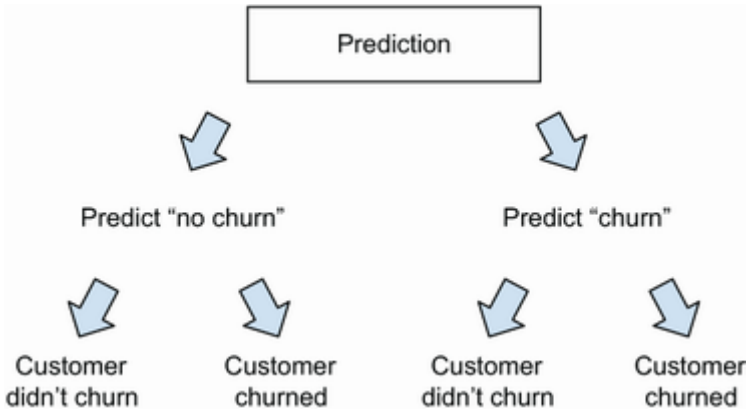


Figure 4.6 There are four possible outcomes: we predict "churn," and the customers either churn or do not, and we predict "no churn," and the customers again either churn or do not.

Two of these situations—the first and last ones—are good: the prediction matched the actual value. The two remaining ones are bad: we didn't make a correct prediction.

Each of these four situations has its own name (figure 4.7):

- True negative (TN): we predict False ("no churn"), and the actual label is also False ("no churn").
- True positive (TP): we predict True ("churn"), and the actual label is True ("churn").
- False negative (FN): we predict False ("no churn"), but it's actually True (the customer churned).
- False positive (FP): we predict True ("churn"), but it's actually False (the customer stayed with us).

Figure 4.7 Each of the four possible outcomes has its own name: true negative, false negative, false positive, and true positive.

It's visually helpful to arrange these outcomes in a table. We can put the predicted classes (False and True) in the columns and the actual classes (False and True) in the rows (figure 4.8).

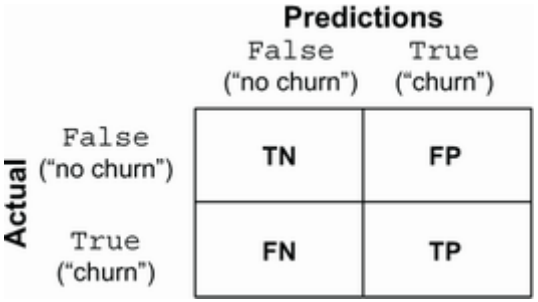


Figure 4.8 We can organize the outcomes in a table—the predicted values as columns and the actual values as rows. This way, we break down all prediction scenarios into four distinct groups: TN (true negative), TP (true positive), FN (false negative), and FP (false positive).

When we substitute the number of times each outcome happens, we get the confusion table for our model (figure 4.9).

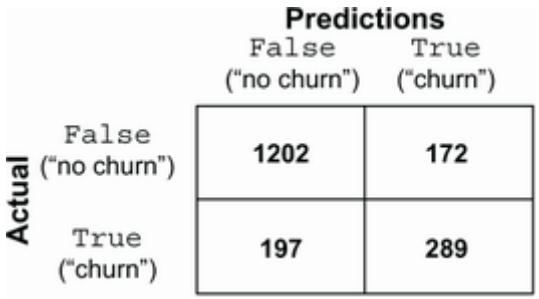


Figure 4.9 In the confusion table, each cell contains the number of times each outcome happens.

Calculating the values in the cells of the confusion matrix is quite easy with NumPy. Next, we see how to do it.

4.2.2 Calculating the confusion table with NumPy

To help us understand our confusion table better, we can visually depict what it does to the validation dataset (figure 4.10).

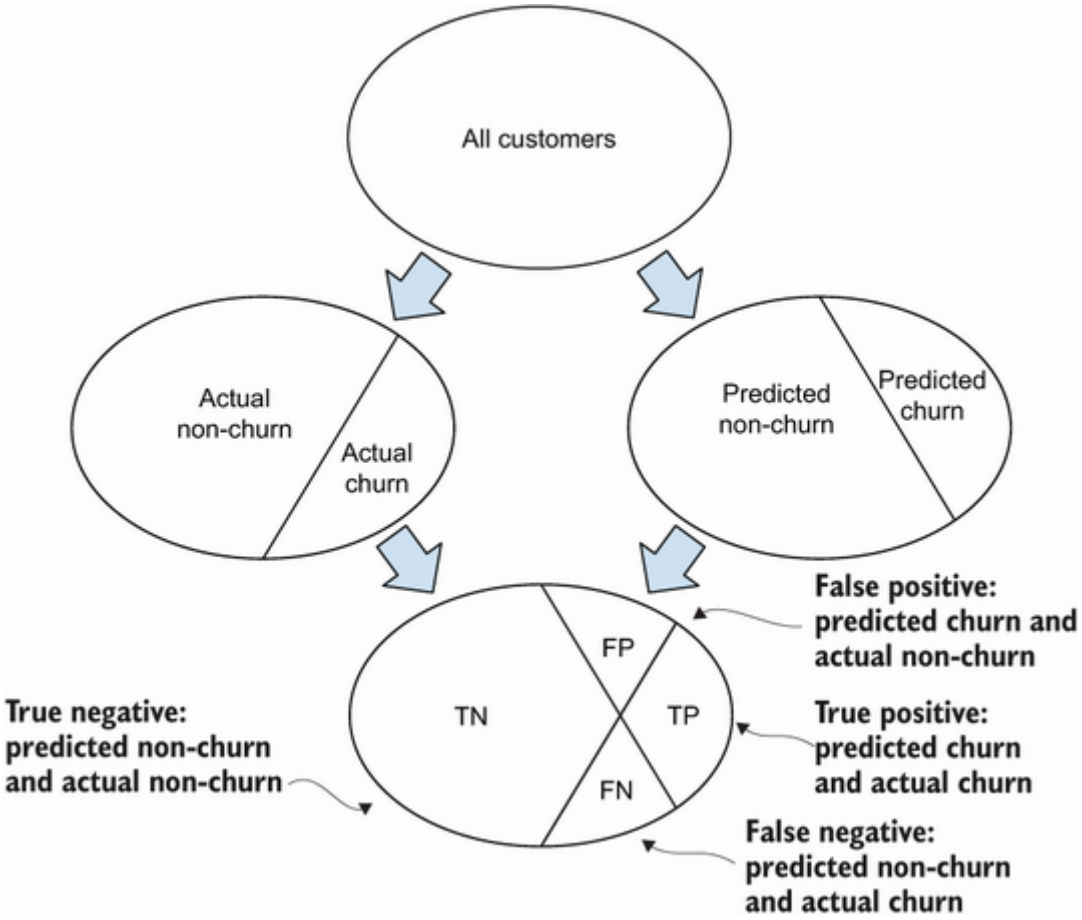


Figure 4.10 When we apply the model to the validation dataset, we get four different outcomes (TN, FP, TP, and FN).

To calculate the confusion table, we need to do these steps:

- First, the predictions split the dataset into two parts: the part for which we predict True ("churn") and the part for which we predict False ("no churn").
- At the same time, the target variable splits this dataset into two different parts: the customers who actually churned ("1" in `y_val`) and the customers who didn't ("0" in `y_val`).

- When we combine these splits, we get four groups of customers, which are exactly the four different outcomes from the confusion table.

Translating these steps to NumPy is straightforward:

```
t = 0.5                                                    ❶
predict_churn = (y_pred >= t)                              ❶
predict_no_churn = (y_pred < t)                            ❶

actual_churn = (y_val == 1)                                ❷
actual_no_churn = (y_val == 0)                             ❷

true_positive = (predict_churn & actual_churn).sum()       ❸
false_positive = (predict_churn & actual_no_churn).sum()   ❹

false_negative = (predict_no_churn & actual_churn).sum()   ❺
true_negative = (predict_no_churn & actual_no_churn).sum() ❻
```

❶ Makes predictions at threshold 0.5

❷ Gets the actual target values

❸ Calculates true positives (cases when we predicted churn correctly)

❹ Calculates false positives (cases when we predicted churn, but the customers didn't churn)

❺ Calculates true negatives (cases when we predicted no churn correctly)

❻ Calculates false negatives (cases when we predicted no churn, but the customers churned)

We begin by making predictions at the threshold of 0.5.

The results are two NumPy arrays:

- In the first array (`predict_churn`), an element is True if the model thinks the respective customer is going to churn and False otherwise.
- Likewise, in the second array (`predict_no_churn`), True means that the model thinks the customer isn't going to churn.

The second array, `predict_no_churn` , is the exact opposite of `predict_churn` : if an element is True in `predict_churn` , it's False in `predict_no_churn` and vice versa (figure 4.11). This is the first split of the validation dataset into two parts—the one that's based on the predictions.

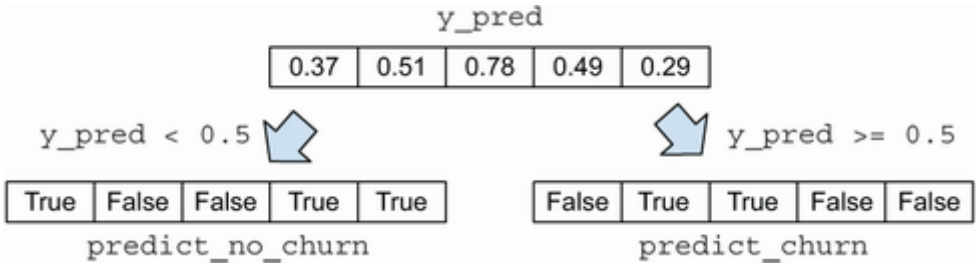


Figure 4.11 Splitting the predictions into two Boolean NumPy arrays: `predict_churn` if the probability is higher than 0.5, and `predict_no_churn` if it's lower

Next, we record the actual values of the target variable in ❷. The results are two NumPy arrays as well (figure 4.12):

- If the customer churned (value “1”), then the respective element of `actual_ churn` is True, and it’s False otherwise.
- For `actual_no_churn` it’s exactly the opposite: it’s True when the customer didn’t churn.

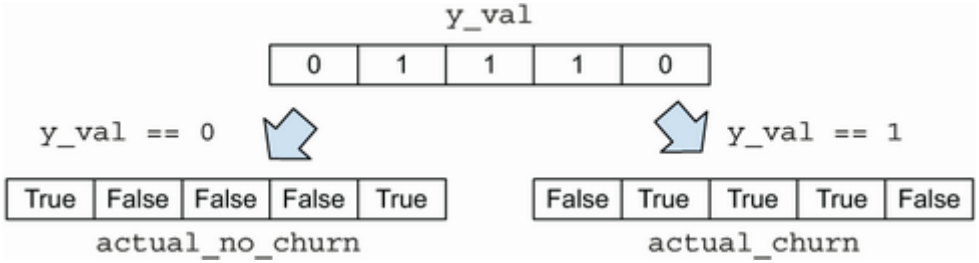


Figure 4.12 Splitting the array with actual values into two Boolean NumPy arrays: `actual_no_churn` if the customer didn’t churn (`y_val == 0`) and `actual_churn` if the customer churned (`y_val == 1`)

That’s the second split of the dataset—the one that’s based on the target variable.

Now we combine these two splits—or, to be exact, these four NumPy arrays.

To calculate the number of true positive outcomes in ❸, we use the logical “and” operator of NumPy (`&`) and the `sum` method:

```
true_positive = (predict_churn & actual_churn).sum()
```

The logical “and” operator evaluates to True only if both values are True. If at least one is False or both are False, it’s False. In case of `true_posi-`

`tive`, it will be True only if we predict "churn" and the customer actually churned (figure 4.13).

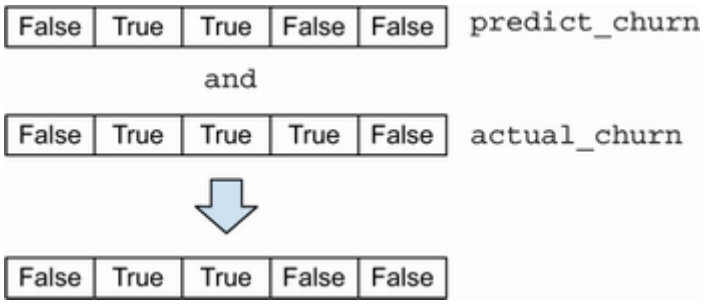


Figure 4.13 Applying the element-wise and operator (`&`) to two NumPy arrays, `predict_churn` and `actual_churn`; this creates another array with True in any position where both arrays contained True and False in all others.

Then we use the `sum` method from NumPy, which simply counts how many `True` values are in the array. It does that by first casting the Boolean array to integers and then summing it (figure 4.14). We already saw similar behavior in the previous chapter when we used the `mean` method.

Figure 4.14 Invoking the `sum` method on a Boolean array: we get the number of elements in this array that are True.

As a result, we have the number of true positive cases. The other values are computed similarly in lines ❹, ❺, and ❻.

Now we just need to put all these values together in a NumPy array:

```
confusion_table = np.array(
 [[true_negative, false_positive],
 [false_negative, true_positive]])
```

When we print it, we get the following numbers:

```
[[1202, 172],
 [ 197, 289]]
```

The absolute numbers may be difficult to understand, so we can turn them into fractions by dividing each value by the total number of items:

```
confusion_table / confusion_table.sum()
```

This prints the following numbers:

```
[[0.646, 0.092],
[0.105, 0.155]]
```

We can summarize the results in a table (table 4.1). We see that the model predicts negative values quite well: 65% of the predictions are true negatives. However, it makes quite a few mistakes of both types: the number of false positives and false negatives is roughly equal (9% and 11%, respectively).

Table 4.1 The confusion table for the churn classifier at the threshold of 0.5. We see that it's easy for the model to correctly predict non-churning users, but it's more difficult for it to identify churning users.

Full model with all features			
		Predicted	
		False	True
Actual	False	1202 (65%)	172 (9%)
	True	197 (11%)	289 (15%)

This table gives us a better understanding of the performance of the model—it's now possible to break down the performance into different components and understand where the model makes mistakes. We actually see that the performance of the model is not great: it makes quite a few errors when trying to identify users that will churn. This is something we couldn't see with the accuracy score alone.

We can repeat the same process for the small model using exactly the same code (table 4.2).

Table 4.2 The confusion table for the small model

Small model with three features	
	Predicted

		False	True
Actual	False	1189 (63%)	185 (10%)
	True	248 (12%)	238 (13%)

When we compare the smaller model with the full model, we see that it's 2% worse at correctly identifying non-churning users (63% versus 65% for true negatives) and 2% worse at correctly identifying churning users (13% versus 15% for true positives), which together accounts for the 4% difference between the accuracies of these two models (76% versus 80%).

The values from the confusion table serve as the basis for many other evaluation metrics. For example, we can calculate accuracy by taking all the correct predictions—TN and TP together—and dividing that number by the total number of observations in all four cells of the table:

accuracy = (TN + TP) / (TN + TP + FN + FP)

Apart from accuracy, we can calculate other metrics based on the values from the confusion table. The most useful ones are precision and recall, which we will cover next.

Exercise 4.1

What is a false positive?

a) A customer for whom we predicted “not churn,” but they stopped using our services

b) A customer for whom we predicted “churn,” but they didn’t churn

c) A customer for whom we predicted “churn,” and they churned

4.2.3 Precision and recall

As already mentioned, accuracy can be misleading when dealing with imbalanced datasets such as ours. Other metrics are helpful to use for such cases: precision and recall.

Both precision and recall are calculated from the values of the confusion table. They both help us understand the quality of the model in cases of class imbalance.

Let’s start with precision. The precision of a model tells us how many of the positive predictions turned out to be correct. It’s the fraction of correctly predicted positive examples. In our case, it’s the number of customers who actually churned (TP) out of all the customers we thought would churn (TP + FP) (figure 4.15):

P = TP / (TP + FP)

For our model, the precision is 62%:

P = 289 / (289 + 172) = 172 / 461 = 0.62

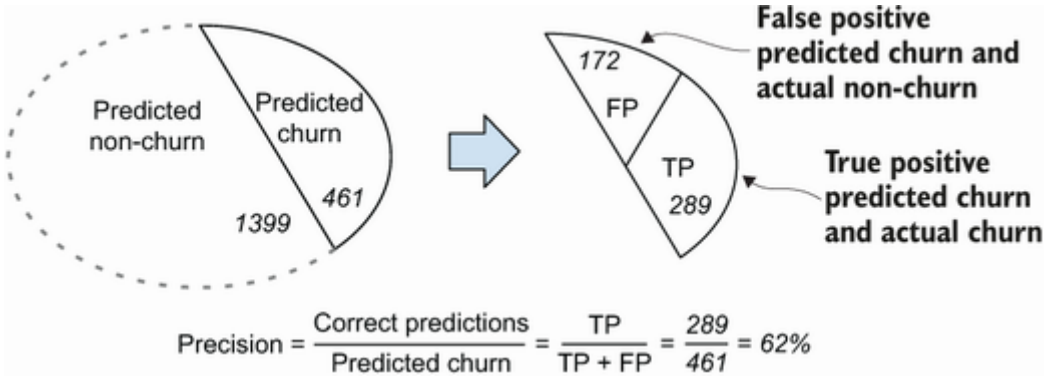


Figure 4.15 The precision of a model is the fraction of correct predictions (TP) among all positive predictions (TP + FP).

Recall is the fraction of correctly classified positive examples among all positive examples. In our case, to calculate recall we first look at all the customers who churned and see how many of them we managed to identify correctly.

The formula for calculating recall is

R = TP / (TP + FN)

Like in the formula for precision, the numerator is the number of true positives, but the denominator is different: it's the number of all positive examples (`y_val == 1`) in our validation dataset (figure 4.16).

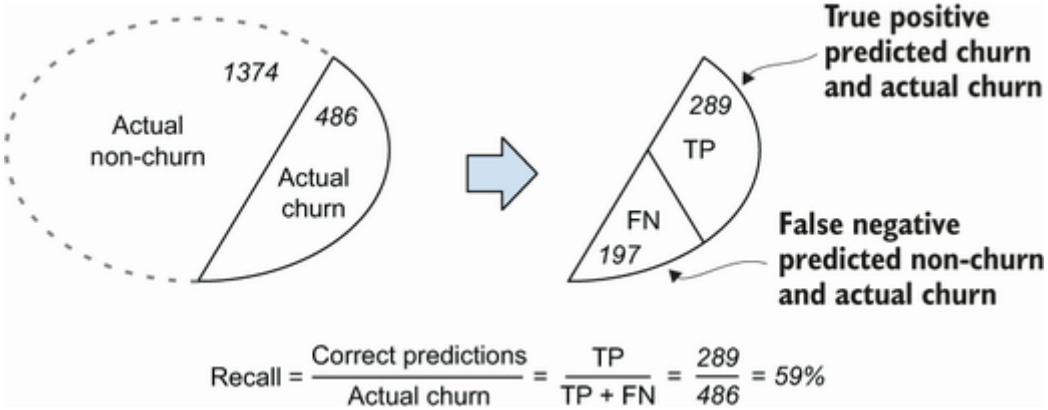


Figure 4.16 The recall of a model is the fraction of correctly predicted churning customers (TP) among all customers who churned (TP + FN).

For our model, the recall is 59%:

R = 286 / (289 + 197) = 289 / 486 = 0.59

The difference between precision and recall may seem subtle at first. In both cases, we look at the number of correct predictions, but the difference is in the denominators (figure 4.17):

- Precision: what's the percent of correct predictions (TP) among customers predicted as churning (TP + FP)?
- Recall: what's the percentage correctly predicted as churning (TP) among all churned customers (TP + FN)?

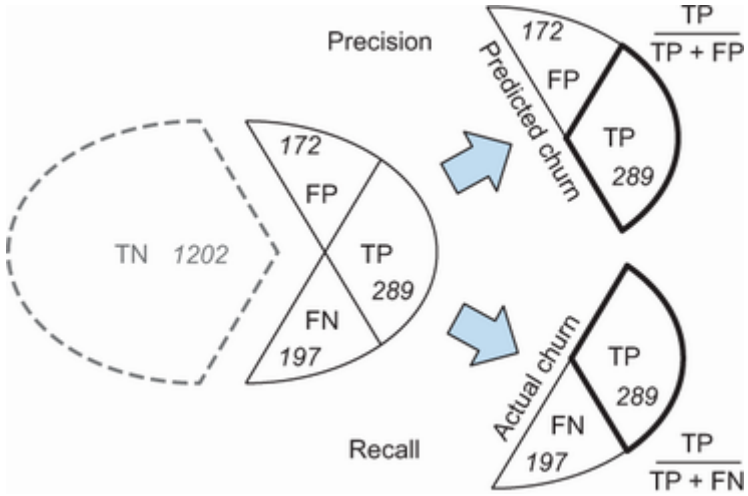


Figure 4.17 Both precision and recall look at the correct predictions (TP), but the denominators are different. For precision, it's the number of customers predicted as churning, whereas for recall, it's the number of customers who churned.

We can also see that both precision and recall don't take true negatives into account (figure 4.17). This is exactly why they are good evaluation metrics for imbalanced datasets. For situations with class imbalance, true negatives typically outnumber everything else—but at the same time, they are also often not really interesting for us. Let's see why.

The goal of our project is to identify customers who are likely to churn. Once we do, we can send them promotional messages in the hopes that they'll change their mind.

When doing this, we make two types of mistakes:

- We accidentally send messages to people who weren't going to churn —these people are the false positives of the model.

- We also sometimes fail to identify people who are actually going to churn. We don't send messages to these people—they are our false negatives.

Precision and recall help us quantify these errors.

Precision helps us understand how many people received a promotional message by mistake. The better the precision, the fewer false positives we have. The precision of 62% means that 62% of the reached customers indeed were going to churn (our true positives), whereas the remaining 38% were not (false positives).

Recall helps us understand how many of the churning customers we failed to find. The better the recall, the fewer false negatives we have. The recall of 59% means that we reach only 59% of all churning users (true positives) and fail to identify the remaining 41% (false negatives).

As we can see, in both cases, we don't really need to know the number of true negatives: even though we can correctly identify them as not churning, we aren't going to do anything with them.

Although the accuracy of 80% might suggest that the model is great, looking at its precision and recall tells us that it actually makes quite a few errors. This is typically not a deal-breaker: with machine learning it's inevitable that models make mistakes, and at least now we have a better and more realistic understanding of the performance of our churn-prediction model.

Precision and recall are useful metrics, but they describe the performance of a classifier only at a certain threshold. Often it's useful to have a metric that summarizes the performance of a classifier for all possible threshold choices. We look at such metrics in the next section.

Exercise 4.2

What is precision?

a) The percent of correctly identified churned customers in the validation dataset

b) The percent of customers who actually churned among the customers who we predicted as churning

---

Exercise 4.3

What is recall?

a) The percent of correctly identified churned customers among all churned customers

b) The percent of correctly classified customers among customers we predicted as churning

3 ROC curve and AUC score

The metrics we have covered so far work only with binary predictions—when we have only True and False values in the output. However, we do

have ways to evaluate the performance of a model across all possible threshold choices. ROC curves is one of these options.

ROC stands for “receiver operating characteristic,” and it was initially designed for evaluating the strength of radar detectors during World War II. It was used to assess how well a detector could separate two signals: whether an airplane was there or not. Nowadays it’s used for a similar purpose: it shows how well a model can separate two classes, positive and negative. In our case, these classes are “churn” and “no churn.”

We need two metrics for ROC curves: TPR and FPR, or true positive rate and false positive rate. Let’s take a look at these metrics.

4.3.1 True positive rate and false positive rate

The ROC curve is based on two quantities, FPR and TPR:

- False positive rate (FPR): the fraction of false positives among all negative examples
- True positive rate (TPR): the fraction of true positives among all positive examples

Like precision and recall, these values are based on the confusion matrix. We can calculate them using the following formulas:

FPR = FP / (FP + TN)

TPR = TP / (TP + FN)

FPR and TPR involve two separate parts of the confusion table (figure 4.18):

- For FPR, we look at the first row of the table: the fraction of false positives among all negatives.
- For TPR, we look at the second row of the table: the fraction of true positives among all positives.

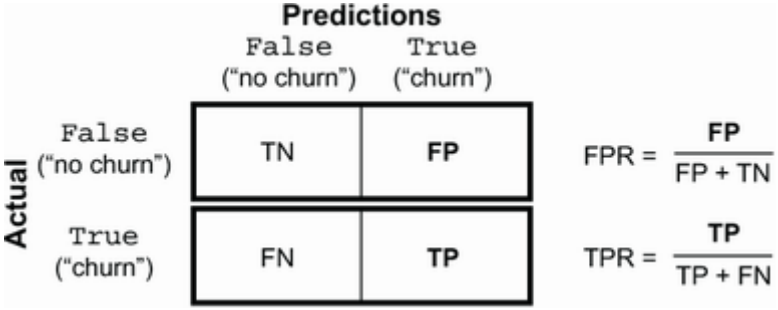


Figure 4.18 For calculating FPR, we look at the first row of the confusion table, and for calculating TPR, we look at the second row.

Let's calculate these values for our model (figure 4.19):

FPR = 172 / 1374 = 12.5%

FPR is the fraction of users we predicted as churning among everybody who didn't churn. A small value for FPR tells us that a model is good—it has few false positives:

TPR = 289 / 486 = 59%

TPR is the fraction of users who we predicted as churning among everybody who actually did churn. Note that TPR is the same as recall, so the

higher the TPR is, the better.

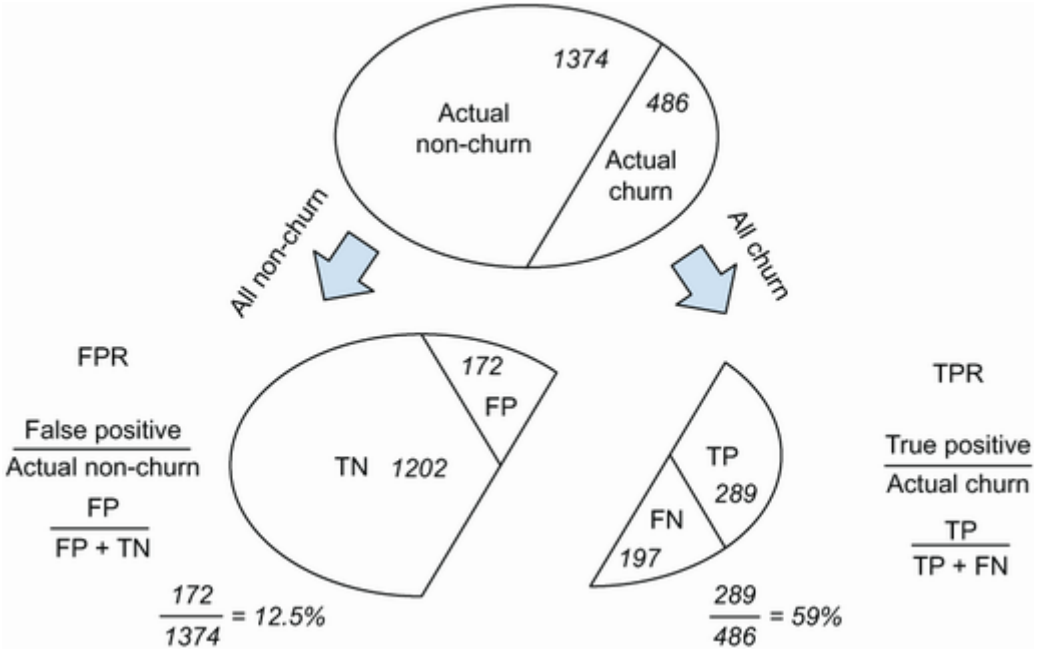


Figure 4.19 FPR is the fraction of false positives among all non-churning customers: the smaller the FPR, the better. TPR is the fraction of true positives among all churning customers: the larger the TPR, the better.

However, we still consider FPR and TPR metrics at only one threshold value—in our case, 0.5. To be able to use them for ROC curves, we need to calculate these metrics for many different threshold values.

4.3.2 Evaluating a model at multiple thresholds

Binary classification models, such as logistic regression, typically output a probability—a score between zero and one. To make actual predictions, we binarize the output by setting some threshold to get only True and False values.

Instead of evaluating the model at one particular threshold, we can do it for a range of them—in the same way we did it for accuracy earlier in this chapter.

For that, we first iterate over different threshold values and compute the values of the confusion table for each.

Listing 4.1 Computing the confusion table for different thresholds

```
scores = []                                          ❶

thresholds = np.linspace(0, 1, 101)                  ❷

for t in thresholds:                                 ❷
    tp = ((y_pred >= t) & (y_val == 1)).sum()        ❸
    fp = ((y_pred >= t) & (y_val == 0)).sum()        ❸
    fn = ((y_pred < t) & (y_val == 1)).sum()         ❸
    tn = ((y_pred < t) & (y_val == 0)).sum()         ❸
    scores.append((t, tp, fp, fn, tn))               ❹
```

❶ Creates a list where we'll keep the results

❷ Creates an array with different threshold values, and loops over them

❸ Computes the confusion table for predictions at each threshold

❹ Appends the results to the scores list

The idea is similar to what we previously did with accuracy, but instead of recording just one value, we record all the four outcomes for the confu-

sion table.

It's not easy to deal with a list of tuples, so let's convert it to a Pandas dataframe:

```
df_scores = pd.DataFrame(scores)                                    ❶
df_scores.columns = ['threshold', 'tp', 'fp', 'fn', 'tn']           ❷
```

❶ Turns the list into a Pandas dataframe

❷ Assigns names to the columns of the dataframe

This gives us a dataframe with five columns (figure 4.20).

```
df_scores[::10]
```

	threshold	tp	fp	fn	tn
0	0.0	486	1374	0	0
10	0.1	458	726	28	648
20	0.2	421	512	65	862
30	0.3	380	350	106	1024
40	0.4	337	257	149	1117
50	0.5	289	172	197	1202
60	0.6	200	105	286	1269
70	0.7	99	34	387	1340
80	0.8	7	1	479	1373
90	0.9	0	0	486	1374
100	1.0	0	0	486	1374

Figure 4.20 The dataframe with the elements of the confusion matrix evaluated at different threshold levels. The `[::10]` expression selects every 10th record of the dataframe.

Now we can compute the TPR and FPR scores. Because the data is now in a dataframe, we can do it for all the values at once:

```
df_scores['tpr'] = df_scores.tp / (df_scores.tp + df_scores.fn)
df_scores['fpr'] = df_scores.fp / (df_scores.fp + df_scores.tn)
```

After running this code, we have two new columns in the dataframe: tpr and fpr (figure 4.21).

```
df_scores[::10]
```

	threshold	tp	fp	fn	tn	tpr	fpr
0	0.0	486	1374	0	0	1.000000	1.000000
10	0.1	458	726	28	648	0.942387	0.528384
20	0.2	421	512	65	862	0.866255	0.372635
30	0.3	380	350	106	1024	0.781893	0.254731
40	0.4	337	257	149	1117	0.693416	0.187045
50	0.5	289	172	197	1202	0.594650	0.125182
60	0.6	200	105	286	1269	0.411523	0.076419
70	0.7	99	34	387	1340	0.203704	0.024745
80	0.8	7	1	479	1373	0.014403	0.000728
90	0.9	0	0	486	1374	0.000000	0.000000
100	1.0	0	0	486	1374	0.000000	0.000000

Figure 4.21 The dataframe with the values of the confusion matrix as well as TPR and FPR evaluated at different thresholds

Let's plot them (figure 4.22):

```
plt.plot(df_scores.threshold, df_scores.tpr, label='TPR')
plt.plot(df_scores.threshold, df_scores.fpr, label='FPR')
plt.legend()
```

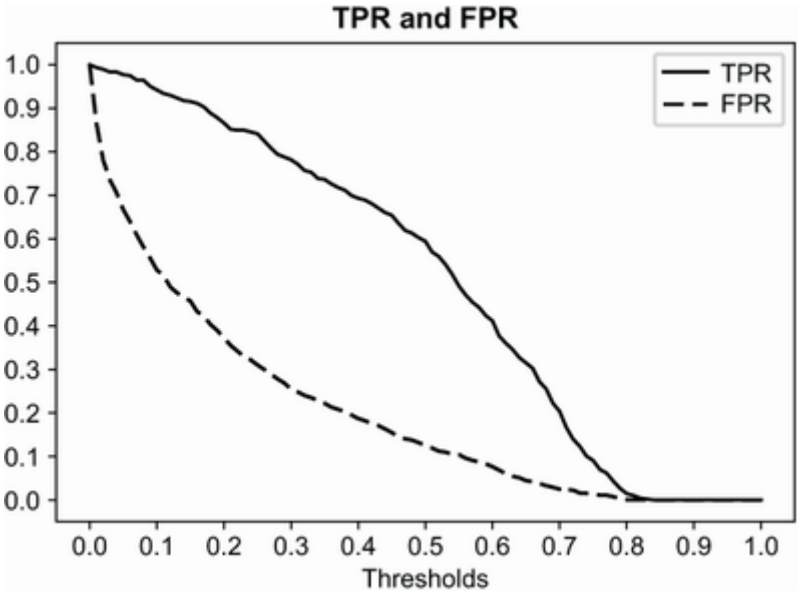


Figure 4.22 The TPR and FPR for our model, evaluated at different thresholds

Both TPR and FPR start at 100%—at the threshold of 0.0, we predict "churn" for everyone:

- FPR is 100% because we have only false positives in the prediction. There are no true negatives: nobody is predicted as non-churning.
- TPR is 100% because we have only true positives and no false negatives.

As the threshold grows, both metrics decline but at different rates.

Ideally, FPR should go down very quickly. A small FPR indicates that the model makes very few mistakes predicting negative examples (false positives).

On the other hand, TPR should go down slowly, ideally staying near 100% all the time: that will mean that the model predicts true positives well.

To better understand what these TPR and FPR mean, let's compare it with two baseline models: a random model and the ideal model. We will start with a random model.

4.3.3 Random baseline model

A random model outputs a random score between 0 and 1, regardless of the input. It's easy to implement—we simply generate an array with uniform random numbers:

```
np.random.seed(1)                                    ❶
y_rand = np.random.uniform(0, 1, size=len(y_val))    ❷
```

❶ Fixes the random seed for reproducibility

❷ Generates an array with random numbers between 0 and 1

Now we can simply pretend that `y_rand` contains the predictions of our "model."

Let's calculate FPR and TPR for our random model. To make it simpler, we'll reuse the code we wrote previously and put it into a function.

Listing 4.2 Function for calculating TPR and FPR at different thresholds

```
def tpr_fpr_dataframe(y_val, y_pred):                                  ❶
    scores = []                                                        ❷

    thresholds = np.linspace(0, 1, 101)                                ❷

    for t in thresholds:                                               ❷
        tp = ((y_pred >= t) & (y_val == 1)).sum()                      ❷
        fp = ((y_pred >= t) & (y_val == 0)).sum()                      ❷
        fn = ((y_pred < t) & (y_val == 1)).sum()                       ❷
        tn = ((y_pred < t) & (y_val == 0)).sum()                       ❷
        scores.append((t, tp, fp, fn, tn))                             ❷
    df_scores = pd.DataFrame(scores)                                   ❸
    df_scores.columns = ['threshold', 'tp', 'fp', 'fn', 'tn']          ❸

    df_scores['tpr'] = df_scores.tp / (df_scores.tp + df_scores.fn)    ❹
    df_scores['fpr'] = df_scores.fp / (df_scores.fp + df_scores.tn)    ❹

    return df_scores                                                   ❺
```

❶ Defines a function that takes in actual and predicted values

❷ Calculates the confusion table for different thresholds

❸ Converts the confusion table numbers to a dataframe

❹ Calculates TPR and FPR using the confusion table numbers

❺ Returns the resulting dataframe

Now let's use this function to calculate the TPR and FPR for the random model:

```
df_rand = tpr_fpr_dataframe(y_val, y_rand)
```

This creates a dataframe with TPR and FPR values at different thresholds (figure 4.23).

```
np.random.seed(1)
y_rand = np.random.uniform(0, 1, size=len(y_val))
df_rand = tpr_fpr_dataframe(y_val, y_rand)
df_rand[::10]
```

	threshold	tp	fp	fn	tn	tpr	fpr
0	0.0	486	1374	0	0	1.000000	1.000000
10	0.1	440	1236	46	138	0.905350	0.899563
20	0.2	392	1101	94	273	0.806584	0.801310
30	0.3	339	972	147	402	0.697531	0.707424
40	0.4	288	849	198	525	0.592593	0.617904
50	0.5	239	723	247	651	0.491770	0.526201
60	0.6	193	579	293	795	0.397119	0.421397
70	0.7	152	422	334	952	0.312757	0.307132
80	0.8	98	302	388	1072	0.201646	0.219796
90	0.9	57	147	429	1227	0.117284	0.106987
100	1.0	0	0	486	1374	0.000000	0.000000

Figure 4.23 The TPR and FPR values of a random model

Let's plot them:

```
plt.plot(df_rand.threshold, df_rand.tpr, label='TPR')
plt.plot(df_rand.threshold, df_rand.fpr, label='FPR')
```

```
plt.legend()
```

We see that both TPR and FPR curves go from 100% to 0%, almost following the straight line (figure 4.24).

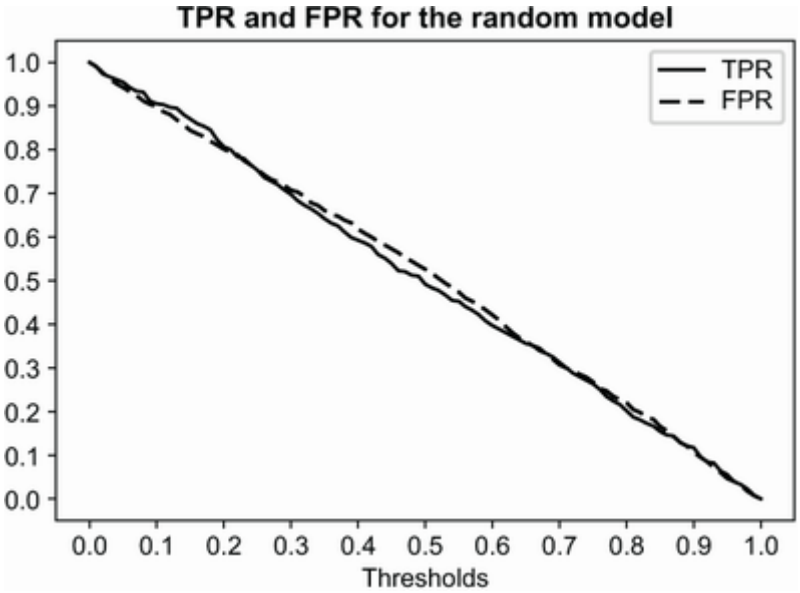


Figure 4.24 Both TPR and FPR of a random classifier decrease from 100% to 0% as a straight line.

At the threshold of 0.0, we treat everybody as churning. Both TPR and FPR are 100%:

- FPR is 100% because we have only false positives: all non-churning customers are identified as churning.
- TPR is 100% because we have only true positives: we can correctly classify all churning customers as churning.

As we increase the threshold, both TPR and FPR decrease.

At the threshold of 0.4, the model with a probability of 40% predicts "non-churn," and with a probability of 60% predicts "churn." Both TPR and FPR are 60%:

- FPR is 60% because we incorrectly classify 60% of non-churning customers as churning.
- TPR is 60% because we correctly classify 60% of churning customers as churning.

Finally, at 1.0, both TPR and FPR are 0%. At this threshold, we predict everybody as non-churning:

- FPR is 0% because we have no false positives: we can correctly classify all non-churning customers as non-churning.
- TPR is 0% because we have no true positives: all churning customers are identified as non-churning.

Let's now move on to the next baseline and see how TPR and FPR look for the ideal model.

1.3.4 The ideal model

The ideal model always makes correct decisions. We'll take it a step further and consider the ideal ranking model. This model outputs scores in such a way that churning customers always have higher scores than non-churning ones. In other words, the predicted probability for all churned ones should be higher than the predicted probability for non-churned ones.

So, if we apply the model to all the customers in our validation set and then sort them by the predicted probability, we first will have all the non-churning customers, followed by the churning ones (figure 4.25).

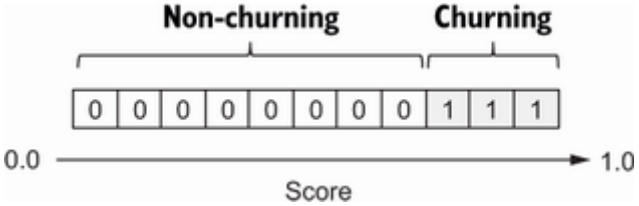


Figure 4.25 The ideal model orders customers such that first we have non-churning customers and then churning ones.

Of course, we cannot have such a model in real life. It's still useful, however: we can use it for comparing our TPR and FPR to the TPR and FPR of the ideal model.

Let's generate the ideal predictions. To make it easier, we generate an array with fake target variables that are already ordered: first it contains only 0s and then only 1s (figure 4.25). As for "predictions," we simply can create an array with numbers that grow from 0 in the first cell to 1 in the last cell using the `np.linspace` function.

Let's do it:

```
num_neg = (y_val == 0).sum()                          ❶
num_pos = (y_val == 1).sum()                          ❶

y_ideal = np.repeat([0, 1], [num_neg, num_pos])       ❷
y_pred_ideal = np.linspace(0, 1, num_neg + num_pos)   ❸
```

```
df_ideal = tpr_fpr_dataframe(y_ideal, y_pred_ideal)    ❹
```

❶ Calculates the number of negative and positive examples in the dataset

❷ Generates an array that first repeats 0s num_neg number of times, followed by 1s repeated num_pos number of times

❸ Generates the predictions of the "model": numbers that grow from 0 in the first cell to 1 in the last

❹ Computes the TPR and FPR curves for the classifier

As a result, we get a dataframe with the TPR and FPR values of the ideal model (figure 4.26). You can read more about `np.linspace` and `np.repeat` functions in appendix C.

	threshold	tp	fp	fn	tn	tpr	fpr
0	0.0	486	1374	0	0	1.000000	1.000000
10	0.1	486	1188	0	186	1.000000	0.864629
20	0.2	486	1002	0	372	1.000000	0.729258
30	0.3	486	816	0	558	1.000000	0.593886
40	0.4	486	630	0	744	1.000000	0.458515
50	0.5	486	444	0	930	1.000000	0.323144
60	0.6	486	258	0	1116	1.000000	0.187773
70	0.7	486	72	0	1302	1.000000	0.052402
80	0.8	372	0	114	1374	0.765432	0.000000
90	0.9	186	0	300	1374	0.382716	0.000000
100	1.0	1	0	485	1374	0.002058	0.000000

Figure 4.26 The TPR and FPR values for the ideal model

Now we can plot it (figure 4.27):

```
plt.plot(df_ideal.threshold, df_ideal.tpr, label='TPR')
plt.plot(df_ideal.threshold, df_ideal.fpr, label='FPR')
plt.legend()
```

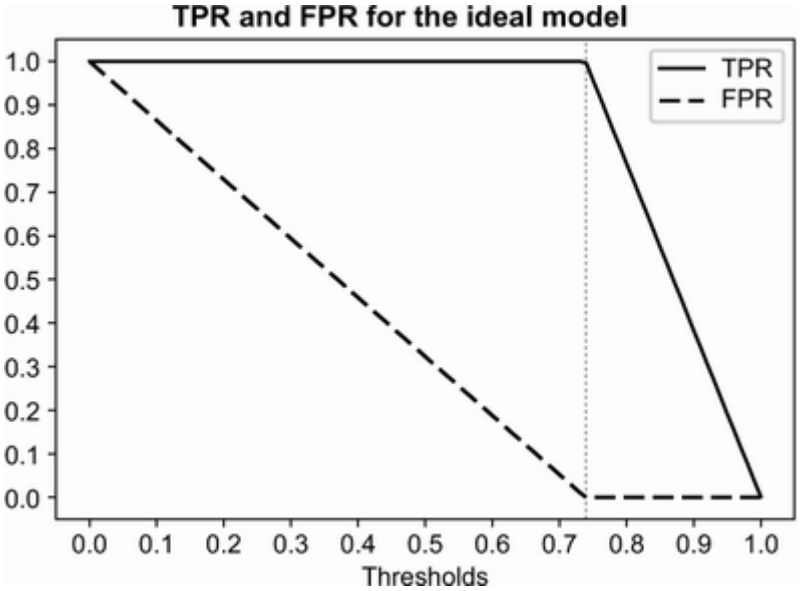


Figure 4.27 The TPR and FPR curves for the ideal model

From the plot, we can see that

- Both TPR and FPR start at 100% and end at 0%.
- For thresholds lower than 0.74, we always correctly classify all churning customers as churning; that's why TRP stays at 100%. On the other hand, we incorrectly classify some non-churning ones as churning—those are our false positives. As we increase the threshold, fewer and fewer non-churning customers are classified as churning, so FPR goes down. At 0.6, we misclassify 258 non-churning customers as churning (figure 4.28, A).
- The threshold of 0.74 is the ideal situation: all churning customers are classified as churning, and all non-churning are classified as non-churning; that's why TPR is 100% and FPR is 0% (figure 4.28, B).

- Between 0.74 and 1.0, we always correctly classify all non-churning customers, so FPR stays at 0%. However, as we increase the threshold, we start incorrectly classifying more and more churning customers as non-churning, so TPR goes down. At 0.8, 114 out of 446 churning customers are incorrectly classified as non-churning. Only 372 predictictions are correct, so TPR is 76% (figure 4.28, C).

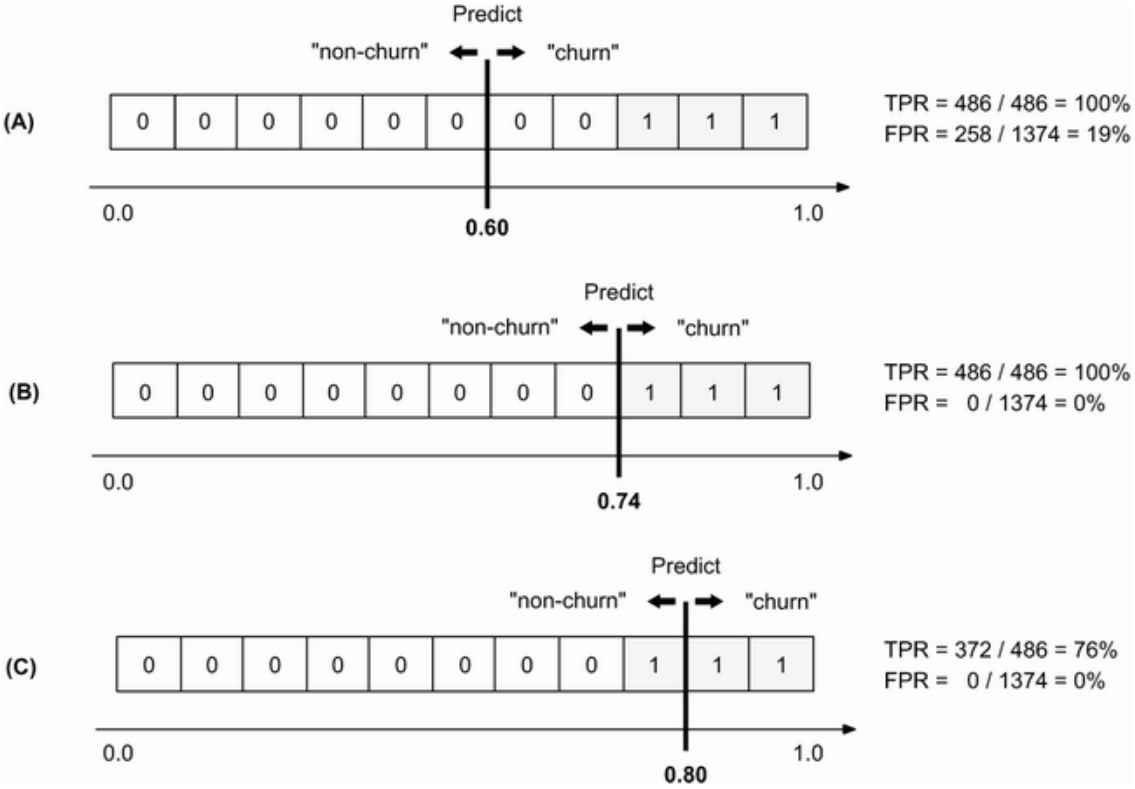


Figure 4.28 TPR and FPR of the ideal ranking model evaluated at different thresholds

Now we're ready to build the ROC curve.

Exercise 4.4

What does the ideal ranking model do?

a) When applied to the validation data, it scores the customers such that for non-churning customers, the score is always lower than for churning ones.

b) It scores non-churning customers higher than churning ones.

4.3.5 ROC Curve

To create an ROC curve, instead of plotting FPR and TPR against different threshold values, we plot them against each other. For comparison, we also add the ideal and random models to the plot:

```
plt.figure(figsize=(5, 5))                                  ❶

plt.plot(df_scores.fpr, df_scores.tpr, label='Model')       ❷
plt.plot(df_rand.fpr, df_rand.tpr, label='Random')          ❷
plt.plot(df_ideal.fpr, df_ideal.tpr, label='Ideal')         ❷

plt.legend()
```

❶ Makes the plot square

❷ Plots the ROC curve for the model and baselines

As a result, we get an ROC curve (figure 4.29). When we plot it, we can see that the ROC curve of the random classifier is an approximately straight line from bottom left to top right. For the ideal model, however, the curve

first goes up until it reaches 100% TPR, and from there it goes right until it reaches 100% FPR.

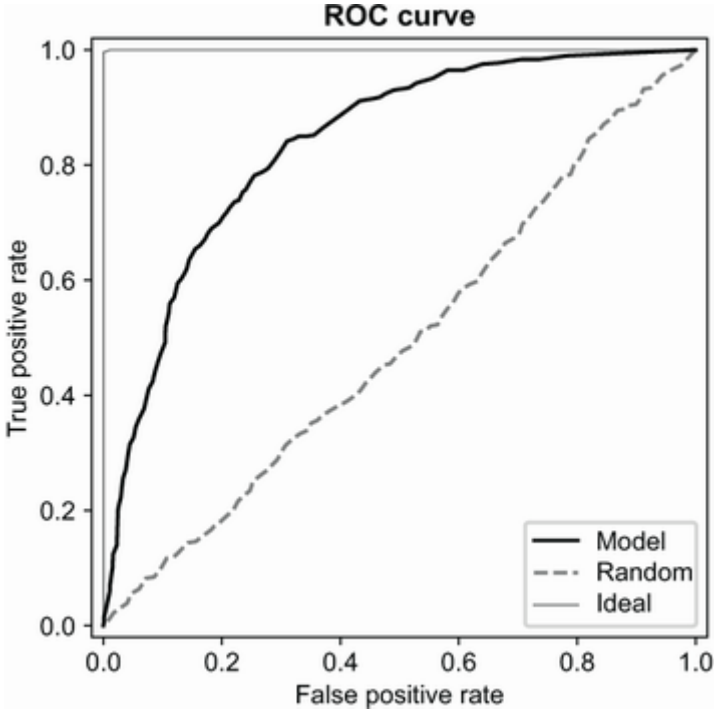


Figure 4.29 The ROC curve shows the relationship between the FPR and TPR of a model.

Our models should always be somewhere between these two curves. We want our model to be as close to the ideal curve as possible and as far as possible from the random curve.

The ROC curve of a random model serves as a good visual baseline—when we add it to the plot, it helps us to judge how far our model is from this baseline—so it's a good idea to always include this line in the plot.

However, we don't really need to generate a random model each time we want to have an ROC curve: we know what it looks like, so we can simply include a straight line from (0, 0) to (1, 1) in the plot.

As for the ideal model, we know that it always goes up to (0, 1) and then goes right to (1, 1). The top-left corner is called the "ideal spot": it's the point when the ideal model gets 100% TPR and 0% FPR. We want our models to get as close to the ideal spot as possible.

With this information, we can reduce the code for plotting the curve to the following:

```
plt.figure(figsize=(5, 5))
plt.plot(df_scores.fpr, df_scores.tpr)
plt.plot([0, 1], [0, 1])
```

This produces the result in figure 4.30.

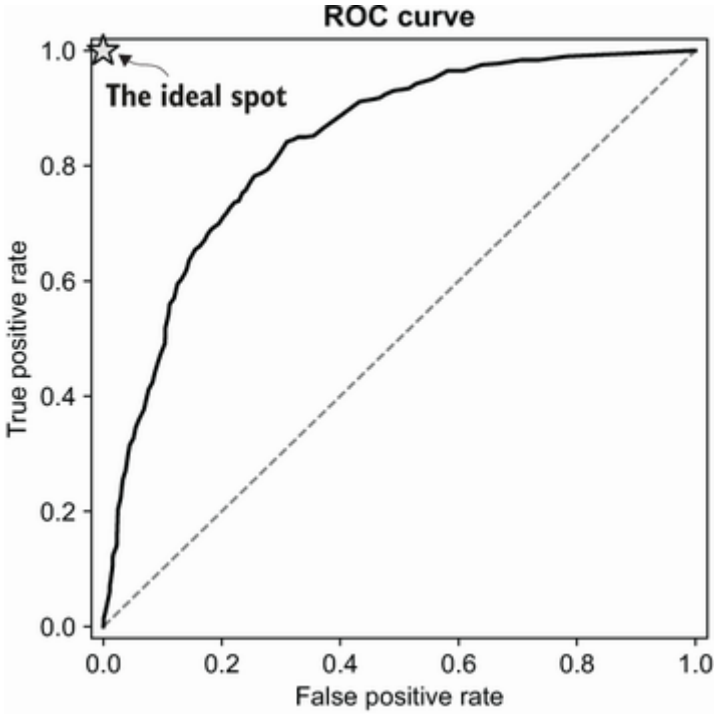


Figure 4.30 The ROC curve. The baseline makes it easier to see how far the ROC curve of our model is from that of a random model. The top-left corner (0, 1) is the "ideal spot": the closer our models get to it, the better.

Although computing all the FPR and TPR values across many thresholds is a good exercise, we don't need to do it ourselves every time we want to plot an ROC curve. We simply can use the `roc_curve` function from the `metrics` package of Scikit-learn:

```
from sklearn.metrics import roc_curve

fpr, tpr, thresholds = roc_curve(y_val, y_pred)

plt.figure(figsize=(5, 5))
```

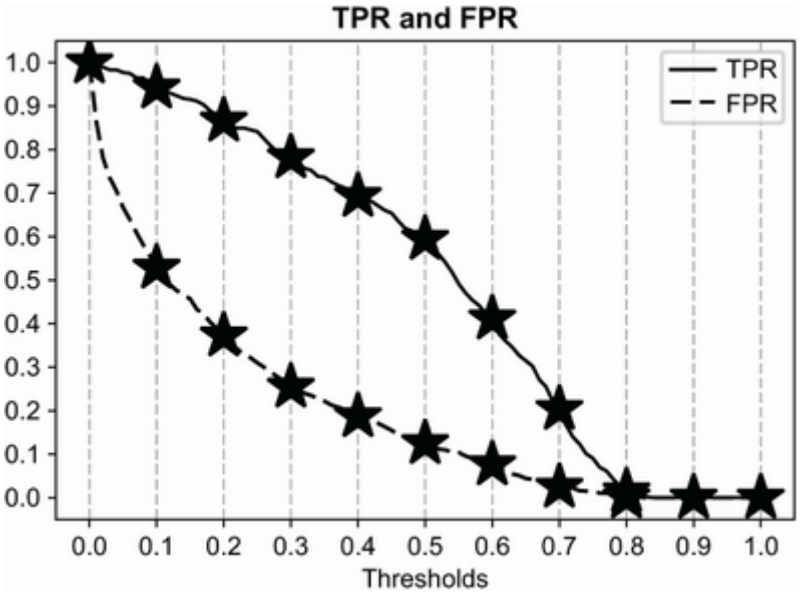
```
plt.plot(fpr, tpr)
plt.plot([0, 1], [0, 1])
```

As a result, we get a plot identical to the previous one (figure 4.30).

Now let's try to make more sense of the curve and understand what it can actually tell us. To do this, we visually map the TPR and FPR values to their thresholds on the ROC curve (figure 4.31).

In the ROC plot, we start from the (0, 0) point—this is the point at the bottom left. It corresponds to 0% FPR and 0% TPR, which happens at high thresholds like 1.0, when no customers are above that score. For these cases we simply end up predicting "no churn" for everyone. That's why our TPR is 0%: we are never correctly predicting churned customers. FPR, on the other hand, is 0% because this dummy model can correctly predict all non-churning customers as non-churning, so there are no false positives.

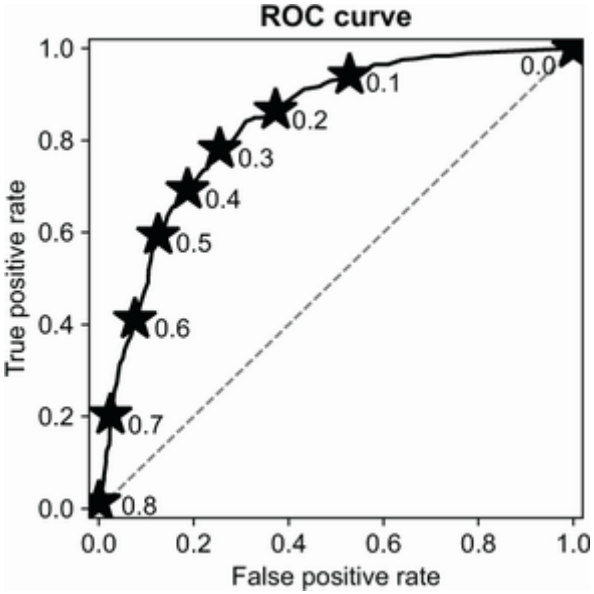
As we go up the curve, we consider FPR and TPR values evaluated at smaller thresholds. At 0.7, FPR changes only slightly, from 0% to 2%, but the TPR increases from 0% to 20% (figure 4.31, B and C).



(A) TPR and FPR at different thresholds

	threshold	fpr	tpr
100	1.0	0.000000	0.000000
90	0.9	0.000000	0.000000
80	0.8	0.000728	0.014403
70	0.7	0.024745	0.203704
60	0.6	0.076419	0.411523
50	0.5	0.125182	0.594650
40	0.4	0.187045	0.693416
30	0.3	0.254731	0.781893
20	0.2	0.372635	0.866255
10	0.1	0.528384	0.942387
0	0.0	1.000000	1.000000

(B) FPR and TPR values of the model for different thresholds



(C) FPR and TPR values for selected thresholds

Figure 4.31 Translation of the TPR and FPR plots against different threshold values (A and B) to the ROC curve (C). In the ROC plot, we start from the bottom left with high threshold values, where most of the customers are predicted as non-churning, and gradually go to the top right with low thresholds, where most of the customers are predicted as churning.

As we follow the line, we keep decreasing the threshold and evaluating the model at smaller values, predicting more and more customers as churning. At some point, we cover most of the positives (churning customers). For example, at the threshold of 0.2, we predict most of the users as churning, which means that many of these predictions are false positives. FPR then starts to grow faster than TPR; at the threshold of 0.2, it's already at almost 40%.

Eventually, we reach the 0.0 threshold and predict that everyone is churning, thus reaching the top-right corner of the ROC plot.

When we start at high threshold values, all models are equal: any model at high threshold values degrades to the constant "model" that predicts False all the time. As we decrease the threshold, we start predicting some of the customers as churning. The better the model, the more customers are correctly classified as churning, resulting in a better TPR. Likewise, good models have a smaller FPR because they have fewer false positives.

Thus, the ROC curve of a good model first goes up as high as it can and only then starts turning right. Poor models, on the other hand, from the start have higher FPRs and lower TPRs, so their curves tend to go to the right earlier (figure 4.32).

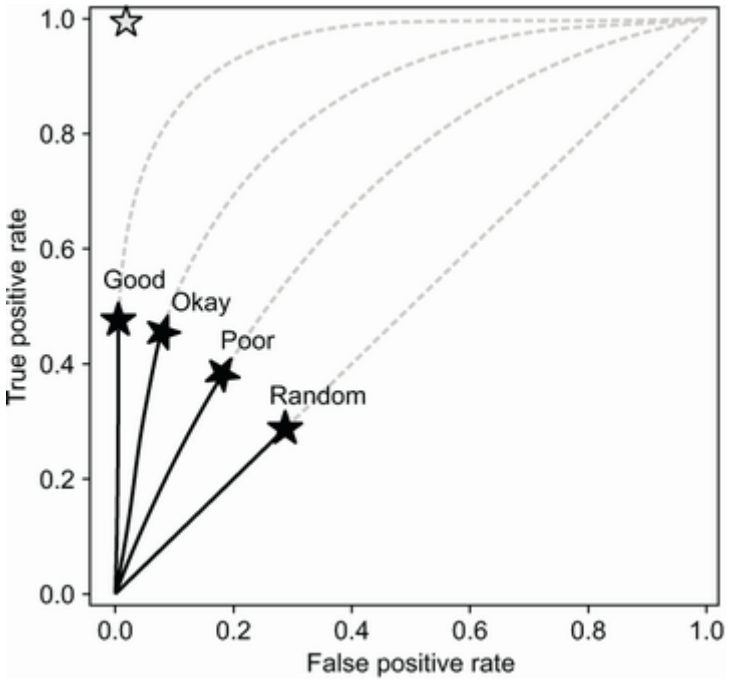


Figure 4.32 ROC curves of good models go up as much as they can before turning right. Poor models, on the other hand, tend to have more false positives from the beginning, so they tend to go right earlier.

We can use this for comparing multiple models: we can simply plot them on the same graph and see which of them is closer to the ideal point of (0, 1). For example, let's take a look at the ROC curves of the large and small models and plot them on the same graph:

```
fpr_large, tpr_large, _ = roc_curve(y_val, y_pred)
fpr_small, tpr_small, _ = roc_curve(y_val, y_pred_small)

plt.figure(figsize=(5, 5))

plt.plot(fpr_large, tpr_large, color='black', label='Large')
plt.plot(fpr_small, tpr_small, color='black', label='Small')
```

```
plt.plot([0, 1], [0, 1])
plt.legend()
```

This way we can get two ROC curves on the same plot (figure 4.33). We can see that the large model is better than the small model: it's closer to the ideal point for all the thresholds.

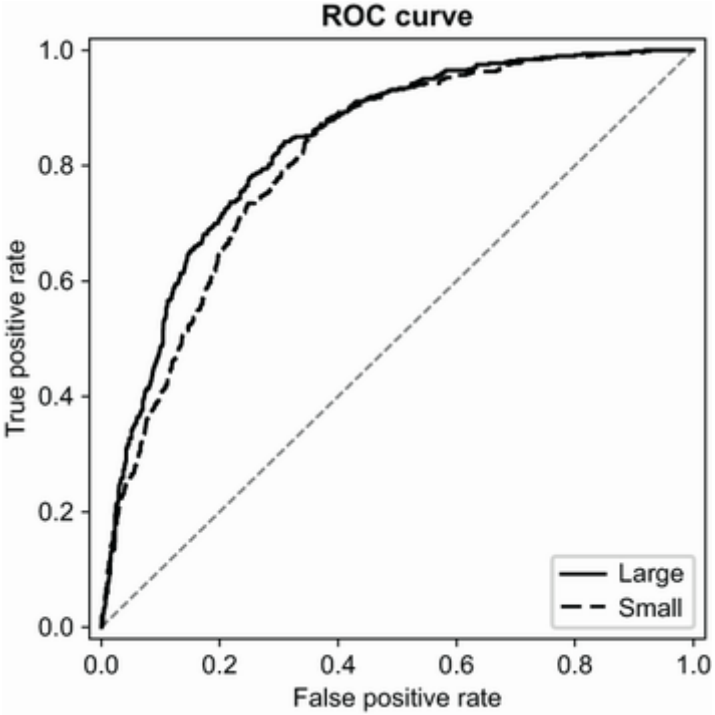


Figure 4.33 Plotting multiple ROC curves on the same graph helps us visually identify which model performs better.

ROC curves are quite useful on their own, but we also have another metric that's based on it: AUC, or the area under the ROC curve.

4.3.6 Area under the ROC curve (AUC)

When evaluating our models using the ROC curve, we want them to be as close to the ideal spot and as far from the random baseline as possible.

We can quantify this "closeness" by measuring the area under the ROC curve. We can use this metric—abbreviated as AU ROC, or often simply AUC—as a metric for evaluating the performance of a binary classification model.

The ideal model forms a 1x1 square, so the area under its ROC curve is 1, or 100%. The random model takes only half of that, so its AUC is 0.5, or 50%. The AUCs of our two models—the large one and the small one—will be somewhere between the random baseline of 50% and the ideal curve of 100%.

IMPORTANT An AUC of 0.9 is indicative of a reasonably good model; 0.8 is okay, 0.7 is not very performant, and 0.6 indicates quite poor performance.

To calculate the AUC for our models we can use `auc`, a function from the `metrics` package of Scikit-learn:

```
from sklearn.metrics import auc
auc(df_scores.fpr, df_scores.tpr)
```

For the large model, the result is 0.84; for the small model, it's 0.81 (figure 4.34). Churn prediction is a complex problem, so an AUC of 80% is quite good.

```
from sklearn.metrics import auc
auc(df_scores.fpr, df_scores.tpr)
```

```
0.8359001084215382
```

```
auc(df_scores_small.fpr, df_scores_small.tpr)
```

```
0.8125475467380692
```

Figure 4.34 The AUC for our models: 84% for the large model and 81% for the small model

If all we need is the AUC, we don't need to compute the ROC curve first. We can take a shortcut and use the `roc_auc_score` function from Scikit-learn, which takes care of everything and simply returns the AUC of our model:

```
from sklearn.metrics import roc_auc_score
roc_auc_score(y_val, y_pred)
```

We get approximately the same results as previously (figure 4.35).

```
from sklearn.metrics import roc_auc_score
roc_auc_score(y_val, y_pred)
```

```
0.8363366398907399
```

```
roc_auc_score(y_val, y_pred_small)
```

```
0.8129354083179088
```

Figure 4.35 Calculating AUC using Scikit-learn's `roc_auc_score` function.

NOTE The values from `roc_auc_score` may be slightly different from AUC computed from the dataframes where we calculated TPR and FPR ourselves: Scikit-learn internally uses a more precise method for creating ROC curves.

ROC curves and AUC scores tell us how well the model separates positive and negative examples. What is more, AUC has a nice probabilistic interpretation: it tells us what the probability is that a randomly selected positive example will have a score higher than a randomly selected negative example.

Suppose we randomly pick a customer that we know churned and a customer who didn't and then apply the model to these customers and see what the score is for each. We want the model to score the churning customer higher than the non-churning one. AUC tells us the probability of that happening: it's the probability that the score of a randomly selected churning customer is higher than the score of a randomly selected non-churning one.

We can verify this. If we do this experiment 10,000 times and then count how many times the score of the positive example was higher than the score of the negative one, the percentage of cases when it's true should roughly correspond to the AUC:

```
neg = y_pred[y_val == 0]                                          ❶
pos = y_pred[y_val == 1]                                          ❷

np.random.seed(1)                                                 ❸
neg_choice = np.random.randint(low=0, high=len(neg), size=10000)  ❹
```

```
pos_choice = np.random.randint(low=0, high=len(pos), size=10000)    ❺
(pos[pos_choice] > neg[neg_choice]).mean()                          ❻
```

❶ Selects the score for all non-churning customers

❷ Selects the score for all churning customers

❸ Fixes the seed to make sure the results are reproducible

❹ Randomly selects 10,000 scores of negative examples (non-churning customers)

❺ Randomly selects 10,000 scores of positive examples (churning customers)

❻ For each of the positive examples, checks if the score is higher than the respective negative example

This prints 0.8356, which is indeed pretty close to the AUC value of our classifier.

This interpretation of AUC gives us additional insight into the quality of our models. The ideal model orders all the customers such that we first have non-churning customers and then churning customers. With this order, the AUC is always 1.0: the score of a randomly chosen churning customer is always higher than the score of a non-churning customer. On the other hand, the random model just shuffles the customers, so the score of a churning customer has only a 50% chance of being higher than the score of a non-churning one.

AUC thus not only gives us a way of evaluating the models at all possible thresholds but also describes how well the model separates two classes: in our case, churning and non-churning. If the separation is good, then we can order the customers such that most of the churning users come first. Such a model will have a good AUC score.

NOTE You should keep this interpretation in mind: it provides an easy way to explain the meaning behind AUC to people without a machine learning background, such as managers and other decision makers.

This makes AUC the default classification metric in most situations, and it's often the metric we use when finding the best parameter set for our models.

The process of finding the best parameters is called "parameter tuning," and in the next section we will see how to do this.

4 Parameter tuning

In the previous chapter, we used a simple hold-out validation scheme for testing our models. In this scheme, we take part of the data out and keep it for validation purposes only. This practice is good but doesn't always give us the whole picture. It tells us how well the model will perform on these specific data points. However, it doesn't necessarily mean the model will perform equally well on other data points. So, how do we check if the model indeed works well in a consistent and predictable manner?

4.4.1 K-fold cross-validation

It's possible to use all the available data to assess the quality of models and get more reliable validation results. We can simply perform validation multiple times.

First, we split the entire dataset into a certain number of parts (say, three). Then we train a model on two parts and validate on the remaining one. We repeat this process three times and at the end get three different scores. This is exactly the idea behind K-fold cross-validation (figure 4.36).

Figure 4.36 K-fold cross-validation (K=3). We split the entire dataset into three equal parts, or folds. Then, for each fold, we take it as the validation dataset and use the remaining K – 1 folds as the training data. After training the model, we evaluate it on the validation fold, and at the end we get k metric values.

Before we implement it, we need to make the training process simpler, so it's easy to run this process multiple times. For that, we'll put all the code

for training into a `train` function, which first converts the data into a one-hot encoding representation and then trains the model.

Listing 4.3 Training the model

```
def train(df, y):
    cat = df[categorical + numerical].to_dict(orient='records')  ❶

    dv = DictVectorizer(sparse=False)                            ❶
    dv.fit(cat)                                                  ❶

    X = dv.transform(cat)                                        ❶

    model = LogisticRegression(solver='liblinear')               ❷
    model.fit(X, y)                                              ❷

    return dv, model
```

❶ Applies one-hot encoding

❷ Trains the model

Likewise, we also put the prediction logic into a `predict` function. This function takes in a dataframe with customers, the vectorizer we "trained" previously—for doing one-hot encoding—and the model. Then we apply the vectorizer to the dataframe, get a matrix, and finally apply the model to the matrix to get predictions.

Listing 4.4 Applying the model to new data

```
def predict(df, dv, model):
    cat = df[categorical + numerical].to_dict(orient='records')    ❶

    X = dv.transform(cat)                                          ❶
    y_pred = model.predict_proba(X)[:, 1]                          ❷

    return y_pred
```

❶ Applies the same one-hot encoding scheme as in training

❷ Uses the model to make predictions

Now we can use these functions for implementing K-fold cross-validation.

We don't need to implement cross-validation ourselves: in Scikit-learn there's a class for doing that. It's called `KFold`, and it lives in the `model_selection` package.

Listing 4.5 K-fold cross-validation

```
from sklearn.model_selection import KFold                          ❶

kfold = KFold(n_splits=10, shuffle=True, random_state=1)           ❷

aucs = []                                                          ❸

for train_idx, val_idx in kfold.split(df_train_full):              ❹
    df_train = df_train_full.iloc[train_idx]                       ❺
    df_val = df_train_full.iloc[val_idx]                           ❺
```

```
        y_train = df_train.churn.values                    ❺
        y_val = df_val.churn.values                        ❺
        dv, model = train(df_train, y_train)               ❻
        y_pred = predict(df_val, dv, model)                ❻

        auc = roc_auc_score(y_val, y_pred)                 ❼
        aucs.append(auc)                                   ❽
```

❶ Imports the KFold class

❷ Uses it to split the data into 10 parts

❸ Creates a list for storing the results

❹ Iterates over the 10 different splits of the data

❺ Splits the data into train and validation sets

❻ Trains the model and makes predictions

❼ Evaluates the quality of the train model on the validation data using AUC

❽ Saves the AUC to the list with the results

Note that when defining the splitting in the `KFold` class in ❷, we set three parameters:

- `n_splits = 10` : That's K, which specifies the number of splits.
- `shuffle = True` : We ask it to shuffle the data before splitting it.

- `random_state = 1` : Because there's randomization in the process (shuffling data), we want the results to be reproducible, so we fix the seed for the random-number generator.

Here we used K-fold cross-validation with K =10. Thus, when we run it, at the end we get 10 different numbers—10 AUC scores evaluated on 10 different validation folds:

```
0.849, 0.841, 0.859, 0.833, 0.824, 0.841, 0.844, 0.822, 0.845, 0.861
```

It's not a single number anymore, and we can think of it as a distribution of AUC scores for our model. We can get some statistics from this distribution, such as the mean and standard deviation:

```
print('auc = %0.3f ± %0.3f' % (np.mean(aucs), np.std(aucs)))
```

This prints "0.842 ± 0.012".

Now, not only do we know the average performance, but we also have an idea of how volatile that performance is, or how far it may deviate from the average.

A good model should be quite stable across different folds: this way, we make sure we don't get a lot of surprises when the model goes live. The standard deviation tells us about that: the smaller it is, the more stable the model is.

Now we can use K-fold cross-validation for parameter tuning: selecting the best parameters.

4.4.2 Finding best parameters

We learned how we can use K-fold cross-validation for evaluating the performance of our model. The model we trained previously was using the default value for the parameter `C`, which controls the amount of regularization.

Let's select our cross-validation procedure for selecting the best parameter `C`. For that, we first adjust the `train` function to take in an additional parameter.

Listing 4.6 Function for training the model with parameter C for controlling regularization

```
def train(df, y, C):                                                    ❶
    cat = df[categorical + numerical].to_dict(orient='records')
    dv = DictVectorizer(sparse=False)
    dv.fit(cat)

    X = dv.transform(cat)

    model = LogisticRegression(solver='liblinear', C=C)                 ❷
    model.fit(X, y)

    return dv, model
```

❶ Adds an extra parameter to the train function

❷ Uses this parameter during training

Now let's find the best parameter `C`. The idea is simple:

- Loop over different values of `C`.
- For each `C`, run cross-validation and record the mean AUC across all folds as well as the standard deviation.

Listing 4.7 Tuning the model: selecting the best parameter C using cross-validation

```
nfolds = 5
kfold = KFold(n_splits=nfolds, shuffle=True, random_state=1)

for C in [0.001, 0.01, 0.1, 0.5, 1, 10]:
    aucs = []

    for train_idx, val_idx in kfold.split(df_train_full):
        df_train = df_train_full.iloc[train_idx]
        df_val = df_train_full.iloc[val_idx]

        y_train = df_train.churn.values
        y_val = df_val.churn.values

        dv, model = train(df_train, y_train, C=C)
        y_pred = predict(df_val, dv, model)

        auc = roc_auc_score(y_val, y_pred)
        aucs.append(auc)

    print('C=%s, auc = %0.3f ± %0.3f' % (C, np.mean(aucs), np.std(aucs)))
```

When we run it, it prints

```
C=0.001, auc = 0.825 ± 0.013
C=0.01, auc = 0.839 ± 0.009
C=0.1, auc = 0.841 ± 0.008
C=0.5, auc = 0.841 ± 0.007
C=1, auc = 0.841 ± 0.007
C=10, auc = 0.841 ± 0.007
```

What we see is that after `C` = 0.1, the average AUC is the same and doesn't grow anymore.

However, the standard deviation is smaller for `C` = 0.5 than for `C` = 0.1, so we should use that. The reason we prefer `C` = 0.5 to `C` = 1 and `C` = 10 is simple: when the `C` parameter is small, the model is more regularized. The weights of this model are more restricted, so in general, they are smaller. Small weights in the model give us additional assurance that the model will behave well when we use it on real data. So we select `C` = 0.5.

Now we need to do the last step: train the model on the entire train and validation datasets and apply it to the test dataset to verify it indeed works well.

Let's use our `train` and `predict` functions for that:

```
y_train = df_train_full.churn.values
y_test = df_test.churn.values

dv, model = train(df_train_full, y_train, C=0.5)    ❶
```

```
y_pred = predict(df_test, dv, model)                    ❷

auc = roc_auc_score(y_test, y_pred)                     ❸
print('auc = %.3f' % auc)                               ❸
```

❶ Trains the model on the full training dataset

❷ Applies it to the test dataset

❸ Evaluates the predictions on the test data

When we execute the code, we see that the performance of the model (AUC) on the held-out test set is 0.858.

That's a little higher than what we had on the validation set, but that's not an issue; it could happen just by chance. What's important is that the score is not significantly different from the validation score.

Now we can use this model for scoring real customers and think about our marketing campaign for preventing churn. In the next chapter, we will see how to deploy this model in a production environment.

5 Next steps

1.5.1 Exercises

Try the following exercises to further explore the topics of model evaluation and model selection:

- In this chapter, we plotted TPR and FPR for different threshold values, and it helped us understand what these metrics mean and also how the performance of our model changes when we choose a different threshold. It's helpful to do a similar exercise for precision and recall, so try to repeat this experiment, this time using precision and recall instead of TPR and FPR.
- When plotting precision and recall for different threshold values, we can see that a conflict exists between precision and recall: when one goes up, the other goes down, and the other way around. This is called the "precision-recall trade-off": we cannot select a threshold that makes both precision and recall good. However, we do have strategies for selecting the threshold, even though precision and recall are conflicting. One of them is plotting precision and recall curves and seeing where they intersect, and using this threshold for binarizing the predictions. Try implementing this idea.
- Another idea for working around the precision-recall trade-off is the F1 score—a score that combines both precision and recall into one value. Then, to select the best threshold, we can simply choose the one that maximizes the F1 score. The formula for computing the F1 score is $F1 = 2 \cdot P \cdot R / (P + R)$, where P is precision and R is recall. Implement this idea, and select the best threshold based on the F1 metric.

- We've seen that precision and recall are better metrics for evaluating classification models than accuracy because they don't rely on false positives, the amount of which could be high in imbalanced datasets. Yet, we saw later that AUC does actually use false positives in FPR. For very highly imbalanced cases (say, 1,000 negatives to 1 positive), AUC may become problematic as well. Another metric works better in such cases: area under the precision-recall curve, or AU PR. The precision-recall curve is similar to ROC, but instead of plotting FPR versus TPR, we plot recall on the x-axis and precision on the y-axis. Like for the ROC curve, we can also calculate the area under the PR curve and use it as a metric for evaluating different models. Try plotting the PR curves for our models, calculating the AU PR scores, and comparing them with those of the random model as well as the ideal model.
- We covered K-fold cross-validation, and we used it to understand what the distribution of AUC scores could look like on a test dataset. When K = 10, we get 10 observations, which under some circumstances might not be enough. However, the idea can be extended to repeated K-fold cross-validation steps. The process is simple: we repeat the K-fold cross-validation process multiple times, each time shuffling the dataset differently by selecting a different random seed at each iteration. Implement repeated cross-validation and perform 10-fold cross-validation 10 times to see what the distribution of scores looks like.

1.5.2 Other projects

You can also continue with the other self-study projects from the previous chapter: the lead scoring project and the default prediction project. Try the following:

- Calculate all the metrics that we covered in this chapter: the confusion table, precision and recall, and AUC. Also try to calculate the scores from the exercises: the F1 score as well as AU PR (the area under the precision-recall curve).
- Use K-fold cross-validation to select the best parameter `C` for the model.

ummary

- A metric is a single number that can be used for evaluating the performance of a machine learning model. Once we choose a metric, we can use it to compare multiple machine learning models with each other and select the best one.
- Accuracy is the simplest binary classification metric: it tells us the percentage of correctly classified observations in the validation set. It's easy to understand and compute, but it can be misleading when a dataset is imbalanced.
- When a binary classification model makes a prediction, we have only four possible outcomes: true positive and true negative (correct answers) and false positive and false negative (incorrect answers). The confusion table arranges these outcomes visually so it's easy to understand them. It gives us the foundation for many other binary classification metrics.

- Precision is the fraction of correct answers among observations for which our prediction is True. If we use the churn model to send promotional messages, precision tells us the percentage of customers who really were going to churn among everybody who received the message. The higher the precision, the fewer non-churning users we incorrectly classify as churning.
- Recall is the fraction of correct answers among all positive observations. It tells us the percentage of churning customers who we correctly identified as churning. The higher the recall, the fewer churning customers we fail to identify.
- The ROC curve analyzes binary classification models at all the thresholds at once. The area under the ROC curve (AUC) tells us how well a model separates positive observations from negative ones. Because of its interpretability and wide applicability, AUC has become the default metric for evaluating binary classification models.
- K-fold cross-validation gives us a way to use all the training data for model validation: we split the data into K folds and use each fold in turn as a validation set, and the remaining K – 1 folds are used for training. As a result, instead of a single number, we have K values, one for each fold. We can use these numbers to understand the performance of a model on average as well as to estimate how volatile it is across different folds.
- K-fold cross-validation is the best way of tuning parameters and selecting the best model: it gives us a reliable estimate of the metric across multiple folds.

In the next chapter we look into deploying our model into a production environment.

nswers to exercises

- Exercise 4.1 B) A customer for whom we predicted “churn,” but they didn’t churn.
- Exercise 4.2 B) The percent of customers who actually churned among the customers who we predicted as churning.
- Exercise 4.3 A) The percent of correctly identified churned customers among all churned customers.
- Exercise 4.4 A) The ideal ranking model always scores churning customers higher than non-churning ones.