Cross-Validation in scikit-learn

Cross-validation is implemented in `scikit-learn` using the `cross_val_score` function from the `model_selection` module. The parameters of the `cross_val_score` function are the model we want to evaluate, the training data, and the ground-truth labels. Let's evaluate `LogisticRegression` on the `iris` dataset:

In[4]:

```
from sklearn.model_selection import cross_val_score
from sklearn.datasets import load_iris
from sklearn.linear_model import LogisticRegression

iris = load_iris()
logreg = LogisticRegression()

scores = cross_val_score(logreg, iris.data, iris.target)
print("Cross-validation scores: {}".format(scores))
```

Out[4]:

```
Cross-validation scores: [ 0.961  0.922  0.958]
```

By default, `cross_val_score` performs three-fold cross-validation, returning three accuracy values. We can change the number of folds used by changing the `cv` parameter:

In[5]:

```
scores = cross_val_score(logreg, iris.data, iris.target, cv=5)
print("Cross-validation scores: {}".format(scores))
```

Out[5]:

```
Cross-validation scores: [ 1.     0.967  0.933  0.9    1.   ]
```

A common way to summarize the cross-validation accuracy is to compute the mean:

In[6]:

```
print("Average cross-validation score: {:.2f}".format(scores.mean()))
```

Out[6]:

```
Average cross-validation score: 0.96
```

Using the mean cross-validation we can conclude that we expect the model to be around 96% accurate on average. Looking at all five scores produced by the five-fold cross-validation, we can also conclude that there is a relatively high variance in the accuracy between folds, ranging from 100% accuracy to 90% accuracy. This could imply that the model is very dependent on the particular folds used for training, but it could also just be a consequence of the small size of the dataset.

Benefits of Cross-Validation

There are several benefits to using cross-validation instead of a single split into a training and a test set. First, remember that `train_test_split` performs a random split of the data. Imagine that we are "lucky" when randomly splitting the data, and all examples that are hard to classify end up in the training set. In that case, the test set will only contain "easy" examples, and our test set accuracy will be unrealistically high. Conversely, if we are "unlucky," we might have randomly put all the hard-to-classify examples in the test set and consequently obtain an unrealistically low score. However, when using cross-validation, each example will be in the training set exactly once: each example is in one of the folds, and each fold is the test set once. Therefore, the model needs to generalize well to all of the samples in the dataset for all of the cross-validation scores (and their mean) to be high.

Having multiple splits of the data also provides some information about how sensitive our model is to the selection of the training dataset. For the `iris` dataset, we saw accuracies between 90% and 100%. This is quite a range, and it provides us with an idea about how the model might perform in the worst case and best case scenarios when applied to new data.

Another benefit of cross-validation as compared to using a single split of the data is that we use our data more effectively. When using `train_test_split`, we usually use 75% of the data for training and 25% of the data for evaluation. When using five-fold cross-validation, in each iteration we can use four-fifths of the data (80%) to fit the model. When using 10-fold cross-validation, we can use nine-tenths of the data (90%) to fit the model. More data will usually result in more accurate models.

The main disadvantage of cross-validation is increased computational cost. As we are now training *k* models instead of a single model, cross-validation will be roughly *k* times slower than doing a single split of the data.

> It is important to keep in mind that cross-validation is not a way to build a model that can be applied to new data. Cross-validation does not return a model. When calling `cross_val_score`, multiple models are built internally, but the purpose of cross-validation is only to evaluate how well a given algorithm will generalize when trained on a specific dataset.

Stratified k-Fold Cross-Validation and Other Strategies

Splitting the dataset into *k* folds by starting with the first one-*k*-th part of the data, as described in the previous section, might not always be a good idea. For example, let's have a look at the `iris` dataset: