02b-model-selection

January 18, 2017

1 Model selection with Scikit-Learn

1.1 Training error

```
In [21]: # Global imports and settings
         from preamble import * # Ignore, this is just to make code cleaner
         HTML('''<style>.CodeMirror{min-width:100% !important;}</style>''') # For slides
         InteractiveShell.ast_node_interactivity = "all"
```

```
Out[21]: <IPython.core.display.HTML object>
```

```
In [22]: from sklearn.neighbors import KNeighborsClassifier
         from sklearn.metrics import zero_one_loss
         from sklearn.datasets import make_blobs

         # Blob data
         X, y = make_blobs(n_samples=1000, centers=20, random_state=123)
         labels = ["b", "r"]
         y = np.take(labels, (y < 10)) # Relabels numeric values to b,r

         clf = KNeighborsClassifier()
         clf.fit(X, y)
         print("Training error =", zero_one_loss(y, clf.predict(X)))
```

```
Out[22]: KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
                    metric_params=None, n_jobs=1, n_neighbors=5, p=2,
                    weights='uniform')
```

```
Training error = 0.108
```

1.2 Test error

Issue: the training error is a **biased** estimate of the generalization error.

Solution: Divide data into two disjoint parts called training and test sets (usually using 70% for training and 30% for test).

- Use the training set for fitting the model;
- Use the test set for evaluation only, thereby yielding an unbiased estimate.

- **The same data should not be used both for training and evaluation.**

```
In [23]: from sklearn.model_selection import train_test_split
         X_train, X_test, y_train, y_test = train_test_split(X, y)
         clf = KNeighborsClassifier()
         clf.fit(X_train, y_train)
         print("Training error =", zero_one_loss(y_train, clf.predict(X_train)))
         print("Test error =", zero_one_loss(y_test, clf.predict(X_test)))
```

```
Out[23]: KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
                    metric_params=None, n_jobs=1, n_neighbors=5, p=2,
                    weights='uniform')
```

```
Training error = 0.0973333333333
Test error = 0.172
```

1.3 Cross-validation

Issue:

- When data is small, training on 70% of the data may lead to a model that is significantly different from a model that would have been learned on the entire set.
- Yet, increasing the size of the training set (resp. decreasing the size of the test set), might lead to an inaccurate estimate of the generalization error.

Solution: K-Fold cross-validation.

- Split data into K small disjoint folds.
- Train on K-1 folds, evaluate the test error one the held-out fold.
- Repeat for all combinations and average the K estimates of the generalization error.

```
In [24]: from sklearn.cross_validation import KFold

         scores = []

         for train, test in KFold(n=len(X), n_folds=5, random_state=42):
             X_train, y_train = X[train], y[train]
             X_test, y_test = X[test], y[test]
             clf = KNeighborsClassifier().fit(X_train, y_train)
             scores.append(zero_one_loss(y_test, clf.predict(X_test)))

         print("CV error = %f +-%f" % (np.mean(scores), np.std(scores)))
```

```
CV error = 0.163000 +-0.010770
```

```
In [25]: # Shortcut
         from sklearn.cross_validation import cross_val_score
         scores = cross_val_score(KNeighborsClassifier(), X, y,
                                  cv=KFold(n=len(X), n_folds=5, random_state=42),
                                  scoring="accuracy")
         print("CV error = %f +-%f" % (1. - np.mean(scores), np.std(scores)))
```

```
CV error = 0.163000 +-0.010770
```

1.4 Metrics

1.4.1 Default score

Estimators come with a built-in default evaluation score

- Accuracy for classification
- R2 score for regression

```
In [26]: y_train = (y_train == "r")
         y_test = (y_test == "r")
         clf = KNeighborsClassifier(n_neighbors=5)
         clf.fit(X_train, y_train)
         print("Default score =", clf.score(X_test, y_test))
```

```
Out[26]: KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
                    metric_params=None, n_jobs=1, n_neighbors=5, p=2,
                    weights='uniform')
```

```
Default score = 0.84
```

1.4.2 Accuracy

Definition: The accuracy is the proportion of correct predictions.

```
In [27]: from sklearn.metrics import accuracy_score
         print("Accuracy =", accuracy_score(y_test, clf.predict(X_test)))
```

```
Accuracy = 0.84
```

1.4.3 Precision, recall and F-measure

$$Precision = \frac{TP}{TP + FP}$$

$$Recall = \frac{TP}{TP + FN}$$

$$F = \frac{2 * Precision * Recall}{Precision + Recall}$$

```
In [28]: from sklearn.metrics import precision_score
         from sklearn.metrics import recall_score
         from sklearn.metrics import fbeta_score
         print("Precision =", precision_score(y_test, clf.predict(X_test)))
         print("Recall =", recall_score(y_test, clf.predict(X_test)))
         print("F =", fbeta_score(y_test, clf.predict(X_test), beta=1))
```

```
Precision = 0.811881188119
Recall = 0.863157894737
F = 0.836734693878
```

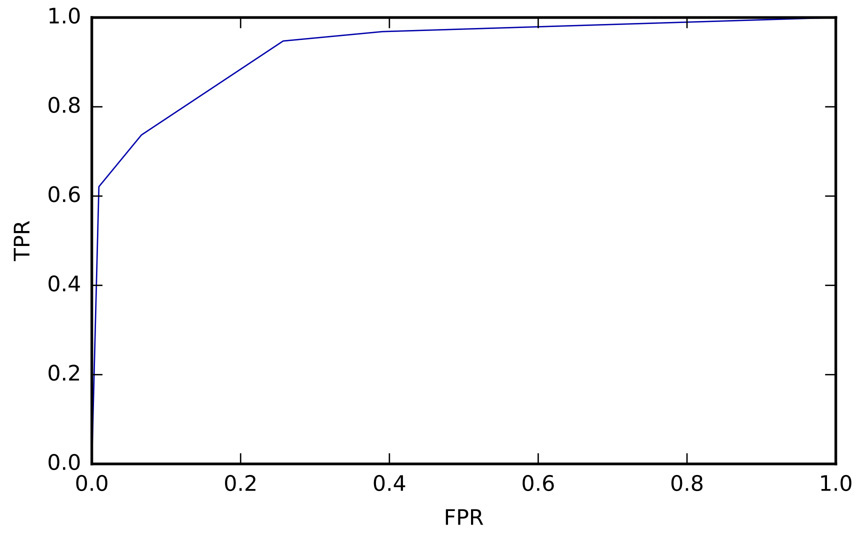
1.4.4 ROC AUC

Definition: Area under the curve of the false positive rate (FPR) against the true positive rate (TPR) as the decision threshold of the classifier is varied.

```
In [29]: from sklearn.metrics import get_scorer
         roc_auc_scorer = get_scorer("roc_auc")
         print("ROC AUC =", roc_auc_scorer(clf, X_test, y_test))

         from sklearn.metrics import roc_curve
         fpr, tpr, thresholds = roc_curve(y_test, clf.predict_proba(X_test)[:, 1])
         plt.plot(fpr, tpr)
         plt.xlabel("FPR")
         plt.ylabel("TPR")
         plt.show()
```

```
ROC AUC = 0.92977443609
```

```
Out[29]: [<matplotlib.lines.Line2D at 0x1155ca2b0>]

Out[29]: <matplotlib.text.Text at 0x110cf92e8>

Out[29]: <matplotlib.text.Text at 0x11559a278>
```



1.4.5 Confusion matrix

Definition: number of samples of class *i* predicted as class *j*.

```
In [30]: from sklearn.metrics import confusion_matrix
         confusion_matrix(y_test, clf.predict(X_test))
```

```
Out[30]: array([[86, 19],
                [13, 82]])
```

2 Transformers, pipelines and feature unions

2.1 Transformers

- Classification (or regression) is often only one or the last step of a long and complicated process;
- In most cases, input data needs to be cleaned, massaged or extended before being fed to a learning algorithm;
- For this purpose, Scikit-Learn provides the `transformer` API.

```
In [31]: class Transformer(object):
             def fit(self, X, y=None):
                 """Fits estimator to data."""
                 # set state of ``self``
                 return self

             def transform(self, X):
                 """Transform X into Xt."""
                 # transform X in some way to produce Xt
```

```
            return Xt

        # Shortcut
        def fit_transform(self, X, y=None):
            self.fit(X, y)
            Xt = self.transform(X)
            return Xt
```

2.2 Pipelines

Transformers can be chained in sequence to form a pipeline.

```
In [32]: from sklearn.pipeline import make_pipeline
         from sklearn.feature_selection import SelectKBest
         from sklearn.ensemble import RandomForestClassifier

         # Get more complex data
         dataset = oml.datasets.get_dataset(337)
         X, y = dataset.get_data(target=dataset.default_target_attribute)
         X_train, X_test, y_train, y_test = train_test_split(X, y)

         # Chain transformers + a classifier to build a new classifier
         clf = make_pipeline(SelectKBest(score_func=f_classif, k=44),
                             RandomForestClassifier())
         clf.fit(X_train, y_train)
         print(clf.predict_proba(X_test)[:5])
```

```
Out[32]: Pipeline(steps=[('selectkbest', SelectKBest(k=44, score_func=<function f_classif at 0x1
                     max_depth=None, max_features='auto', max_leaf_nodes=None,
                     min_impurity_split=1e-07...imators=10, n_jobs=1, oob_score=False, random_st
                     verbose=0, warm_start=False))])
```

```
[[ 0.4  0.6]
 [ 0.4  0.6]
 [ 0.1  0.9]
 [ 0.9  0.1]
 [ 0.7  0.3]]
```

2.3 Optimizing parameters

Search for the best hyperparameter settings

```
In [33]: # Hyper-parameters can be accessed using step names
         print("K =", clf.get_params()["selectkbest__k"])
```

```
K = 44
```

```
In [34]: from sklearn.grid_search import GridSearchCV
         grid = GridSearchCV(clf,
                             param_grid={"selectkbest__k": [1, 10, 20, 30, 40],
                                         "randomforestclassifier__max_features": [0.1, 0.25, 0.5
         grid.fit(X_train, y_train)

         print("Best params =", grid.best_params_)

Out[34]: GridSearchCV(cv=None, error_score='raise',
                estimator=Pipeline(steps=[('selectkbest', SelectKBest(k=44, score_func=<function
                     max_depth=None, max_features='auto', max_leaf_nodes=None,
                     min_impurity_split=1e-07...imators=10, n_jobs=1, oob_score=False, random_st
                     verbose=0, warm_start=False))]),
                fit_params={}, iid=True, n_jobs=1,
                param_grid={'selectkbest__k': [1, 10, 20, 30, 40], 'randomforestclassifier__max_
                pre_dispatch='2*n_jobs', refit=True, scoring=None, verbose=0)

Best params = {'selectkbest__k': 40, 'randomforestclassifier__max_features': 0.25}
```

2.4 Final remarks

- Scikit-learn has many more preprocessing techniques. Check the documentation
- There are better ways to optimize hyperparameters:
  - RandomSearch
  - Bayesian Optimization (see auto-sklearn library)