Model selection: choosing estimators and their parameters

Score, and cross-validated scores

As we have seen, every estimator exposes a `score` method that can judge the quality of the fit (or the prediction) on new data. **Bigger is better**.

```
>>> from sklearn import datasets, svm
>>> digits = datasets.load_digits()
>>> X_digits = digits.data
>>> y_digits = digits.target
>>> svc = svm.SVC(C=1, kernel='linear')
>>> svc.fit(X_digits[:-100], y_digits[:-100]).score(X_digits[-100:], y_digits[-100:])
0.97999999999999998
```

To get a better measure of prediction accuracy (which we can use as a proxy for goodness of fit of the model), we can successively split the data in *folds* that we use for training and testing:

```
>>> import numpy as np
>>> X_folds = np.array_split(X_digits, 3)
>>> y_folds = np.array_split(y_digits, 3)
>>> scores = list()
>>> for k in range(3):
...     # We use 'list' to copy, in order to 'pop' later on
...     X_train = list(X_folds)
...     X_test  = X_train.pop(k)
...     X_train = np.concatenate(X_train)
...     y_train = list(y_folds)
...     y_test  = y_train.pop(k)
...     y_train = np.concatenate(y_train)
...     scores.append(svc.fit(X_train, y_train).score(X_test, y_test))
>>> print(scores)
[0.93489148580968284, 0.95659432387312182, 0.93989983305509184]
```

This is called a `KFold` cross validation

Cross-validation generators

The code above to split data in train and test sets is tedious to write. Scikit-learn exposes cross-validation generators to generate list of indices for this purpose:

```
>>> from sklearn import cross_validation
>>> k_fold = cross_validation.KFold(n=6, n_folds=3)
>>> for train_indices, test_indices in k_fold:
...      print('Train: %s | test: %s' % (train_indices, test_indices))
Train: [2 3 4 5] | test: [0 1]
Train: [0 1 4 5] | test: [2 3]
Train: [0 1 2 3] | test: [4 5]
```

The cross-validation can then be implemented easily:

```
>>> kfold = cross_validation.KFold(len(X_digits), n_folds=3)
>>> [svc.fit(X_digits[train], y_digits[train]).score(X_digits[test], y_digits[test])
...          for train, test in kfold]
[0.93489148580968284, 0.95659432387312182, 0.93989983305509184]
```

To compute the `score` method of an estimator, the sklearn exposes a helper function:

```
>>> cross_validation.cross_val_score(svc, X_digits, y_digits, cv=kfold, n_jobs=-1)
array([ 0.93489149,  0.95659432,  0.93989983])
```

n_jobs=-1 means that the computation will be dispatched on all the CPUs of the computer.

Cross-validation generators

`KFold` (n, k)	`StratifiedKFold` (y, k)	`LeaveOneOut` (n)	`LeaveOneLabelOut` (labels)
Split it K folds, train on K-1 and then test on left-out	It preserves the class ratios / label distribution within each fold.	Leave one observation out	Takes a label array to group observations

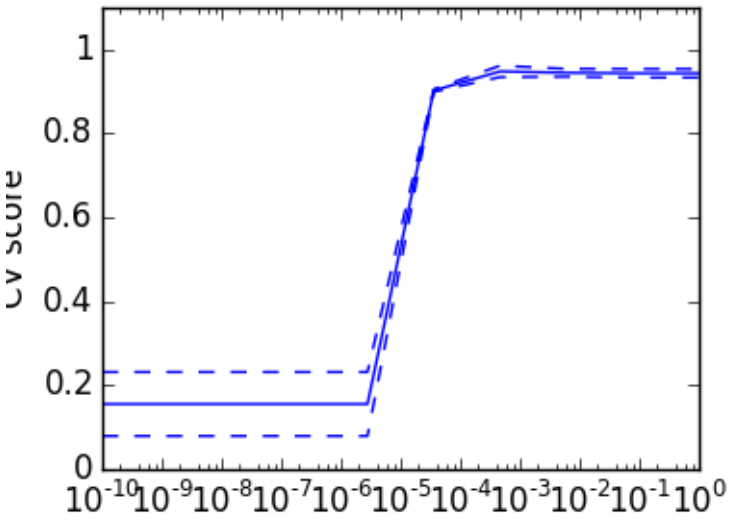
Exercise

On the digits dataset, plot the cross-validation score of a `SVC` estimator with an linear kernel as a function of parameter `C` (use a logarithmic grid of points, from 1 to 10).

```
import numpy as np
from sklearn import cross_validation,

digits = datasets.load_digits()
X = digits.data
y = digits.target

svc = svm.SVC(kernel='linear')
C_s = np.logspace(-10, 0, 10)
```



Solution: *Cross-validation on Digits Dataset Exercise*

Grid-search and cross-validated estimators

Grid-search

The sklearn provides an object that, given data, computes the score during the fit of an estimator on a parameter grid and chooses the parameters to maximize the cross-validation score. This object takes an estimator during the construction and exposes an estimator API:

```
>>> from sklearn.grid_search import GridSearchCV
>>> Cs = np.logspace(-6, -1, 10)
>>> clf = GridSearchCV(estimator=svc, param_grid=dict(C=Cs),
...                    n_jobs=-1)
```

```
>>> clf.fit(X_digits[:1000], y_digits[:1000])
GridSearchCV(cv=None,...
>>> clf.best_score_
0.925...
>>> clf.best_estimator_.C
0.0077...

>>> # Prediction performance on test set is not as good as on train set
>>> clf.score(X_digits[1000:], y_digits[1000:])
0.943...
```

By default, the `GridSearchCV` uses a 3-fold cross-validation. However, if it detects that a classifier is passed, rather than a regressor, it uses a stratified 3-fold.

Nested cross-validation

```
>>> cross_validation.cross_val_score(clf, X_digits, y_digits)
...
array([ 0.938...,  0.963...,  0.944...])
```

Two cross-validation loops are performed in parallel: one by the `GridSearchCV` estimator to set `gamma` and the other one by `cross_val_score` to measure the prediction performance of the estimator. The resulting scores are unbiased estimates of the prediction score on new data.

Warning: You cannot nest objects with parallel computing (`n_jobs` different than 1).

Cross-validated estimators

Cross-validation to set a parameter can be done more efficiently on an algorithm-by-algorithm basis. This is why for certain estimators the sklearn exposes *Cross-validation: evaluating estimator performance* estimators that set their parameter automatically by cross-validation:

```
>>> from sklearn import linear_model, datasets
>>> lasso = linear_model.LassoCV()
>>> diabetes = datasets.load_diabetes()
>>> X_diabetes = diabetes.data
>>> y_diabetes = diabetes.target
>>> lasso.fit(X_diabetes, y_diabetes)
LassoCV(alphas=None, copy_X=True, cv=None, eps=0.001, fit_intercept=True,
    max_iter=1000, n_alphas=100, n_jobs=1, normalize=False, positive=False,
    precompute='auto', random_state=None, selection='cyclic', tol=0.0001,
    verbose=False)
>>> # The estimator chose automatically its lambda:
>>> lasso.alpha_
0.01229...
```

These estimators are called similarly to their counterparts, with ‘CV’ appended to their name.

Exercise

On the diabetes dataset, find the optimal regularization parameter alpha.

Bonus: How much can you trust the selection of alpha?

```
from sklearn import cross_validation, datasets, linear_model

diabetes = datasets.load_diabetes()
X = diabetes.data[:150]
```

```
y = diabetes.target[:150]

lasso = linear_model.Lasso()
alphas = np.logspace(-4, -.5, 30)
```

Solution: *Cross-validation on diabetes Dataset Exercise*