Hyper-parameter search

In addition to the "learned" parameters (e.g., Θ) there are a number of parameters to the learning process itself. Among the ones we've seen so far

- Strength of regularization penalty
- Number of folds for cross validation
- Degree of the polynomial features

How do we choose values for these hyper parameters?

One way is by searching through a space of possible values.

sklearn makes this easy via the GridSearchCV method, which we briefly describe.

<u>sklearn</u> <u>GridSearchCV documentation (https://scikit-learn.org/stable/auto_examples/model_selection/plot_grid_search_digits.html)</u>

Set the parameters by cross-validation tuned_parameters = [{'kernel': ['rbf'], 'gamma': [1e-3, 1e-4], 'C': [1, 10, 100, 1000]}, {'kernel': ['linear'], 'C': [1, 10, 100, 1000]}] scores = ['precision', 'recall'] clf = GridSearchCV(SVC(), tuned_parameters, cv=5, scoring='%s_macro' % score)

GridSearchCV will create an object (which turns out to be an estimator).

In creating this object, we specify

- an instance *e* of an estimator
- a dictionary
 - ullet whose keys are names of parameters to e
 - whose values are a list of possible values for the parameters

clf.fit(X_train, y_train)

Fitting the GridSearchCV estimator does the following

- it creates every possible combination of parameter values in the dictionary
- $\bullet\,$ for each combination, it performs Cross Validated fitting of the estimator e

So it fits estimator e many times, one for each possible parameter combination across the multi-dimensional space of hyper-parameters.

Hence the name: Grid Search.

One can then have Grid Search report summaries as well as the best combination of parameters.

Randomized search in sklearn

RandomizedSearchCV documentation (https://scikit-learn.org/stable/modules/grid_search.html#randomized-parameter-optimization)

GridSearchCV searches the entire multi-dimensional space of hyper-parameters, which can be very large and therefore time consuming.

sklearn implements a randomized version of the exploration of the multidimensional space.

Instead of searching the grid exhaustively, it randomly samples combinations of hyperparameters to try.

The user specifies how many samples are taken.

Alternative to Randomized Search

The assumption underlying Randomized Search is that all points in the multidimensional space of hyper-parameters are equally likely candidates for being the best.

Like any other optimization problem, experience tells us this is not likely to be the case:

- Some parameters have less impact on the Performance Metric than others
- The values for a particular hyper-parameter that lead to high performance tend to be clustered rather than evenly distributed

Is there a way to improve Randomized Search?

One idea is to partition the space of possible values of a hyper-parameter unevenly.
One can then try an equal number of values of the hyper-parameter in each partition
 the increment between values of a large partition are larger than for a small partition

For example suppose the range for hyper-parameter p is $\left[0,1000\right]$

- we create partitions using a logarithmic scale:
 - **[**0,.001]
 - **.** [.001, .01]
 - •
 - **•** [100, 1000]

This would be consistent with our belief that the best values for p are extremely small.

So we explore small values in smaller increments than the values between $100\,\mathrm{and}$ and 1000.

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