Evaluating and using ML classifiers: model selection using cross validation and data snooping
Reminder: Cross validation

Cross validation:

- Randomly partition the data into \( k \) parts ("folds").
- Set one fold aside for evaluation and train a model on the remaining \( k-1 \) folds and evaluate it on the held-out fold.
- Repeat until each fold has been used for evaluation

Stratified-cross validation aims at achieving roughly the same class distribution in each fold.

\[
E_{cv} = \frac{1}{N} \sum_{n=1}^{N} \left( \hat{y}_n - y_n \right)^2 - H(\lambda) \]

\[
H(\lambda) = Z(Z^t Z + \lambda I)^{-1} Z^t.
\]
Model selection

You have been tasked with deploying a classifier for a given task and you have some labeled data to work with.

You would like to compare several classification methods and choose the best one. Each classifier has one or more hyperparameters (e.g. SVM soft margin constant and kernel parameter).

Approach:
For each classifier compare the accuracy of the best parameter setting (estimated using cross-validation or a test set).
Using cross-validation

Now we have to ask ourselves how well do we expect that classifier to perform: $E_{cv}$ is a biased estimate of performance of the classifier trained using the chosen parameters.
Model selection

The task:
For each classifier compare the accuracy of the best parameter setting (estimated using cross-validation or a test set)

So, assuming we are comparing two classifiers, this means we are making the following comparison:

$$\max(s_1,\ldots,s_m) \text{ vs } \max(t_1,\ldots,t_m)$$

In computing the maximum we are using information about the test set labels!

Cross validation tells you how well the classifier is performing on a given setting of classifier parameters.
Two ways of doing cross validation

External cross validation:
- Perform cross validation across various settings of classifier parameters and report the best result you got

Internal cross validation (nested CV):
- For each fold, perform cross-validation on the training data, and train a classifier on the best set of parameters for that fold
- This evaluates the training procedure
Table 8: Error rate estimates for kernel ridge regression over thirteen benchmark data sets, for model selection schemes that are internal and external to the cross-validation process. The results for each approach and the relative bias are presented in the form of the mean error rate over for 100 realisations of each data set (20 in the case of the image and splice data sets), along with the associated standard error.
Internal cross-validation

Notice that each train/test fold may get different parameter settings.
That’s fine!

This results in a “parameterless” algorithm that internally sets parameters for each data set it gets.
What to do for the system you are deploying

Use external cross-validation to determine good parameters
Train your model on ALL the data.

Provide your “customer” with the results of internal-cross validation as estimates of future performance.
Data snooping

Do a cross-validation study to set parameters
Do another cross-validation study, using the best parameters, to estimate future accuracy
  - How will this relate to the “true” future accuracy?
  - Likely to be an overestimate

What about:
1. Do a proper internal cross-validation experiment
2. Improve your algorithm; goto 1
Over-estimates in algorithm development

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(Machine Learning’s dirty secret!)
Training/validation/test

If you have a lot of data you can substitute internal cross-validation with use of a training/validation/test set.

For each parameter setting, train on the training set, and choose the parameter setting that gives best performance on the validation set. Retrain using those parameters on the training + validation sets and report accuracy on the test set.
Correct classifier evaluation

When running experiments consider the following question:

On each fold of cross-validation, did I ever access in any way the label of a test case?

Any preprocessing done over entire data set (feature selection, parameter tuning, threshold selection) must not use labels.
Using repository data for classifier evaluation

Pros:
- Very easy to implement
- Data from real applications
- Facilitates replication and comparison of results

Cons:
- Not representative of the data mining process which involves many steps other than classification.
- Community experiment/multiplicity effect: since so many experiments are run on the same data set, by chance, some will yield interesting (though meaningless) results
Model selection in scikit-learn

Is nested cross-validation difficult in scikit-learn?

NO!