

Chapter 5

Hyperopt-Sklearn

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Abstract

Hyperopt-sklearn is a software project that provides automatic algorithm configuration of the Scikit-learn machine learning library. Following Auto-Weka, we take the view that the choice of classifier and even the choice of preprocessing module can be taken together to represent a single large hyperparameter optimization problem. We use Hyperopt to define a search space that encompasses many standard components (e.g. SVM, RF, KNN, PCA, TFIDF) and common patterns of composing them together. We demonstrate, using search algorithms in Hyperopt and standard benchmarking data sets (MNIST, 20-Newsgroups, Convex Shapes), that searching this space is practical and effective. In particular, we improve on best-known scores for the model space for both MNIST and Convex Shapes at the time of release.

5.1 Introduction

Relative to deep networks, algorithms such as Support Vector Machines (SVMs) and Random Forests (RFs) have a small-enough number of hyperparameters that manual tuning and grid or random search provides satisfactory results. Taking a step back though, there is often no particular reason to use either an SVM or an RF when they are both computationally viable. A model-agnostic practitioner may simply prefer to go with the one that provides greater accuracy. In this light, the choice of classifier can be seen as hyperparameter alongside the C-value in the SVM and the max-tree-depth of the RF. Indeed the choice and configuration of preprocessing components may likewise be seen as part of the model selection / hyperparameter optimization problem.

The Auto-Weka project [18] was the first to show that an entire library of machine learning approaches (Weka [8]) can be searched within the scope of a single run of hyperparameter tuning. However, Weka is a GPL-licensed Java

library, and was not written with scalability in mind, so we feel there is a need for alternatives to Auto-Weka. Scikit-learn [15] is another library of machine learning algorithms. It is written in Python (with many modules in C for greater speed), and is BSD-licensed. Scikit-learn is widely used in the scientific Python community and supports many machine learning application areas.

This chapter introduces Hyperopt-Sklearn: a project that brings the benefits of automatic algorithm configuration to users of Python and scikit-learn. Hyperopt-Sklearn uses Hyperopt [3] to describe a search space over possible configurations of scikit-learn components, including preprocessing, classification, and regression modules. One of the main design features of this project is to provide an interface that is familiar to users of scikit-learn. With very little changes, hyperparameter search can be applied to an existing code base. This chapter begins with a background of Hyperopt and the configuration space it uses within scikit-learn, followed by example usage and experimental results with this software.

5.2 Background: Hyperopt for Optimization

The Hyperopt library [3] offers optimization algorithms for search spaces that arise in algorithm configuration. These spaces are characterized by a variety of types of variables (continuous, ordinal, categorical), different sensitivity profiles (e.g. uniform vs. log scaling), and conditional structure (when there is a choice between two classifiers, the parameters of one classifier are irrelevant when the other classifier is chosen). To use Hyperopt, a user must define/choose three things:

- A search domain,
- An objective function,
- An optimization algorithm.

The search domain is specified via random variables, whose distributions should be chosen so that the most promising combinations have high prior probability. The search domain can include Python operators and functions that combine random variables into more convenient data structures for the objective function. Any conditional structure is defined within this domain. The objective function maps a joint sampling of these random variables to a scalar-valued score that the optimization algorithm will try to minimize.

An example search domain using Hyperopt is depicted below.

```
from hyperopt import hp

space = hp.choice('my_conditional',
[
    ('case 1', 1 + hp.lognormal('c1', 0, 1)),
    ('case 2', hp.uniform('c2', -10, 10))
])
```

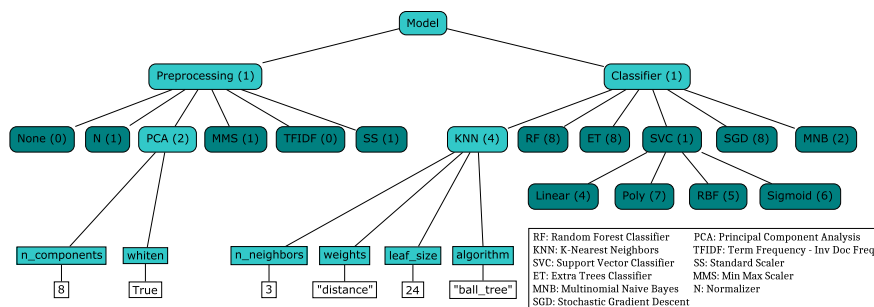


Figure 5.1: An example hyperopt-sklearn search space consisting of a preprocessing step followed by a classifier. There are 6 possible preprocessing modules and 6 possible classifiers. Choosing a model within this configuration space means choosing paths in an ancestral sampling process. The highlighted light blue nodes represent a (PCA, K-Nearest Neighbor) model. The white leaf nodes at the bottom depict example values for their parent hyperparameters. The number of active hyperparameters in a model is the sum of parenthetical numbers in the selected boxes. For the PCA+KNN combination, 8 hyperparameters are activated.

```
1) ('case 3', hp.choice('c3', ['a', 'b', 'c']))
```

Here there are four parameters, one for selecting which case is active, and one for each of the three cases. The first case contains a positive valued parameter that is sensitive to log scaling. The second case contains a bounded real valued parameter. The third case contains a categorical parameter with three options.

Having chosen a search domain, an objective function, and an optimization algorithm, Hyperopt's `fmin` function carries out the optimization, and stores results of the search to a database (e.g. either a simple Python list or a MongoDB instance). The `fmin` call carries out the simple analysis of finding the best-performing configuration, and returns that to the caller. The `fmin` call can use multiple workers when using the MongoDB backend, to implement parallel model selection on a compute cluster.

5.3 Scikit-Learn Model Selection as a Search Problem

Model selection is the process of estimating which machine learning model performs best from among a possibly infinite set of options. As an optimization problem, the search domain is the set of valid assignments to the configuration parameters (hyperparameters) of the machine learning model. The objective function is typically the measure of success (e.g. accuracy, F1-Score, etc) on held-out examples. Often the negative degree of success (loss) is used to set up

the task as a minimization problem, and cross-validation is applied to produce a more robust final score. Practitioners usually address this optimization by hand, by grid search, or by random search. In this chapter we discuss solving it with the Hyperopt optimization library. The basic approach is to set up a search space with random variable hyperparameters, use scikit-learn to implement the objective function that performs model training and model validation, and use Hyperopt to optimize the hyperparameters.

Scikit-learn includes many algorithms for learning from data (classification or regression), as well as many algorithms for preprocessing data into the vectors expected by these learning algorithms. Classifiers include for example, K-Nearest-Neighbors, Support Vector Machines, and Random Forest algorithms. Preprocessing algorithms include transformations such as component-wise Z-scaling (Normalizer) and Principle Components Analysis (PCA). A full classification algorithm typically includes a series of preprocessing steps followed by a classifier. For this reason, scikit-learn provides a pipeline data structure to represent and use a sequence of preprocessing steps and a classifier as if they were just one component (typically with an API similar to the classifier). Although hyperopt-sklearn does not formally use scikit-learn's pipeline object, it provides related functionality. Hyperopt-sklearn provides a parameterization of a search space over pipelines, that is, of sequences of preprocessing steps and classifiers or regressors.

The configuration space provided at the time of this writing currently includes 24 classifiers, 12 regressors, and 7 preprocessing methods. Being an open-source project, this space is likely to expand in the future as more users contribute. Upon initial release, only a subset of the search space was available, consisting of six classifiers and five preprocessing algorithms. This space was used for initial performance analysis and is illustrated in Figure 5.1. In total, this parameterization contains 65 hyperparameters: 15 boolean variables, 14 categorical, 17 discrete, and 19 real-valued variables.

Although the total number of hyperparameters in the full configuration space is large, the number of active hyperparameters describing any one model is much smaller: a model consisting of PCA and a RandomForest for example, would have only 12 active hyperparameters (1 for the choice of preprocessing, 2 internal to PCA, 1 for the choice of classifier and 8 internal to the RF). Hyperopt description language allows us to differentiate between conditional hyperparameters (which must always be assigned) and non-conditional hyperparameters (which may remain unassigned when they would be unused). We make use of this mechanism extensively so that Hyperopt's search algorithms do not waste time learning by trial and error that e.g. RF hyperparameters have no effect on SVM performance. Even internally within classifiers, there are instances of conditional parameters: KNN has conditional parameters depending on the distance metric, and LinearSVC has 3 binary parameters (loss, penalty, and dual) that admit only 4 valid joint assignments. Hyperopt-sklearn also includes a blacklist of (preprocessing, classifier) pairs that do not work together, e.g. PCA and MinMaxScaler were incompatible with MultinomialNB, TF-IDF could only be used for text data, and the tree-based classifiers were not compatible with the

sparse features produced by the TF-IDF preprocessor. Allowing for a 10-way discretization of real-valued hyperparameters, and taking these conditional hyperparameters into account, a grid search of our search space would still require an infeasible number of evaluations (on the order of 10^{12}).

Finally, the search space becomes an optimization problem when we also define a scalar-valued search objective. By default, Hyperopt-sklearn uses scikit-learn's score method on validation data to define the search criterion. For classifiers, this is the so-called "Zero-One Loss": the number of correct label predictions among data that has been withheld from the data set used for training (and also from the data used for testing after the model selection search process).

5.4 Example Usage

Following Scikit-learn's convention, hyperopt-sklearn provides an Estimator class with a fit method and a predict method. The fit method of this class performs hyperparameter optimization, and after it has completed, the predict method applies the best model to given test data. Each evaluation during optimization performs training on a large fraction of the training set, estimates test set accuracy on a validation set, and returns that validation set score to the optimizer. At the end of search, the best configuration is retrained on the whole data set to produce the classifier that handles subsequent predict calls.

One of the important goals of hyperopt-sklearn is that it is easy to learn and to use. To facilitate this, the syntax for fitting a classifier to data and making predictions is very similar to scikit-learn. Here is the simplest example of using this software.

```
from hpsklearn import HyperoptEstimator

# Load data
train_data, train_label, test_data, test_label = load_my_data()

# Create the estimator object
estim = HyperoptEstimator()

# Search the space of classifiers and preprocessing steps and their
# respective hyperparameters in scikit-learn to fit a model to the
# data
estim.fit(train_data, train_label)

# Make a prediction using the optimized model
prediction = estim.predict(test_data)

# Report the accuracy of the classifier on a given set of data
score = estim.score(test_data, test_label)

# Return instances of the classifier and preprocessing steps
```

```
model = estim.best_model()
```

The HyperoptEstimator object contains the information of what space to search as well as how to search it. It can be configured to use a variety of hyperparameter search algorithms and also supports using a combination of algorithms. Any algorithm that supports the same interface as the algorithms in hyperopt can be used here. This is also where you, the user, can specify the maximum number of function evaluations you would like to be run as well as a timeout (in seconds) for each run.

```
from hpsklearn import HyperoptEstimator
from hyperopt import tpe
estim = HyperoptEstimator(algo=tpe.suggest,
                          max_evals=150,
                          trial_timeout=60)
```

Each search algorithm can bring its own bias to the search space, and it may not be clear that one particular strategy is the best in all cases. Sometimes it can be helpful to use a mixture of search algorithms.

```
from hpsklearn import HyperoptEstimator
from hyperopt import anneal, rand, tpe, mix
# define an algorithm that searches randomly 5% of the time,
# uses TPE 75% of the time, and uses annealing 20% of the time
mix_algo = partial(mix.suggest, p_suggest=[
    (0.05, rand.suggest),
    (0.75, tpe.suggest),
    (0.20, anneal.suggest)])
estim = HyperoptEstimator(algo=mix_algo,
                          max_evals=150,
                          trial_timeout=60)
```

Searching effectively over the entire space of classifiers available in scikit-learn can use a lot of time and computational resources. Sometimes you might have a particular subspace of models that they are more interested in. With hyperopt-sklearn it is possible to specify a more narrow search space to allow it to be explored in greater depth.

```
from hpsklearn import HyperoptEstimator, svc

# limit the search to only SVC models
estim = HyperoptEstimator(classifier=svc('my_svc'))
```

Combinations of different spaces can also be used.

```
from hpsklearn import HyperoptEstimator, svc, knn
```

```

from hyperopt import hp

# restrict the space to contain only random forest,
# k-nearest neighbors, and SVC models.
clf = hp.choice('my_name',
    [random_forest('my_name.random_forest'),
     svc('my_name.svc'),
     knn('my_name.knn')])
estim = HyperoptEstimator(classifier=clf)

```

The support vector machine provided by scikit-learn has a number of different kernels that can be used (linear, rbf, poly, sigmoid). Changing the kernel can have a large effect on the performance of the model, and each kernel has its own unique hyperparameters. To account for this, hyperopt-sklearn treats each kernel choice as a unique model in the search space. If you already know which kernel works best for your data, or you are just interested in exploring models with a particular kernel, you may specify it directly rather than going through the svc.

```

from hpsklearn import HyperoptEstimator, svc_rbf
estim = HyperoptEstimator(classifier=svc_rbf('my_svc'))

```

It is also possible to specify which kernels you are interested in by passing a list to the svc.

```

from hpsklearn import HyperoptEstimator, svc
estim = HyperoptEstimator(
    classifier=svc('my_svc',
        kernels=['linear',
                 'sigmoid']))

```

In a similar manner to classifiers, the space of preprocessing modules can be fine tuned. Multiple successive stages of preprocessing can be specified through an ordered list. An empty list means that no preprocessing will be done on the data.

```

from hpsklearn import HyperoptEstimator, pca
estim = HyperoptEstimator(preprocessing=[pca('my_pca')])

```

Combinations of different spaces can be used here as well.

```

from hpsklearn import HyperoptEstimator, tfidf, pca
from hyperopt import hp
preproc = hp.choice('my_name',

```

```
[[pca('my_name.pca')],
 [pca('my_name.pca'), normalizer('my_name.norm')],
 [standard_scaler('my_name.std_scaler')],
 []])
estim = HyperoptEstimator(preprocessing=preproc)
```

Some types of preprocessing will only work on specific types of data. For example, the TfidfVectorizer that scikit-learn provides is designed to work with text data and would not be appropriate for other types of data. To address this, hyperopt-sklearn comes with a few pre-defined spaces of classifiers and preprocessing tailored to specific data types.

```
from hpsklearn import HyperoptEstimator, \
    any_sparse_classifier, \
    any_text_preprocessing
from hyperopt import tpe
estim = HyperoptEstimator(
    algo=tpe.suggest,
    classifier=any_sparse_classifier('my_clf')
    preprocessing=any_text_preprocessing('my_pp')
    max_evals=200,
    trial_timeout=60)
```

So far in all of these examples, every hyperparameter available to the model is being searched over. It is also possible for you to specify the values of specific hyperparameters, and those parameters will remain constant during the search. This could be useful, for example, if you knew you wanted to use whitened PCA data and a degree-3 polynomial kernel SVM.

```
from hpsklearn import HyperoptEstimator, pca, svc_poly
estim = HyperoptEstimator(
    preprocessing=[pca('my_pca', whiten=True)],
    classifier=svc_poly('my_poly', degree=3))
```

It is also possible to specify ranges of individual parameters. This is done using the standard hyperopt syntax. These will override the defaults defined within hyperopt-sklearn.

```
from hpsklearn import HyperoptEstimator, pca, sgd
from hyperopt import hp
import numpy as np
sgd_loss = hp.pchoice('loss',
    [(0.50, 'hinge'),
     (0.25, 'log'),
     (0.25, 'huber')])
sgd_penalty = hp.choice('penalty',
```

```

                                ['12', 'elasticnet'])
sgd_alpha = hp.loguniform('alpha',
                           low=np.log(1e-5),
                           high=np.log(1) )
estim = HyperoptEstimator(
    classifier=sgd('my_sgd',
                  loss=sgd_loss,
                  penalty=sgd_penalty,
                  alpha=sgd_alpha) )

```

All of the components available to the user can be found in the `components.py` file. A complete working example of using hyperopt-sklearn to find a model for the 20 newsgroups data set is shown below.

```

from hpsklearn import HyperoptEstimator, tfidf, any_sparse_classifier
from sklearn.datasets import fetch_20newsgroups
from hyperopt import tpe
import numpy as np
# Download data and split training and test sets
train = fetch_20newsgroups(subset='train')
test = fetch_20newsgroups(subset='test')
X_train = train.data
y_train = train.target
X_test = test.data
y_test = test.target
estim = HyperoptEstimator(
    classifier=any_sparse_classifier('clf'),
    preprocessing=[tfidf('tfidf')],
    algo=tpe.suggest,
    trial_timeout=180)
estim.fit(X_train, y_train)
print(estim.score(X_test, y_test))
print(estim.best_model())

```

5.5 Experiments

We conducted experiments on three data sets to establish that hyperopt-sklearn can find accurate models on a range of data sets in a reasonable amount of time. Results were collected on three data sets: MNIST, 20-Newsgroups, and Convex Shapes. MNIST is a well-known data set of 70K 28x28 greyscale images of hand-drawn digits [11]. 20-Newsgroups is a 20-way classification data set of 20K newsgroup messages ([12] , we did not remove the headers for our experiments). Convex Shapes is a binary classification task of distinguishing pictures of convex white-colored regions in small (32x32) black-and-white images [10].

Figure 5.2 (left) shows that there was no penalty for searching broadly. We performed optimization runs of up to 300 function evaluations searching the

MNIST		20 Newsgroups	
Approach	Accuracy	Approach	F-Score
Committee of convnets	99.8%	CFC	0.928
hyperopt-sklearn	98.7%	hyperopt-sklearn	0.856 %
libSVM grid search	98.6%	SVMTorch	0.848 %
Boosted trees	98.5%	LibSVM	0.843

Convex Shapes	
Approach	Accuracy
hyperopt-sklearn	88.7%
hp-dbnnet	84.6%
dbn-3	81.4%

Table 5.1: Hyperopt-sklearn scores relative to selections from literature on the three data sets used in our experiments. On MNIST, hyperopt-sklearn is one of the best-scoring methods that does not use image-specific domain knowledge (these scores and others may be found at <http://yann.lecun.com/exdb/mnist/>). On 20 Newsgroups, hyperopt-sklearn is competitive with similar approaches from the literature (scores taken from [7]). In the 20 Newsgroups data set, the score reported for hyperopt-sklearn is the weighted-average F1 score provided by sklearn. The other approaches shown here use the macro-average F1 score. On Convex Shapes, hyperopt-sklearn outperforms previous automatic algorithm configuration approaches [6] and manual tuning [10].

subset of the space depicted in Figure 5.1, and compared the quality of solution with specialized searches of specific classifier types (including best known classifiers).

Figure 5.2 (right) shows that search could find different, good models. This figure was constructed by running hyperopt-sklearn with different initial conditions (number of evaluations, choice of optimization algorithm, and random number seed) and keeping track of what final model was chosen after each run. Although support vector machines were always among the best, the parameters of best SVMs looked very different across data sets. For example, on the image data sets (MNIST and Convex) the SVMs chosen never had a sigmoid or linear kernel, while on 20 newsgroups the linear and sigmoid kernel were often best.

Sometimes researchers not familiar with machine learning techniques may simply use the default parameters of the classifiers available to them. To look at the effectiveness of hyperopt-sklearn as a drop-in replacement for this approach, a comparison between the performance of the default scikit-learn parameters and a small search (25 evaluations) of the default hyperopt-sklearn space was conducted. The results on the 20 Newsgroups dataset are shown in Figure 5.3. Improved performance over the baseline is observed in all cases, which suggests that this search technique is valuable even with a small computational budget.

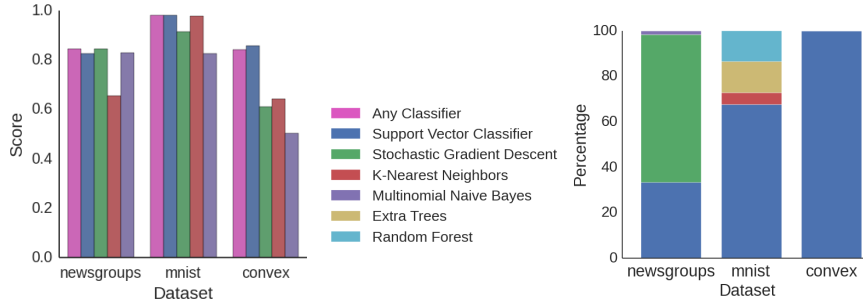


Figure 5.2: Left: Best Model Performance. For each data set, searching the full configuration space (“Any Classifier”) delivered performance approximately on par with a search that was restricted to the best classifier type. Each bar represents the score obtained from a search restricted to that particular classifier. For the “Any Classifier” case there is no restriction on the search space. In all cases 300 hyperparameter evaluations were performed. Score is F1 for 20 Newsgroups, and accuracy for MNIST and Convex Shapes.

Right: Model Selection Distribution. Looking at the best models from all optimization runs performed on the full search space (Any Classifier, using different initial conditions, and different optimization algorithms) we see that different data sets are handled best by different classifiers. SVC was the only classifier ever chosen as the best model for Convex Shapes, and was often found to be best on MNIST and 20 Newsgroups, however the best SVC parameters were very different across data sets.

5.6 Discussion and Future Work

Table 5.1 lists the test set scores of the best models found by cross-validation, as well as some points of reference from previous work. Hyperopt-sklearn’s scores are relatively good on each data set, indicating that with hyperopt-sklearn’s parameterization, Hyperopt’s optimization algorithms are competitive with human experts.

The model with the best performance on the MNIST Digits data set uses deep artificial neural networks. Small receptive fields of convolutional winner-take-all neurons build up the large network. Each neural column becomes an expert on inputs preprocessed in different ways, and the average prediction of 35 deep neural columns to come up with a single final prediction [4]. This model is much more advanced than those available in scikit-learn. The previously best known model in the scikit-learn search space is a radial-basis SVM on centered data that scores 98.6%, and hyperopt-sklearn matches that performance [14].

The CFC model that performed quite well on the 20 newsgroups document classification data set is a Class-Feature-Centroid classifier. Centroid approaches are typically inferior to an SVM, due to the centroids found during training being far from the optimal location. The CFC method reported here uses a

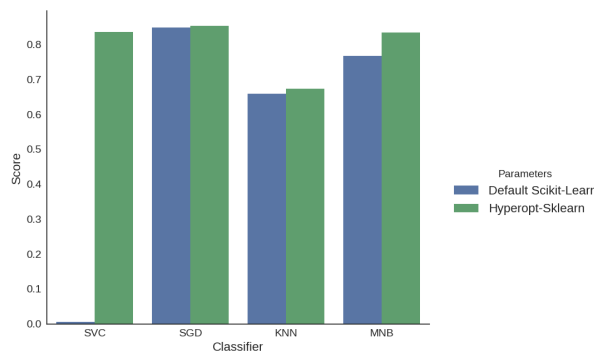


Figure 5.3: Comparison of F1-Score on the 20 Newsgroups dataset using either the default parameters of scikit-learn or the default search space of hyperopt-sklearn. The results from hyperopt-sklearn were obtained from a single run with 25 evaluations, restricted to either Support Vector Classifier, Stochastic Gradient Descent, K-Nearest Neighbors, or Multinomial Naive Bayes.

centroid built from the inter-class term index and the inner-class term index. It uses a novel combination of these indices along with a denormalized cosine measure to calculate the similarity score between the centroid and a text vector [7]. This style of model is not currently implemented in hyperopt-sklearn, and our experiments suggest that existing hyperopt-sklearn components cannot be assembled to match its level of performance. Perhaps when it is implemented, Hyperopt may find a set of parameters that provides even greater classification accuracy.

On the Convex Shapes data set, our Hyperopt-sklearn experiments revealed a more accurate model than was previously believed to exist in any search space, let alone a search space of such standard components. This result underscores the difficulty and importance of hyperparameter search.

Hyperopt-sklearn provides many opportunities for future work: more classifiers and preprocessing modules could be included in the search space, and there are more ways to combine even the existing components. Other types of data require different preprocessing, and other prediction problems exist beyond classification. In expanding the search space, care must be taken to ensure that the benefits of new models outweigh the greater difficulty of searching a larger space. There are some parameters that scikit-learn exposes that are more implementation details than actual hyperparameters that affect the fit (such as `algorithm` and `leaf_size` in the KNN model). Care should be taken to identify these parameters in each model and they may need to be treated differently during exploration.

It is possible for a user to add their own classifier to the search space as long as it fits the scikit-learn interface. This currently requires some understanding of how hyperopt-sklearn’s code is structured and it would be nice to improve the

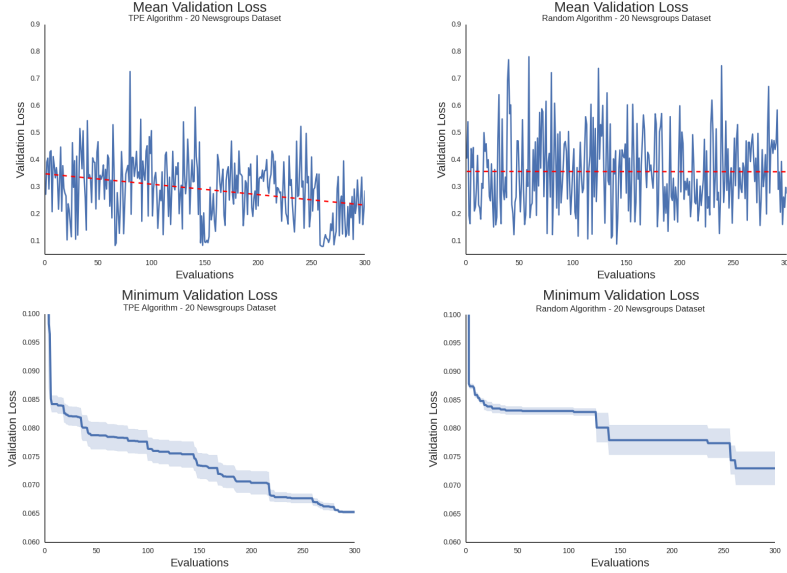


Figure 5.4: Validation loss of models found for each successive parameter evaluation using the 20 Newsgroups dataset and the Any Classifier search domain. **Upper Left:** Mean validation loss at each step across different random number seeds for the TPE algorithm. Downward trend indicates more promising regions are explored more often over time. **Upper Right:** Mean validation loss for the random algorithm. Flat trend illustrates no learning from previous trials. Large variation in performance across evaluations indicates the problem is very sensitive to hyperparameter tunings. **Lower Left:** Minimum validation loss of models found so far for the TPE algorithm. Gradual progress is made on 20 Newsgroups over 300 iterations and gives no indication of convergence. **Lower Right:** Minimum validation loss for the random algorithm. Progress is initially rapid for the first 40 or so evaluations and then settles for long periods. Improvement still continues, but becomes less likely as time goes on.

support for this so minimal effort is required by the user. It is also possible for the user to specify alternate scoring methods besides the default accuracy or F-measure, as there can be cases where these are not best suited to the particular problem.

We have shown here that Hyperopt’s random search, annealing search, and TPE algorithms make Hyperopt-sklearn viable, but the slow convergence in Figure 5.4 suggests that other optimization algorithms might be more call-efficient. The development of Bayesian optimization algorithms is an active research area, and we look forward to looking at how other search algorithms interact with hyperopt-sklearn’s search spaces. Hyperparameter optimization opens up a new art of matching the parameterization of search spaces to the strengths of search algorithms.

Computational wall time spent on search is of great practical importance, and hyperopt-sklearn currently spends a significant amount of time evaluating points that are un-promising. Techniques for recognizing bad performers early could speed up search enormously [17, 5].

5.7 Conclusions

This chapter has introduced Hyperopt-sklearn, a Python package for automatic algorithm configuration of standard machine learning algorithms provided by Scikit-Learn. Hyperopt-sklearn provides a unified interface to a large subset of the machine learning algorithms available in scikit-learn and with the help of Hyperopt’s optimization functions it is able to both rival and surpass human experts in algorithm configuration. We hope that it provides practitioners with a useful tool for the development of machine learning systems, and automatic machine learning researchers with benchmarks for future work in algorithm configuration.

Acknowledgements

This research was supported by the NSERC Banting Fellowship program, the NSERC Engage Program and by D-Wave Systems. Thanks also to Hristijan Bogoevski for early drafts of a hyperopt-to-scikit-learn bridge.

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