Search Based Code Generation for Machine Learning Programs

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ABSTRACT
Machine Learning (ML) has revamped every domain of life as it provides powerful tools to build complex systems that learn and improve from experience and data. Our key insight is that to solve a machine learning problem, data scientists do not invent a new algorithm each time, but evaluate a range of existing models with different configurations and select the best one. This task is laborious, error-prone, and drains a large chunk of project budget and time. In this paper we present a novel framework inspired by programming by Sketching [8] and Partial Evaluation [4] to minimize human intervention in developing ML solutions. We templatize machine learning algorithms to expose configuration choices as holes to be searched. We share code and computation between different algorithms, and only partially evaluate configuration space of algorithms based on information gained from initial algorithm evaluations. We also employ hierarchical and heuristic based pruning to reduce the search space. Our initial findings indicate that our approach can generate highly accurate ML models. Interviews with data scientists show that they feel our framework can eliminate sources of common errors and significantly reduce development time.

1 INTRODUCTION
Machine Learning (ML) is a set of techniques that give computers the ability to learn specific tasks from the data without being explicitly programmed. We are living in the golden age of machine learning—ML algorithms have defeated humans in chess, learned to drive autonomously, beat humans in Jeopardy, and out performed humans in fundamentally innate tasks of image recognition as well as speech understanding. While most of these battles are won by well funded teams of highly trained engineers, machine learning tools remain prohibitively expensive for average users and domain experts. In this paper we present software engineering techniques that make machine learning algorithms more usable by reducing the time to specify them and making them less costly to build.

Sculley et al. [7], based on their experience at Google, observe that software engineers developing ML code often have less time to write high quality code or explore the best solutions. Fernández-Delgado et al. [3] in a large scale study of various classifiers and datasets note that even well trained data scientists choose only classifiers from a range of familiar classifiers and do not necessarily pick the best ones. Moreover, the developers are susceptible to various machine learning pitfalls that existing APIs and frameworks do not protect against [2]. As more and more applications move to incorporate machine learning components in them, there is a need to provide better software engineering and tool support to developers.

Solar-Lezama [8] presented the Sketching framework to synthesize and generate code automatically from partial implementation i.e. a high level specifications with holes. To generally express the models as templates, we use a similar approach used by sketches. Searching mechanisms fill the holes to specify the models for specific data and hyperparameters. Sketching uses SAT-based inductive synthesis but our framework uses heuristics guided searching to fill the holes. To reduce the search space and runtime, we exploit partial evaluation [4]. While searching optimal hyperparameters, we can treat a previously trained model as partial evaluated and can update it for new combinations of hyperparameters. Thornton et al. used Bayesian optimization in Auto-Weka [9] to search for models and hyperparameters for given dataset and integrated it with Weka [5]. The focus of their technique is to optimize and automate the model searching mechanism using a statistical approach i.e. Bayesian optimization. By contrast, we show that we can develop a comprehensive machine learning framework using software engineering techniques such as sketching, partial evaluation, and searching using rule based decision.

In this paper we present a proof of concept implementation of our machine learning pipeline. We have selected a set of supervised1 learning algorithms and stored their templates, similar to sketches with holes. The user can setup the problem by providing a data source, its format, and select the column with class labels. Our approach preprocesses the data, normalizes it, and analyzes the data for its classes and features. We use a systematic search to find the best hyperparameter configuration that fill the "holes" for each classification algorithm. We only partially evaluate the search space and employ heuristics to prune our search space. Our approach ranks the algorithms based on their accuracy and returns the top candidate.

Contributions: We make various novel contributions in this work. We are the first to employ code synthesis and compiler optimization techniques to generate machine learning code. Existing model selection techniques [9] do not prune search space and simply attempt to find an optimum value based on a given criteria, and they do not work across various algorithms. We borrow meticulous engineering steps traditionally used in compiler optimization to prune the search space as well as transfer computation and information across algorithms.

2 ILLUSTRATIVE EXAMPLES
In this section we demonstrate how our prototype classifies real life datasets by selecting the right model with optimal hyperparameters and pruning search space using partial-evaluation and

1Supervised machine learning algorithms assume that the training data has class labels available
rules. Suppose we want to determine labels of ‘Glass Identification’ dataset from UCI repository [1]. We call the program as:

```
metaClassifier(format=’CSV’, source=’/glass.csv’,
              verbose=True, hasHeader=True)
```

Some arguments like data source are mandatory while others like data format are optional which are either inferred like data format or can be set as default such as default verbose=False. The arguments are parsed and the program is initialized. The holes of data acquisition sketches are filled by determining the data source and format and the potential search space is built i.e. classifiers and their hyperparameters’ candidate space. By default, the size of search space for classification is more than a thousand i.e. the sum of the combinations of hyperparameters of all classifiers under consideration. In case of the SVC, the hyperparameters’ candidate space is given below having forty combinations of hyperparameters:

$$
CSV_{candSpace} = \begin{cases} 
    \{ \text{kernel} \in \{ \text{linear, rbf, sigmoid} \} \} \\
    \{ C \in \{ 1, 10, 100, 1000, 10000 \} \} \\
    \{ \text{kernel} \in \{ \text{poly} \} \} \\
    \{ C \in \{ 1, 10, 100, 1000, 10000 \} \} \\
    \{ \text{degree} \in \{ 3, 4, 5, 6, 7 \} \}
\end{cases}
$$

The dataset is analyzed to determine that it has ten features and two hundreds and fourteen instances and six classes implying it is multiclass dataset and prune out all classifiers or hyperparameters from candidate space specific to binary-class datasets like for Logistic Regression, multi_class \( \in \{ \text{multinomial} \} \) instead of multi_class \( \in \{ \text{multinomial, ovr} \} \), because ovr repeatedly uses a binary approach to fit multiclass datasets. Next, ‘linearly separable test’ using perceptron is carried out. Its code is generated by filling the holes of perceptron with default parameters (penalty=None, alpha=0.0001 etc.) to classify the dataset and the accuracy is computed which is 43% (< 50%). Concluding that data is not linearly separable, the search space is updated by removing linear classifiers such as linearSVC, and hyperparameters such as liblinear from solvers for Logistic Regression and linear from kernels of SVC. This reduces the search space to about 80% of the original.

After preliminary pruning, the program begins to search the best model and optimal hyperparameters while dynamically pruning the remaining search space. It starts from the sketch of SVC:

```
SVC(C=??, kernel=??, degree=??)
```

by filling the holes from the above given candidate space e.g. C=1, kernel=rbf. Linear kernel is pruned and degree is needed only if kernel=polynomial. Next it tries kernel=rbf, C={10, 100} and determines that by increasing C beyond 10, the accuracy is not increasing so rules out higher values of C. Same rule applies to max_iter and some other numeric hyperparameters to reduce search space. Further models and their hyperparameters are tried while pruning out the search space. Search space reduces to about 60% of the original and when it exhausts, the model configuration with highest accuracy is selected to predict the labels, which is \( \text{SVC(C=10, kernel=rbf)} \) in this case. Consider another example of ‘Wisconsin Breast Cancer Dataset’ from UCI dataset repository which is linearly separable binary class dataset. Passing the linear separability test i.e. running perceptron, LinearSVC should be tried on this dataset along with Logistic Regression for binary classification using the liblinear solver and rule out all non-linear options.

### 3 APPROACH

Our approach to develop the framework is similar to fundamental ML pipeline. Every module of the pipeline automates the work to mitigate the human intervention and reduces the space wherever possible. Figure 1 demonstrates our pipeline approach. Module A acquires the datasets from given source provided by user as arguments. The test and training datasets are fed to Module B for data preparation without any human intervention to standardize the data like predicting the missing values and data transformation. After common preprocessing, framework inspects data in Module D to get its size i.e. the number of instances and features, number of classes, and also run some simple tests like linearly separable test. Using the results of inspection and heuristics, Module E reduces the by including or excluding the linear models and their hyperparameters by building the lists of classifiers C and the list of their corresponding hyperparameters H.

After preparation, the labeled (training) datasets is used for model-selection using stratified K-fold cross validation where the framework selects the best model without user intervention and reduces the using heuristics. In Module C, labeled dataset is split in K stratified folds i.e. \( D_{labeled} = \{ D_1, D_2, ..., D_k \} \). Module F picks the classifier sketch C and its hyperparameters’ candidate space H from search space and generates code by filling the holes of sketch and the generated model is trained using train set i.e. \( D_{labeled} \). In Module G, the labels are predicted for test features i.e. \( D_t \) using model testing. Accuracy is computed using predicted labels and actual labels in Module H, Model Evaluation. After each model evaluation, heuristics are gathered to update and prune the search space for example if accuracy is not increased by increasing the value of max_iter in Logistic Regression, we can remove all combinations with higher values of max_iter and same other hyperparameters. When search space exhausts, framework selects the model with highest accuracy to predict the labels of unlabeled (test) dataset in Module I and the predicted labels are output to user.

Algorithm 1 outlines our framework to solve classification problems automatically. The framework takes minimum information like data source and format, labels’ information, time budget, etc. as args. It parses the args and sets the fields of options (line 2); a dictionary holding global variables and behavior of the framework.

#### 3.1 Model Selection, Hyperparameters Optimization and Feature Selection

Our framework prototype treats the classification problem as a meta-search – the combined selection of classifier, its best hyperparameters and features selection. Suppose we have a set of classifiers, \( C = \{ C_1, C_2, ..., C_n \} \) and their respective hyperparameters spaces as \( \mathcal{H} = \{ \mathcal{H}_1, \mathcal{H}_2, ..., \mathcal{H}_n \} \). Algorithm 1 from line 8 to 17 iterates over the search space while updating and reducing. The search continues until interruption due to resource budget constraints or the search space \( \mathcal{S} = \sum_i |\mathcal{H}_i|\) exhausts. In time constraints, where \( \mathcal{S} \) does not exhaust, to find the potentially best model, the searching algorithm takes some decisions based on previous observations (explained in §3.2). In a given dataset, each feature/attribute doesn’t contribute to a solution equally. Line 9 selects best features of the dataset for C. From line 10 to 15, the algorithm iterates over all feasible combinations of hyperparameters of \( \mathcal{H}_i \) for a given classifier.
Algorithm 1 Meta Classifier

```
procedure metaClassifier(args)
  options ← parse(args)  // options is global dictionary
  D_train, D_test ← acquireData()
  preprocess(D_train, D_test)  // Common preprocessing
  inspectData(D_train, D_test)  // Inspect and run basic test
  Build list C and corresponding H  // based on data tests
  results ← φ  // To hold results of cross validation
  while not interrupted And C ← C.removeHead() do
    D_train, features ← selectFeatures(C, D_train)
    while H_C not exhausts do  // H_C is the grid of C
      Initialize C with H_C^j  // Set j^{th} combination
      acc, std = evaluateModel(C, D_train)
      results.Add(acc, std, C, H_C^j, features)
      Update H_C
    end while
    Update C and H
  end while
  Get appropriate model i.e with max(acc) and min(std)
  y = model.predict(D_test)
  return y
end procedure
```

\( C_i \) and using stratified cross validation, the scores (accuracy and std. deviation) are calculated and recorded in results.

### 3.2 Optimizations

The naïve searching mechanism can end up owing limited time budget and in those cases, sometime the searched model may not be the best one. To mitigate these situations, we used software engineering techniques. In this subsection, we describe the non-exhaustive list of the optimization tactics used in our prototype framework.

**Sharing of Code and Computation:** Machine learning models solving similar problems like classification have tendency to share code and computation to a reasonable extent. For example, instead of loading data from either local storage or remote server for every model separately, an obvious optimization is to load data once and make some common preprocessing before executing some model on it.

**Templatization and Code Generation:** For generalization of the models, we define them as templates in the same fashion of sketches for program synthesis [8]. The partial implementation of models is generic enough to synthesize (generate) the final code with specific data and hyperparameters.

**Partial Evaluation:** While searching the best hyperparameters of a model, for two consecutive combinations (where usually, the value of one hyperparameter is changed), we can use the previously fitted model as a partially evaluated module and update it. For example, finding the optimal number of epochs for stochastic gradient descent used by many ML models, instead of restarting iteration and initializing coefficients to zeros, we can resume iterations by retaining the coefficients. Moreover, different hyperparameters of a model usually control independent properties of underlying algorithm.

**Heuristics** Previous execution of a model with a combination of hyperparameters may, in some cases, omit other combinations. For example, while searching for best hyperparameters of logistic regression, if the accuracy does not improve with increase of max_iter (but keeping all other hyperparameters constant), we can skip all combinations of hyperparameters with higher values of max_iter. Similarly, the observations derived from the executions of one model can lead to prioritization of other models. This raises the probability that the best model is selected despite interruption due to time constraints. For example, if we run SGDClassifier and its accuracy with loss=perceptron is very low, we should try classifier Perceptron at the end. We continue updating our search space i.e. the list C and hyperparameters H based on observations to reduce the search space and prioritize models.

**Rule Based Optimization:** The knowledge and insight of data scientists guiding the search for the best performing model can be, in fact, translated into a long rule-based list, thereby automating the human decision making process, as in rule based expert systems. Following are a few examples:

- **Linearly Separable Test:** We should start the search using SVM classifier (i.e. C_1 = SVM) without any kernel or with linear kernel. If the score/accuracy is reasonably high, we can conclude that data is potentially linearly separable and we should first try other linear classifiers such as SVM with fine tuning.

- **Each Hyperparameter is not used in every combination.** Thus, we can ignore these to reduce the search space. For instance, in case of scikit-learn’s logistic regression, n_jobs and warm_start Hyperparameters are ignore if solver is set to liblinear. Similarly, in case of sklearn.svm.SVC, the Hyperparameter degree is ignored for all kernels except kernel=linear.
| Dataset     | Best Model | Hyperparameters | Accu |
|-------------|------------|-----------------|------|
| Breast Cancer | LR         | solver=l2, max_iter=10, penalty=1, C=1 | 0.98 |
| Iris         | LR         | solver=newton-cg, max_iter=100, multi_class=multinomial, pen=12, C=100 | 1    |
| Glass        | SVC        | kernel=rbf, C=10 | 0.76 |
| Ionosphere   | SVC        | kernel=rbf, C=10 | 0.88 |
| Diabetes     | SVC        | kernel=linear, C=1 | 0.78 |
| Sonar        | SVC        | kernel=rbf, C=1 | 0.82 |

Table 1: Best Models with Hyperparameters and Accuracy

4 IMPLEMENTATION AND EVALUATION

In order to evaluate our proposed framework, we implemented a prototype having the following classifiers: Logistic Regression, Perceptron, Support Vector Machine (SVM) Classifier, Linear SVM Classifier and Perceptron. Instead of implementing these classifiers from scratch, we used scikit-learn [6] as the underlying models along with some basic preprocessing and grid search to find the optimal hyperparameters. Our framework is designed generically to further incorporate other classifiers such as Naïve Bayes, as well as preprocessing techniques and optimization insights. In the same fashion, we can scale it for other machine learning problems such as regression, clustering etc.

We evaluated the prototype on some common datasets from UCI Machine Learning Repository [1] Table 1 shows the best model with optimal hyperparameters, accuracies and execution time of the test suit. In order to evaluate usability, we are interviewing ML practitioners to gather data on the time, effort and cost splurged in writing and debugging code. So far, we have anecdotal evidence that even experienced ML users fall into common pitfalls such as not using stratification, not identifying outliers, forgetting to normalize, or using different scales on train and test sets resulting in loss of precious time and effort. We plan to carry out a full scale qualitative and quantitative usability study and anticipate that ML users and particularly domain experts would benefit from the implementation support and ML insights provided by the framework.

5 FUTURE DIRECTIONS

Search based software engineering can revolutionize the field of machine learning. We strongly believe that work presented in this paper will be foundational in a massive effort to democratize machine learning and enable average users and domain experts to take full advantage of the technology. We have abstracted and templated ML algorithms thus exposing interfaces for searching it. We foresee many promising future direction arising from our work: Self Application of Machine Learning: One key observation of our work is that we can apply machine learning to discover and find better machine learning solutions. The curse of dimensionality and search space explosion have been a key hindrance in applying machine learning to itself. Initial approaches attempted to explore the entire space or approach it with random searching. We have presented a more systematic method that prunes the space based on human insights, which is comparable to how data scientists make decision and produce equivalent results. We believe this provides an avenue to explore other ML techniques to pick the best ML algorithm. For example, a Deep Neural Network (DNN) which decides which ML approach will work best for the given data and classification problem.

Transfer Learning among ML Algorithms: When data scientist run a machine learning algorithm, they naturally select the parameters and hyperparameters based on earlier runs of other algorithms or prior runs on a smaller dataset. This transfer of knowledge is the key to reducing the state space. In this paper we have used heuristics to transfer information, but in the future we are working on analytical solutions to this problem. The key advantage of an analytical solution is that it allows us to initialize the parameters of the algorithms optimally thus reducing the time for algorithm convergence.

Searching for Algorithm Architecture: We also see the possibility of extending our work to directly search the architecture of ML algorithm, chaining different algorithms and composing them like software modules. A simple example of compositional search would be to have a DNN that combines DNNs to find nose, ears, lips and eyes to find a face. This creates a possibility of building Wide Neural Networks where parts are searched in parallel.

Optimizing for Commodity Hardware: MapReduce and Spark have demonstrated the power of distributed system in exploring large search spaces in fraction of seconds. We believe that search based ML will become main stream as we port our search to exploit large scale distributed systems.

6 CONCLUSION

In this work we have demonstrated that software engineering techniques can make machine learning accessible to average users. We are able to represent ML algorithms with holes that our approach can efficiently and optimally fill with rules guided systematic search.

We have also implemented a machine learning pipeline to search across different ML algorithms and transfer knowledge between models being evaluated to minimize the human effort. The ultimate objective of our research is to build an end-to-end machine learning solution that can find the best model without any human intervention. The work presented here is a very promising first step in this direction.

REFERENCES

[1] A. Asuncion and D.H. Newman. 2007. UCI Machine Learning Repository. (2007). http://archive.ics.uci.edu/ml
[2] Cheng-Tao Chu. 2015. 7 common mistakes when doing Machine Learning. (March 2015). http://www.kdnuggets.com/2015/03/machine-learning-data-science-common-mistakes.html [Online; posted 01-March-2015].
[3] Manuel Fernández-Delgado, Eva Cernadas, Senén Barro, and Dinanl Amorim. 2014. Do We Need Hundreds of Classifiers to Solve Real World Classification Problems? J. Mach. Learn. Res. 15, 1 (Jan. 2014), 3133–3181. http://dl.acm.org/citation.cfm?id=2627435.2697065
[4] Yoshishiro Putamura. 1983. Partial computation of programs. In RMS Symposium on Software Science and Engineering. Springer, 1–35.
[5] Geoffrey Holmes, Andrew Donkin, and Ian H Witten. 1994. Weka: A machine learning workbench. In Intelligent Information Systems, 1994. Proceedings of the 1994 Second Australian and New Zealand Conference on. IEEE, 357–361.
[6] Fabian Pedregosa, Gael Varoquaux, Alexandre Gramfort, Vincent Michel, Bertrand Thirion, Olivier Grisel, Mathieu Blondel, Peter Prettenhofer, Ron Weiss, Vincent Dubourg, et al. 2011. Scikit-learn: Machine learning in Python. Journal of Machine Learning Research 12, Oct (2011), 2825–2830.
[7] D. Sculley, Gary Holt, Daniel Golovin, Alexandre Gramfort, Vincent Michel, Bertrand Thirion, Olivier Grisel, Mathieu Blondel, Peter Prettenhofer, Ron Weiss, Vincent Dubourg, et al. 2011. Scikit-learn: Machine learning in Python. Journal of Machine Learning Research 12, Oct (2011), 2825–2830.
[8] Chris Thornton, Frank Hutter, Holger H Hoos, and Kevin Leyton-Brown. 2013. Auto-WEKA: Combined selection and hyperparameter optimization of classification algorithms. In Proceedings of the 19th ACM SIGKDD international conference on Knowledge discovery and data mining. ACM, 847–855.