Why is Differential Evolution Better than Grid Search for Tuning Defect Predictors?

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Abstract

Context: One of the black arts of data mining is learning the magic parameters which control the learners. In software analytics, at least for defect prediction, several methods, like grid search and differential evolution (DE), have been proposed to learn these parameters, which has been proved to be able to improve the performance scores of learners.

Objective: We want to evaluate which method can find better parameters in terms of performance score and runtime cost.

Methods: This paper compares grid search to differential evolution, which is an evolutionary algorithm that makes extensive use of stochastic jumps around the search space.

Results: We find that the seemingly complete approach of grid search does no better, and sometimes worse, than the stochastic search. When repeated 20 times to check for conclusion validity, DE was over 210 times faster than grid search to tune Random Forests on 17 testing data sets with F-Measure.

Conclusions: These results are puzzling: why does a quick partial search be just as effective as a much slower, and much more, extensive search? To answer that question, we turned to the theoretical optimization literature. Bergstra and Bengio conjecture that grid search is not more effective than more randomized searchers if the underlying search space is inherently low dimensional. This is significant since recent results show that defect prediction exhibits very low intrinsic dimensionality—an observation that explains why a fast method like DE may work as well as a seemingly more thorough grid search. This suggests, as a future research direction, that it might be possible to peek at data sets before doing any optimization in order to match the optimization algorithm to the problem at hand.

Keywords: Defect prediction, tuning, differential evolution, grid search, intrinsic dimensionality.

1. Introduction

Given the large amount of data now available to analysts, many researchers in empirical software engineering are now turning to automatic data miners to help them explore the data [1, 2]. These learners come with many “magic numbers” which, if tuned, can generate better predictors for particular data spaces. For example, Fu et al. [3] showed that, with parameter tuning, the precision of software defect predictors learned from static code metrics can grow by 20% to 60%.

Since tuning is so effective, it is tempting to enforce tuning for all data mining studies. However, there is a problem: tuning can be slow. For example, in this paper, one of our tuners used 27.5 days of CPU time to perform 20 repeats of tuning Random Forests [4] for one tuning goal with 17 test data sets. Other researchers also comment that tuning may require weeks, or more, of CPU time [5]. One dramatic demonstration of the slowness of tuning (not for defect prediction) comes from Wang et al. [6] where the study required 15 years of CPU to explore 9.3 million candidate configurations for software clone detectors.

One way to address the cost of tuning data miners is to use cloud-based CPU farms. The advantage of this approach is that it is simple to implement (just buy the cloud-based CPU time). For example, such cloud resources were used in this paper. But uses of cloud-based resources have several disadvantages:

- Cloud computing environments are extensively monetized so the total financial cost of tuning can be prohibitive.

- The CPU time is wasted if there is a faster and more effective way.

It turns out that the last point is indeed the case—at least for tuning defect predictors learned from static code attributes. The case study of this paper compares two tuning methods: the grid search as used by Tantithamthavorn et al. [7] and differential evolution as used by Fu et al. [3]. Both papers investigate the impacts of tunings on defect predictors and find that parameter tuning can improve the learner performance by different methods. However, little is known which method can find better parameters in terms of performance scores and runtime cost. In this study, we would like to investigate the following questions:

- **RQ1:** Does tuning improve learners’ performance?

The case study shows that parameter tuning does improve learners’ performance. Hence, this suggests all the future
empirical study involving with data mining methods should not use “off-the-shelf” data mining tools.

- **RQ2:** Is grid search statistically better than DE in terms of performance scores (AUC & AUC$_{20}$ & precision & F-Measure)? The case study shows that grid search just performs statistically better in 6 out of 17 data sets for CART (Classification And Regression Tree) with precision evaluation measure. Other than that, grid search works just as well as DE for Random Forests and CART.

- **RQ3:** Is DE a more efficient tuner than grid search in terms of runtime cost? The case study show that DE runs much faster than grid search.

To answer the research questions, we build defect predictors with CART and Random Forests, and then conduct parameter tuning with DE, grid search and random search. After that, we evaluate the untuned learners, DE tuned learners, grid search tuned learners, and random search tuned learners on 17 test data sets in terms of AUC, AUC$_{20}$, precision and F-Measure. We also record the start and end time when each tuner running. This study makes the following contributions:

- To the best of our knowledge, this is the first such comparison of these two techniques for the purposes of tuning defect predictors;
- We show that differential evolution is just as effective as grid search for improving defect predictors, while being one to two orders of magnitude faster;
- Hence, we offer a strong recommendation to use evolutionary algorithms (like DE) for tuning defect predictors;
- Lastly, we propose a prediction method that would allow future analysts to match the optimization method to the data at hand.

The rest of this paper is organized as follows. Section 2 describes background, how defect predictors can be generated by data miners, and how tuning can affect the effectiveness of the learners. Section 3 defines and compares differential evolution and grid search as tuners. Section 4 presents the results from the case study. Section 5 is a discussion on why DE is effective and faster than grid search by showing how intrinsic dimensionality of the tuning search space help stochastic search method, like DE, to converge faster than more exhaustive methods like grid search. Section 6 discusses the potential threats to validity of this paper. Section 7 concludes this paper and discusses the future work.

While the specific conclusion of this paper relates to defect prediction, this work has broader implications across data science. Many researchers in software engineering (SE) explore hyper-parameter tuning \cite{8, 9, 10, 11, 12, 13, 7, 6} (for details, see Section 2.3). Within the group, grid search is the most commonly used tuner. Such studies can be tediously slow, often requiring days to weeks of CPU time. The success of differential evolution to tune defect predictors raises the possibility that tuning research could be greatly accelerated by a better selection of tuning algorithms. This could be a very productive avenue for future research.

2. Background

2.1. Defect Prediction

Human programmers are clever, but flawed. Along with functionality coding add defects. Hence, software sometimes crashes (perhaps at the most awkward or dangerous moment) or delivers the wrong functionality.

Since programming inherently introduces defects into programs, it is important to test them before they are used. Testing is expensive. According to Lowry et al. \cite{14}, software assessment budgets are finite while assessment effectiveness increases exponentially with assessment effort. Exponential costs quickly exhaust finite resources so the standard practice is to apply the best available resources only on code sections that seem most critical. Any method that focuses on parts of the code can miss defects in other areas, which means some sampling policy should be used to explore the rest of the system. This sampling policy will always be incomplete, but it is the only option when amount of resources available prevents a complete assessment of everything.

One of such sampling policies is defect predictors learned from static code attributes. Given software described in the attributes like Table 1, data miners can infer where software defects mostly occur. This is useful since static code attributes can be automatically collected, even for very large systems. Other methods, like manual code reviews, are slower and more labor-intensive \cite{15}. There is an increasing number of work to build defect predictors based on static code attributes \cite{16, 17, 18} and it can localize 70% (or more) of the defects in code. \cite{2}. They also perform well compared to certain widely-used automatic methods. Rahman et al. \cite{19} compared (a) static code analysis tools FindBugs, Jlint, and Pmd with (b) static code defect predictors. They found no significant differences in the cost-effectiveness of these approaches. This is interesting since static code defect prediction can be quickly adapted to new languages by building lightweight parsers that extract attributes described in Table 1. The same is not true for static code analyzers which need extensive modification before they can be used on new languages.

2.2. Data Mining

Data miners produce summaries of data and they are efficient since they employ various heuristics in order to reduce their search space for finding summaries. For examples, CART and Random Forests tree learners. These algorithms divide a data set, then recursively split on each node until some stop criterion is satisfied. In the case of building defect predictors,
these learners reflect on the number of issue reports \( d_i \) raised for each class in a software system where the issue counts are converted into binary “yes/no” decisions via Equation (1), where \( T \) is a threshold number.

\[
\text{inspect} = \begin{cases} 
  d_i \geq T \rightarrow \text{Yes} \\
  d_i < T \rightarrow \text{No,}
\end{cases}
\]

For the specific implementation in Scikit-learn [20], the splitting process is controlled by numerous tuning parameters listed in Table 2 where the default parameters for CART and Random Forest are set by the Scikit-learn authors except for \( n_{\text{estimators}} \), as recommended by Witten et al. [21], we used 100 trees as default instead of 10. If data contains more than \( \text{min}\_\text{sample}\_\text{split} \), then a split is attempted. On the other hand, if a split contains no more than \( \text{min}\_\text{samples}_\text{leaf} \), then the recursion stops.

These learners use different techniques to explore the splits:

- CART finds the attributes of the dataset whose ranges contain rows (samples of data) with least variance in the number of defects; if an attribute ranges \( i \) is found in \( n_i \) rows, each with a defect count variance of \( v_i \), then CART seeks the attributes whose ranges minimizes \( \sum_i (\sqrt{n_i} \times n_i / (\sum n_i)) \).

- Random Forests divides data like CART then builds number of \( F \) trees \((F>1)\), each time using some random subset of the attributes.

Note that some tuning parameters are learner specific. \( \text{max}\_\text{feature} \) is used by CART and Random Forests to select the number of attributes used to build one tree. CART’s default is to use all the attributes while Random Forests usually selects the square root of the number of attributes. Also, \( \text{max}\_\text{leaf}\_\text{nodes} \) is the upper bound on leaf nodes generated in a Random Forests. Lastly, \( \text{max}\_\text{depth} \) is the upper bound on the depth of the CART tree.

2.3. Parameter Tuning

Parameter tuning for evolutionary algorithms was studied by Arcuri et al. [5] and presented at SSSBE’11. Using the grid search method (described below), they found that different parameter settings for evolutionary programs cause very large variance in their performance. Also, while default parameter settings perform relatively well, they are far from optimal on particular problem instances.

Tuning is now explored in many parts of the SE research literature. Apart for defect prediction, tuning is used in the hyper-parameter optimization literature exploring better combinatorial search methods for software testing [8] or the use of genetic algorithms to explore 9.3 million different configurations for clone detection algorithms [6].

Other researchers explore the effects of parameter tuning on topic modeling [9]. Like Arcuri et al. [5], that work showed that the performance of the LDA (Latent Dirichlet Allocation) topic modeling algorithm was greatly effected by the choice of four parameters that configure LDA. Furthermore, Agrawal et.al [22] demonstrate that more stable topics can be generated by tuning LDA parameters using differential evolution algorithm.

Tuning is also used for software effort estimation; e.g. using tabu search for tuning SVM [10]; or genetic algorithms for tuning ensembles [11]; or as an exploration tool for checking if parameter settings affect the performance of effort estimators (and what learning machines are more sensitive to their parameters) [12]. The latter study explored Random Forests, kth-nearest neighbor methods, MLPs (MultiLayer Perceptrons), and bagging. This was another grid search paper that explored a range of tunings parameters and the corresponding value ranges were divided into 5 bins.

For defect prediction, we have performed a literature review starting with the key words “software engineering” and “defect prediction” and “data mining” [3] (more details can be found at https://goo.gl/Inl9nF). After sorting by the citation count and...
discarding the non-SE papers (and those without a pdf link), we read over this sample of 52 highly-cited SE defect prediction papers. What we found in that sample was that few authors acknowledged the impact of tunings (exceptions: [23, 13, 7, 3]). As shown in Figure 1 about 80% of papers in our sample did not mention any parameter tuning and just use the “off-the-shelf” configuration of the data miner (e.g. [2, 24, 25]). Lessmann et al. [13] used grid search to tune parameters as part of their extensive analysis of different algorithms for defect prediction. Strangely, they only tuned a small set of their learners while for most of them, they used the default settings. This is an observation we cannot explain but our conjecture is that the overall cost of their grid search tuning was so expensive that they restricted it to just the hardest choices. Gao et al. [23] acknowledged the impacts of the parameter tuning and they set some parameters within the learner, like set \( k = 30 \) for KNN. However, they did not provide any further explanation.

There are two recent work investigating the effects of parameter tuning on defect prediction by Tantithamthavorn et al. [7] and Fu et al. [3]: the former used grid search while the latter used differential evolution (both these techniques are detailed, below). These two teams worked separately using completely different scripts (written in “R” or in Python). Yet for tuning defect predictors, both groups reported the same results as follows:

- Across a range of performance measures (AUC, precision, recall, F-Measure), tuning rarely makes performance worse;
- Tuning offers a median improvement of 5% to 15% for most measures;
- For a third of data sets exploration, tuning can result in performance improvements of 30% to 50%.

Also, in a result that echoes one of the conclusions of Arcuri & Fraser, Fu et al. [3] report that different data sets require different tunings.

What was different between Fu et al. [3] and Tantithamthavorn et al. [7] was the computational costs of the two studies. Fu et al. [3] used a single desktop machine and all their runs terminated in 2 hours for one tuning goal. On the other hand, the grid search of Tantithamthavorn et al. [7] used 43 high-performance computing machines with 24 hyper-threads times 43 machines = 1,032 hyper-threads. Their total runtime were not reported— but as shown below, such tuning with grid search can take over a day just to learn one defect predictor.

### 3. Case Study: Grid Search vs. Differential Evolution

Tantithamthavorn et al. [7] and Fu et al. [3] use different methods to tune defect predictors. Neither offer a comparison of their preferred tuning method to any other. This section offers such a case study: specifically, a comparison of grid search and different evolution for tuning defect predictors.

#### 3.1. Algorithms

**Grid search** is simply picking a set of values for each configuration parameter and evaluating all the combinations of these values, then return the best one as the final optimal result. This can be simply implemented by nested for-loops. For example, for Naive Bayes, two loops might explore different values from the Laplace and M-estimator while a third loop might explore what happens when numeric values are divided into, say, \( 2 \leq b \leq 10 \) bins.

Bergstra and Bengio [26] comment on the popularity of grid search: (a) Such a simple search gives researchers some degree of insight into it; (b) There is little technical overhead or barrier to its implementation; (c) As to automating grid search, it is simple to implement and parallelization is trivial; (d) According to Bergstra and Bengio [26], grid search (on a computing cluster) can find better tunings than sequential optimization (in the same amount of time).

Since it’s easy to understand and implement and, to some extent, also has good performance, grid search has been available in most popular data mining and machine learning tools, like caret package in the R and GridSearchCV module in Scikit-learn [20].

**Differential evolution** is included in many optimization toolkits, like JMetal in Java [28]. But given its implementation simplicity, it is often written from scratch using the researcher’s preferred scripting language. Differential evolution just randomly picks three different vectors \( B, C, D \) from a list called \( F \) (the frontier) for each parent vector \( A \) in \( F \) [29]. Each pick generates a new vector \( E \) (which replaces \( A \) if it scores better according to the tuning goal). \( E \) is generated as follows:

\[
\forall i \in A, E_i = \begin{cases} 
B_i + f \ast (C_i - D_i) & \text{if } \mathcal{R} < cr \\
A_i & \text{otherwise}
\end{cases}
\]

where \( 0 \leq \mathcal{R} \leq 1 \) is a random number, and \( f, cr \) are constants (following Storn et al. [29], we use \( cr = 0.3 \) and \( f = 0.75 \)). Also, one \( A_i \) value (picked at random) is moved to \( E_i \) to ensure that \( E \) has at least one unchanged part of an existing vector.

![Figure 1: Literature review about parameter tuning on 52 top cited defect prediction papers](image-url)
As a sanity check, we also provide random search as a third optimizer to tune the parameters. Random search is nothing but randomly generate a set of different candidate parameters, and always evaluate them against the current “best” one. If better, then it will replace the “best” one. The process is repeated until the stop condition meets. In this case study, we set maximum iterations for random search the same as median number of evaluations in DE. The parameter will be randomly generated from the same tuning range as in Table 2. Grid search is much slower than DE since DE explores fewer options. Grid search’s execution of X loops exploring N options takes time $O(N^X)$, where $X$ is the number of parameters being tuned. Hence, Tantithamthavorn et al. [7] required 1000s of hyperthreads to complete their study in less than a day [7].

The grid search of Arcuri & Fraser [5] took weeks to terminate, even using a large computer cluster. In the following study, our grid search times took 27.5 days of total CPU time for Random Forests with F-Measure.

On the other hand, DE’s runtime is much faster since it is linear on the size of the frontiers, i.e. $O(|F|)$.

### 3.2. Data Miners

This study uses Random Forests and CART, for the following reason. Firstly, they were two of the learners studied by Tantithamthavorn et al. [7] and Fu et al. [3]. Secondly, they are interesting learners in that they represent two ends of a performance spectrum for defect predictors. CART and Random Forests were mentioned in a recent IEEE TSE paper by Lessmann et al. [13] that compared 22 learners for defect prediction. That study ranked CART as the worst learning technique and Random Forests as the best one. In a demonstration of the impact of tuning, Fu et al. [3] showed that they could refute the conclusions of Lessmann et al. [13] in the sense that, after tuning, CART performs just as well as Random Forests.

### 3.3. Tuning Parameters

The DE and grid search explored the parameter space as described Table 2. Specifically, since Tantithamthavorn et al. [7] divide each tuning range into 5 bins (if applicable), we also use the same policy here. For example, we pick values [50, 75, 100, 125, 150] for $n_{estimators}$. Other parameters grid will be generated in the same way. As to why we used the “Tuning Range” shown in Table 2 and not some other ranges, we note that (1) those ranges included the defaults; (2) the results shown below show that by exploring those ranges, we achieved large gains in the performance of our defect predictors. This is not to say that larger tuning ranges might not result in greater improvements.

#### 3.4. Data

Our defect data, shown in Table 3, comes from SEACRAFT repository so is available for others to replicate our results [30]. This data pertains to open source Java systems defined in terms of Table 1: ant, camel, ivy, jedit, log4j, lucene, poi, synapse, velocity and xerces.

We selected these data sets since they have at least three consecutive releases (where release $i + 1$ was built after release $i$). This will allow us to build defect predictors based on the past data and then predict (test) defects on future version projects, which will be a more practical scenario.

More specifically, when tuning a learner:

- Release $i$ was used for training a learner with tunings generated by grid search or differential evolution.
- During the search, each candidate has to be evaluated by some model, which we build using CART or Random Forests from release $i + 1$.
- After grid search or DE terminated, we tested the tunings found by those methods on CART or Random Forests and applied to release $i + 2$.

For comparison purposes, CART and Random Forests were also trained (with default tunings) on releases $i$ and $i + 1$, then tested on release $i + 2$.

In Table 3, we list all the data sets used for our case study. The fractions denote defects/total. E.g., given antV0 data sets, we have training, tuning and testing data. Specifically, the training data data set has 20 defective instances out of 125 total.

#### 3.5. Optimization Goals

Our optimizers explore tuning improvements for precision, AUC, $AUC_20$ and the F-Measure, defined as follows. Note that all these scores, the better scores are larger.

$$
\text{Precision} = \frac{\text{True Positive}}{\text{True Positive} + \text{False Positive}}
$$

$$
\text{Recall} = \frac{\text{True Positive}}{\text{True Positive} + \text{False Negative}}
$$

$$
F - \text{Measure} = \frac{2 \times \text{Precision} \times \text{Recall}}{\text{Recall} + \text{Precision}}
$$

### Table 2: List of parameters tuned by this paper.

| Learner Name | Parameters     | Default | Tuning Range      | Description                                                                 |
|--------------|---------------|---------|-------------------|-----------------------------------------------------------------------------|
| CART         | threshold     | 0.5     | [0.01, 1]         | The value to determine defective or not.                                    |
|              | max_feature   | None    | [0.01, 1]         | The number of features to consider when looking for the best split.         |
|              | min_samples_splits | 2   | [2, 20]          | The minimum number of samples required to split an internal node.            |
|              | min_samples_leaf | 1    | [1, 20]          | The minimum number of samples required to be at a leaf node.                |
|              | max_depth     | None    | [1, 50]           | The maximum depth of the tree.                                             |
| Random Forests | threshold     | 0.5     | [0.01, 1]         | The value to determine defective or not.                                    |
|              | max_feature   | None    | [0.01, 1]         | The number of features to consider when looking for the best split.         |
|              | max_leaf_nodes| None    | [1, 20]           | Grow trees with max_leaf_nodes in best-first fashion.                       |
|              | min_samples_splits | 2   | [2, 20]          | The minimum number of samples required to split an internal node.            |
|              | min_samples_leaf | 1    | [1, 20]          | The minimum number of samples required to be at a leaf node.                |
|              | n_estimators  | 100     | [50, 150]        | The number of trees in the forest.                                         |
**3.6. 20 Random Runs:**

All our studies were repeated 20 times to check for the stability of conclusions across different random biases. Initially, we planned for 30 repeats but grid search proved to be so slow that, for pragmatic reasons, we used 20 repeats. To be clear, the random seed is different for each data set in each repeat, but it will be the same across learners built by grid search and DE as well as random search for the same data set.

The reason that we believe this is the right thing to do is the search bias for a particular training/tuning/testing run is always the same. For the same training/tuning/testing data set, searching algorithms will start from the same random seed. With this approach, it is important to note that different triplets have different seed values (so this case study does sample across a range of search biases).

**3.7. Statistical Tests**

For each data set, the results of grid search and DE were compared across the 20 repeats. Statistical differences were tested by the Scott-Knott test [36] that used the Efron & Tibshirani bootstrap procedure [37] and the Vargha and Delaney A12 effect size test [38] to confirm that sub-cluster of the treatments are statistically different by more than a small effect. We used these statistical tests since they were recently endorsed in the SE literature by Mittas & Angelis (for Scott-Knott) in TSE’13 [39] and Acura & Briand (for A12) at ICSE’11 [40].

**4. Results**

In this section, we present the results from the above designed case studies. To answer the research questions, we build defect predictors based on CART and Random Forests. Then, we apply DE, random search and grid search on the learners to tune the parameters listed in Table 2 according different tuning goals, precision, F-Measure, AUC and AUC$_{20}$, respectively. Then, the performance of these learners are evaluated based on these measures accordingly.

**RQ1: Does tuning improve learners’ performance?**

The performance scores of untuned learner and tuned learners (by DE, random search and grid search) in terms of precision, F-Measure, AUC and AUC$_{20}$ are shown in Figure 2, Figure 3, Figure 4 and Figure 5 respectively. As a note, all these four figures are generated by four separate case studies with tuning goals of precision, F-Measure, AUC and AUC$_{20}$, respectively. In those figures: (a) The blue squares show the DE results; (b) The green diamonds show the results of running a learner using the default parameter settings; (c) The yellow triangles show the random search results; (d) The red dots show the grid search results.
Grid search results are denoted by the red dots. In this study, to compare whether grid search is statistically better than DE, we apply Scott Knott test on evaluation scores over 20 repeats. Based the Scott Knott results, (a) when tuning CART, grid search performs statistically better than DE only on velocityV0 for AUC and six test data sets (i.e., camelV0, jeditV0, jeditV1, log4jV0, poiV0, xercesV1) for precision. However, grid search is never better than DE for F-Measure. Furthermore, grid search works even worse than the default leaner for AUC20 scores on almost all data sets. (b) when tuning Random Forests, grid search only works statistically better than DE on log4jV0 test data for precision score. Other than that, grid search never outperforms DE for any evaluation measure.

Note that Figure 2 to Figure 5 also contain results that echoes conclusions from Arcuri & Fraser in SSBSE’11 [5]: (a) Default parameter settings perform relatively well. Note that there exists several cases where the tuned results (blue squares or red dots) are not much different to the results from using the default parameters (the green diamonds). (b) But they are far from optimal on particular problem instances. Note all the results where the red dots and blue squares are higher than green, particularly in the results where we are tuning for precision.

The comparisons between DE and grid search in terms of different evaluation measures suggest that:

Differential evolution is just as effective as grid search for improving defect predictors.

**RQ3: Is DE a more efficient tuner than grid search in terms of runtime cost?**

Figure 6 and Figure 7 show the runtime cost of grid search, random search and DE over 17 data sets including precision, F-Measure, AUC and AUC20 as optimization objectives. The Figure 6 shows the raw runtime (in seconds) of our entire tuning process in terms of 4 evaluation measures. In that plot, firstly, we see that tuning CART is faster than tuning Random Forests. Specifically, 20 repeats of a grid search of Ran-
dom Forests required 109 days of CPU time for all 4 evaluation measures; Secondly, DE is faster than grid search: it takes $10^5$ seconds for both DE to tune CART and Random Forests, while $10^5$ and $10^7$ seconds for grid search to complete the tuning. DE runs as fast as random search for both CART and RF and there’s no significant difference between DE and random search in terms of runtime.

The Figure 7 shows the same information as Figure 6 but in the ratio form. In that plot, each bar represents the runtime of the learner with the corresponding tuning technique to running learner without tuning. From Figure 7 we observe that grid search is 1,000 to 10,000 times slower than just running the default learners, while DE adds a factor of $10^2$ to the default (untuned) runtime cost. Overall, both Figure 6 and Figure 7 suggest that:

Differential evolution runs much faster than grid search.

According to the above results, we summarize the conclusions as: (a) Both DE and random search as well as grid search can improve learners’ performance for most cases; (b) Compared to DE, grid search runs far too long for too little additional benefit; (c) Both DE and random search require the same amount of runtime. But for some cases, DE has better performance than random search. (d) There are many cases where DE outperforms grid search.

5. Discussion

5.1. Why does DE perform better than grid search?

How to explain the suprising success of DE over grid search? Surely a thorough investigation of all options (via grid search) must do better than a partial exploration of just a few options (via DES).

It turns out that grid search is not a thorough exploration of all options. Rather, it jumps through different parameter settings between some min and max value of pre-defined tuning range. If the best options lie in between these jumps, then grid search will skip the critical tuning values. That means, the selected grid points will finally determine what kind of tunings we can get and good tunings require a lot of expert knowledge.

Note that DE is less prone to skip since, as shown in Equation 2 tuning values are adjusted by some random amount that is the difference between two randomly selected vectors. Further, if that process results in a better candidate, then this new randomly generated value might be used as the start point of a subsequent random selection of data. Hence DE is more likely than grid search to “fill in the gaps” between an initially selected values.

Another important difference between DE and grid search is the nature of their searches:

• All the grid points in the pre-defined grids are independently evaluated. This is useful since it makes grid search highly suited for parallelism (just run some of the loops on different processors). That said, this independence has a drawback: any lessons learned midway by grid search cannot affect (improve) the inferences made in the remaining runs.

• DE’s candidates (equivalent to grid points) do “transfer knowledge” to candidates in the new generation. Since DE is an evolutionary algorithms, the better candidates will be inherited by the following generations. That said, DE’s discoveries of better vectors accumulate in the frontier—which means new solutions (candidates) are being continually built from increasingly better solutions cached in the frontier. That is, lessons learned midway through a DE run can improve the inferences made in the remaining runs.

Bergstra and Benigo [26] offer a more formal analysis for why random searches (like DEs) can do better than grid search. They comment that grid search will be expected to fail if the region containing the useful tunings is very small. In such a search space: (a) Grid search can waste much time exploring an irrelevant part of the space. (b) Grid search’s effectiveness is limited by the curse of dimensionality.
Bergstra and Benigo reasons for the second point are as follows. They compared deep belief networks configured by a thoughtful combination of manual search and grid search, and purely random search over the same 32-dimensional configuration space. They found found statistically equal performance on four of seven data sets, and superior performance on one of seven. A Gaussian process analysis of their systems revealed that for most data sets only a few of the tuning really matter, but that different hyper-parameters are important on different data sets. They comment that a grid with sufficient granularity to tune for all data sets must consequently be inefficient for each individual data set because of the curse of dimensionality: the number of wasted grid search trials is exponential in the number of search dimensions that turn out to be irrelevant for a particular data set. Bergstra and Benigo add:

... in contrast, random search thrives on low effective dimensionality. Random search has the same efficiency in the relevant subspace as if it had been used to search only the relevant dimensions.

Our previous results in Section 4 also verified Bergstra and Benigo’s conclusion that random search is much better than grid search for exploring defect prediction data space, where random search is as good as DE in most data sets. But grid search rarely outperformed DE and random search in terms of performance scores (F-Measure, Precision, AUC and AUC$_{20}$). However, grid search just wastes a lot of time to explore unnecessary space.

5.2. When (not) to use DE?

How can we assess the external validity of the above results? Is it possible to build some predictor when DEs might and might not work well?

To explore these questions we use Bergstra and Benigo’s comments to define the conditions when we would expect DEs to work better than grid search for defect prediction. According to the argument above, DE works well for tuning since: (a) DE tends to favor the small number of intrinsic dimensions relevant to tuning; (b) The space of tunings for defect predictors is inherently low dimensional.

In defence of the first point, recall that Equation 2 says that DE repeatedly compares an existing tuning $A$ against another candidate $E$ that is constructed by taking a small step between three other candidates $B, C, D$. DE runs over a list of old candidates, $n$ times. For $n > 1$, the invariant is that members of that list are not inferior to at least one other example. If a new candidate $E$ is created that is orthogonal to the relevant dimensions, it will be no better than the candidates $B, C, D$ it was created from. Hence, the invariant for any successful $E$ replacement of $A$ is that it has moved over the relevant dimensions.

As to the second point about the low dimensional nature of tuning defect predictors, we first assume that the dimensionality of the tuning problem is linked to the dimensionality of the data explored by the learners. Our argument for this assumption is (1) learners like CART and Random Forests divide the data into regions with similar properties (specifically, those with and without defects); (2) when we tune those learners, we are constraining how they make those divisions over that data.

Given that assumption, exploring the space of tunings for defect predictors really means exploring the dimensionality of defect prediction data. Two studies strongly suggest that this data is inherently low-dimensionality. Papakroni 31 combined instance selection and attributes pruning for defect prediction. Using some information theory, he was able to prune 75% of the attributes of Table 1 as uninformative. He then clustered the remaining data, replacing each cluster with one centroid. This two-phase pruning procedure generated small data sets with, e.g., 24 columns (attributes) and 800 rows (instances) to a table of 6 columns and 20 rows. To test the efficacy of that reduced space, Papakroni built defect predictors by extrapolating between the two nearest centroids in the reduced space, for each test case. Papakroni found that those estimates from that small space worked just as well as those generated by state-of-the-art learners (Random Forests and Naive Bayes) using all the data 41. That is, according to Papakroni, the signal in these data sets can be found in a handful of attributes and a few dozen instances.

In order to formalize the findings of the Papakroni study, Provence 42 explored the intrinsic dimensionality of defect data sets. Intrinsic dimensionality measures the number of dimensions $m$ used by data within an $n$ dimensional space. For example, the “B” data shown at right spreads over a $n = 2$ dimensional space. but the “A” data does not use all the available dimensions. Hence, the intrinsic dimensionality of the “A” data is $m = 1$.

Like Provence, we use correlation dimension to calculate the intrinsic dimensionality of the datasets. Euclidean distance is
used to compute the distance between the independent decisions $d$ within each candidate solution; all $d_i$ values are normalized by $max - min$. Next, we use the distance measure as part of the correlation dimension defined by by Grassberger and Procaccia [33]. This correlation dimension of a data set with $k$ items is found by plotting the number of items found at distance within radius $r$ from any other item against $r$ (where $r$ is actually a distance, as defined in the last paragraph). Then we normalize this by the number of connections between $k$ items to find the expected number of neighbors at distance $r$ is $C(r) = \frac{2}{k(k-1)} \sum_{i=1}^{k} \sum_{j=i+1}^{k} I\{||x_i, x_j|| < r\}$.

Given a dataset with $k$ items and min, max distance of $r_{min}$ and $r_{max}$, we estimate the intrinsic dimensionality as the mean value of the slope of $\ln(C(r))$ vs $\ln(r)$ by evaluating $C(r)$ for $r$ in $\{r_0, ..., r_n\}$, such that $\{r_0, ..., r_n\}$ is sufficient for a good estimation of slope, and $r_n << r_{max}$.

Figure 8 shows the intrinsic dimensions for the data sets used in this study. Note the low intrinsic dimensionality (median value, shown as the dashed line, nearly $1.2$). By way of comparison, the intrinsic dimensions reported by other researchers in their data sets (not from SE) is often much larger; e.g. 5 to 10, or more; see [43].

From all this, Provence concluded that the effects reported by Papakroni were due to the underlying low dimensionality of the data. Extending his result, we conjecture that our conclusion (that DEs do better than grid search for tuning data miners) are externally valid when the data miners are exploring data with low intrinsic dimensionality.

6. Threats to Validity

Threats to construct validity concern the extent to which the observed phenomena correspond to what is intended to be observed. Some of evaluation measures (precision, F-Measure, AUC) used in this paper to access defect predictors are widely used in defect prediction literature. In addition, we use AUC to characterize how the models could predicts defects when taking account of efforts required to inspect the predicted files. We find that grid search works quite bad under this evaluation measure. Another threat is that the data set used in paper is from SEACRAFT (previously as PROMISE), which might include noise and have errors. To mitigate such threats, we will compare DE with grid search to tune defect predictors on other defect prediction data in the future work.

Threats to conclusion validity concern the relationship between the treatment and the results. In addition to compare the median values of 20 repeats of DE and grid search for tuning defect predictors, we also use Scott Knott (non-parametric test) to determine if the difference in the performance of 20 repeats DE and grid search is significant.

Threats to internal validity concern the consistency of the results obtained from the result. In our study, to investigate why differential evolution performs better than grid search for parameter tuning, we select defect prediction, which is a well explored research problem in software engineering filed as a case study. To mitigate the threats to internal validity, we carefully examine the data sets used in this study and all the data sets used in this study are also publicly available [30] for other researchers to repeat, improve and refute our results. Another threats to the internal validity might be the raw runtime cost for DE and grid search. Different implementations of data loading and processing methods would have different runtime cost. However, the data loading and processing methods implemented in this study are used by all models (e.g., DE and grid search). Therefore, the relative runtime cost comparison between DE and grid search still hold.

Threats to external validity represent if the results are of relevance for other cases, or the ability to generalize the observations in a study. In this study, we use ten widely used open source JAVA software project data from SEACRAFT as the subject. As only the metrics listed in Table 2 are used as the attributes to build defect predictors, we can not guarantee that our findings can be directly generalized to other projects that using different metrics, like code change metrics [35]. Meanwhile, we can not guarantee that our conclusion could be generalized to defect prediction on other projects. Therefore, the future work might include verify our findings on other software project with different metrics. Also, we only take defect prediction as a case study to compare the performance of differential evolution and grid search as parameter tuner, we can not guarantee that our conclusions can be generated to other software analytics. However, those other software analytics tasks often apply machine learning methods [45] and so it is quite possible that the conclusion (DE is better than grid search as a parameter optimizer) would be widely applicable, elsewhere.

7. Conclusion and Future Work

When the parameters of data miners are tuned to the local data, the performance of the resulting learners can be greatly increased. Such tuning are very computationally expensive, especially when done with grid search. For some software engineering tasks, it is possible to avoid those very long runtime. When tuning defect predictors learned from static code attributes, a simple evolutionary strategy (differential evolution) runs one to two orders of magnitude faster that grid search. Further the tunings found in this way work as well, or better, than those found via grid search. We explain this result using the (1) Bergstra and Benigo argument that random search works best in low-dimensional data sets and (2) the empirical results of Papakroni and Provence that defect data sets are very low dimensional in nature.

As to testing the external validity of this paper’s argument, the next steps are clear:

- Sort data sets by how well a simple evolutionary algorithm like DE can improve the performance of data miners executing on that data;
- Explore the difference in the worst and best end of that sort.
- If the intrinsic dimensionalities are very different at both ends of this sort, then that would support with the claims of this paper.
• Else, this paper’s claims would not be supported and we would need to seek other difference between the best and worst data sets.

Note that we offer these four items as future work, rather than reported results, since so far all the defect data sets we have tried had responded best to DE. For a time, we did consider trying this with artificially generated data (where we control how many dimensions were contained in the data). However, prior experience with using artificial data sets [46] suggested to us that such arguments are not widely convincing since the issue is not how often an effect holds in artificial data, but how often it holds in real data. Hence, in future work, we will look further afield for radically different (real world) data sets.

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