

Autotune: A Derivative-free Optimization Framework for Hyperparameter Tuning

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ABSTRACT

Machine learning applications often require hyperparameter tuning. The hyperparameters usually drive both the efficiency of the model training process and the resulting model quality. For hyperparameter tuning, machine learning algorithms are complex black-boxes. This creates a class of challenging optimization problems, whose objective functions tend to be nonsmooth, discontinuous, unpredictably varying in computational expense, and include continuous, categorical, and/or integer variables. Further, function evaluations can fail for a variety of reasons including numerical difficulties or hardware failures. Additionally, not all hyperparameter value combinations are compatible, which creates so called hidden constraints. Robust and efficient optimization algorithms are needed for hyperparameter tuning. In this paper we present an automated parallel derivative-free optimization framework called **Autotune**, which combines a number of specialized sampling and search methods that are very effective in tuning machine learning models despite these challenges. Autotune provides significantly improved models over using default hyperparameter settings with minimal user interaction on real-world applications. Given the inherent expense of training numerous candidate models, we demonstrate the effectiveness of Autotune’s search methods and the efficient distributed and parallel paradigms for training and tuning models, and also discuss the resource trade-offs associated with the ability to both distribute the training process and parallelize the tuning process.

CCS CONCEPTS

• **Computer systems organization** → **Distributed architectures**; • **Mathematics of computing** → **Optimization with randomized search heuristics**;

KEYWORDS

Derivative-free Optimization; Stochastic Optimization; Bayesian Optimization; Hyperparameters; Distributed Computing System

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1 INTRODUCTION

The approach to finding the ideal values for hyperparameters (tuning a model for a particular data set) has traditionally been a manual effort. For guidance in setting these values, researchers often rely on their past experience using these machine learning algorithms to train models. However, even with expertise in machine learning algorithms and their hyperparameters, the best settings of these hyperparameters will change with different data; it is difficult to prescribe the hyperparameter values based on previous experience. The ability to explore alternative configurations in a more guided and automated manner is needed.

A typical approach to generating alternative model configurations is through a grid search. Each hyperparameter of interest is discretized into a desired set of values to be studied, and models are trained and assessed for all combinations of the values across all hyperparameters. Although easy to implement, a grid search is quite costly because the computational expense grows exponentially with the number of hyperparameters and the number of discrete levels of each. While three hyperparameters with three levels each requires only 27 model configurations to be evaluated, six hyperparameters with five levels each would require 15,625 models to be trained. Even with a substantial cluster of compute resources, training these many models is prohibitive in most cases, especially with the computation cost of modern machine learning algorithms and massive data sets associated with applications like image recognition and natural language processing.

A simple yet surprisingly effective alternative to performing a grid search is to train and assess candidate models by using random combinations of hyperparameter values. As demonstrated in Bergstra and Bengio[1], given the disparity in the sensitivity of model accuracy to different hyperparameters, a set of candidates that incorporates a larger number of trial values for each hyperparameter will have a much greater chance of finding effective values for each hyperparameter. Because some of the hyperparameters might actually have little to no effect on the model for certain data

sets, it is prudent to avoid wasting the effort to evaluate all combinations, especially for higher-dimensional hyperparameter spaces. Still, the effectiveness of evaluating purely random combinations of hyperparameter values is subject to the size and uniformity of the sample. Candidate combinations can be concentrated in regions that completely omit the most effective combination of values of the hyperparameters, and it is still likely to generate fewer improved configurations. A recent variation on random search called Hyperband focuses on speeding up random search by terminating ill-performing hyperparameter configurations (Li et al. [15]). This approach allows more configurations to be evaluated in a given time period, increasing the opportunity to identify improved configurations.

A approach similar to random search but more structured is to use a random Latin hypercube sample (LHS) (McKay [18]), an experimental design in which samples are exactly uniform across each hyperparameter but random in combinations. These so-called low-discrepancy point sets attempt to ensure that points are approximately equidistant from one another in order to fill the space efficiently. This sampling ensures coverage across the entire range of each hyperparameter and is more likely to find good values of each hyperparameter which can then be used to identify good combinations. Other experimental design procedures can also be quite effective at ensuring equal density sampling throughout the entire hyperparameter space, including optimal Latin hypercube sampling as proposed by Sacks et al. [23].

Exploring alternative model configurations by evaluating a discrete sample of hyperparameter combinations, whether randomly chosen or through a more structured experimental design approach, is certainly straightforward. However, true optimization of hyperparameters should facilitate a complete search of continuous parameter space in addition to discrete parameter space, and make use of information from previously evaluated configurations to increase the number of alternate configurations that show improvement. Discrete samples are unlikely to identify even a local accuracy peak or error valley in the hyperparameter space; searching between these discrete samples can uncover good combinations of hyperparameter values. The search is based on an objective of minimizing the model validation error, so each “evaluation” from the optimization algorithm’s perspective is a full cycle of model training and validation. Optimization methods are designed to make intelligent use of fewer evaluations and thus save on the overall computation time. Optimization algorithms that have been used for hyperparameter tuning include Broyden-Fletcher-Goldfarb-Shanno (BFGS) (Konen et al. [14]), covariance matrix adaptation evolution strategy (CMA-ES) (Konen et al. [14]), particle swarm (PS) (Renukadevi and Thangaraj [22]; Gomes et al. [6]), tabu search (TS) (Gomes et al. [6]), genetic algorithms (GA) (Lorena and de Carvalho [17]), and more recently surrogate-based Bayesian optimization (Denwanker et al. [3]).

However, because machine learning training and scoring algorithms are a complex black-box to the tuning algorithm, they create a class of challenging optimization problems. Note that optimization variables are hyperparameters here. Figure 1 illustrates several of these challenges:

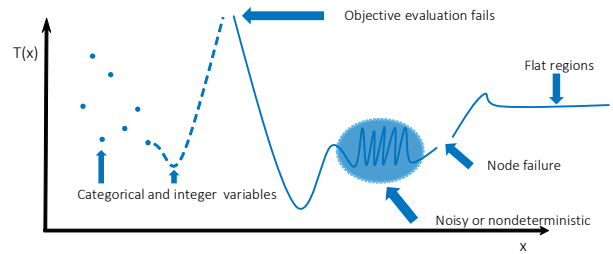


Figure 1: Challenges in applying optimization to hyperparameter tuning.

- Machine learning algorithms typically include not only continuous variables, but also categorical and integer variables, leading to a very discrete objective space.
- In some cases, the variable space is discontinuous, and the objective evaluation fails.
- The space can also be very noisy and nondeterministic, for example, when distributed data are moved around because of unexpected rebalancing.
- Objective evaluations can fail because of numerical difficulties or hardware failures, which can derail a search process.
- Often the search space contains many flat regions where multiple configurations produce very similar models and an optimizer can fail to find a direction of improvement.

An additional challenge is the unpredictable computational expense of training and validating predictive models using different hyperparameter values. Adding hidden layers and neurons to a neural network, for example, can significantly increase the training and validation time, resulting in widely ranging potential objective expense. Given these challenges, a very flexible and efficient search strategy is needed. As with machine learning algorithms, the no free lunch theorem applies to optimization algorithms (Wolpert [28]; Wolpert and Macready [29]), i.e., no single algorithm can overcome all these challenges and work well for all data sets. Also, the strengths of sampling methods cannot be overlooked.

In the next section, we introduce our automated parallel derivative-free optimization framework **Autotune** that concurrently exploits the strengths of sampling methods and multiple derivative-free optimization algorithms, which are very effective for hyperparameter tuning. Given the inherent expense of training numerous candidate models, we then discuss efficient distributed and parallel paradigms for training and tuning models, and also discuss the resource tradeoffs associated with the ability to both distribute the training process and parallelize the tuning process. Finally, we report benchmark tuning results, present two case studies, and conclude with contributions and future work.

2 DERIVATIVE-FREE OPTIMIZATION FRAMEWORK

In this section, we describe the derivative-free optimization framework Autotune, the search methods incorporated, and its default search method. Autotune is a product within SAS® Visual Data Mining and Machine Learning [27], and operates on SAS® Viya® [24],

which is designed to enable distributed analytics and to support cloud computing. Autotune is able to tune the hyperparameters of various machine learning models including decision trees, forests, gradient boosted trees, neural networks, support vector machines, factorization machines, and Bayesian network classifiers.

2.1 System Overview

Autotune is designed to perform optimization of general nonlinear functions over both continuous and integer variables. The functions do not need to be expressed in analytic closed form, black-box integration is supported, and they can be non-smooth, discontinuous, and computationally expensive to evaluate. Problem types can be single-objective or multiobjective. The system is designed to run in either single-machine mode or distributed mode.

Because of the limited assumptions that are made about the objective function and constraint functions, Autotune takes a parallel hybrid derivative-free approach similar to those used in Taddy et al. [26]; Plantenga [21]; Gray, Fowler, and Griffin [8]; Griffin and Kolda [10]. Derivative-free methods are effective whether or not derivatives are available, provided that the dimension of x is not too large (Gray and Fowler [7]). As a rule of thumb, derivative-free algorithms are rarely applied to black-box optimization problems that have more than 100 variables. The term “black-box” emphasizes that the function is used only as a mapping operator and makes no implicit assumption about or requirement on the structure of the functions themselves. In contrast, derivative-based algorithms commonly require the nonlinear objectives and constraints to be continuous and smooth and to have an exploitable analytic representation.

Autotune has the ability to simultaneously apply multiple instances of global and local search algorithms in parallel. This streamlines the process of needing to first apply a global algorithm in order to determine a good starting point to initialize a local algorithm. For example, if the problem is convex, a local algorithm should be sufficient, and the application of the global algorithm would create unnecessary overhead. If the problem instead has many local minima, failing to run a global search algorithm first could result in an inferior solution. Rather than attempting to guess which paradigm is best, the system simultaneously performs global and local searches while continuously sharing computational resources and function evaluations. The resulting run time and solution quality should be similar to having automatically selected the best global and local search combination, given a suitable number of threads and processors. Moreover, because information is shared among simultaneous searches, the robustness of this hybrid approach can be increased over other hybrid combinations that simply use the output of one algorithm to hot-start the second algorithm.

Inside Autotune, integer and categorical variables are handled by using strategies and concepts similar to those in Griffin et al. [9]. This approach can be viewed as a genetic algorithm that includes an additional “growth” step, in which selected points from the population are allotted a small fraction of the total evaluation budget to improve their fitness score (that is, the objective function value) by using local optimization over the continuous variables.

This Autotune framework supports:

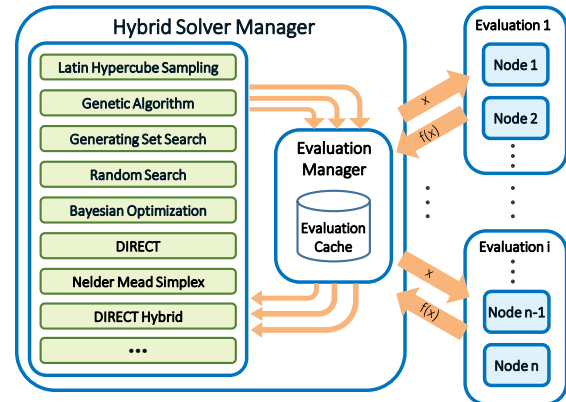


Figure 2: The Autotune framework.

- Running in distributed mode on a cluster of machines that distribute the data and the computations
- Running in single-machine mode on a server
- Exploiting all the available cores and concurrent threads, regardless of execution mode

A pictorial illustration of this framework is shown in Figure 2. An extendable suite of search methods (also called solvers) are driven by the Hybrid Solver Manager that controls concurrent execution of the search methods. New search methods can easily be added to the framework. Objective evaluations are distributed across multiple worker nodes in a compute grid and coordinated in a feedback loop that supplies data from running search methods.

Execution of the system is iterative in its processing, with each iteration containing the following steps:

- (1) Acquire new points from the solvers
- (2) Evaluate each of those points by calling the appropriate black-box functions (model training and validation)
- (3) Return the evaluated point values (model accuracy) back to the solvers
- (4) Repeat

For each solver in the list, the evaluation manager exchanges points with that solver. During this exchange, the solver receives back all the points that were evaluated in the previous iteration. Based upon those evaluated point values, the solver generates a new set of points it wants evaluated and those new points get passed to the evaluation manager to be submitted for evaluation. For any solvers capable of “cheating”, they may look at evaluated points that were submitted by a different solver. As a result, search methods can learn from each other, discover new opportunities, and increase the overall robustness of the system.

2.2 Search Methods

Autotune is designed to support multiple search methods, which not only can be run concurrently but they also can be combined to create new hybrid methods. In addition to the sampling methods (random and LHS) already discussed and the default search method

to be introduced in the next session, the set of supported search methods include the following:

2.2.1 Genetic Algorithm (GA). GAs are a family of search algorithms that seek optimal solutions to problems by applying the principles of natural selection and evolution (Goldberg [5]). Genetic algorithms can be applied to almost any optimization problem and are especially useful for problems for which other calculus-based techniques do not work, such as when the objective function has many local optima, when the objective function is not differentiable or continuous, or when solution elements are constrained to be integers or sequences. In most cases, genetic algorithms require more computation than specialized techniques that take advantage of specific problem structures or characteristics. However, for optimization problems for which no such techniques are available, genetic algorithms provide a robust general method of solution.

2.2.2 Generating Set Search (GSS). This type of method is designed for problems that have continuous variables and have the advantage that, in practice, they often require significantly fewer evaluations to converge than an exploratory search method like GA (Griffin and Kolda [11]). GSS can provide a measure of local optimality that is very useful in performing multimodal optimization. It may add additional “growth steps” to an exploratory search method for continuous variables.

2.2.3 Bayesian Optimization. The Bayesian optimization method in Autotune employs a Gaussian process surrogate model [12]. LHS is used to initialize the surrogate model, which is then used to generate new evaluations that minimize the approximate function. These new evaluations are executed using the real black-box function and potentially added to the surrogate model for increased accuracy until a certain maximum number of points are in the approximate model. Confidence levels between samples and an exploration parameter allows generations of trials in new regions to avoid converging on lower accuracy models.

2.2.4 DIRECT. This method is an implicit branch and bound type algorithm that divides the hyper-rectangle defined by the variable bounds into progressively smaller rectangles where the relevance of a given rectangle is based on its diameter and the objective value at the center point [13]. The former is used to quantify uncertainty, the latter is used to estimate the best value within. A Pareto set is maintained for these two quantities and used to select which of the hyper-rectangles to trisect at the next iteration.

2.2.5 Nelder-Mead. This method is a variable shape simplex direct-search optimization method that maintains the objective values of the vertices of a polytope whose number is one greater than the dimension being optimized [20]. It then predicts new promising vertices for the simplex based on current values using a variety of simplex transformation operations.

2.2.6 DIRECT Hybrid. This hybrid method first uses DIRECT principles to divide and sort the feasible regions into a set of hyper-rectangles of varying dimension based on the likelihood of containing a global minimizer. As the hyper-rectangles are divided, the size of the rectangles as measured by the distance between its center and corners reduces. When this size is small enough, then a

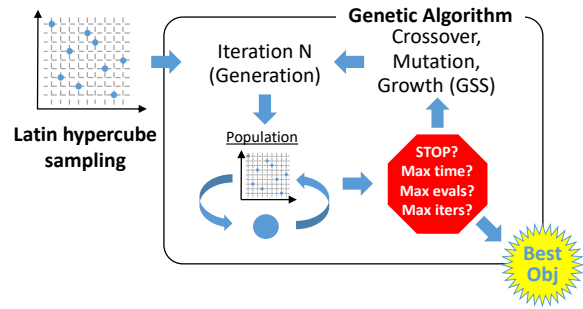


Figure 3: The tuning process of the default search method used by Autotune.

Nelder-Mead optimization is executed based on the small hyper-rectangle to further refine the search and the small hyper-rectangle is no longer considered for division. The best value found by a small hyper-rectangle's Nelder-Mead optimizer is then used to represent that given rectangle.

2.3 Default Search Method

Algorithm 1 Default Search Method in Autotune

Require: Population size n_p , and evaluation budget n_b .

Require: Number of centers $n_c < n_p$ and initial step-size $\hat{\Delta}$.

Require: Sufficient decrease criterion $\alpha \in (0, 1)$.

- ```

1: Generate initial parent-points \mathcal{P} using LHS with $|\mathcal{P}| = n_p$.
2: Evaluate \mathcal{P} asynchronously in parallel.
3: Populate reference cache-tree, \mathcal{R} , with unique points from \mathcal{P} .
4: Associate each point $p \in \mathcal{P}$ with step Δ_p initialized to $\hat{\Delta}$.
5: while ($|\mathcal{R}| \leq n_b$) do
6: Select $\mathcal{A} \subset \mathcal{P}$ for local search, such that $|\mathcal{A}| = n_c$.
7: for $p \in \mathcal{A}$ do ▷ Search along compass directions
8: Set $\mathcal{T}_p = \{\}$
9: for $e_i \in I$ do
10: $\mathcal{T}_p = \mathcal{T}_p \cup \{p + \Delta_p e_i\} \cup \{p - \Delta_p e_i\}$
11: end for
12: end for
13: Generate child-points C via crossover and mutations on \mathcal{P} .
14: Set $\mathcal{T} = C \cup_{p \in \mathcal{A}} \mathcal{T}_p$.
15: Evaluate $\mathcal{T} \cap \mathcal{R}$ using fast tree-search look-up on \mathcal{R} .
16: Evaluate remaining $\mathcal{T} - \mathcal{R}$ asynchronously in parallel.
17: Add unique points from $\mathcal{T} - \mathcal{R}$ to cache-tree \mathcal{R} .
18: Update \mathcal{P} with new generation C and initial step $\hat{\Delta}$.
19: for $p \in \mathcal{A}$ do
20: if $\min_{y \in \mathcal{T}_p} f(y) < f(p) - \alpha \Delta_p^2$ then
21: Set $p = y$ ▷ Pattern search success
22: else
23: Set $\Delta_p = \Delta_p / 2$ ▷ Pattern search failure
24: end if
25: end for
26: end while

```



As illustrated in Figure 3 and explained by the pseudocode in Algorithm 1, the default search method used by Autotune is a *hybrid* method that begins with a Latin hypercube sample of the hyperparameter space. The best configurations from the LHS are then used to generate the initial population for the GA, which crosses and mutates the best samples in an iterative process to generate a new population of model configurations at each iteration.

In addition to the crossover and mutation operations of a classic GA, Autotune adds an additional "growth" step to each iteration of the GA. This permits the GSS algorithm to perform local search in a neighborhood of select members from the current GA population. This can improve convergence to a good minimum once the GA is sufficiently near the corresponding basin or region of attraction. Typically the best point in the GA population is continuously optimized. If sufficient computing resources are available, other points may be optimized simultaneously by, for example, selecting points randomly from the Pareto-front comparing the population's objective function and distance to the nearest neighbor.

The default search method in Autotune essentially combines the elements of LHS, GA and GSS methods. The strengths of this hybrid method include handling of continuous, integer, and categorical variables; handling nonsmooth, discontinuous spaces; and ease of parallelizing the search. All are prevalent and critical for the hyperparameter tuning problem.

Autotune uses a specified model accuracy measure (misclassification, mean squared error, multiclass log loss, AUC, KS coefficient, etc.) as objective values. This measure is calculated on validation data, otherwise the autotuning process would likely overfit the training data. Validation is an additional, but necessary, expense during tuning when training many alternative model configurations. Ideally a cross-validation process is applied to incorporate all data in training and validation, with separate "folds". However, evaluation of each fold for each model configuration significantly increases the training expense and thus the tuning expense, making it prohibitive for big data applications. Fortunately, it is often unnecessary and undesirable to run each training process to completion when tuning. Given information about the current best configurations, it is possible to abort running model configurations after a subset of all folds if the estimated model quality is not near the current best. This is one form of early stopping that is supported by Autotune.

Even with aborting of bad models, many datasets are still too large for cross-validation. In this case, a single validation partition is used. To ensure that the training subset and the validation subset are both representative of the original data set, stratified sampling is used when possible (nominal target). With very large data sets, subsampling can also be employed to reduce the training and validation time during tuning, and again stratified sampling helps ensure the data partitions remain representative. The biggest increase in efficiency, however, comes from the evaluation of alternate model configurations in parallel - a process that comes with its own set of challenges. The parallel hyperparameter tuning implementation in Autotune is detailed in the next section.

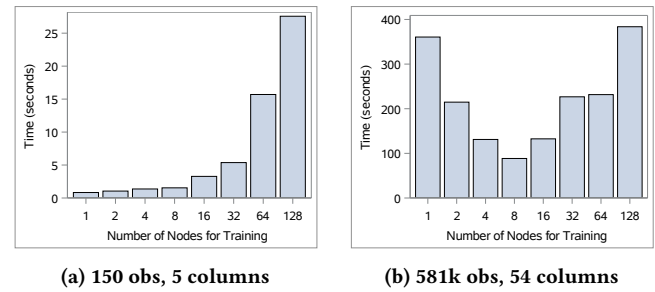


Figure 4: Training times with different number of computing nodes on two data sets.

### 3 PARALLEL HYPERPARAMETER TUNING

The training of a model by a machine learning algorithm is often computationally expensive. As the size of a training data set grows, not only does the expense increase, but the data (and thus the training process) must often be distributed among compute nodes because the data exceed the capacity of a single computer. Also, the configurations to be considered during tuning are independent, making a sequential tuning process not only expensive but unnecessary, given a grid of compute resources.

While some systems only support assigning worker nodes to either the training process or the tuning process (sequential tuning with each model trained on all workers or parallel training of multiple models each on one worker), the Autotune system presented here supports both assigning multiple worker nodes to each model to be trained and training multiple models in parallel. The challenge is to determine the best usage of available worker nodes for the tuning process as a whole.

For small data sets data distribution is not necessary, but it may not be clear that it can actually be detrimental, reducing performance. In Figure 4a, a tree based gradient boosting algorithm is applied to train a model to the popular iris data set (containing only 150 observations) using a number of different worker nodes ranging from 1 to 128. The communication cost required to coordinate data distribution and model training increases continuously as the number of worker nodes increases. The training time grows from less than 1 second on a single machine to nearly half a minute on 128 nodes. In this case, a model tuning process would benefit more from parallel tuning (training different model configurations in parallel) than from distributed/parallel training of each model; with a grid of 128 nodes, 128 models could be trained in parallel without overloading the grid.

As shown in Figure 4b, for larger data sets, distributing the data and the training process reduces the training time; here gradient boosting and covtype<sup>1</sup> data set are used. The covtype data set contains over 581K observations and 54 features. However, the benefit of data distribution and parallel training does not continue to increase with an increasing number of worker nodes. At some point the cost of communication again outweighs the benefit of parallel processing for model training. Here the time for training increases beyond 8 worker nodes, to a point where 32 and 64 nodes

<sup>1</sup>The Forest Covtype dataset is Copyrighted 1998 by Jock A. Blackard and Colorado State University.

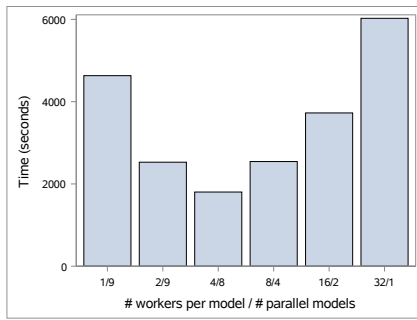
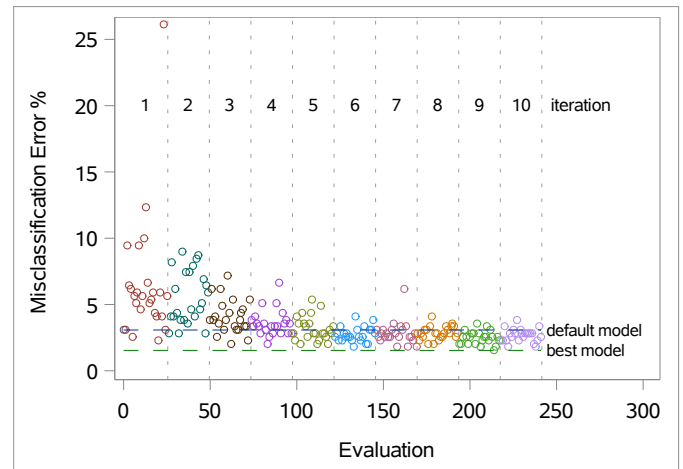


Figure 5: A tuning resource allocation example.

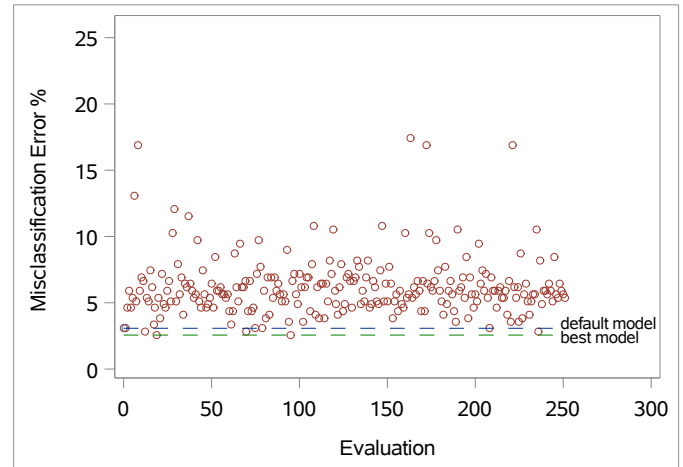
are more costly than 2 nodes and using all 128 is more costly than using only 1 node.

Determining the best worker node allocation for the tuning process is more challenging than determining the most efficient training process. In Figure 4b, the training process is most efficient with 8 worker nodes. However, a grid of 128 nodes would support 16 different model configurations trained in parallel during tuning if each uses 8 worker nodes (without overloading the grid). The training expense is not half with 8 worker nodes compared to with 4 worker nodes, and so it may make more sense to train each model with 4 worker nodes, allowing 32 model configurations to be trained in parallel. In fact, if the data fits on one worker node, 128 model configurations trained in parallel on 1 worker each may be more efficient than 4 batches of 32 models each trained on 4 workers. For very large data sets, the data must be distributed, but training multiple models in parallel typically leads to larger gains in tuning efficiency than training each model faster by using more worker nodes for each model configuration. The performance gain becomes nearly linear as the number of nodes increases because each trained model is independent during tuning, so no communication is required between the different configurations being trained. Determining the right resource allocation then depends on the size of the data set, the size of the compute grid, and the tuning method taken. Note that an iterative search strategy limits the size of each parallel batch (for example, the population size at each iteration of the genetic algorithm).

Allocating resources to both the model training process and the model tuning process requires very careful management of the data, the training process, and the tuning process. Multiple alternate model configurations are submitted concurrently by the framework, and the individual model configurations are trained and validated on a subset of available worker nodes in isolated processes. This allows multiple nodes to be used to manage large training data when necessary, speeding up each individual training process. Figure 5 shows a tuning time comparison for tuning the gradient boosting model to the covtype data set. The tuning process consists of 5 iterations of 10 models and uses the default search method on a compute grid of 32 workers. In this case, 4 workers for each model configuration, with 8 parallel configurations is most efficient. However, up to 16 configurations could be evaluated in parallel with 2 workers rather than 8 with 4 workers, nearly doubling the



(a) The default hybrid search history



(b) Random search history

Figure 6: The tuning history for the default hybrid search and random search on an image recognition data set.

total number of configurations over 5 iterations without doubling the tuning time.

When it comes to choosing a search method for automated parallel hyperparameter tuning, time, available compute resources, and tuning goals drive the choice. Random search is popular for two main reasons: a) the hyperparameter space is often discrete, which random search naturally accommodates, and b) random search is simple to implement and all hyperparameter configurations could potentially be evaluated concurrently because they are all independent and can be pre-specified. The latter reason is a strong argument when a limited number of configurations is considered or a very large compute grid is available. Figure 6 illustrates the tuning history of Autotune’s default search method and random search using an image recognition data set. Here 10 iterations of 25 configurations are performed with the default hybrid approach and a single sample of 250 configurations for random search. The

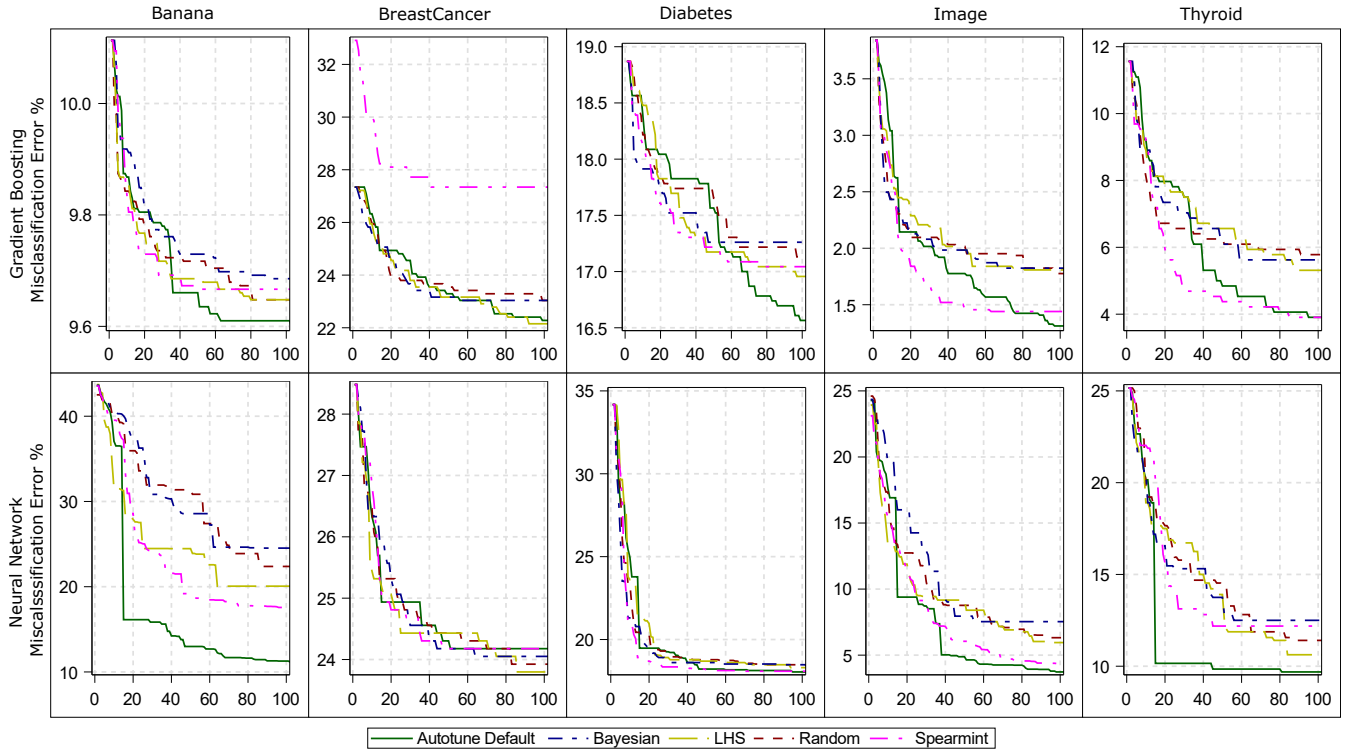


Figure 7: Benchmark experiment results.

learning occurring through the optimization strategy can clearly be seen in Figure 6a. The initial iteration contains configurations most of which are worse than the initial/default, but as the iterations progress, more and more improvements are found with the last iteration containing mostly improved configurations. In the case of random sampling, the results are fairly uniform across the history of 250 configurations chosen, as expected; however, many fewer improvements are identified. If the final “best” models are similar and 250 grid nodes are available, and the data can fit on one worker node, the random search will be more efficient. However, if less than 250 grid nodes are available and/or if a comparison and selection among top improved models is sought, the hybrid search method that learns the more effective configurations across multiple iterations is more effective.

## 4 EXPERIMENTS

To evaluate the performance of Autotune and the effectiveness of each search method, we conducted a benchmark experiment by applying the Autotune system to a set of five familiar benchmark data sets. The five data sets are taken from *mldata.org* [19], and include *banana*, *breast cancer*, *diabetes*, *image* and *thyroid*. All problems are tuned with a 30% single partition for error validation during tuning. For the default hybrid search method and Bayesian search method, 10 iterations with 10 hyperparameter configurations per iteration are used; for random search and LHS, the sample size is 100. All problems are run 10 times, and the results obtained are averaged to better assess behavior of the search methods. We also

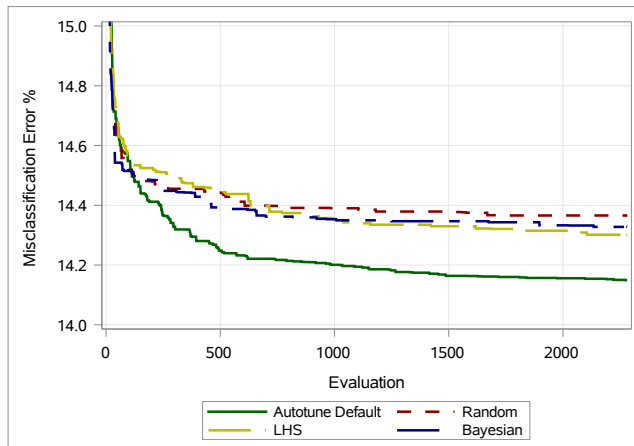
use the open source Spearmint Bayesian optimization package [25] for comparison.

Two model types are used in this experiment. For tree-based gradient boost models, six hyperparameters are tuned: *number of trees*, *number of inputs to try when splitting*, *learning rate*, *sampling rate*, *lasso*, and *ridge regularization*. For fully connected neural network models, seven hyperparameters are tuned: *number of hidden layers (0-2)*, *number of neurons in each hidden layer*, *L1 and L2 regularization*, *learning rate*, and *annealing rate*.

Results for tuning both model types are shown in Figure 7. For tuning the gradient boosting models, the default method performs better on three of the five data sets; LHS or Spearmint is each slightly better than the default on one data set. For tuning the neural network model, again, the default method performs better on three of the five data sets, and LHS or Spearmint each wins one. These results show that the default method used by Autotune is very competitive and robust, and an effective hyperparameter tuning system needs to employ a suite of diversified search methods to cover a wide range of problems. Furthermore, integrating/combining different search methods is an effective way to create powerful hybrid methods.

## 5 CASE STUDIES

Autotune has been deployed in many real-world applications. Here we report the use of Autotune to find better models in two applications.



**Figure 8: The autotune results of the bank product promotion data set. The gradient boost model error with default hyperparameter settings is nearly 20%. For clarity of convergence comparisons only the last percent of improvement, below 15%, is shown here.**

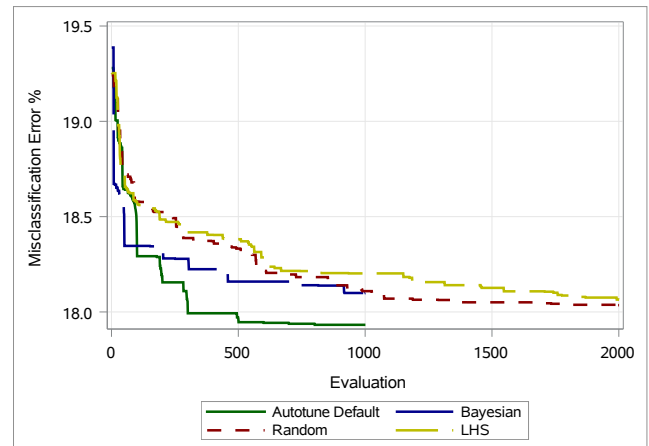
### 5.1 Bank Product Promotion Campaign

The bank data set [4] consists of anonymized and transformed observations taken from a large financial services firm’s accounts, and contains 1,060,038 observations and 21 features. Accounts in the data represent attributes describing the customer’s propensity to buy products, RFM (recency, frequency, and monetary value) of previous transactions, and characteristics related to profitability and creditworthiness. The goal is to predict which customers to target as the most likely to purchase new bank products in a promotional campaign.

The compute grid available for this study contains 40 machines: a controller node and 39 worker nodes. Each model train uses 2 worked nodes, which allows 19 hyperparameter configurations to be evaluated in parallel without overloading the grid.

In this study, we investigate the convergence properties of different search methods. Due to the long running time of Spearmint Bayesian method on large data sets, it is not included in our case studies. The default search method is configured with a population size of 115 (resulting in 6 batches of 19 plus the default/best configuration). The number of iterations is set to 20, resulting in up to 2281 model configurations evaluated. Random search and LHS are set to the same total sample size of 2280 plus default. The Bayesian search method is configured to run 60 iterations of 38, allowing model updating after two parallel batches of 19, with a matching maximum number of evaluations of 2280. Each search method is executed 10 times to average random effects. We use a tree-based gradient boosting model and tune six of its hyperparameters as listed in Section 4. For each search method, the tuning takes from 1 to 3 hours, so it takes roughly 1 full day to run each 10 times.

Tuning results for the bank data are shown in Figure 8. It is clear that all the tested methods are able to find better hyperparameter configurations quickly. The errors are reduced from 20% to 15% during the first few batches of evaluations. The last percent of



**Figure 9: The autotune results of wine quality data set.**

improvement happens gradually over the remaining 2200+ evaluations, at different rates and with different final ‘best’ results for each search method. After around 100 evaluations, the Bayesian search, random search, and LHS begin to stagnate while the default method continues to learn and reduce the model error and outperforms the other methods.

It is important to note here that the ‘2X random’ approach that has also become a popular basis for comparison is not relevant in this case. Since we can only run 19 models in parallel, and are doing so for all search methods, 2X random will not be more efficient. It may or may not find equivalent or better solutions, but will take twice as long given this grid configuration. Academically, the argument is valid: if we had 4000 machines, running 2000 configurations in parallel with 2 worker nodes each would be the most efficient. Realistically, most data scientists do not have access to that many resources, and must share the resources that are available. Also, for this study, 1000 evaluations used in the default search method result in a better model than 2000 random samples; even at this level of resource allocation, the intelligent search methods are able to find improvement beyond those found by twice as many random samples.

### 5.2 Wine Quality

The wine quality data set is a prepared and extended version of a data set obtained from the UCI machine learning repository [16]. The data set is a collection of red and white variants of the Portuguese “Vino Verde” wine [2], with 6,497,000 observations and 11 features representing the physiochemical properties of the wines and a quality rating for each wine. For the purposes of this study, the quality ratings were binned such that quality  $\leq 6$  was labelled as “Economy”, and quality  $> 6$  was labeled as “Premium”, making it a binary classification problem to predict the new QualityGrp category. In addition, the data set was augmented to make it 1000 times larger by synthesizing variations of each observation with random perturbations of each attribute value while maintaining the QualityGrp value.

The compute grid used for the wine data study contains 145 machines: a controller node and 144 worker nodes. Here 4 worker



nodes are used for each model training, and a limit of 25 hyperparameter configurations is allowed to be evaluated concurrently. The default Autotune search method is configured with a population size of 101 (resulting in 4 batches of 25 plus the initial/best configuration). The number of iterations is set to 10, resulting in up to 1001 hyperparameter configurations evaluated (including the initial configuration). Random search is set to 2000 plus the initial configuration for a 2X random comparison. Bayesian search is performed with 20 iterations of 50, updating the approximated model after two parallel batches of 25, with a matching maximum number of evaluations of 1000. For this study, we use a neural network model and tune the seven hyperparameters as listed in Section 4. Each search method is executed 10 times to average random effects. For each search method, the tuning time ranges from 2 to 6 hours, and ten repeats of each runs for over 1 day.

Tuning results for the wine data are shown in Figure 9. The Autotune default search strategy converges at a higher rate and to a lower error than the other search methods. The Bayesian search method beats the default search method for the first 150 evaluations, after which its rate of improvement slows. It should be noted here that the Gaussian process model is limited in the number of evaluations used to build the model; in this case due to the high expense of tuning, with the total of 10 repeats taking over 50 hours, the model size is limited to 300 evaluations used in the model. The Bayesian search method still finds better solutions than random search through its 1000 evaluations, after which random search exceeds the capability of the limited model used for Bayesian search. The best solution found by the default search method is better than that found by twice as many random search evaluations.

## 6 CONCLUSIONS

In this paper, we have presented the hybrid derivative-free optimization framework Autotune for automated parallel hyperparameter tuning. The system implementation supports multi-level parallelism where objective evaluations (different model configurations to be trained and validated) can be evaluated in parallel across different worker nodes in a grid environment while each objective evaluation also uses multiple worker nodes for model training, allowing scaling to large data sets and increased training efficiency. One lesson learned in applying the system is that the most efficient distributed grid configuration for a single model train is usually not the most efficient grid configuration for model tuning. More gains are seen from training many models in parallel than making each model train as efficient as possible; careful resource allocation and management of parallel processes is necessary. Furthermore, the framework facilitates concurrent, parallel execution of search methods, sharing of objective evaluations across search methods, easy addition of new search methods, and combining of search methods to create new hybrid strategies, exploiting the strengths of each method. This powerful combination has shown promising numerical results for hyperparameter tuning, where black-box machine learning algorithm complexities include mixed variable types, stochastic and discontinuous objective functions, and the potential for high computational cost. Combining sampling, local and global search has shown to be more robust than applying a single method, and is the main reason why the default search method

in Autotune consistently performs better than other search methods. Future work to further enhance Autotune includes improving Autotune's Bayesian search method, handling early stopping of unpromising model configurations more effectively, and supporting multi-objective tuning where trade-offs between model quality and model complexity can be explored.

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