Learning Certifiably Optimal Rule Lists: A Case For Discrete Optimization in the 21st Century

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BY
NICHOLAS L. LARUS-STONE
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Thesis advisor: Professor Margo Seltzer Nicholas L. Larus-Stone

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Abstract

We demonstrate a new algorithm, CORELS, for constructing rule lists. It finds the optimal rule list and produces proof of that optimality. Rule lists, which are lists composed of *if-then* statements, are similar to decision trees and are useful because each step in the model's decision making process is understandable by humans. CORELS uses the discrete optimization technique of branch-and-bound to eliminate large parts of the search space and turn this into a computationally feasible problem. We use three types of bounds: bounds inherent to the rules themselves, bounds based on the current best solution, and bounds based on symmetries between rule lists. In addition, we use efficient data structures to minimize the memory usage and runtime of our algorithm on this exponentially difficult problem. Our algorithm demonstrates the feasibility of finding optimal solutions in a search space using discrete optimization on modern computers. Our algorithm therefore allows for the discovery and analysis of optimal solutions to problems requiring human-interpretable algorithms.

Contents

Acknowledgments

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1 Introduction

As computing power continues to grow, combinatorial optimization problems that may not have been possible using less powerful hardware can now be reliably completed on a commodity laptop. The goal of this thesis is to discuss a number of data structure optimizations that allow for the completion of medium to large scale combinatorial optimization problems. This work builds off of the theoretical bounds and implementation found in Angelino et al.[2] While the techniques found in this thesis are applied to the machine learning technique of rule lists, it is our hope that they can be generalized to other combinatorial optimization problems.

We work in the realm of machine learning, specifically focusing on the interpretability of predictive models. Our algorithm produces models that are highly predictive, but in which each step of the model's decision making process can also be understood by humans. Machine learning models, such as neural nets or support vector machines, can achieve stunning predictive accuracy, but the reasons for their predictions remain unintelligible to a human user. This lack of interpretability is important, because models that are not understood by humans may have hidden bias in their predictive decision making. A recent ProPublica article found racial bias in the use of a black box machine learning model used to create risk assessments intended to help judges with criminal sentencing[19].

Northepointe, the company providing COMPAS (the black box model), argues that they need to use a black box model in order to achieve higher accuracy. This thesis is part of a body of work that showing that it is possible to build interpretable machine learning models without sacrificing accuracy.

There are negative repercussions for applying biased models, so it is preferable to have a model that can be understood by the people applying it. For some problems, though, interpretable models are less accurate than black box models. So, it is important to know the limit of interpretable models. Finding the optimal solution for an interpretable model provides an important upper bound on the accuracy of that model. This helps decision makers decide whether or not a problem can be solved using interpretable models or whether a black box model really does achieve better accuracy.

To achieve interpretability, we use *rule lists*, also known as decision lists, which are lists comprised of *if-then* statements[33]. This structure allows for predictive models that can be easily interpreted, because each prediction is explained by examining which rule is satisfied. Given a set of rules associated with a dataset, every possible ordering of rules produces a unique rule list. Since most data points can be classified by multiple rules, changing the order of rules could lead to the same data point being predicted differently; therefore, different orderings have differing accuracies. Rule list generation algorithms attempt to maximize predictive accuracy through the discovery of different rule lists. In our case, we are searching for the rule list with the highest accuracy—the optimal rule list. A brute force solution to find the the optimal rule list is computationally prohibitive due to the exponential number of rule lists. Our algorithm uses combinatorial optimization to find the optimal rule list in a reasonable amount of time.

Recent work on generating rule lists[23,38] instead uses probabilistic approaches to generating rule lists. These approaches achieve high accuracy quickly. However, despite the apparent accuracy of the rule lists generated by these algorithms, there is no way to determine if the generated rule list is optimal or how close to optimal it is. Our model, called Certifiably Optimal RulE ListS (CORELS), finds the optimal rule list and also allows us to investigate the accuracy of near

optimal solutions*. The benefits of this model are two-fold: first, we are able to generate the best rule list on a given data set and therefore will have the most accurate predictions that a rule list can give. Second, since CORELS generates the entire space of potential solutions, we can evaluate the quality of rule lists generated by other algorithms. In particular, we can determine if the rule lists from probabilistic approaches are nearly optimal or whether those approaches sacrifice too much accuracy for speed. This will allow us to bound the accuracy on important problems and determine if interpretable methods should be used.

CORELS achieves these results by optimizing an objective function and placing a set of bounds on the best objective that a rule list can achieve in the future. This allows us to prune that rule list if those bounds are worse than the objective value of the best rule list that we have already examined. We continue to examine rule lists until we have either examined every rule list or eliminated all but one from consideration. Thus, when the algorithm terminates, we have found the rule list with the best possible accuracy. Our use of this branch and bound technique leads to massive pruning of the search space of potential rule lists and allows our algorithm to find the optimal rule list on real data sets.

Due to our interest in interpretability, the amount of data each rule captures informs the value of that rule. We want our rule lists to be understandable by humans, so shorter rule lists are more optimal. Therefore, we use an objective function that takes into account both accuracy and the length of the rule list to prevent overfitting. This means we may not always find the highest accuracy rule list—our optimality is over both accuracy and length of rule lists. This requires each rule to classify a minimum amount of data correctly to make it worth the penalty of making a rule list longer. This limits the overall length of our rule lists and avoids overfitting, as well as preventing us from investigating rule lists containing useless rules.

The exponential nature of the problem means that the efficacy of CORELS is largely dependent on how much our bounds allow us to prune. There are three classes of bounds that allow us to drastically prune our search space. The first type of bound is intrinsic to the rules themselves. This category includes bounds such as the bound described above that ensures that rules capture enough

* Code can be found at github.com/nlarusstone/corels.

data correctly to overcome a regularization parameter. Our second type of bound compares the best future performance of a given rule list to the best solution encountered so far. We can avoid examining parts of the search space whose maximum possible accuracy is less than the accuracy of our current best solution. Finally, our last class of bounds compares similar rule lists and uses a symmetry-aware map to prune all but the best permutation of any given set of rules.

To keep track of all of these bounds for each rule list, we implemented a modified trie that we call a prefix tree. Each node in the prefix tree represents an individual rule; thus, each path in the tree represents a rule list where the final node in the path contains metrics about that rule list such as its accuracy and the number of data points classified. This tree structure facilities the use of multiple different selection algorithms including breadth-first search, a priority queue based on a custom function that trades off exploration and exploitation, and a stochastic selection process. In addition, we are able to limit the number of nodes in the tree and thereby achieve a way of tuning space-time tradeoffs in a robust manner. This tree structure is a useful way of organizing the generation of rule lists and it allows the implementation of CORELS to be easily parallelized.

We applied CORELS to two problems that have had black box models accused of racial bias. First, we investigate the problem of predicting criminal recidivism on the COMPAS dataset. Larson et al. examines the problem of predicting recidivism and shows that a black box model, specifically the COMPAS score from the company Northpointe, leads to racially biased predictions[19]. Black defendants are misclassified at a higher risk for recidivism than occurs in practice, while white defendants are misclassified at a lower risk. The model that produces the COMPAS scores is a black box algorithm, which is not interpretable, and therefore the model does not provide a way for human input to correct for these racial biases. We also explore the problem of predicting whether or not someone is carrying a weapon using the Stop and Frisk dataset. This dataset, released by the New York Civil Liberties Union, has been analyzed by Goel et al. to show that black individuals are stopped disproportionately often. We propose that the rule list generated by CORELS could be used as a heuristic for NYC police officers who need to decide whether or not to make a

stop. On both problems, our model produces accuracies that are similar to standard black-box predictive models while maintaining interpretability and having no evidence of racial bias.

CORELS demonstrates a novel approach towards generating interpretable models by identifying and certifying the optimal rule list. While searching for that optimal list, we are able to discover near-optimal solutions that provide insight into how effective other interpretable methods might be. Rule lists have been around for 30 years[33], but computational power has been too limited to use discrete optimization to attack problems of reasonable scale.

There are two major contributions of this work. First, it shows that discrete optimization techniques are computationally feasible with today's hardware. Additionally, the optimizations performed on our tree and symmetry-aware map can be generalized and applied more broadly to other discrete optimization problems.

Chapter 2 provides an overview of related work in the fields of interpretable models, rule lists, and discrete optimization. Chapter 3 proves definitions and explanations of the terminology used in the rest of this thesis. Chapter 4 describes the implementation and architecture of CORELS, paying special attention to the data structures used to make this problem tractable. Chapter 5 explains the data structure optimizations performed and exhibits the experiments used to measure and validate these optimizations.

This thesis arose out of joint work with Elaine Angelino, Daniel Alabi, Margo Seltzer, and Cynthia Rudin. This joint work involved the development of the implementation of CORELS as well as proofs of the theoretical bounds upon which this work is based. However, the papers about the joint work focus more on the theoretical bounds than the data structure optimizations performed. Therefore, my thesis is intended to provide a different perspective on this work—focusing on the implementation details and trying to generalize to other types of systems.

2

Related Work

The use of classification models is popular in a number of different fields from image recognition[21] to churn prediction[22]. Oftentimes, however, simply receiving a prediction from software is not enough–it is important to have a predictive model that humans can investigate and understand[6,32,34,27,12]. For example, in fields such as medical diagnoses[4] and criminal sentencing[19], it is important to be able to investigate the reasons behind a model's predictions. One reason is that medical experts are unlikely to trust the predictions of these models if they are unable to understand why the model is making certain predictions[20]. Interpretable models also allow users to examine predictions to detect systemic biases in the model. This is especially important in classification problems, such as criminal recidivism prediction, where there are often race-related biases[19] or credit scoring where a justification is necessary for the denial of credit[3].

Tree structured classifiers are a popular technique that combines interpretability with high predictive accuracy. Also called decision trees, these trees are often used as either classification or regression tools. Every node in the tree classifier splits the data into two subsets; these subsets are then recursively split by nodes lower in the tree. Nodes are constructed by choosing an attribute that splits the data to minimize a certain metric. This metric differs from algorithm to algorithm, but it is usually focused on separating similar items into their own

groups.Trees are constructed by recursively performing splits on the child subsets until the resulting subset is either entirely homogenous according to the metric or small enough according to some threshold. Methods for constructing decision trees differ primarily based on how they define this metric and what attributes they choose for each node. Breiman et al. laid out an seminal algorithm, CART, to create such trees[7]. CART tries to minimize Gini impurity which is a measure of the probability that any random element taken from a node is mislabeled. Another popular algorithm, C4.5, uses the idea of information gain to make its splits instead[31]. In C4.5, nodes are chosen such that each split minimizes the amount of information necessary to reconstruct the original data. Both algorithms grow the initial tree greedily. However, this leads to extremely large trees, so they perform a post-processing step of pruning to avoid overfitting and maintain interpretability.

The problem of constructing the optimal binary decision tree has been shown to be NP-Complete[15], where optimal means the fewest number of nodes. So, while most decision trees are constructed greedily, and thus provide no guarantees on optimality, there has been some work on constructing optimal decision trees[28]. There has even been the use of a branch and bound technique in an attempt to construct more optimal decision trees. Garofalakis et al. introduce an algorithm to generate more interpretable decision trees by allowing constraints to be placed on the size of the decision tree[14]. They use the branch and bound technique to constrain the size of the search space and limit the eventual size of the decision tree. During tree construction, they bound the possible Minimum Description Length (MDL) cost of every different split at a given node. If every split at that node leads to a more expensive tree than the MDL cost of the current subtree, then that node can be pruned. In this way, they were able to prune the tree while constructing it instead of just constructing the tree and then pruning at the end. However, even with the added bounds, this approach does not guarantee globally optimal decision trees, because they constrain the number of nodes in the tree.

Whereas decision trees are always grown from the top downwards, decision lists are built while considering the entire pool of rules. Thus, while decision trees are often unable to achieve optimal performance even on simple tasks such

as determining the winner of a tic-tac-toe game, decision lists can achieve globally optimal performance. Decision lists are a generalization of decision trees since any decision tree can be converted to a decision list through the creation of rules to represent the leaves of the decision tree[33]. Thus, decision list algorithms are a direct competitor to the popular interpretable methods detailed above: CART and C4.5. Indeed, decision list algorithms are being used for a number of real world applications including stroke prediction[23], suggesting medical treatments[40], and text classification[24].

Work in the field of decision lists focuses both on the generation of new theoretical bounds and new algorithms to generate rule lists. Both approaches share the end goal of improving the predictive accuracy of models using rule lists. Recent work on improving accuracy has led to the creation of probabilistic decision lists that generate a distribution over the space of potential decision lists[23,38]. These methods achieve good accuracy while maintaining a small execution time. In addition, these methods improve on existing methods, such as CART or C4.5, by optimizing over the global space of decision lists as opposed to searching for rules greedily and getting stuck at local optima. Letham et al. are able to do this by pre-mining rules, which reduces the search space from every possible split of the data to a discrete number of rules. Rule mining generates rules by creating boolean clauses that represent common features in the dataset. We take the same approach towards optimizing over the global search space, though we don't use probabilistic techniques because we want a guarantee on the optimality of our solution. We also want to work in a regime with a discrete number of rules, thus we use the same rule mining framework from Letham et al. to generate the rules for our data sets[23]. This framework creates features from the raw binary data and then builds rules out of those features. Yang et al. builds on Letham et al., improving runtime and accuracy, by placing additional bounds on the search space and creating a fast low-level framework for computation, specifically a high performance bit vector manipulation library. We use that bit vector manipulation library to help perform computations involving calculating accuracy of rules[38].

In addition to these recent practical improvements in rule list generation, there has been a wide body of literature on the theoretical aspects of rule lists.

Rivest introduced decision lists[33] soon after Valiant published his theory of learnability[37]. Much of the work in the years immediately following the invention of decision lists were focused on issues of learnability and complexity rather than practical implementations. Some of this work has focused on the attribute efficiency of various algorithms[5,9], while others have focused on the relationship between decision lists and classes of boolean functions such as DNF or CNF[33,11]. Other authors focused on a specific case of decision lists such as homogenous decision lists[35] or a more general cases of the decision list problem such as decision committees[30]. Much of the research into rule lists has improved the complexity of both the number of training examples necessary and the worst case runtime of rule list algorithms[16]. Despite discussing that the difficulty surrounding learning accurate decision lists, there has been little work trying to solve the optimality problem. Due to the intrinsic computational difficulty fo the problem, researchers have not applied discrete optimization techniques with regards to the problem of decision lists. We hypothesize that hardware limitations severely constrained the size of the problems that could be solved using these techniques, contributing to this gap in the literature.

Branch and bound was a technique originally developed to solve linear programming problems[18]. The branch and bound algorithm recursively splits the data into subgroups, yielding a tree-like structure. Using a value corresponding to the end goal of the algorithm, the algorithm can guarantee that some branches of the tree will be worse in every case than another branch and therefore can be pruned. By repeating these two steps of branching and bounding, the algorithm quickly reduces the search space. For decades, it has been used to great effect in the realm of mixed integer programming[25]. It has also been applied to other NP-hard problems such as the Traveling Salesman Problem[26] and the Knapsack Problem[17]. More recently, it has been applied to machine learning problems such as feature subset selection[29] and clustering[13]. However, over the past few decades, its popularity has declined in favor of convex optimization methods such as SVMs. These optimization methods have allowed researchers to achieve high accuracy on large datasets without running into the computational difficulties of branch and bound. However, the continual improvements in computer hardware have led to a recent resurgence in the use of branch and

bound techniques[10].

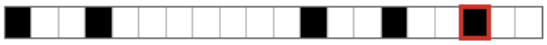
3 Definitions

We present definitions and explanations of concepts and terms that are used throughout this work. Throughout this chapter, we provide examples from a hypothetical dataset, Computer. We will use Computer to answer the problem of predicting whether someone uses a Mac or a PC. Computer is a dataset comprised of 20 individuals, whether they use a Mac or PC, and other personal details that may help with the prediction.

3.1 Rules

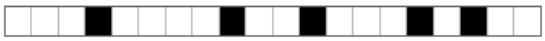
A *rule* is an *if-then* statement consisting of a boolean antecedent and a classification label. We are working in the realm of binary classification, so the label is either a 0 or a 1 (or an equivalent label). The boolean antecedents are generated from the rule mining mechanism of Letham et al.[23] and are a conjunction of boolean features. These antecedents are *satisfied* by some data points (also called *samples*) and not for others. We say a rule *classifies* a given data point when the antecedent is satisfied for that data point. A rule's *support* is comprised of all of the data points that are classified by a rule. Rules therefore have an inherent accuracy based on their support. Fig 3.1 provides an example of 4 rules that could be mined from the Computer dataset. Rule 1, has a support of

Rule 1: **if** $age < 25$ **then predict** Mac



Rule 2**: if** $(education = college)$ **then predict** Mac

Rule 3**: if** $age > 45 \wedge \neg(job = software\ engineer)$ **then predict** PC



Rule 4**: if** $\neg(residence = california)$ **then predict** PC

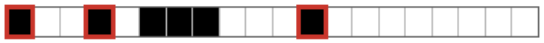


Figure 3.1: Example rules from the Computer dataset . The bit vector below the rule is a visual representation of the rule---each box is a data point. Black boxes represent data points that are classified by a rule. Data points that are classified incorrectly are outlined in red.

Rule List 1
if $age < 25$ **then predict** Mac
else if $\neg(residence = california)$ **then predict** PC
else predict PC

Rule List 2
if $\neg(residence = california)$ **then predict** PC
else if $age < 25$ **then predict** Mac
else predict PC

Figure 3.2: Example rule lists from the Computer dataset made using Rule 1, Rule 4, and a default rule. As in Fig 3.1, black boxes represent data points captured by the rules in the rule list and red marks incorrect classification. All of the white boxes are classified by the default rule. Rule 4 has an accuracy of 50% in Rule List 2, but an accuracy of 100% in Rule List 1 when it comes after Rule 1. Thus, despite the two rule lists being permutations of each other, Rule List 1 performs much better than Rule List 2.

5 but only classifies 4 of those samples correctly—thus its inherent accuracy is 80%.

3.2 Rule Lists

A *rule list* is an ordered collection of rules. As defined above, rules have an inherent accuracy based on what data they classify and how they predict the la-

bel. As we combine these rules into rule lists, however, only the first rule that classifies any given data point can make a prediction for that data point. Thus, we say a rule *captures* a given data point if it is the first rule in a rule list to classify that data point. Therefore, when rules are placed into a rule list, their accuracy is based on what data they capture—which is not necessarily the same as what data they classify. They can perform better or worse than their inherent accuracy depending on what rules come before them in a given rule list. For example, we can see in Fig 3.2 that even though Rule 4 only has an inherent accuracy of 50%, in Rule List 1 it has an accuracy of 100% because it is placed below Rule 1.

Our algorithm is focused on finding the list that combines rules in an order that maximizes predictive accuracy. A rule list also has a *default rule*, placed at the end of any rule list, that classifies all data points and predicts the majority label. This allows a rule list to make predictions for all points because any point not captured by the pre-mined rules is captured by the default rule. We refer to the length of a rule list as the number of pre-mined rules, without including the default rule. The rule lists in Fig 3.2 are both of length 2. We define a *prefix* as any subset of the rules at the beginning of a rule list. We will often use prefix to refer to the list of all rules in a rule list except for the default rule.

3.3 Objective Function

Rule lists have a loss function based on the number of points that are misclassified by the rules in the rule list—including misclassifications due to the default rule. We define our *objective* function to be the sum of that loss and a *regularization term*, which is a constant times the length of the rule list. This has the effect of preventing overfitting on training datasets as well as discouraging extremely long, and therefore uninterpretable, rule lists. While the objective is related to accuracy (a higher accuracy means a lower objective), we will be minimizing over the objective function instead of maximizing the accuracy to reap the benefits of the regularization term. Let RL be a rule list, then:

$$objective(RL) = loss(RL) + \lambda * len(RL)$$

We can calculate the objective for Rule List 1 in Fig 3.2 as follows. The loss from rules 1 and 4 is 0.05, while the loss from the default rule is 0.05. Assuming a regularization constant of $\lambda = 0.01$, the objective for Rule List 1 is $0.05+0.05+2*0.01 = 0.12$.

3.4 Bounds

For a set of n rules, there are $n!$ possible rule lists. Finding the optimal rule list using a brute force approach is infeasible for any problem of reasonable size. Our algorithm uses the discrete optimization technique of branch-and-bound to solve this combinatorially difficult problem of finding an optimal rule list. This requires tight bounds that allow us to prune as much of the search space as possible. These bounds are formalized and proved in Angelino et al.[2] and are reproduced in Appendix A. For clarity, we present informal summaries of the important bounds here.

3.4.1 Lower Bound

We use the term *lower bound* to mean the best possible outcome for the objective function for a given prefix. We do this by calculating the loss of the prefix and assuming that any points not captured by the prefix will be predicted correctly. This is equivalent to creating a hypothetical default rule that captures all points perfectly. Because any future extensions of the prefix can never do better than this perfect default rule, we will be able to use this bound to prune our exploration. The lower bound also increases monotonically—any rules we add can only make mistakes that this perfect default rule does not make. Much of the work on CORELS has focused on creating bounds that are as close to the true lower bound as possible. The smaller the difference between our bounds and the true lower bound, the easier it is to prune sub-optimal rule lists.

$$lower\ bound(prefix) = loss(prefix) + \lambda * len(prefix)$$

The lower bound for Rule List 1 is therefore $0.05 + 2 * 0.01 = 0.07$, which is less than its objective. This is due to the fact that the objective function includes the error made by the default rule, but the lower bound has to assume that we

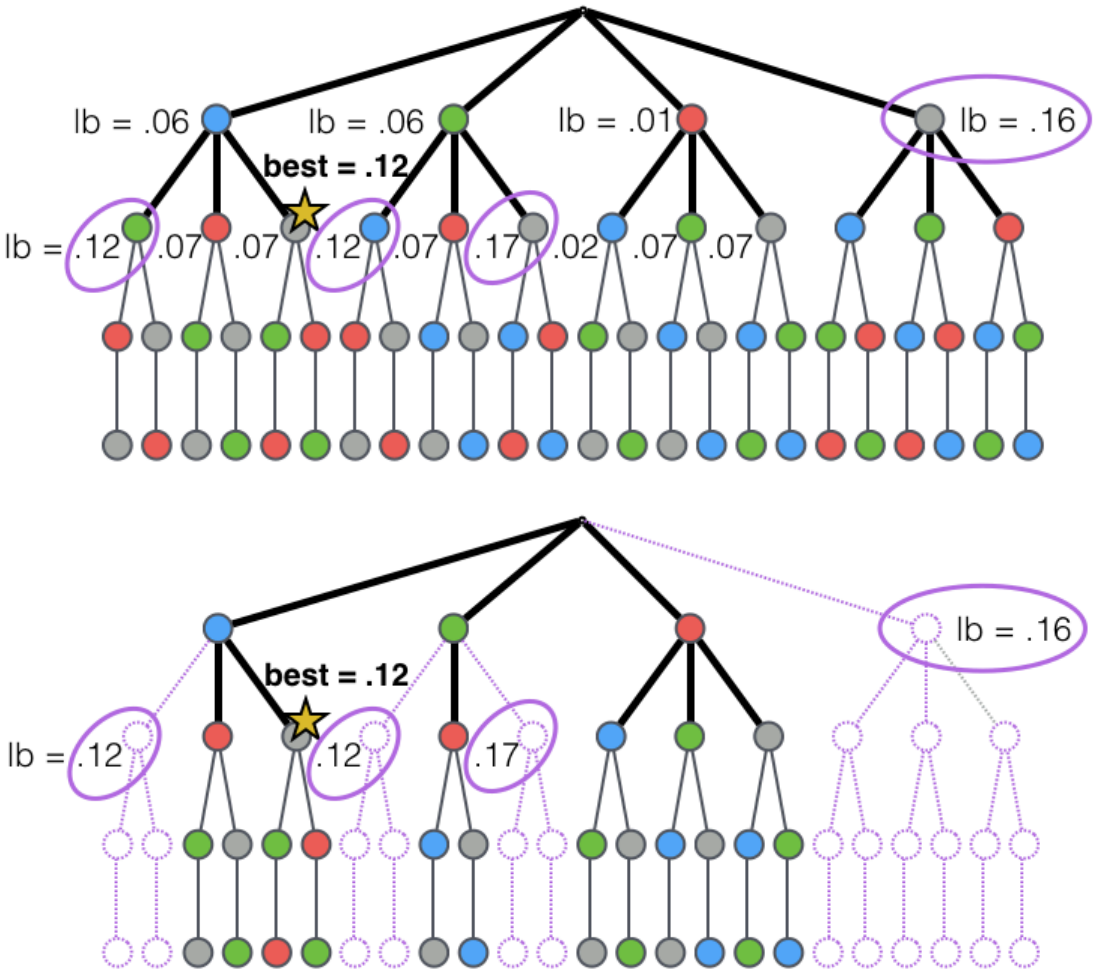


Figure 3.3: This tree shows the hierarchical objective bound in action. Each color represents one of our 4 rules from Fig 3.1: blue = Rule 1, green = Rule 2, red = Rule 3, and gray = Rule 4. Thus, each path in the tree represents a rule list. Our best objective seen is the rule list (1, 4, default) with an objective of 0.12. Any prefixes with lower bound greater than this objective---all prefixes beginning with (4), (1, 2), (2, 1), or (2, 4)---can be pruned and not examined. The bottom tree shows the pruned prefixes, marked in purple.

could add a rule that would correctly classify the data point that is misclassified by the default rule.

3.4.2 Hierarchical Objective Bound

The main bound for our algorithm is the *hierarchical objective bound*. It says that we do not need to pursue a rule list if it has a lower bound that is worse than the best objective we have already seen. This follows from the fact that lower bounds increase monotonically, so if the lower bound of Rule List 2 is equal to or worse than the objective of Rule List 1, any extensions of Rule List 2 can never be better than Rule List 1. This allows us to prune large parts of the search space by not pursuing rule lists that could never be better than something we have already seen. Fig 3.3 provides an example of our pruning mechanism in action. It shows how an exploration of the search space leads to a difference in the best observed objective and the lower bounds of some rule lists. Our algorithm will use that difference to prune parts of the search space and reduce a combinatorially large problem into a tractable one.

3.4.3 Permutation Bound

As defined above, every sample is captured by precisely one rule—in the prefix (1, 4), any sample that is captured by rule 1 cannot be captured by rule 4. Now consider a *permutation* of the prefix (1, 4): the prefix (4, 1). Any samples that are captured by either rule 1 or 4 but not both will be captured identically in both rule lists. Samples that are captured by both rules will again be captured the same in both rule lists, though they may be predicted differently in the two rule lists. Thus, regardless of the order in which the rules appear, prefixes (1, 4) and (4, 1) will capture exactly the same set of data—this can be seen in the bit vectors of Fig 3.2. They will differ only in which rules capture which samples, so their accuracies may differ. We can use this knowledge to create a bound that we call the *permutation bound*. If we know that the lower bound of the prefix (1, 4) is better than the lower bound of (4, 1), we can eliminate from consideration all rule lists beginning with (4, 1). This is due to the fact that any rule list beginning with (1, 4) will capture exactly the same samples as the equivalent rule list beginning with (4, 1), but will have a better objective score. Fig 3.4 demonstrates the pruning process with the prefixes (1, 4) and (4, 1). Since (1, 4) has a lower bound of 0.07 while (4, 1) has a lower bound of 0.16, we can prune (4, 1) and not pursue any of its children.

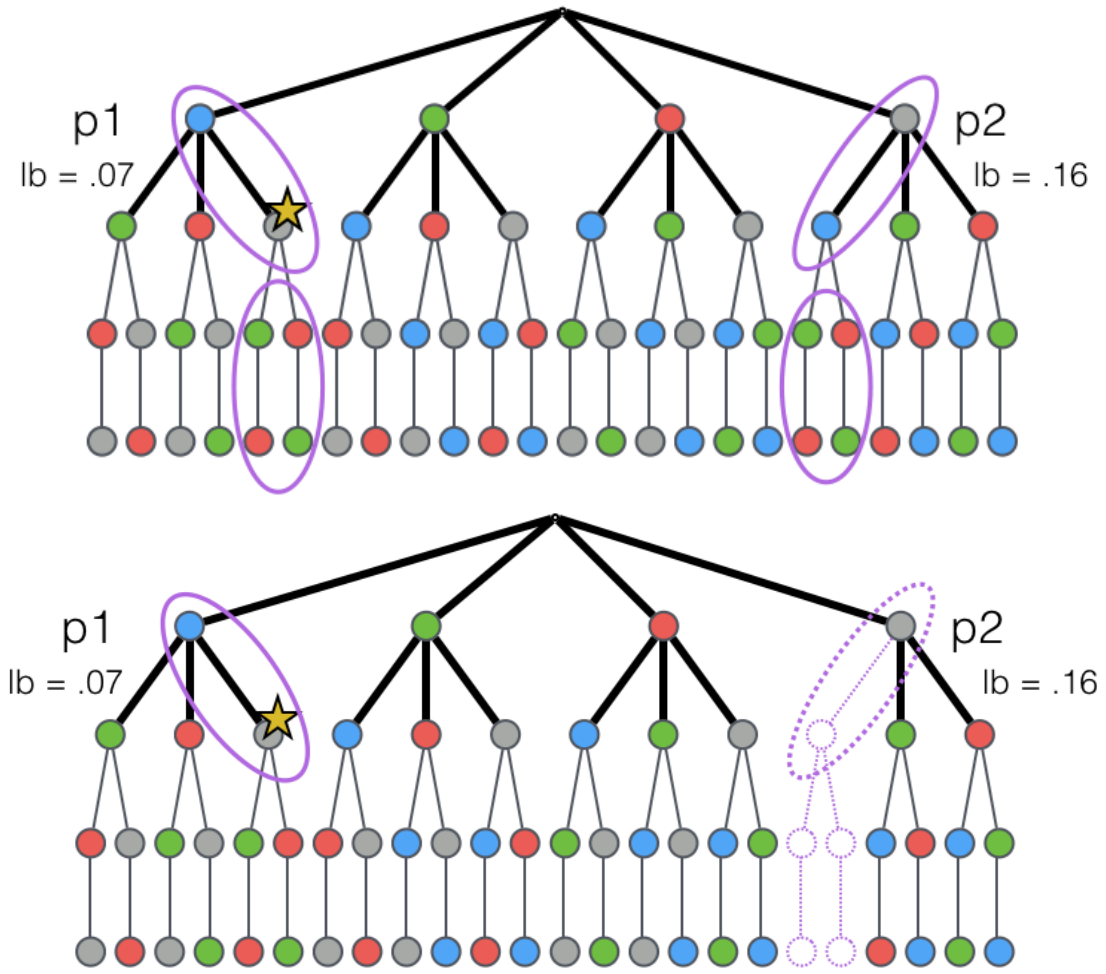


Figure 3.4: This tree shows the use of the permutation bound in action. Prefixes (1, 4) and (4, 1) are permutations of each other, so they capture identical data (see Fig 3.2). When we compare their lower bounds, we see the prefix (1, 4) has a better lower bound. Any rule list beginning with (4, 1) would be worse than the corresponding rule list beginning with (1, 4), so (4, 1) can be pruned and none of its children have to be examined.

Generalizing this principle allows us to eliminate all but one permutation of a given set of rules. When we are dealing with these permutations, it is helpful to map all permutations to a single ordering by ordering the rules in numerical order. We call this the *canonical ordering* of a prefix. For example, the prefixes (1, 4) and (4, 1) both map to the canonical ordering (1, 4).

3.4.4 Support Bounds

Due to the regularization term in our objective function, adding a rule that does little to improve accuracy will harm the overall objective score. This allows us to place bounds that rely on the support of the rules we add. It never makes sense to add a rule that increases the objective function, so we consider adding only those rules that capture sufficiently many points correctly to overcome the regularization penalty. By definition, rules that do not capture enough of the remaining points cannot capture them correctly, so this provides us with two closely related bounds. As our rule lists grow, many rules do not capture enough points and this bound begins to play a larger role.

3.4.5 Equivalent Points Bound

This bound relies on the similarities within the structure of our dataset. In our dataset, we may encounter two data points that have the same features but different labels. We call the set of these data points *equivalence points* and describe the label that occurs less often as the *minority* label. Since equivalence points have identical features, any rule that classifies one point in an equivalence class will also classify all other points in that class. However, it is impossible to correctly predict equivalence points with different labels using a single rule. So, for a given class of equivalence points, we know that we will mispredict all of the points with a minority label. We can thus update our lower bound to be tighter than just assuming that the default rule will capture all remaining points correctly. Now, we assume that any remaining points with a minority label will be captured incorrectly. This gives us much tighter lower bounds and, in practice, allows us to prune more efficiently.

In our Computer dataset, for instance, we might have 3 people who are in college and form an equivalence class. Now, 2 of those people use Macs and will be correctly classified by Rule 1. However, we will never correctly classify that 3rd person who uses a PC because any rule will always predict Mac to maximizes its accuracy. So, our lower bound should take into account the fact that we will always mispredict that person.

3.5 Curiosity

There are a number of different ways to explore the search space (see Section 4.3). Some methods, such as BFS, prioritize exploration—looking at all rule lists of a given length before proceeding to the next length. Others, such as ordering by lower bound, focus purely on exploiting the best prefixes that we have seen. We define a new metric, *curiosity*, that combines exploration and exploitation. Lower values of curiosity mark prefixes that we explore first. Curiosity is a function of both the lower bound and the number of samples captured. This prioritizes rule lists that still have many samples left to capture (exploration) while also pursuing rule lists with promising lower bounds (exploitation).

$$curiosity(RL) = (lowerBound(RL) - minority) * (nsamples/|captured(RL)|)$$

Assuming a minority value of 0, we can see that the curiosity of Rule List 1 is $(.07 - 0) * (20/8) = 0.175$, while the curiosity of Rule List 2 is $(.22 - 0) * (20/8) = 0.55$. Thus, curiosity prioritizes extending the more promising rule list.

3.6 Remaining Search Space

One metric for tracking the efficacy of our optimizations will be observing how quickly we reduce the remaining search space. We start with a combinatorially large search space, but quickly reduce it using our bounds. We calculate the remaining search space by determining how much each prefix could be expanded. We do this for every prefix we have evaluated and not eliminated. Due to our regularization term, we are able to bound the maximum length of any optimal rule list as our best objective gets updated. This upper bound on the maximum length of an optimal rule list allows us to place an upper bound on the remaining search space as well. The search space of our problem can be visualized as a tree with fanout n–depth. From the root, there are n rules we can add, and then we can add $n - 1$ rules to each of those rules, and so forth. However, as the best objective we have seen gets better, there are more paths of the tree that we can eliminate and so our search tree grows smaller.

3.7 Datasets

All of our datasets are split into a training set and a test dataset to test for accuracy. We then divide the dataset 90-10 for training and test sets. In addition, we split our training and test sets into 10 folds to perform cross validation. For our analysis that does not involve accuracy calculations, our performance numbers come from running on a single fold.

The COMPAS dataset is a list of criminal offenders and information about them and their records. The classification problem that we're trying to solve is whether or not a given offender will commit another crime within 2 year of being arrested. As mentioned in the introduction, this problem is currently being handled through the use of a black box model because the authors of that model claim that adding interpretability would harm accuracy. This black box model has been accused of racially biased predictions[19]. We explore this dataset with the goal of providing an interpretable, non-biased model that has accuracy comparable to state of the art black-box models.

The COMPAS dataset has 7214 individuals, meaning our training set has 6489 data points. 2947 (45.1%) of these individuals are labeled "yes", meaning they have committed a second crime after being arrested—while the other 3542 (54.9%) individuals are labeled "no". On this particular dataset, COMPAS scores achieve 61% accuracy for predicting recidivism. The creator of the COMPAS score, Tim Brennan, has previously shown an AUC of .68 for predicting any offense on a smaller dataset of 2300 individuals[8]. He also claims that it's difficult to get good accuracy without using racially influenced features, saying:

> "it is difficult to construct a score that does not include items that can be correlated with race such as poverty, joblessness and social marginalization. 'If those are omitted from your risk assessment, accuracy goes down', [Brennan] said."[19]

We are able to extract 155 rules from the dataset, including rules that involve the race of the individual.

The Stop and Frisk dataset is a list of stops made by the New York City Police Department (NYPD) that contains information about the outcome of that stop: whether an individual was frisked, searched, or found carrying a weapon.

The classification problem that we are trying to solve are whether someone is carrying a weapon when stopped (which we refer to from now on as Weapon). Stop and Frisk has been a controversial program and recent work has alleged that blacks and Hispanics are disproportionately stopped[36]. The authors of that work further suggest that it would be ideal to provide police officers with a simple heuristic about whether or not to make a stop. We hope to provide a model that is short and easy to remember, but also has high predictive accuracy when it comes to finding weapons or other contraband.

This dataset is composed of 45787 individuals of whom 3.3% are carrying a weapon. We are able to extract 46 rules, some of which include features involving the race of the individual.

4

Implementation

This chapter lays out the design and implementation of the system used to generate optimal rule lists. We begin by providing an overview of our algorithm. Next, we explore the details of each of the three main data structures used to run our algorithm—a prefix trie, a symmetry-aware map, and a queue. We conclude with a more thorough walkthrough of the implementation of our main algorithm, including a discussion of our garbage collection and memory tracking.

4.1 Algorithm overview

Algorithm 1 details a pseudocode version of our branch-and-bound algorithm. First, we perform the branching step where we choose a new branch to explore on our search tree by selecting the next rule list to evaluate. Next, we evaluate the objective and bounds on this rule list and prune it if possible, allowing us to prune some rule lists and not examine the entire search space. Finally, we update the optimal rule list if this rule list is better than the best rule list we have seen—this allows us to perform the bounding step more efficiently. We continue with these 3 steps until we have no more prefixes to evaluate. At the

Algorithm 1 Branch-and-bound Algorithm for Rule Lists

Input: A dataset and a binary classification problem.
Output: The best rule list and its objective

initialize data structures
while rule lists to examine **do**
    get next rule list
    evaluate rule list bounds, discard if possible
    if rule list is better than previous best **then**
        update best rule list
        garbage collection
return best rule list, best objective

```
class Node {
  protected:
    std::map<unsigned short, Node*> children_;
    Node* parent_;
    double lower_bound_;
    double objective_;
    double minority_;
    size_t depth_;
    size_t num_captured_;
    unsigned short id_;
    bool prediction_;
    bool default_prediction_;
    bool done_;
    bool deleted_;
};
```

Figure 4.1: Our custom C++ class defining a node in the prefix trie.

end of execution, we return the optimal rule list, which is the rule list with the best objective.

4.2 Prefix Trie

The prefix trie is a custom C++ class and is used as a cache to keep track of rule lists we have already evaluated. Each node represents a rule—see Fig 4.1

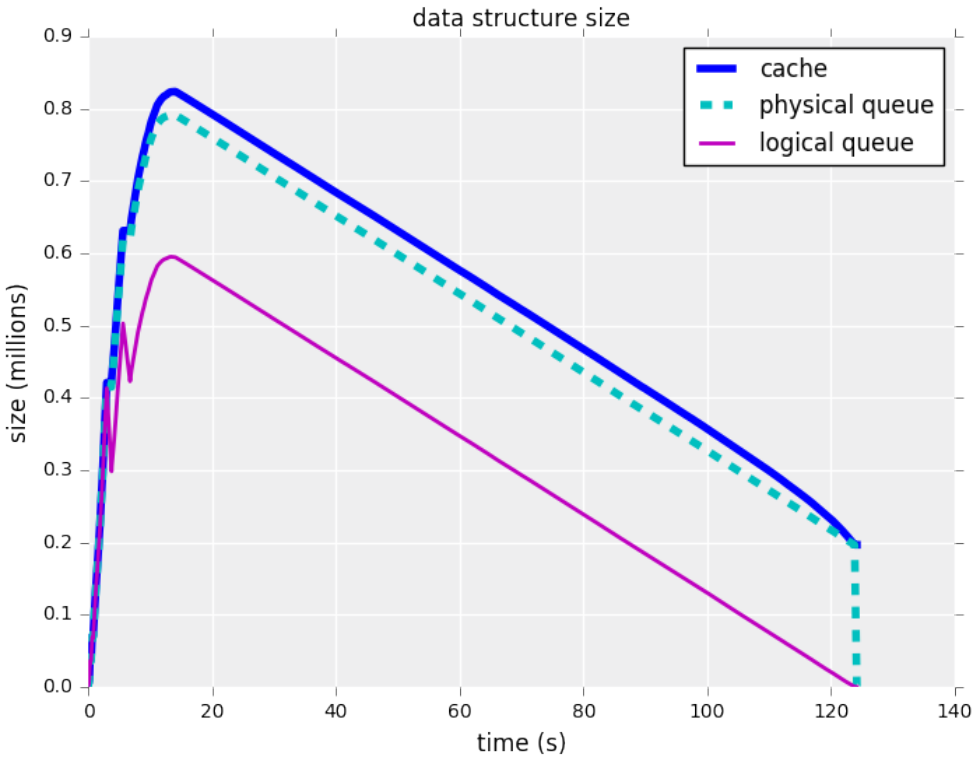


Figure 4.2: Size of prefix trie, logical queue, and physical queue over the execution of our algorithm on the COMPAS dataset. This dataset has 155 rules and 6489 samples (see Section 3.7). The gap between the logical queue and the physical queue is due to our lazy garbage collection.

for our class definition of a node—that contains the id and prediction for the rule that the node represents. Nodes in the trie also contain the metadata associated with that corresponding rule list. This metadata includes the following bookkeeping information: which child rule lists are viable, lower bound, objective, minority misclassification, length, number captured, prediction for default rule, and whether or not this node should be pruned. In addition to our base trie class, we also implemented a different node types that we use in our algorithm. We implemented a sub-class that has an additional field that tracks the curiosity of a given prefix as defined in Section 3.5. Curiosity is one of several ways we use to order our search space. Since the curiosity field is just a double, the memory overhead is minimal.

4.3 Queue

The queue is a worklist that orders our exploration over the search space of possible rule lists. We implement a number of different scheduling schemes including a stochastic exploration process, BFS, DFS, and priority metrics of curiosity, objective, or lower bound. Our queue contains pointers to leaves in the trie to leverage incremental computation. The search process involves selecting which leaf node to explore. The stochastic exploration process bypasses the use of a queue by performing random walks on the trie until a leaf is reached. Our other scheduling schemes use a STL C++ priority queue to hold and order all of the leaves of the trie that still need to be explored. Our priority metrics can be ordered by curiosity, the objective, or the lower bound. We find that using an exploitation strategy, such as ordering by lower bound, usually leads to a faster runtime than using BFS.

In C++ the priority queue is a wrapper container that prevents access to the container underlying the queue. Therefore we cannot access elements in the middle of the queue, even if we have know the value that we're trying to access. Thus, we run into a problem where we may delete something in the prefix trie that is currently in the queue, as we have no way to update the queue without iterating over every element. We address this by lazily marking nodes as deleted in the prefix trie without deleting the physical node until it has been removed from the queue. Fig 4.2 shows that this leads to a situation where our logical queue is actually smaller than the physical queue. However, the difference is minimal and the alternative of iterating over the queue would be very slow.

4.4 Symmetry-aware map

We implement our symmetry-aware map as an STL unordered_map, to apply the permutation bound described in Section 3.4.3. We have two different versions of the map with different key types that allow permutations to be compared and pruned. In both cases, the values consist of the best lower bound and the actual ordering of the rules that is best for that permutation. In the first version, keys to the map are represented as the canonical order of the rules, called PrefixKeys. The second version has keys that represent what data has

Algorithm 2 CORELS

Input: A dataset and a binary classification problem.
Output: The best rule list and its objective.

```
opt ← NULL
T ← initializeTree()
Q ← queue( [T.root() ])
P ← map({})
while Q not empty or niter == termination do
    prefix ← Q.pop( )
    newObj ← incremental(prefix, T, Q, P)        ▷ Finds possible extensions
                                                   of prefix (defined below)
    if newObj < T.minObjective( ) then
        opt ← T.bestRuleList( )
        T.garbageCollect( )
return opt, T.minObjective( )
```

been captured, which we call CapturedKeys. Our permutation bound is based on the fact that different permutations capture the same data, so both types of key will mark the rule lists (1, 4) and (4, 1) as permutations. CapturedKeys could potentially match more permutations since two prefixes may not be permutations of each other but might capture the same data points and therefore fall under the permutation bound. However, our analysis in Section 5.3, shows that this increase in matches is not enough to offset the massive amount of memory needed by the CapturedKeys. Despite supporting only one bound, the symmetry-aware map plays a significant role in our memory usage.

4.5 Incremental execution

Algorithm 2 shows the macrostructure of our algorithm. It is very similar to the general structure provided in Algorithm 1, but it replaces the pseudocode with our specific data structures. Our program terminates when all leaves of the trie have been explored and there is nothing else in our queue. We can also opt for early termination based on the number of leaves in the trie. This prevents us from achieving the certificate of optimality, but can still lead to us finding a

good or even optimal rule list. Most executions find the optimal rule list quickly, but then certification requires a long time and a large amount of memory. Early termination allows us to trade the guarantee of optimality for lower time and memory costs.

While there are still leaves of the trie to be explored, we use our scheduling policy to select the next prefix to evaluate. We pass that prefix to our incremental function, detailed in Algorithm 3. For every rule that is not already in this prefix, i.e. rules that we could potentially add to the list, we calculate whether adding that rule to that prefix would create a viable rule list. First, we compute how many points the new rule would capture and how many of those it would capture correctly to determine if it passes our support bound. Then, we calculate the lower bound and prune this rule list if the lower bound is larger than the best objective we have seen. Next, we determine the rule list's objective and update our current best objective if necessary. If our lower bound is large enough that adding any additional rule will cause the lower bound to be larger than our current best objective, we apply the lookahead bound and do not add the rule list to any of our data structures. Finally, we try to add the rule list to our various data structures. The symmetry-aware map will take care of the permutation bound, so we only insert the rule list into the prefix trie and queue if it successfully passes the permutation bound. Otherwise, we do not insert it into any of our data structures, and we continue to the next potential rule. After evaluating all of the rules we could add to the current rule list, we return to the main loop and examine the next element in the queue. Upon clearing our queue, we return the optimal rule list and its objective value.

4.6 Garbage Collection

Every time we update the minimum objective, we garbage collect the trie by traversing from the root to the leaves. Any time we encounter a node with a lower bound larger than the minimum objective, we delete its entire subtree. In addition, if we encounter a node with no children, we prune upwards—deleting that node and recursively traversing the tree towards the root, deleting any childless nodes. This garbage collection allows us to limit the memory usage of the trie. In practice, though, the minimum objective is not updated that often,

so garbage collection is triggered only rarely.

4.7 Memory tracking

Throughout our development of CORELS, we often ran into the problem that larger datasets would run us out of memory. Therefore, we wanted to institute data structure optimizations that would reduce the memory burden of our algorithm. In order to achieve this goal, we needed to implement a way of tracking how much memory our program was using and where it was being used. We track memory through the use of C++11 custom allocators. Our allocators are simple malloc wrappers that log which data structure the allocation is coming from—the trie, the map, or the queue. We validated the accuracy of this memory tracking by running the program under Valgrind's Massif heap profiler tool and comparing the outputs. Our outputs matched Valgrind's to within a few tenths of a percentage points, so we concluded that our memory tracking was successful: on a limited run of the COMPAS dataset, Valgrind's tool Massif reported that we used 98.7 MB, while our data structure tracking recorded 98.5 MB, a difference of 0.2% which can be explained by heap allocations not related to our main data structures. The heap profiling of Valgrind has a large overhead, while our memory logging has minimal overhead. Our custom memory logging allows us to output our memory usage per data structure on a regular basis without incurring the large overhead of Valgrind.

Algorithm 3 Incremental evaluation of a prefix

Input: Node to be evaluated *parent*, prefix tree T, queue Q, symmetry-aware map P
Output: Best objective found

$bestObj = 1.0$
$prefix \leftarrow parent$.prefix( )
$t \leftarrow c \cdot nsamples$ ▷ This forms the threshold for our support bounds
for $rule \notin prefix$ **do**
  $rlist \leftarrow prefix$.append($rule$)
  $cap \leftarrow parent$.notCaptured( ) $\wedge$ $rule$.captured( )
  if $|cap| < t$ **then** ▷ Minimum support bound
    continue
  $capZero \leftarrow cap \wedge T$.zeroLabel( ) ▷ Record how many zeros the new rule captures
  $corr \leftarrow max\{|capZero|, |cap| - |capZero|\}$
  if $corr < t$ **then** ▷ Minimum correct support bound
    continue
  $lb = parent$.bound( ) $-$ $parent$.minority( ) $+$ $\frac{|cap| - corr}{nsamples} + c$ ▷ Lower bound is equal to parent's lower bound plus the number of mistakes made by the new rule.
  if $lb >= T$.minObjective( ) **then** ▷ Objective bound
    continue
  $notCap \leftarrow parent$.notCaptured( ) $\wedge \neg cap$
  $notCapZero \leftarrow notCap \wedge T$.zeroLabel( )
  $defaultCorr \leftarrow max\{|notCapZero|, |notCap - notCapZero|\}$
  $obj \leftarrow lb + \frac{|notCap| - defaultCorr}{nsamples}$ ▷ Calculate objective based on lower bound and default rule
  $bestObj = min\{bestObj, obj\}$
  if $obj < T$.minObjective( ) **then** ▷ Update minimum objective
    $T.minObjective(obj)$
  if $lb + c >= T$.minObjective( ) **then** ▷ Lookahead bound
    continue
  $n \leftarrow P.insert(rlist)$ ▷ Symmetry-aware map handles permutation bound for us
  if n **then** ▷ n will be NULL if it failed the permutation bound check
    T.insert(n)
    Q.push(n)
return $bestObj$

5
Experiments

The following experiments were executed on a commodity laptop, a MacBook Air with a 1.4 GHz Intel Core i5 processor and 8GB of RAM. The lowend nature of our platform illustrates the potential ubiquity of using discrete optimization techniques. In addition, we hope that this accessibility will allow our model to be used in places that typically lack advanced computing resources such as police departments, courts, and hospitals.

We first examine the accuracy of our algorithm on each of our datasets and compare it to other interpretable and non-interpretable methods. Then, we demonstrate that without our algorithmic and data structure improvements, it would be intractable to solve a real-world problem. We also show that even with our improvements, this algorithm would not have been able to be run just 25 years ago. Next, we examine the improvements made to our symmetry-aware map to reduce the memory overhead on our algorithm. Then, we discuss the benefits of implementing our algorithm using templates as opposed to inheritance. Finally, we describe a parallel implementation and some of the issues that complicate a parallel implementation.

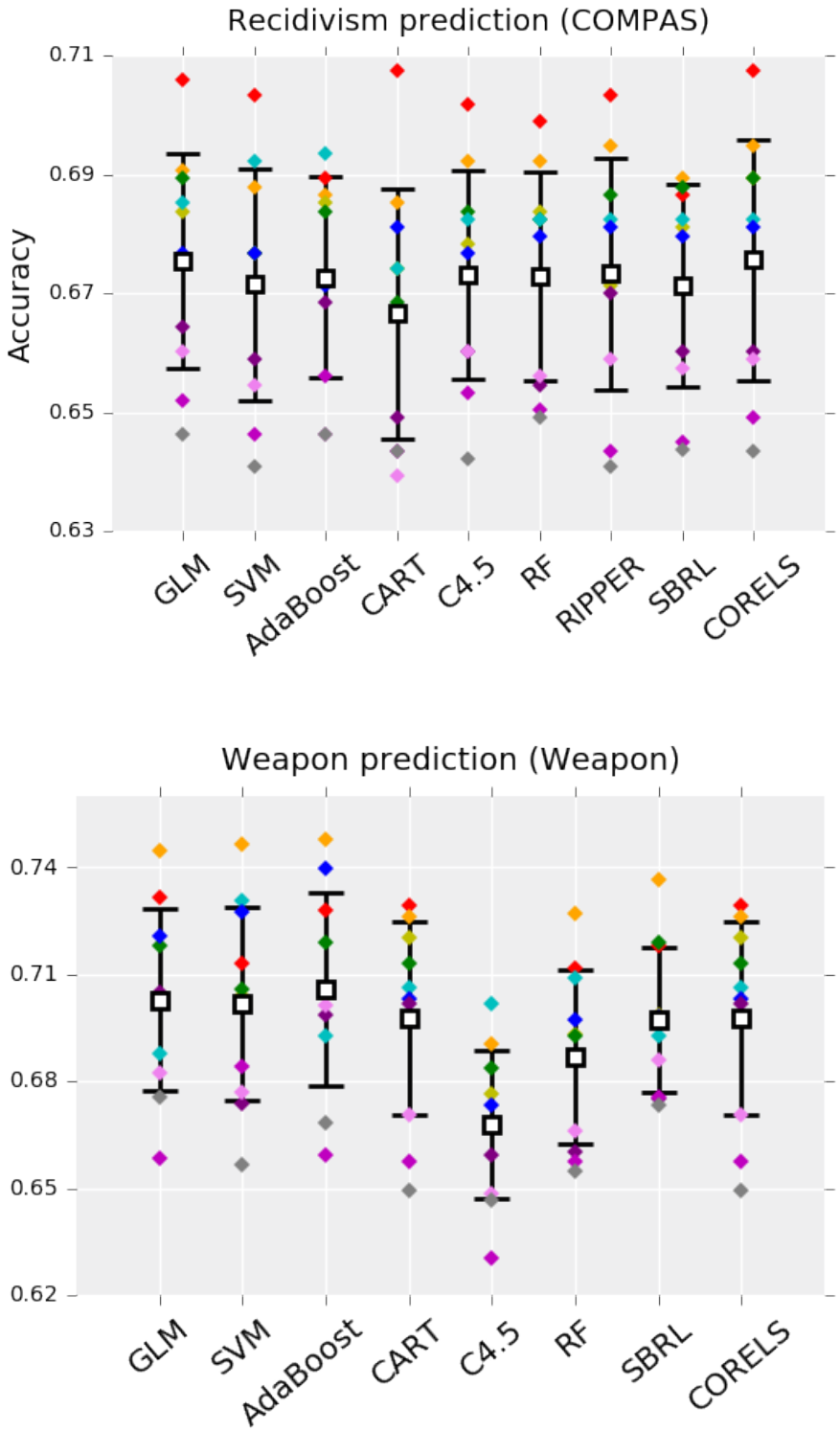


Figure 5.1: 10-fold cross validation of various machine learning models on the COMPAS and Weapon datasets. CORELS performs as well as or better than equivalent interpretable and black-box models. Method type from left to right: Logistic Regression, Support Vector Machine, Boosted Decision Tree, Decision Tree, Decision Tree, Random Forest, (Rule Set), Rule List, Rule List. Note that RIPPER (a Rule Set algorithm) is absent in the Weapon dataset.

Optimal COMPAS rule list
if $(age = 23\text{–}25) \wedge (priors = 2\text{–}3)$ **then predict** yes
else if $(age = 18\text{–}20)$ **then predict** yes
else if $(sex = male) \wedge (age = 21\text{–}22)$ **then predict** yes
else if $(priors > 3)$ **then predict** yes
else predict no

Optimal Weapon rule list
if $stop\ reason = suspicious\ object$ **then predict** yes
else if $location = transit\ authority$ **then predict** yes
else if $stop\ reason = suspicious\ bulge$ **then predict** yes
else predict no

Figure 5.2: Top: The optimal rule list that predicts two-year recidivism for a fold of the COMPAS dataset, found by CORELS. Bottom: The optimal rule list that predicts whether or not someone who is stopped by the NYPD has a weapon for one fold of the Stop and Frisk dataset, found by CORELS.

5.1 Accuracy

We tested CORELS for accuracy on the COMPAS and Weapon datasets. In addition to CORELS, we tested other interpretable rule based methods such as RIPPER and SBRL, tree methods such as CART, C4.5, and Adaboost, and less interpretable algorithms such as random forests, logistic regression, and SVMs. Fig 5.1 shows that CORELS performs just as well as any other predictive method that we tested on the COMPAS and Weapon datasets. Both of these problems are difficult, so no model is able to capture all of the nuances of human behavior perfectly. We see that CORELS performs slightly better than other rule based methods such as SBRL and RIPPER, but that these other methods are not far from optimal. In addition, we see no increase in accuracy granted by using a non-interpretable method instead of an interpretable method such as CORELS. This provides evidence against the claim that predictive accuracy on these problems will suffer if an interpretable algorithm is used.

Fig 5.2 shows the optimal rule lists for the COMPAS and Weapon datasets. Neither of the optimal rule lists includes a race related rule. Both datasets were mined for rules pertaining to race, which means that those rules were not predictive enough to be in the optimal rule list. This shows that it is possible to get

models with state of the art accuracy that do not rely on race to make their predictions. Thus, the excuse that using a racially biased model is more predictive does not hold true. In addition, these rule lists are short and accurate and therefore would be useful as a racially unbiased heuristic aid for judges and police officers.

5.2 Isolated Optimization Analysis

We wished to determine how helpful each theoretical bound and data structure optimization was. We ran a number of experiments where we took out a single component from our system and measured the effects on the runtime and memory usage of our algorithm. We find that, depending on the structure of our problem, different bounds have differing importance.

In addition, we wanted to find out how much of an overall speed-up CORELS gave compared to a naive implementation. On the COMPAS dataset, where $n = 155$, naively evaluating all prefixes of up to length 5 would require examining 84,382,025,575 different prefixes. However, with our solution, we examine only 83,357,673 prefixes in total—a reduction of 1012x. Note that this is a lower bound on the reduction since any brute force solution would have to examine prefixes of longer than length 5 to certify optimality. It takes us about 2μs to evaluate a single prefix. A naive solution would take 168,764s—about 2 days—while CORELS takes only 2 minutes. While the naive solution will eventually complete for this dataset, it is clear that brute force wouldn't scale to larger problems.

However, if we look at how processor speeds have changed over the last 25 years, we can see that computers are about 1,000,000 faster now than they were in 1993[Sup]. Even with our algorithmic and data structural improvements, CORELS would have run in over 120,000,000s in 1993—an unreasonable amount of time. Thus, our advances are only meaningful because we can run them on a modern system. Combining our algorithmic improvements with the increase in modern processor speeds, our algorithm runs more than 1 billion times faster than a naive implementation would have in 1993.

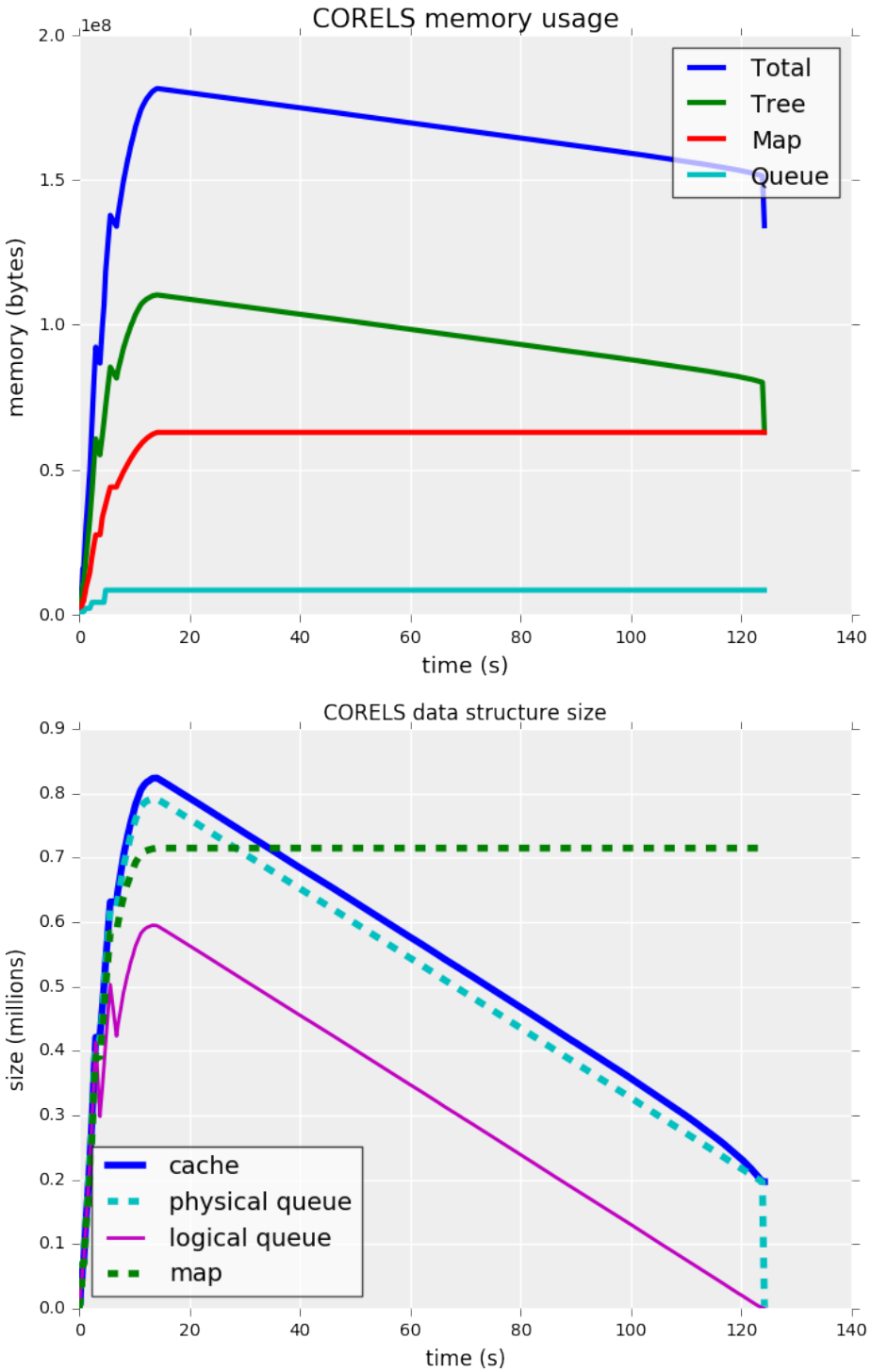


Figure 5.3: Memory usage of full CORELS system on the COMPAS dataset. Our prefix tree accounts for the bulk of the memory usage. The size (in number of items) of each of our main data structures. Corresponds to the amount of memory used.

5.2.1 Full CORELS system

The algorithm with all of our improvements is called the CORELS system. Running the full CORELS system on the Weapon dataset yields the optimal solution and certificate within 142s. COMPAS is slightly faster, allowing us to discover and certify optimality within 124s. Fig 5.3 shows the growth of our data structures and memory usage throughout the execution of our algorithm on the COMPAS dataset. The maximum memory usage is 170MB, with the majority of that coming from our prefix trie. With about 1 million items active at the peak, this comes out to about 170 bytes per item. This includes copies of that item that are kept across the prefix trie, symmetry-aware map, and queue. For a modern machine, this is not very much memory, demonstrating further that our algorithm can be run without undue memory pressure.

We also run CORELS on the Weapon dataset, which has fewer rules but many more individuals. This will cause optimizations that limit the depth of our search—the equivalent points bound, the lookahead bound—to be less important than ones that allow us to prune more aggressively—the priority queue and symmetry-aware map. The following sections demonstrate that while individual optimizations may play a larger role in certain datasets, the entirety of the system allows for speedy computation and certification of the optimal solution.

5.2.2 Priority Queue

One of our first optimizations was the use of a priority queue to utilize different exploration techniques. On the COMPAS dataset, using BFS instead of a priority queue does not seem to harm our performance at all, Removing the priority queue from the Weapon dataset, however, slows down our performance by a factor of 2. The queue requires very little memory and can give us a significant speed-up on certain types of problems.

5.2.3 Support Bounds

The support bounds are intrinsic to the rules and are the first bounds we check in our execution, because they are the simplest to compute. Despite this ease

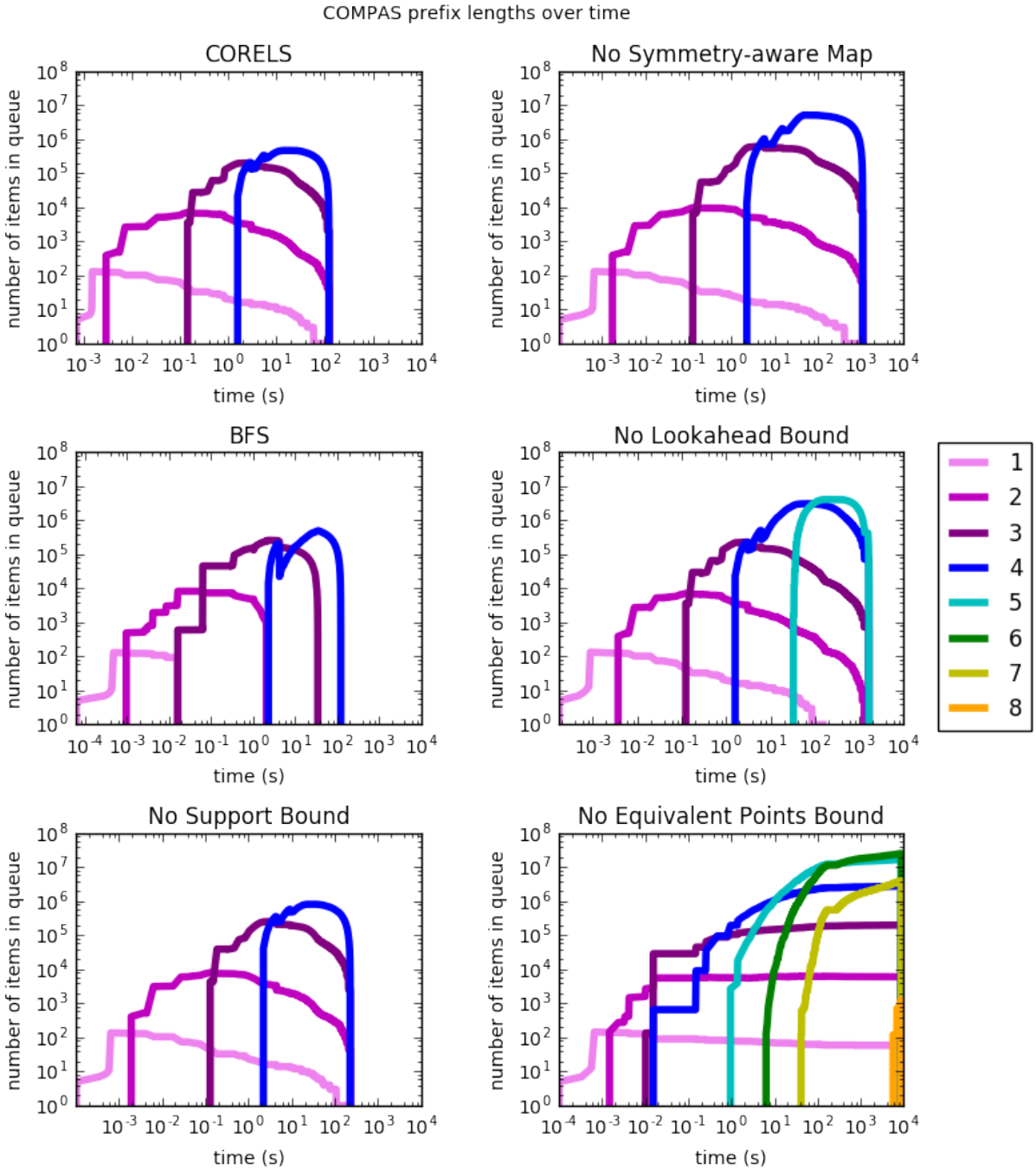


Figure 5.4: Tracks the number of prefixes of a given length active in the queue for our system when running on the COMPAS dataset. Each color represents a different length prefix. Each graph represents an experiment run without one of our bounds or data structures. This allows us to isolate the critical improvement(s) for a given class of problem. The equivalent points bound is especially important for datasets with a large number of rules and relatively few data points. Without that bound we our runtime increases dramatically and we examine much longer prefixes.

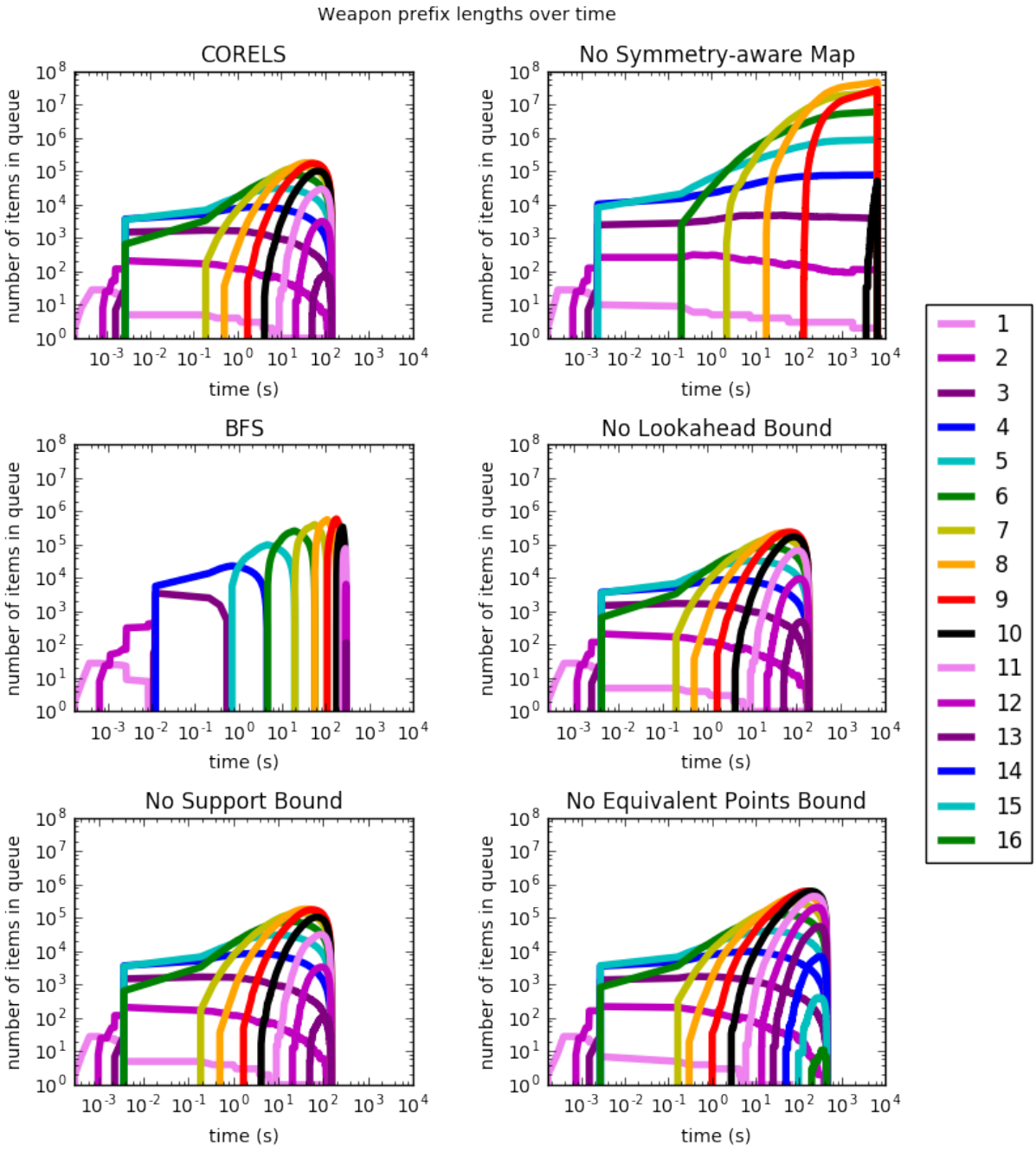


Figure 5.5: Tracks the number of prefixes of a given length active in the queue for our system when running on the Weapon dataset. Each graph represents an experiment run without one of our bounds or data structures. This allows us to isolate the critical improvement(s) for a given class of problem. For datasets with few rules but many data points, the symmetry-aware map and permutation bound play a crucial role.

Removed component	t_{total} (s)	t_{opt} (s)	i_{total} ($\times 10^6$)	$Q_{\max}$ ($\times 10^6$)	$K_{\max}$	t/t_{CORELS}
none (CORELS)	142	0.002	1.15	0.67	13	1
priority queue (BFS)	297	0.012	2.40	0.68	13	2.09
support bounds	153	0.003	1.21	0.69	13	1.08
symmetry-aware map	> 6400	>0.002	>114	≥ 108	≥ 10	>45
lookahead bound	186	0.004	1.56	0.9	13	1.31
equivalent pts bound	443	0.002	4.85	2.7	16	3.32

Table 5.1: Per-component performance improvement. The columns report total execution time, time to optimum, number of queue insertions, maximum queue size, and maximum evaluated prefix length. The first row shows CORELS; subsequent rows show variants that each remove a specific implementation optimization or bound. (We are not measuring the cumulative effects of removing a sequence of components.) All rows represent complete executions, except for the symmetry-aware map row, in which each execution was terminated due to memory constraints

of computation, these bounds prevent the pursuit of useless rules. Without these bounds we complete the certification in 229s (1.8x) for COMPAS and 153s (1.08x) for Weapon. So, these bounds are not crucial for the completion of our algorithm, but they do provide some speed-up.

5.2.4 Symmetry-aware map

The symmetry-aware map is a novel way of approaching branch-and-bound, and it plays a large role in our elimination of search space. Using the symmetry-aware map means that we are able to pursue only one prefix out of all of its permutations. As our prefixes grow to length 4, for example, that means we can eliminate at least 23 additional prefixes. For a problem like COMPAS, where we typically examine prefixes up to length 5 (we examine prefixes of length 5 even though Fig 5.4 only shows prefixes up to length 4 being placed in the queue), this can be a very important bound. However, we can see the true importance of the symmetry-aware map on the Weapon dataset in Table 5.1 where we are unable to even finish the problem without the symmetry-aware map. This problem requires us to look at rule lists of length 10 or more, so the permutation bound helps eliminate millions of prefixes.

Removed component	t_{total} (s)	t_{opt} (s)	i_{total} ($\times 10^6$)	$Q_{\max}$ ($\times 10^6$)	$K_{\max}$	t/t_{CORELS}
none (CORELS)	124	5.6	0.84	0.59	4	1.0
priority queue (BFS)	121	4.22	0.99	0.50	4	0.98
support bounds	229	9.1	1.3	0.98	4	1.8
symmetry-aware map	1118	15	6.5	5.6	4	9.0
lookahead bound	1646	6.2	7.6	6.9	5	13
equivalent pts bound	>8780	>21	>50	>50	$\geq$8	> 71

Table 5.2: Per-component performance improvement. The columns report total execution time, time to optimum, number of queue insertions, maximum queue size, and maximum evaluated prefix length. The first row shows CORELS; subsequent rows show variants that each remove a specific implementation optimization or bound. (We are not measuring the cumulative effects of removing a sequence of components.) All rows represent complete executions, except for the final row, in which each execution was terminated due to memory constraints

5.2.5 Lookahead Bound

Our lookahead bound is useful for preventing us from examining longer prefixes than we need to. From running our full CORELS system on COMPAS, we know that our optimal rule list is of length 4. With our lookahead bound, we never have to place prefixes of length 5 into our queue. However, removing that bound means that we do place prefixes of length 5 into our queue and therefore have to examine prefixes of length 6. This drastically slows our computation to 1646s, a 13x slowdown over our full CORELS system. However, this bound is much less important on the Weapon dataset where we are already examining long rule lists.

5.2.6 Equivalent points bound

The equivalent points bound is our optimization that provides the largest benefit when we have a large number of rules. Since all of our other bounds eliminate prefixes contingent on the lower bound, the equivalent points bound is important because it tightens the lower bound. Removing this bound typically makes it impractical to complete real world problems. For COMPAS, Table 5.2 demonstrates that even after halting execution after multiple hours (8780s), there is still a large portion of the search space to be explored. This bound plays less of a role for the Weapon dataset, but still remains an important op-

timization by giving us a 4x speedup.

5.3 Symmetry-aware Map Optimization

As one of our two main data structures, the memory usage of our symmetry-aware map is something that was very important to us. In early versions of this algorithm, the symmetry-aware map was the most memory-intensive data structure and we would often run out of memory before certifying the optimal rule list. Section 5.2.4 shows us that running without a symmetry-aware map leads to a much longer runtime, so we needed to find a way to use the symmetry-aware map while reducing memory usage. In the course of a normal execution, our permutation map would grow to be hundreds of thousands or millions of entries large. Thus, carrying a lot of memory overhead with each node led to excess memory usage and ran us out of memory. This section explores some of the techniques we used to address this memory bloat.

Our first instantiation of the symmetry-aware map was an STL map with STL sets as keys and a pair of an STL vector and a double as the values. One problem is that the STL map is implemented as a red-black tree, meaning every node had the overhead of multiple pointers pointing to its children. This can be solved using a STL unordered map, which is implemented as a hashtable. That has some overhead, since it will allocate more buckets than are filled, but it has much less overhead than the two pointers per node of overhead of the STL map.

Our original scheme also used the 8 byte size_t to represent rule ids. By assuming that we'll never have more than 65,000 rules—which would be intractable for our algorithm anyways—we were able to use 2 byte unsigned shorts for our rule ids. This means that our key type, value type, and our node type were able to use only 2 bytes per rule id instead of 8 bytes. Since our prefixes often get to be length 5 or greater, saving 6 bytes per rule in every representation of the prefix led to large space savings.

After these initial optimizations, we worked on optimizing our key type. The only criteria for our key type is that two different prefixes that are permutations of each other should map to the same key. We began by using a STL set as the key because it allowed us to easily determine if two prefixes were permutations of each other by simply converting the prefix into a set. However, this carries a

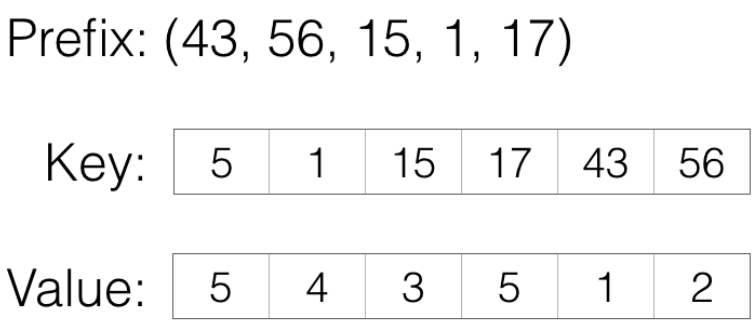


Figure 5.6: An example prefix (43, 56, 15, 1, 17) and the associated representations in the key and the value types. The key is an array of 6 unsigned shorts where the first entry demarcates the length of the prefix. Each the rest of the array are the rule ids of the prefix in canonical order. The value is an array of 6 unsigned chars where the first entry again represents the length of the prefix. The remaining entries in the array map the rule ids in the canonical order to their actual order in the prefix. For instance, the first entry in the key is 1 and the first entry in the value is 4, so rule 1 is the 4th rule in the prefix.

lot of overhead because a set needs to support insertions, lookups, and deletions in $O(\log n)$ time. This overhead varies between compilers, but my machine allocated 32 bytes for each 2 byte item inserted into the set, plus 24 bytes for the set itself. For a prefix of length 5, the corresponding key therefore takes up 160 bytes.

Sets support far more operations than we need, though, so we transitioned to a sorted STL vector. This still allows us to compare prefixes as permutations, and it reduced overhead because a STL vector is essentially just a dynamically resizing array with a little bit of extra bookkeeping information. This translates to a prefix of length 5 taking up only 40 bytes. However, STL vectors still support a broader range of operations than we needed because they need to know when to allocate more space. All we needed was some way to compare the canonical orders and determine if they were the same. We created a custom key class by allocating a chunk of memory that held the length of the prefix and the sorted order of the ids. This kept the same idea that the STL vector had in order to compare two prefixes, but it removed the overhead. In the end, we use only 12 bytes for the key for a prefix of length 5.

We went through a similar process with our values for the symmetry-aware map. Our only requirement for the values were that they keep track of which

Map version	Key version	Value version	Total Memory (MB)	t_{total} (s)
Map	Set (size_t)	Vector (size_t)	190.7	139
Unordered Map	Set (size_t)	Vector (size_t)	185.9	135
Unordered Map	Set (short)	Vector (short)	148.6	133
Unordered Map	Vector (short)	Vector (short)	68.7	132
Unordered Map	Custom Key	Custom Value	62.9	124

Table 5.3: Symmetry aware map improvements when running on the COMPAS dataset. The columns report the type of map, type of key, type of value, total memory used by the symmetry-aware map, and time of execution. Each row represents a different version of the symmetry aware map that we tested. We see that each optimization reduced the total memory consumption while maintaining or slightly reducing the overall runtime. Short refers to unsigned short and Vector refers to STL Vector.

prefix was the current best for the given permutation. We began with a STL vector to keep track of the actual order of the rules in the prefix, but we again wanted to remove the overhead incurred by the fact that STL containers need to support a wider array of operations than we needed. We reduced our memory usage through a similar technique of what we did with the key type: we moved from a STL vector to a chunk of memory. However, we realized that we could do even better because we already had the rule ids—all we need in the value was the ordering of those rules. Since we don't need to represent the rule ids, we can use unsigned chars instead of unsigned shorts to record the actual ordering of the rule ids stored in the key type. Fig 5.6 demonstrates how a prefix can be converted into the custom key and value classes that we designed.

In total, Table 5.3 shows us that these improvements give us a 3x memory reduction on this problem. These reductions take the symmetry-aware map from being the largest data structure to being smaller than the prefix trie. Reducing the memory footprint of CORELS was helpful for running on COMPAS, but on larger problems this memory improvement is even more pronounced.

In Section 4.4 we described two different key types for the symmetry-aware map: PrefixKeys and CapturedKeys. All of the above optimizations pertained only to the PrefixKey type, so dealing with the CapturedKey type required a different approach. To keep track of what data points a rule list captured, we used the bit vector manipulation library from Yang et al.[38] which was built on top of the GMP library. These bit vectors are of the GMP defined type mpz_t,

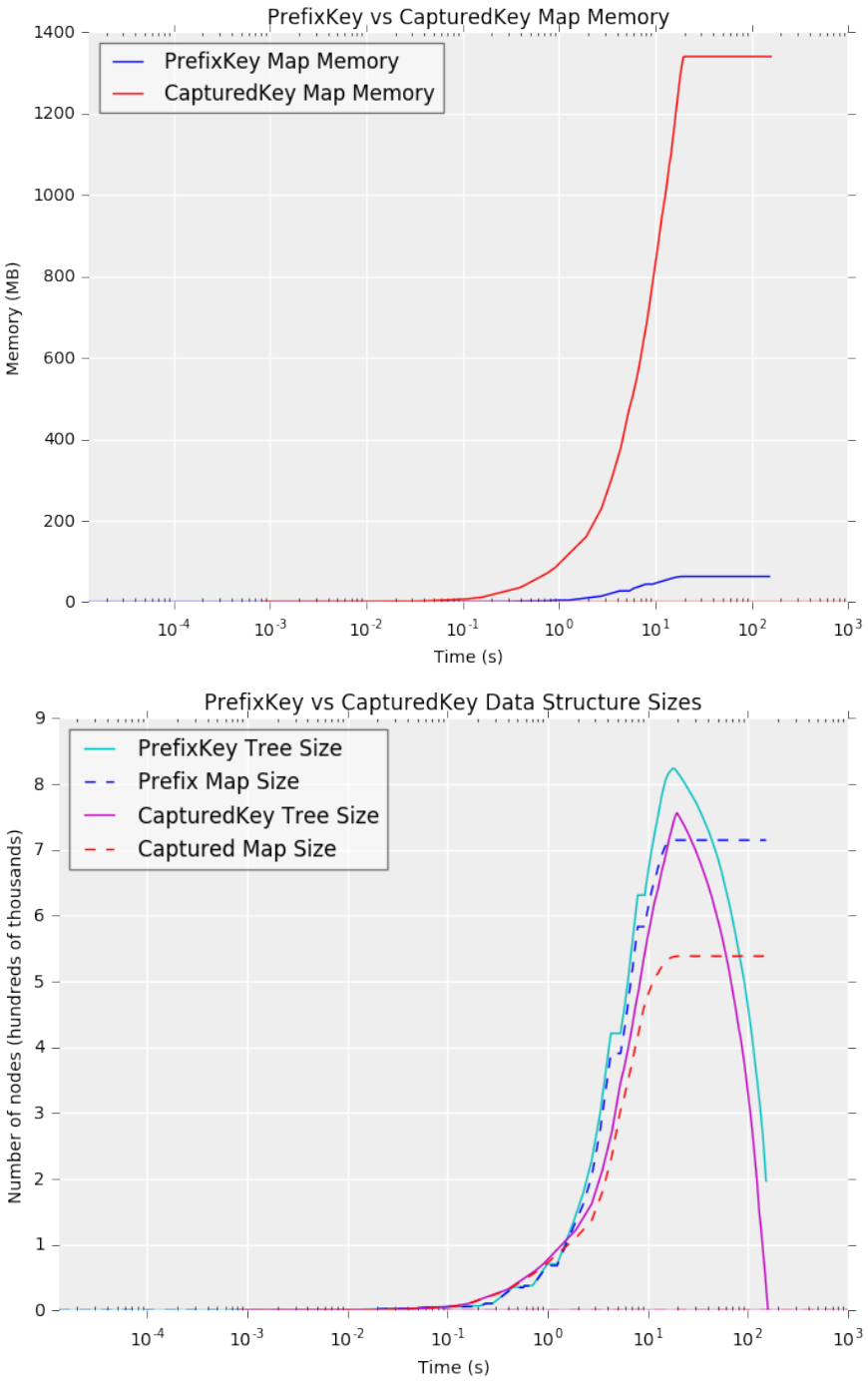


Figure 5.7: This graph shows the memory usage of the map when using CapturedKeys and PrefixKeys on the COMPAS dataset. We see that CapturedKeys cost much more memory than PrefixKeys despite the slight decrease in the number of nodes inserted into the trie.

which stands for multiple precision integer. This type allows us represent and perform operations with very large bit vectors in an efficient manner. Since unordered_map is implemented as a hash table, it requires a custom hash for non built-in types. We initially wrote a function to convert between mpz_t and a STL vector containing bools so that we could use STL's built-in hash function. This conversion turned out to be very slow, especially when we were running on data sets with many samples. These mpz_t types were fairly large, so copying the information from one place to another was inefficient and impractical. Instead, we adapted the sdbm hash function to our mpz_t type.[Yigit]. Once we used our own hash function and didn't have to copy between types, CapturedKeys became much faster. Fig 5.7 shows that despite these optimizations, CapturedKeys were still less space efficient that PrefixKeys. CapturedKeys have to store all of the data points instead of just a few rules, so we used PrefixKeys for our later analyses.

5.4 Templates vs Inheritance

Our system has many modular parts—various priority metrics, symmetry-aware map types, and different types of information stored in trie nodes. Since we were using C++, we took advantage of its templating system to achieve this modularity. We initially believed that it would be the easiest way to switch out different components of the system. Due to code duplication, however, templates can lead to a much larger executable. Indeed, with a pure templating system, our executable was 253,732 bytes and execution time took about 126s on the COMPAS data set.

An alternative way to maintain modularity was to take advantage of C++'s class system and use inheritance and polymorphism. Instead of having a template argument for each data structure, we have a base data structure type and then implement each of our extensions as subclasses. Therefore, we can write all of our functions to take the base class as arguments and then pass in the specialized subclasses based on command line arguments. This requires the use of virtual functions, which are potentially a bit slower than regular functions, because they require a vtable lookup. A vtable, or virtual method table, is how C++ deals with the fact that the compiler might not know what class a vari-

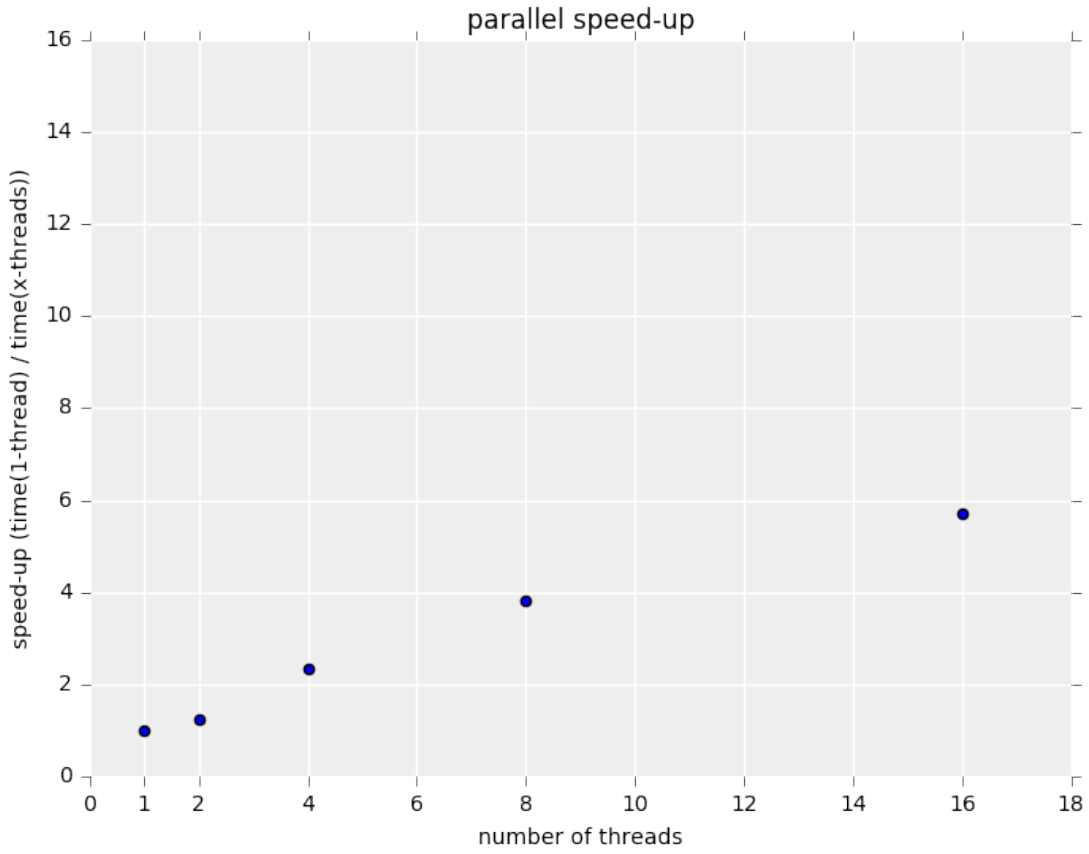


Figure 5.8: This graph shows the speedup of our parallel implementation as we add more threads. We see a sub-linear speedup, likely due to cache misses. However, we are able to get up to a 6x speedup with 16 cores. This puts some large problems that were previously unfeasible in the realm of completion.

able is at compile time. At runtimem the vtable is used to run the appropriate function, but this requires a bit of overhead. With a pure inheritance framework, our executable was 171,288 bytes. However, even with the inheritance framework, the runtime of our algorithm (124s) was not significantly different from the template runtime (126s). Thus, since inheritance provided a much cleaner code base to work with, we decided to switch to an inheritance based framework.

5.5 Parallelization

Almost every modern machines supports parallelism through the use of multiple cores or simultaneous multi-threading. This is a crucial fact that modern discrete optimization programs can use to their advantage. We show that the structure of our branch and bound algorithm nicely supports a parallel implementation. Furthermore, we show that we get significant, though not linearly-scaling, speed-up with our parallel implementation. This set of experiments was executed on Harvard's Odyssey cluster to take advantage of multi-core machines.

Analysis of our log files showed that the majority of the time of our program is spent in the incremental section of our execution, shown in Algorithm 3. So, we began by trying to parallelize this inner loop of our incremental evaluation. This inner loop involves trying to extend a prefix by calculating the bounds for all possible rules we could add to this prefix. In order to add these child rules, though, we need to calculate the bounds based on characteristics of the parent prefix. Without locking the parent, we run into a race condition where one thread is trying to insert a child rule into the parent's representation of the children and another thread is trying to read the parent's representation of the children. This leads to a segfault in the STL code and could be fixed by locking the appropriate fields in the parent. Locking the parent has too much contention, however, because all of our threads needed to own the parent lock at the same time—essentially rendering the loop sequential.

We realized, however, that the tree structure of our search space, encapsulated by our prefix trie, lends itself nicely to parallelization. Instead of parallelizing the evaluation of a single prefix, we can parallelize our search over the tree itself. We do this by creating the tree in the master thread and then spawning worker threads to work in different parts of the tree. Thus, there is no contention on parent nodes since only one thread can access a node at a time. The shared state only consists of the minimum objective and the symmetry-aware map, and these are kept in the master thread. We lock the symmetry-aware map on insertions and lookups because insertions can trigger a rehash of the underlying hashtable, which is problematic if multiple threads are accessing the map. Deletion and garbage collection are handled by the master thread as well.

Fig 5.8 shows that parallelizing our implementation did lead to a significant speed-up, but we see diminishing returns as we increase the number of threads. One theory we had was that since we had to add locking to the symmetry-aware map, there might be contention that is slowing down the multi-threaded implementation. However, when we preallocate a large symmetry-aware map (avoiding the need to rehash) and don't lock, we see the same type of slowdown, implying that contention is not the issue. An alternative explanation is that increasing the number of threads leads to cache thrashing because the appropriate parts of the tree can no longer be kept in memory.

6
Conclusion

Through the use of tight theoretical bounds and clever data structure optimizations, we are able to find and certify the optimal rule list on real-world problems. We have also shown that other rule list methods produce rule lists which are close to optimal. On two problems plagued by racially biased models in the real world, we show that interpretable methods achieve comparable accuracy to black-box models, refuting the claim that black-box models lead to better performance. The rule lists generated by our algorithm had no race-related factors, supporting their use over racially biased, uninterpretable models.

We also showed that careful analysis of where memory is allocated is especially important for combinatorial optimization problems. Even with a good branch and bound algorithm and a modern machine, large datasets will test the memory constraints of that machine. We have provided an novel data structure, the symmetry-aware map, for future combinatorial optimization problems. Potential future optimizations for the map include distance sensitive hashing or bit-packing to reduce runtime and memory usage further.

This work has also provided a parallel implementation of CORELS. The techniques used to parallelize this algorithm are not rule list specific and could be applied to any branch and bound algorithm. Even with a sub-linear speedup, the parallel implementation of CORELS provides large runtime savings and

could be useful when applying CORELS to real world problems. Further work remains to be done on the analysis of the slowdown as well as potentially parallelizing the implementation across machines.

Discrete optimization has become less popular as other techniques such as convex optimization or stochastic gradient descent dominate the machine learning landscape. However, we showed that due to dramatic increases in processor speed and computer memory, discrete optimization techniques can be applied to real problems and complete them in a reasonable amount of time. In particular, we hope that this work will inspire further work on discrete optimization techniques for other methods such as decision trees or SVMs.

Some of the computations in this paper were run on the Odyssey cluster supported by the FAS Division of Science, Research Computing Group at Harvard University.

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A

Proof of Bounds

The following bounds and proofs are adapted from the joint work upon which this thesis is based[2].

A.1 Rule lists for binary classification

We restrict our setting to binary classification.

Let $\{(x_n, y_n)\}_{n=1}^N$ denote training data, where $x_n \in \{0,1\}^J$ are binary features and $y_n \in \{0,1\}$ are labels. Let $\mathbf{x} = \{x_n\}_{n=1}^N$ and $\mathbf{y} = \{y_n\}_{n=1}^N$, and let $x_{n,j}$ denote the j-th feature of x_n.

A rule list $d = (r_1, r_2, \ldots, r_K, r_0)$ of length $K \geq 0$ is a $(K+1)$-tuple consisting of K distinct association rules, $r_k = p_k \to q_k$, for $k = 1, \ldots, K$, followed by a default rule r_0.

An association rule $r = p \to q$ is an implication corresponding to the conditional statement, "if p, then q." In our setting, an antecedent p is a Boolean assertion that evaluates to either true or false for each datum x_n, and a consequent q is a label prediction. For example, $(x_{n,1} = 0) \wedge (x_{n,3} = 1) \to (y_n = 1)$ is an association rule. The final default rule r_0 in a rule list can be thought of as an association rule $p_0 \to q_0$ whose antecedent p_0 simply asserts true.

Let $d = (r_1, r_2, \ldots, r_K, r_0)$ be a rule list where $r_k = p_k \to q_k$ for each $k = 0, \ldots, K$.

We introduce a useful alternate rule list representation: $d = (d_p, \delta_p, q_0, K)$, where we define $d_p = (p_1, \ldots, p_K)$ to be d's prefix, $\delta_p = (q_1, \ldots, q_K) \in \{0,1\}^K$ gives the label predictions associated with d_p, and $q_0 \in \{0,1\}$ is the default label prediction.

Let $d_p = (p_1, \ldots, p_k, \ldots, p_K)$ be an antecedent list, then for any $k \leq K$, we define $d_p^k = (p_1, \ldots, p_k)$ to be the k-prefix of d_p. For any such k-prefix d_p^k, we say that d_p starts with d_p^k. For any given space of rule lists, we define $\sigma(d_p)$ to be the set of all rule lists whose prefixes start with d_p:

$$\sigma(d_p) = \{(d'_p, \delta'_p, q'_0, K') : d'_p \text{ starts with } d_p\}. \tag{A.1}$$

If $d_p = (p_1, \ldots, p_K)$ and $d'_p = (p_1, \ldots, p_K, p_{K+1})$ are two prefixes such that d'_p starts with d_p and extends it by a single antecedent, we say that d_p is the parent of d'_p and that d'_p is a child of d_p.

A rule list d classifies datum x_n by providing the label prediction q_k of the first rule r_k whose antecedent p_k is true for x_n. We say that an antecedent p_k of antecedent list d_p captures x_n in the context of d_p if p_k is the first antecedent in d_p that evaluates to true for x_n.

A prefix captures those data captured by its antecedents; for a rule list $d = (d_p, \delta_p, q_0, K)$, data not captured by the prefix d_p are classified according to the default label prediction q_0.

Let β be a set of antecedents. We define $\text{cap}(x_n, \beta) = 1$ if an antecedent in β captures datum x_n, and 0 otherwise. For example, let d_p and d'_p be prefixes such that d'_p starts with d_p, then d'_p captures all the data that d_p captures:

$$\{x_n : \text{cap}(x_n, d_p)\} \subseteq \{x_n : \text{cap}(x_n, d'_p)\}$$

Now let d_p be an ordered list of antecedents, and let β be a subset of antecedents in d_p. Let us define $\text{cap}(x_n, \beta \,|\, d_p) = 1$ if β captures datum x_n in the context of d_p, *i.e.*, if the first antecedent in d_p that evaluates to true for x_n is an antecedent in β, and 0 otherwise. Thus, $\text{cap}(x_n, \beta \,|\, d_p) = 1$ only if $\text{cap}(x_n, \beta) = 1$; $\text{cap}(x_n, \beta \,|\, d_p) = 0$ either if $\text{cap}(x_n, \beta) = 0$, or if $\text{cap}(x_n, \beta) = 1$ but there is an antecedent α in d_p, preceding all antecedents in β, such that $\text{cap}(x_n, \alpha) = 1$. For

example, if $d_p = (p_1, \ldots, p_k, \ldots, p_K)$ is a prefix, then

$$\operatorname{cap}(x_n, p_k \,|\, d_p) = \left(\bigwedge_{k'=1}^{k-1} \neg \operatorname{cap}(x_n, p_{k'}) \right) \wedge \operatorname{cap}(x_n, p_k) \tag{A.2}$$

indicates whether antecedent p_k captures datum x_n in the context of d_p. Now, define $\operatorname{supp}(\beta, \mathbf{x})$ to be the normalized support of β,

$$\operatorname{supp}(\beta, \mathbf{x}) = \frac{1}{N} \sum_{n=1}^{N} \operatorname{cap}(x_n, \beta), \tag{A.3}$$

and similarly define $\operatorname{supp}(\beta, \mathbf{x} \,|\, d_p)$ to be the normalized support of β in the context of d_p,

$$\operatorname{supp}(\beta, \mathbf{x} \,|\, d_p) = \frac{1}{N} \sum_{n=1}^{N} \operatorname{cap}(x_n, \beta \,|\, d_p), \tag{A.4}$$

Next, we address how empirical data constrains rule lists. Given training data $(\mathbf{x}, \mathbf{y})$, an antecedent list $d_p = (p_1, \ldots, p_K)$ implies a rule list $d = (d_p, \delta_p, q_0, K)$ with prefix d_p, where the label predictions $\delta_p = (q_1, \ldots, q_K)$ and q_0 are empirically set to minimize the number of misclassification errors made by the rule list on the training data. Thus for $1 \leq k \leq K$, label prediction q_k corresponds to the majority label of data captured by antecedent p_k in the context of d_p, and the default q_0 corresponds to the majority label of data not captured by d_p. In the remainder of our presentation, whenever we refer to a rule list with a particular prefix, we implicitly assume these empirically determined label predictions.

Finally, we note that our approach leverages pre-mined rules, following the methodology taken by[23] and[38]. One of the results we later prove implies a constraint that can be used as a filter during rule mining – antecedents must have at least some minimum support (Theorem 5).

A.2 Objective Function

Define a simple objective function for a rule list $d = (d_p, \delta_p, q_0, K)$:

$$R(d, \mathbf{x}, \mathbf{y}) = \ell(d, \mathbf{x}, \mathbf{y}) + \lambda K \tag{A.5}$$

This objective function is a regularized empirical risk; it consists of a loss $\ell(d, \mathbf{x}, \mathbf{y})$, measuring misclassification error, and a regularization term that penalizes longer rule lists. $\ell(d, \mathbf{x}, \mathbf{y})$ is the fraction of training data whose labels are incorrectly predicted by d. In our setting, the regularization parameter $\lambda \geq 0$ is a small constant; *e.g.*, $\lambda = 0.01$ can be thought of as adding a penalty equivalent to misclassifying 1% of data when increasing a rule list's length by one.

A.3 Optimization framework

Our objective has structure amenable to global optimization via a branch-and-bound framework. In particular, we make a series of important observations that each translates into a useful bound, and that together interact to eliminate large parts of the search space. We will discuss these in depth throughout the following sections:

- Lower bounds on a prefix also hold for every extension of that prefix. (§A.4, Theorem 1)
- We can sometimes prune all rule lists that are longer than a given prefix, even without knowing anything about what rules will be placed below that prefix. (§A.4, Lemma 1)
- We can calculate *a priori* an upper bound on the maximum length of an optimal rule list. (§A.5, Theorem 3)
- Each rule in an optimal rule list must have support that is sufficiently large. This allows us to construct rule lists from frequent itemsets, while preserving the guarantee that we can find a globally optimal rule list from pre-mined rules. (§A.7, Theorem 5)
- Each rule in an optimal rule list must predict accurately. In particular, the number of observations predicted correctly by each rule in an optimal rule list must be above a threshold. (§A.7, Theorem 6)

- We need only consider the optimal permutation of antecedents in a prefix; we can omit all other permutations. (§A.8, Theorem 7 and Corollary 2)
- If multiple observations have identical features and opposite labels, we know that any model will make mistakes. In particular, the number of mistakes on these observations will be at least the number of observations with the minority label. (§A.8.3, Theorem 9)

A.4 Hierarchical objective lower bound

We can decompose the misclassification error into two contributions corresponding to the prefix and the default rule:

$$\ell(d, \mathbf{x}, \mathbf{y}) \equiv \ell_p(d_p, \delta_p, \mathbf{x}, \mathbf{y}) + \ell_0(d_p, q_0, \mathbf{x}, \mathbf{y}), \tag{A.6}$$

where $d_p = (p_1, \ldots, p_K)$ and $\delta_p = (q_1, \ldots, q_K)$;

$$\ell_p(d_p, \delta_p, \mathbf{x}, \mathbf{y}) = \frac{1}{N} \sum_{n=1}^{N} \sum_{k=1}^{K} \operatorname{cap}(x_n, p_k \,|\, d_p) \wedge \mathbb{1}[q_k \neq y_n] \tag{A.7}$$

is the fraction of data captured and misclassified by the prefix, and

$$\ell_0(d_p, q_0, \mathbf{x}, \mathbf{y}) = \frac{1}{N} \sum_{n=1}^{N} \neg \operatorname{cap}(x_n, d_p) \wedge \mathbb{1}[q_0 \neq y_n] \tag{A.8}$$

is the fraction of data not captured by the prefix and misclassified by the default rule. Eliminating the latter error term gives a lower bound $b(d_p, \mathbf{x}, \mathbf{y})$ on the objective,

$$b(d_p, \mathbf{x}, \mathbf{y}) \equiv \ell_p(d_p, \delta_p, \mathbf{x}, \mathbf{y}) + \lambda K \leq R(d, \mathbf{x}, \mathbf{y}), \tag{A.9}$$

where we have suppressed the lower bound's dependence on label predictions δ_p because they are fully determined, given $(d_p, \mathbf{x}, \mathbf{y})$. Furthermore, as we state next in Theorem 1, $b(d_p, \mathbf{x}, \mathbf{y})$ gives a lower bound on the objective of *any* rule list whose prefix starts with d_p.

Theorem 1 (Hierarchical objective lower bound)**.** *Define*

$$b(d_p, \mathbf{x}, \mathbf{y}) = \ell_p(d_p, \delta_p, \mathbf{x}, \mathbf{y}) + \lambda K$$

Also, define $\sigma(d_p)$ to be the set of all rule lists whose prefix starts with d_p, as in (A.1)*. Let $d = (d_p, \delta_p, q_0, K)$ be a rule list with prefix d_p, and let $d' = (d'_p, \delta'_p, q'_0, K') \in \sigma(d_p)$ be any rule list such that its prefix d'_p starts with d_p and $K' \geq K$, then $b(d_p, \mathbf{x}, \mathbf{y}) \leq R(d', \mathbf{x}, \mathbf{y})$.*

To generalize, consider a sequence of prefixes such that each prefix starts with all previous prefixes in the sequence. It follows that the corresponding sequence of objective lower bounds increases monotonically. This is precisely the structure required and exploited by branch-and-bound.

Specifically, the objective lower bound in Theorem 1 enables us to prune the state space hierarchically. While executing branch-and-bound, we keep track of the current best (smallest) objective R^c, thus it is a dynamic, monotonically decreasing quantity. If we encounter a prefix d_p with lower bound $b(d_p, \mathbf{x}, \mathbf{y}) \geq R^c$, then by Theorem 1, we needn't consider *any* rule list $d' \in \sigma(d_p)$ whose prefix d'_p starts with d_p. For the objective of such a rule list, the current best objective provides a lower bound, *i.e.*,

$$R(d', \mathbf{x}, \mathbf{y}) \geq b(d'_p, \mathbf{x}, \mathbf{y}) \geq b(d_p, \mathbf{x}, \mathbf{y}) \geq R^c$$

, and thus d' cannot be optimal.

Next, we state an immediate consequence of Theorem 1.

Lemma 1 (Objective lower bound with one-step lookahead)**.** *Let d_p be a K-prefix and let R^c be the current best objective. If $b(d_p, \mathbf{x}, \mathbf{y}) + \lambda \geq R^c$, then for any K'-rule list $d' \in \sigma(d_p)$ whose prefix d'_p starts with d_p and $K' > K$, it follows that $R(d', \mathbf{x}, \mathbf{y}) \geq R^c$.*

Therefore, even if we encounter a prefix d_p with lower bound $b(d_p, \mathbf{x}, \mathbf{y}) \leq R^c$, if $b(d_p, \mathbf{x}, \mathbf{y}) + \lambda \geq R^c$, then we can prune all prefixes d'_p that start with and are longer than d_p.

A.5 Upper bounds on prefix length

Proposition 1 (Trivial upper bound on prefix length)**.** *Consider a state space of all rule lists formed from a set of M antecedents, and let $L(d)$ be the length of rule list d. M provides an upper bound on the length of any optimal rule list $d^* \in \operatorname{argmin}_d R(d, \mathbf{x}, \mathbf{y})$, i.e., $L(d) \leq M$.*

At any point during branch-and-bound execution, the current best objective R^c implies an upper bound on the maximum prefix length we might still have to consider.

Theorem 2 (Upper bound on prefix length)**.** *Consider a state space of all rule lists formed from a set of M antecedents. Let $L(d)$ be the length of rule list d and let R^c be the current best objective. For all optimal rule lists $d^* \in \operatorname{argmin}_d R(d, \mathbf{x}, \mathbf{y})$*

$$L(d^*) \leq \min\left(\lfloor R^c/\lambda \rfloor, M\right), \tag{A.10}$$

where λ is the regularization parameter.

Corollary 1 (Simple upper bound on prefix length)**.** *For all optimal rule lists $d^* \in \operatorname{argmin}_d R(d, \mathbf{x}, \mathbf{y})$,*

$$L(d^*) \leq \min\left(\lfloor 1/2\lambda \rfloor, M\right). \tag{A.11}$$

For any particular prefix d_p, we can obtain potentially tighter upper bounds on prefix length for all prefixes that start with d_p.

Theorem 3 (Prefix-specific upper bound on prefix length)**.** *Let*

$$d = (d_p, \delta_p, q_0, K)$$

be a rule list, let $d' = (d'_p, \delta'_p, q'_0, K') \in \sigma(d_p)$ be any rule list such that d'_p starts with d_p, and let R^c be the current best objective. If d'_p has lower bound $b(d'_p, \mathbf{x}, \mathbf{y}) < R^c$, then

$$K' < \min\left(K + \left\lfloor \frac{R^c - b(d_p, \mathbf{x}, \mathbf{y})}{\lambda} \right\rfloor, M\right). \tag{A.12}$$

We can view Theorem 3 as a generalization of our one-step lookahead bound (Lemma 1), as (A.12) is equivalently a bound on $K' - K$, an upper bound on the number of remaining 'steps' corresponding to an iterative sequence of single-rule extensions of a prefix d_p.

A.6 Upper bounds on prefix evaluations

In this section, we use Theorem 3's upper bound on prefix length to derive a corresponding upper bound on the number of prefix evaluations made by

Algorithm 1. We present Theorem 4, in which we use information about the state of Algorithm 2's execution to calculate, for any given execution state, upper bounds on the number of additional prefix evaluations that might be required for the execution to complete. This number of remaining evaluations is equal to the number of prefixes that are currently in or will be inserted into the queue. The relevant execution state depends on the current best objective R^c and information about prefixes we are planning to evaluate, *i.e.*, prefixes in the queue Q of Algorithm 2.

Theorem 4 (Upper bound on the number of remaining prefix evaluations)**.** *Consider a state space of all rule lists formed from a set of M antecedents, and consider Algorithm 2 at a particular instant during execution. Let R^c be the current best objective, let Q be the queue, and let $L(d_p)$ be the length of prefix d_p. Define $\Gamma(R^c, Q)$ to be the number of remaining prefix evaluations, then*

$$\Gamma(R^c, Q) \leq \sum_{d_p \in Q} \sum_{k=0}^{f(d_p)} \frac{(M - L(d_p))!}{(M - L(d_p) - k)!}, \tag{A.13}$$

$$\textit{where} \quad f(d_p) = \min\left(\left\lfloor \frac{R^c - b(d_p, \mathbf{x}, \mathbf{y})}{\lambda} \right\rfloor, M - L(d_p) \right). \tag{A.14}$$

Proof. The number of remaining prefix evaluations is equal to the number of prefixes that are currently in or will be inserted into queue Q. For any such prefix d_p, Theorem 3 gives an upper bound on the length of any prefix d'_p that starts with d_p:

$$L(d'_p) \leq \min\left(L(d_p) + \left\lfloor \frac{R^c - b(d_p, \mathbf{x}, \mathbf{y})}{\lambda} \right\rfloor, M \right) \equiv U(d_p). \tag{A.15}$$

This gives an upper bound on the number of remaining prefix evaluations:

$$\Gamma(R^c, Q) \leq \sum_{d_p \in Q} \sum_{k=0}^{U(d_p) - L(d_p)} P(M - L(d_p), k). \tag{A.16}$$

□

The proposition below is a naïve upper bound on the total number of prefix evaluations over the course of Algorithm 2's execution. It only depends on the number of rules and the regularization parameter λ; *i.e.*, unlike Theorem 4, it does not use algorithm execution state to bound the size of the search space.

Proposition 2 (Upper bound on the total number of prefix evaluations)**.** *Define $\Gamma_{\text{tot}}(S)$ to be the total number of prefixes evaluated by Algorithm 2, given the state space of all rule lists formed from a set S of M rules. For any set S of M rules,*

$$\Gamma_{\text{tot}}(S) \leq \sum_{k=0}^{K} \frac{M!}{(M-k)!}, \quad \textit{where} \quad K = \min(\lfloor 1/2\lambda \rfloor, M). \tag{A.17}$$

Proof. By Corollary 1, $K \equiv \min(\lfloor 1/2\lambda \rfloor, M)$ gives an upper bound on the length of any optimal rule list. We obtain (A.17) by viewing our problem as finding the optimal selection and permutation of k out of M rules, over all $k \leq K$. □

A.7 Lower bounds on antecedent support

In this section, we give two lower bounds on the normalized support of each antecedent in any optimal rule list; both are related to the regularization parameter λ.

Theorem 5 (Lower bound on antecedent support)**.** *Let*

$$d^* = (d_p, \delta_p, q_0, K) \in \operatorname*{argmin}_d R(d, \mathbf{x}, \mathbf{y})$$

be any optimal rule list, with objective R^*. For each antecedent p_k in prefix $d_p = (p_1, \ldots, p_K)$, the regularization parameter provides a lower bound, $\lambda < \text{supp}(p_k, \mathbf{x} \,|\, d_p)$, on the normalized support of p_k.

Thus, we can prune a prefix d_p if any of its antecedents do not capture more than a fraction λ of data, even if $b(d_p, \mathbf{x}, \mathbf{y}) < R^*$. The bound in Theorem 5 depends on the antecedents, but not the label predictions, and thus doesn't account for misclassification error. Theorem 6 gives a tighter bound by leveraging this information.

Theorem 6 (Lower bound on accurate antecedent support)**.** *Let*

$$d^* \in \operatorname*{argmin}_d R(d, \mathbf{x}, \mathbf{y})$$

be any optimal rule list, with objective R^*; let $d^* = (d_p, \delta_p, q_0, K)$, with prefix $d_p = (p_1, \ldots, p_K)$ and labels $\delta_p = (q_1, \ldots, q_K)$. For each rule $p_k \to q_k$ in d^*, define a_k to be the fraction of data that are captured by p_k and correctly classified:

$$a_k \equiv \frac{1}{N} \sum_{n=1}^{N} \text{cap}(x_n, p_k \,|\, d_p) \wedge \mathbb{1}[q_k = y_n]. \tag{A.18}$$

The regularization parameter provides a lower bound, $\lambda < a_k$.

Thus, we can prune a prefix if any of its rules do not capture and correctly classify at least a fraction λ of data. While the lower bound in Theorem 5 is a sub-condition of the lower bound in Theorem 6, we can still leverage both – since the sub-condition is easier to check, checking it first can accelerate pruning. In addition to applying Theorem 5 in the context of constructing rule lists, we can furthermore apply it in the context of rule mining. Specifically, it implies that we should only mine rules with normalized support greater than λ; we need not mine rules with a smaller fraction of observations. In contrast, we can only apply Theorem 6 in the context of constructing rule lists; it depends on the misclassification error associated with each rule in a rule list, thus it provides a lower bound on the number of observations that each such rule must correctly classify.

A.8 Equivalent support bound

Let D_p be a prefix, and let $\xi(D_p)$ be the set of all prefixes that capture exactly the same data as D_p. Now, let d be a rule list with prefix d_p in $\xi(D_p)$, such that d has the minimum objective over all rule lists with prefixes in $\xi(D_p)$. Finally, let d' be a rule list whose prefix d'_p starts with d_p, such that d' has the minimum objective over all rule lists whose prefixes start with d_p. Theorem 7 below implies that d' also has the minimum objective over all rule lists whose prefixes start with *any* prefix in $\xi(D_p)$.

Theorem 7 (Equivalent support bound)**.** *Define $\sigma(d_p)$ to be the set of all rule lists whose prefix starts with d_p, as in* (A.1)*. Let $d = (d_p, \delta_p, q_0, K)$*

be a rule list with prefix $d_p = (p_1, \ldots, p_K)$*, and let* $D = (D_p, \Delta_p, Q_0, \kappa)$ *be a rule list with prefix* $D_p = (P_1, \ldots, P_\kappa)$*, such that* d_p *and* D_p *capture the same data, i.e.,*

$$\{x_n : \text{cap}(x_n, d_p)\} = \{x_n : \text{cap}(x_n, D_p)\}. \tag{A.19}$$

If the objective lower bounds of d *and* D *obey* $b(d_p, \mathbf{x}, \mathbf{y}) \leq b(D_p, \mathbf{x}, \mathbf{y})$*, then the objective of the optimal rule list in* $\sigma(d_p)$ *gives a lower bound on the objective of the optimal rule list in* $\sigma(D_p)$*:*

$$\min_{d' \in \sigma(d_p)} R(d', \mathbf{x}, \mathbf{y}) \leq \min_{D' \in \sigma(D_p)} R(D', \mathbf{x}, \mathbf{y}). \tag{A.20}$$

Thus, if prefixes d_p and D_p capture the same data, and their objective lower bounds obey $b(d_p, \mathbf{x}, \mathbf{y}) \leq b(D_p, \mathbf{x}, \mathbf{y})$, Theorem 7 implies that we can prune D_p. Next, in Sections A.8.1 and A.8.2, we highlight and analyze the special case of prefixes that capture the same data because they contain the same antecedents.

A.8.1 Permutation bound

Let $P = \{p_k\}_{k=1}^K$ be a set of K antecedents, and let Π be the set of all K-prefixes corresponding to permutations of antecedents in P. Now, let d be a rule list with prefix d_p in Π, such that d has the minimum objective over all rule lists with prefixes in Π. Finally, let d' be a rule list whose prefix d'_p starts with d_p, such that d' has the minimum objective over all rule lists whose prefixes start with d_p. Corollary 2 below, which can be viewed as special case of Theorem 7, implies that d' also has the minimum objective over all rule lists whose prefixes start with *any* prefix in Π.

Corollary 2 (Permutation bound)**.** *Let* π *be any permutation of* $\{1, \ldots, K\}$*, and define* $\sigma(d_p)$ *to be the set of all rule lists whose prefix starts with* d_p*, as in* (A.1)*. Let* $d = (d_p, \delta_p, q_0, K)$ *and* $D = (D_p, \Delta_p, Q_0, K)$ *denote rule lists with prefixes* $d_p = (p_1, \ldots, p_K)$ *and* $D_p = (p_{\pi(1)}, \ldots, p_{\pi(K)})$*, respectively, i.e., the antecedents in* D_p *correspond to a permutation of the antecedents in* d_p*. If the objective lower bounds of* d *and* D *obey* $b(d_p, \mathbf{x}, \mathbf{y}) \leq b(D_p, \mathbf{x}, \mathbf{y})$*, then the objective of the optimal rule list in* $\sigma(d_p)$ *gives a lower bound on*

the objective of the optimal rule list in $\sigma(D_p)$:

$$\min_{d' \in \sigma(d_p)} R(d', \mathbf{x}, \mathbf{y}) \leq \min_{D' \in \sigma(D_p)} R(D', \mathbf{x}, \mathbf{y}). \tag{A.21}$$

Thus if prefixes d_p and D_p have the same antecedents, up to a permutation, and their objective lower bounds obey $b(d_p, \mathbf{x}, \mathbf{y}) \leq b(D_p, \mathbf{x}, \mathbf{y})$, Corollary 2 implies that we can prune D_p. We call this symmetry-aware pruning, and we illustrate the subsequent computational savings next in §A.8.2.

A.8.2 Upper bound on prefix evaluations with symmetry-aware pruning

Here, we present an upper bound on the total number of prefix evaluations that accounts for the effect of symmetry-aware pruning (§A.8.1). Since every subset of K antecedents generates an equivalence class of $K!$ prefixes equivalent up to permutation, symmetry-aware pruning dramatically reduces the search space. Algorithm 2 describes a breadth-first exploration of the state space of rule lists. Now suppose we integrate symmetry-aware pruning into our execution of branch-and-bound, so that after evaluating prefixes of length K, we only keep a single best prefix from each set of prefixes equivalent up to a permutation.

Theorem 8 (Upper bound on the total number of prefix evaluations with symmetry-aware pruning)**.** *Consider a state space of all rule lists formed from a set S of M antecedents, and consider the branch-and-bound algorithm with symmetry-aware pruning. Define $\Gamma_{\text{tot}}(S)$ to be the total number of prefixes evaluated. For any set S of M rules,*

$$\Gamma_{\text{tot}}(S) \leq 1 + \sum_{k=1}^{K} \frac{1}{(k-1)!} \cdot \frac{M!}{(M-k)!}, \tag{A.22}$$

where $K = \min(\lfloor 1/2\lambda \rfloor, M)$.

Proof. By Corollary 1, $K \equiv \min(\lfloor 1/2\lambda \rfloor, M)$ gives an upper bound on the length of any optimal rule list. The algorithm begins by evaluating the empty prefix, followed by M prefixes of length $k = 1$, then $P(M, 2)$ prefixes of length $k = 2$, where $P(M, 2)$ is the number of size-2 subsets

of $\{1, \ldots, M\}$. Before proceeding to length $k = 3$, we keep only $C(M, 2)$ prefixes of length $k = 2$, where $C(M, k)$ denotes the number of k-combinations of M. Now, the number of length $k = 3$ prefixes we evaluate is $C(M, 2)(M - 2)$. Propagating this forward gives

$$\Gamma_{\text{tot}}(S) \leq 1 + \sum_{k=1}^{K} C(M, k-1)(M - k + 1). \tag{A.23}$$

□

Pruning based on permutation symmetries thus yields significant computational savings. Let us compare, for example, to the naïve number of prefix evaluations given by the upper bound in Proposition 2. If $M = 100$ and $K = 5$, then the naïve number is about 9.1×10^9, while the reduced number due to symmetry-aware pruning is about 3.9×10^8, which is smaller by a factor of about 23. If $M = 1000$ and $K = 10$, the number of evaluations falls from about 9.6×10^{29} to about 2.7×10^{24}, which is smaller by a factor of about 360,000. While 10^{24} seems infeasibly enormous, it does not represent the number of rule lists we evaluate. As we show in (§5.2.4), our permutation bound in Corollary 2 and our other bounds together conspire to reduce the search space to a size manageable on a single computer. The choice of $M = 1000$ and $K = 10$ in our example above corresponds to the state space size our efforts target. $K = 10$ rules represents a (heuristic) upper limit on the size of an interpretable rule list, and $M = 1000$ represents the approximate number of rules with sufficiently high support (Theorem 5) we expect to obtain via rule mining.

A.8.3 Equivalent points bound

The bounds in this section quantify the following: If multiple observations that are not captured by a prefix d_p have identical features and opposite labels, then no rule list that starts with d_p can correctly classify all these observations. For each set of such observations, the number of mistakes is at least the number of observations with the minority label within the set.

Consider a dataset $\{(x_n, y_n)\}_{n=1}^N$ and a set of antecedents $\{s_m\}_{m=1}^M$. Define distinct datapoints to be equivalent if they are captured by exactly the

same antecedents, *i.e.*, $x_i \neq x_j$ are equivalent if

$$\frac{1}{M}\sum_{m=1}^{M} \mathbb{1}[\text{cap}(x_i, s_m) = \text{cap}(x_j, s_m)] = 1. \tag{A.24}$$

Notice that we can partition a dataset into sets of equivalent points; let $\{e_u\}_{u=1}^{U}$ enumerate these sets. Now define $\theta(e_u)$ to be the normalized support of the minority class label with respect to set e_u, *e.g.*, let

$$e_u = \{x_n : \mathbb{1}[\text{cap}(x_n, s_m) = \text{cap}(x_i, s_m)]\}$$

, and let q_u be the minority class label among points in e_u, then

$$\theta(e_u) = \frac{1}{N}\sum_{n=1}^{N} \mathbb{1}[x_n \in e_u] \wedge \mathbb{1}[y_n = q_u]. \tag{A.25}$$

The existence of equivalent points sets with non-singleton support yields a tighter objective lower bound that we can combine with our other bounds; as our experiments demonstrate (§5.2.6), the practical consequences can be dramatic. First, for intuition, we present a global bound in Proposition 3; next, we explicitly integrate this bound into our framework in Theorem 9.

Proposition 3 (Global equivalent points bound)**.** *Let d be any rule list, then $R(d, \mathbf{x}, \mathbf{y}) \geq \sum_{u=1}^{U} \theta(e_u)$.*

Now, recall that to obtain our lower bound $b(d_p, \mathbf{x}, \mathbf{y})$ in (A.9), we simply deleted the default rule misclassification error $\ell_0(d_p, q_0, \mathbf{x}, \mathbf{y})$ from the objective $R(d, \mathbf{x}, \mathbf{y})$. Theorem 9 obtains a tighter objective lower bound via a tighter lower bound $0 \leq b_0(d_p, \mathbf{x}, \mathbf{y}) \leq \ell_0(d_p, q_0, \mathbf{x}, \mathbf{y})$ on the default rule misclassification error.

Theorem 9 (Equivalent points bound)**.** *Let d be a rule list with prefix d_p and lower bound $b(d_p, \mathbf{x}, \mathbf{y})$, then for any rule list $d' \in \sigma(d)$ whose prefix d_p starts with d_p,*

$$R(d', \mathbf{x}, \mathbf{y}) \geq b(d_p, \mathbf{x}, \mathbf{y}) + b_0(d_p, \mathbf{x}, \mathbf{y}), \quad \textit{where} \tag{A.26}$$

$$b_0(d_p, \mathbf{x}, \mathbf{y}) = \frac{1}{N} \sum_{u=1}^{U} \sum_{n=1}^{N} \neg \operatorname{cap}(x_n, d_p) \wedge \nVdash [x_n \in e_u] \wedge \nVdash [y_n = q_u].$$