DiversiTREE: A New Method to Efficiently Compute Diverse Sets of Near-Optimal Solutions to Mixed-Integer Optimization Problems

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Abstract
While most methods for solving mixed-integer optimization problems compute a single optimal solution, a diverse set of near-optimal solutions can often be more useful. We present a new method for finding a set of diverse solutions by emphasizing diversity within the search for near-optimal solutions. Specifically, within a branch-and-bound framework, we investigate parameterized node selection rules that explicitly consider diversity. Our results indicate that our approach significantly increases diversity of the final solution set. When compared with two existing methods, our method runs with similar runtime as regular node selection methods and gives a diversity improvement of up to 140%. In contrast, popular node selection rules such as best-first search gives an improvement in diversity of no more than 40%. Further, we find that our method is most effective when diversity in node selection is continuously emphasized after reaching a minimal depth in the tree and when the solution set has grown sufficiently large. Our method can be easily incorporated into integer programming solvers and has the potential to significantly increase diversity of solution sets.

Keywords integer programming · near-optimal solutions · diversity · node-selection rules

1 Introduction

It is often useful to find sets of near-optimal solutions to optimization problems rather than a single solution. In particular, for these multiple near-optimal solutions to be usable, they should be diverse, to ensure that decision makers are presented with a variety of options.

One class of methods for generating diverse sets of near-optimal solutions to mixed-integer optimization (MIO) problems uses a two-phase approach. In the first solution generation phase, an oracle finds a set of near-optimal solutions without considering diversity. For example, [Danna et al. (2007)] developed the ONE TREE oracle for this purpose. In the second diverse subset selection phase the output set from the first phase is processed by heuristics (e.g., [Glover et al. (2000)], [Danna and Woodruff (2009)]) or an optimization algorithm (e.g., [Danna and Woodruff (2009)]) to select a small subset of the input set with maximum diversity. While this approach works well for problems with a small number of near-optimal solutions, for MIOs with a very large set of near-optimal solutions it is not practical to find the complete set. As a result, the first phase can only compute a subset of near-optimal solutions. Unfortunately, because existing first-phase methods do not consider diversity, the near-optimal sets they generate often lack diversity...
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A subset of solutions that are computed by the first phase may lack diversity. To address this problem, we developed a method — **DIVERSITREE** — to emphasize diversity in the first phase (solution generation). The output from our solution generation oracle can be used by itself or as a more diverse input set for the second phase in which a for diverse subset is computed.

### 1.1 Motivation

There has been increasing awareness of finding not only one but multiple optima due to increased computational capabilities in the last two decades (Bertsimas et al. (2016)). Some specific applications in which it is desirable to find multiple near-optimal solutions to optimization problems include the correct identification of metabolic activity of cells and tissues in metabolic networks (Rodríguez-Mier et al. 2021), identifying alternative near-optimal structural designs (He et al. 2020), providing policies that are more robust to data changes in reinforcement learning and machine learning (Kumar et al. 2020, Eysenbach et al. 2018), enabling exploration and mapping searches to broader but specific solutions in large search spaces by including near-optimal search results in search requests (Mouret and Clune 2015, Zahavy et al. 2021), adding more artistic alternatives to structural topology optimization (Cai et al. 2021, He et al. 2020), providing competitive alternatives to facility location and location routing problems (Church and Baez 2020, Schittekat and Sörensen 2009), diversifying software deployment to enable stronger computer software security (Tsoupidi et al. 2020), aiding motif finding in computational molecular biology (Zaslavsky and Singh 2006), generating multiple near-optimal group preferences in computational social choice analysis (Boehmer and Niedermeier 2021), and broadening architectural testing in processor design (Van Hentenryck et al. 2009).

Many of these applications have a large number of near-optimal solutions (see Table 2 in Appendix A). For instance, both the routing problem from Ceria et al. (1998) and the multi-period facility location problem studied in Eckstein (1996) are known to have more than 10,000 solutions with objective value within 1% of optimality. In problems with many near-optimal solutions, there is a need to identify a small subset of near-optimal solutions that is representative of the whole. One measure of how well a subset represents the whole is the diversity of the subset. Unfortunately, methods for finding near-optimal solutions such as ONE TREE find near-optimal sets consisting of solutions that are not very diverse (see example provided in §5).

There are several important contexts in which it is useful to have a diverse set of near-optimal solutions. First, in some design problems decision makers seek a set of designs from which to choose, for the purpose of considering other difficult-to-model factors when selecting a single design (Joseph et al. 2015). A similar context is in statistical model selection for a specific domain. Presenting a domain expert with a diverse set of models with similar fit allows the expert to select the model that best matches intuition. Several new studies hypothesize that for many machine learning tasks a set of models exist with near-minimal loss (Semenova et al. 2019; also see §9 of Rudin et al. 2022). Second, using optimization for decision problems can often be an iterative process in which a MIP solution is first presented to a decision maker, only to have the decision maker identify that the solution violates an important side constraint that was not included in the model. If the decision maker is only given a single solution, the model must be re-solved after adding the side constraint. However, if a diverse set of near-optimal solutions were readily available, the decision maker may be able to find a good solution in the set that does not violate the side constraint, avoiding the need to re-solve the model. Third, in contexts in which solutions are implemented repeatedly, it can be useful to alternate between a diverse set of near-optimal solutions. For example, one may use MIP to match workers to jobs to minimize total completion time, but regularly implement different near-optimal matchings to increase cross-training. Lastly, a set of near-optimal solutions can be used to measure and explain the importance of variables in applications such as statistical model selection (see §9 of Rudin et al. 2022). If a feature is present in a large number of diverse near-optimal solutions, this provides additional evidence that the feature is an important predictor of the response variable.

In two-phase approaches the output of the solution generation phase is the input to the diverse subset selection phase (see, e.g., Danna et al. 2007, Silva et al. 2007). Solution generation methods that do not include diversity in the solution generation phase would use this approach with the intent of collecting enough solutions to cover the solution space in the first phase and hence a diverse set in the second phase. Apart from the additional time this takes, if the solution set
computed in the solution generation phase lacks diversity, then the subset computed by the *diverse subset selection* phase will lack diversity. To address this gap, this research explores methods that encourage diversity during the solution generation phase.

1.2 Related Work

Although there exists some work on finding near-optimal solutions to continuous optimization problems (see Lavine (2019)), most of the work has been in relation to mixed-integer optimization (MIO) problems and, in particular, with respect to (binary) integer variables.

There are a number of different algorithms for generating a set of near-optimal solutions to a MIO problem. Achterberg et al. (2008) developed an approach for generating all feasible solutions to an MIO problem called *branch-and-count*. This approach is based on detecting “unrestricted subtrees” in the branching tree. This method can also be used to find all solutions within a certain threshold of the optimal objective value, if known. Other methods have been proposed for finding all optimal solutions; an example is the work by Lee et al. (2000) which uses a recursive MIP algorithm to find all alternate optima. Serra (2020) used weighted decision diagrams to compactly represent all near-optimal solutions generated for an integer programming problem. The compact representation eases resolves and information retrieval from all generated solutions. Also, the ONETREE method (currently implemented in GAMS-CPLEX) given by Danna et al. (2007) which extends the branching tree used to solve the MIP problem to generate near-optimal solutions. In addition, approaches have been developed for specific classes of problems including using dynamic programming to generate multiple solutions to graph-based problems (Baste et al. (2023)), methods to represent near-optimal solutions compactly (Serra and Hooker (2020)) and algorithms specific to topology optimization problems (Wang et al. (2018)). While these methods are effective at finding near-optimal solutions, they do not necessarily compute solution sets that are diverse. One of the few papers that discusses balancing diversity and optimality is Zhou et al. (2016). They developed a Dual Diverse Competitive Design (DDCD) method that formulates balancing optimality and diversity as an optimization problem that maximizes diversity, subject to constraints on the performance penalty. While their method specifically focuses on generating competitive designs that would give diverse solutions, the goal of this article is a method for general MIO problems.

There are a number of different approaches for finding a diverse set of near-optimal solutions to an optimization problem. In the *sequential* approach (Danna et al. (2007)), the optimization problem is solved multiple times, and after each solve a constraint is added that requires the next optimal solution be different from the previous. The sequential approach is also used in Trapp and Konrad (2015) to select diverse solutions to binary integer linear problems and in Petit and Trapp (2015) in the context of constraint programming. Both methods consider maximizing a metric that is the ratio of diversity of solutions to loss in objective function. Petit and Trapp (2019) extend these ideas further by including the notion of solution quality when generating diverse near-optimal solutions. The *variable copy* approach adds $k$ copies of the variables, one copy for each near-optimal solution desired, in an optimization model and adds constraints to enforce that the solutions differ (Cameron et al. (2021)). Greistorfer et al. (2008) compared the sequential and variable copy approaches for the problem of finding two diverse near-optimal solutions and found that the sequential approach usually required less computation time and yielded solutions that were nearly as good as the simultaneous approach. Further, population-based *metaheuristics* are a natural approach for finding diverse sets of solutions because these algorithms operate on a set of solutions. For instance, Glover et al. (2000) used a scatter-search algorithm to find a diverse set of solutions to MIPs. While metaheuristics are often effective in practice, their main drawback is their inability to guarantee that the entire set of near-optimal solutions has been found. Finally, *two-phase* approaches use an oracle such as the ONETREE algorithm (Danna et al. (2007)) to find a (not necessarily diverse) set of near-optimal solutions. Then the second phase inputs this set of near-optimal solutions and chooses a subset that maximizes diversity. Regarding the second phase, Danna and Woodruff (2009) developed exact and heuristics algorithms to find a diverse subset. The work by Glover et al. (1998) which proposed four different heuristics algorithms for generating the most diverse solutions from a larger set does not consider how close they are to the optimal objective value. Kuo et al. (1993) proposed two different methods that use linear...
programming to select the most diverse solutions from a solution set. Schwind et al. (2020) developed methods for computing a small subset of solutions that represent the larger set using bi-objective optimization. The authors of Danna et al. (2007) found that the sequential and simultaneous methods do not scale as the number of solutions that are been generated increases. The approach developed in this article combines both phases of the two-phase approach, emphasizing diversity while searching for a near-optimal set.

1.3 Contributions and Findings

This article examines how using different node selection rules within a branch-and-bound framework affects the diversity of the computed near-optimal solution set. In addition, we also present experimental results for new node selection rules that prioritize solution diversity. We select random problems from MIPLIB and split them into a training set (75\% of the number of problems) and a test set (25\% of the problems). We learn the optimal parameters for DIVERSITREE on the training set and evaluate these parameters on the problems in the test set. Our specific contributions are the following:

1. *Diversity of solution sets computing by existing node selection rules.* We investigated the diversity of near-optimal sets generated using popular node selection rules within a branch-and-bound algorithm. We found that, while the effect of node selection rules on solution set diversity is problem specific, the best-first search rule typically gave better diversity solutions overall.

2. *A new node selection rule that emphasizes solution set diversity.* We investigated a new node selection rule used within a branch-and-bound framework that selects new nodes in the tree based on a criteria that infuses a diversity metric into the traditional node relaxation value.

3. *Best parameters for diversity-emphasizing node selection rules.* We investigated several different parameterized node selection rules for finding diverse solution sets, including the depth of a node within the branch-and-bound tree and the number of solutions currently in the solution set. We found that the greatest diversity is obtained when waiting to emphasize diversity until a number of solutions is gathered or when selecting solutions deeper in the tree.

4. *Benefits of emphasizing diversity in node selection.* Using 36 problem instances randomly selected from MIPLIB (2003, 2010 and 2017), we found that using our new diversity-emphasizing node selection results in solution sets that are up to 140\% more diverse than the ONETREE algorithm—a leading method for finding near-optimal sets currently implemented in GAMS. Regarding runtime, we found that our method of emphasizing diversity within the node selection procedure runs within ±15\% of the time used by regular node selection methods that do not emphasize diversity and results in a better tradeoff between runtime and solution diversity than competing approaches. Importantly, we found that the parameter settings that performed best on a training set of problems also performed well even when applied to a “test set” of problems.

1.4 Outline of the paper

The remainder of this article first gives mathematical and algorithmic preliminaries in §2 followed by a description of the diversity-emphasizing node selection rules tested in this work in §3. Experimental results on the training and test set data is discussed in §4 while §5 illustrates the use of DIVERSITREE on real data prior to concluding in §6.

2 Mathematical and Algorithmic Preliminaries

We consider finding a diverse set of near-optimal solutions to the following problem:

\[
\begin{align*}
    z^* &= \min_{x \in X} c^T x \\
    X &= \{ x \in \mathbb{R}^d : Ax \geq b, x_i \in \mathbb{Z}, \forall i \in \mathbb{I} \subseteq \{1, \ldots, d\} \}
\end{align*}
\]
**DiversiTee**

Let \( S_q = \{ x \in X : c^T x \leq (1 + q)z^* \} \) denote a set of \( q \)-optimal solutions to (1), \( q \geq 0 \). While mixed-integer programs are considered, diversity is only computed over binary integer variables. If \( |S_q| \) is small, it may be sufficient to use a near-optimal solution generation algorithm such as ONE TREE (Danna et al. (2007)) to generate the entire set \( S_q \) for presentation to a decision maker. In the case in which \( |S_q| \) is large but not very large, not more than 1,000 elements, the following two-phase approach may be used. In the first phase, a solution generation algorithm is used to obtain the complete set of near-optimal solutions \( S_q \). Then in the second phase, use a diverse subset selection algorithm (see, e.g., Danna and Woodruff 2009) to find a small subset of \( S_q \) of cardinality \( p \), solving the following problem:

\[
\max_{S \subseteq S_q, |S| = p} D(S).
\]  

(2)

where \( D(S) \) is a measure of the diversity of solution set \( S \).

In many cases, however, the set \( S_q \) has very many elements, perhaps 10,000 or more. In particular, for about half of the instances tested in Danna and Woodruff (2009), \( |S_q| > 10,000 \). For these instances, the authors limited the input to the second phase to a subset of \( S_q \) consisting of the first 10,000 solutions obtained by the ONE TREE algorithm Danna et al. (2007). That is, the first phase finds a subset \( \bar{S} \subseteq S_q \) (\( |\bar{S}| = 10,000 \)) without explicit consideration of diversity, while the second phase solves:

\[
\max_{S \subseteq \bar{S}, |S| = p} D(S).
\]  

(3)

These problem instances with very large \( S_q \) present two issues:

- **Computational.** These problems could not be solved to optimality in the second-phase of the two-phase approach due to memory limitations or exceeding a 10-day time limit (Danna and Woodruff 2009). As a result, heuristics were employed. For smaller problems these heuristics appear to produce solutions that nearly maximize diversity. However, it is not known whether the heuristics produce good solutions to any of the larger problems.

- **Solution quality.** Using the subset \( \bar{S} \) as an input to the second phase rather than the complete set \( S_q \) could result in a loss of diversity if there is insufficient diversity in the input subset to either of the heuristic or exact methods.

To address these issues, we seek to solve (3) directly rather than via a two-phase approach. Specifically, we examine how to modify the exploration strategy of the solution generation phase to increase the diversity of the subset \( \bar{S} \).

### 2.1 Computing near-optimal sets

Given a mixed integer programming problem, we assume the existence of an oracle capable of enumerating a set of all or a sufficiently high number of near-optimal solutions for the problem. We use the branch-and-count method as the oracle due to its significant speed at enumerating near-optimal solutions by detecting and pruning infeasible subtrees (Achterberg et al. 2008). The branch-and-count method is implemented in SCIP (Gamrath et al. 2020), which provides access to, as well as modification privileges for, the branching tree and implementation methods of the oracle.

The branch-and-count algorithm is an extension of the branch-and-cut algorithm, a variant of branch-and-bound that adds valid inequalities to the formulation during the traversal of the tree so as to strengthen the LP relaxation. Branch-and-cut operates by going through the entire search tree generated during the regular branch-and-cut process, collecting all feasible solutions at each node if that node is detected to represent an unrestricted subtree. The authors prove that the subtree at a node in the search tree is unrestricted if all constraints at that subtree are satisfied by all possible variable assignments of values in the domain of that subtree, that is, the constraints are locally redundant at that node. This way, they can construct solution vectors for that subtree while avoiding traversing every node in that subtree. This significantly reduces the number of nodes this algorithm visits. The pseudocode is given in Algorithm 1.
To use this algorithm to generate the set $\bar{S}$, we first solve equation (1) to global optimality to find an optimal objective value $z^*$. Next, we pass the number of near-optimal solutions requested ($p_1$) as input to the algorithm and add the constraint $c^T x \leq (1 + q)z^*$ to equation (1) and solve using the branch-and-count algorithm.

**Algorithm 1 Branch and Count Pseudocode**

1: **INPUT** $p_1, MIP$
2: **ADD** constraint $c^T x \leq (1 + q)z^*$ to initial MIP problem
3: $Q \leftarrow \emptyset$
4: **ADD** initial MIP problem to queue of active nodes $Q$
5: $\bar{S} \leftarrow \emptyset$
6: **while** $Q$ is not empty and $|\bar{S}| < p_1$ **do**
7: **Use** node selection rule to dequeue node $i'$ from list $Q$
8: **if** node $i'$ is unrestricted **then**
9: Add solution to $\bar{S}$
10: **else if** node $i'$ is infeasible **then**
11: Prune
12: **end if**
13: **Use** regular branching rule to discover more nodes and add to list $Q$
14: **end while**
15: **return** $\bar{S}$

### 2.2 Node Selection Rules.

During line 6 of the branch-and-count search outlined in Algorithm [1], the node selection rule decides which node from the queue of active nodes is selected as the next node. Popular node selection rules include:

- **Best-First Search (BestFS).** Selects the node with the best bound, that is, for minimization problems, select $i'$ as the next node according to

\[
i' \in \arg \min_{i \in Q} \{ LB_i \},
\]

where $LB_i$ is the lower bound for node $i$.

- **Depth First Search (DFS).** Nodes encountered as the branch and bound search tree is traversed are added to a queue and are selected in Last In First Out (LIFO) order.

- **Breadth First Search (BrFS).** Nodes are added to a queue and processed using the First In First Out (FIFO) order.

- **Upper Confidence Bounds for Trees (UCT)** [Gamrath et al. (2020)]. Selects the next node $i'$ as a node with the best UCT_score, that is:

\[
i' \in \arg \min_{i \in Q} \{ UCT_{Score} i \},
\]

$UCT_{score}$ is calculated as:

\[
UCT_{Score} i = LB_i + \rho \frac{V_i}{v_i}
\]
where \(v_i\) and \(V_i\) are the number of times the algorithm has visited node \(i\) and its parent, respectively. \(\rho\) is a weight parameter chosen by the user.

- **Hybrid Estimate (HE)** (Gamrath et al. (2020)). Selects the next node \(i'\) as a node having the best HE_Score, i.e.:

\[
i' \in \arg\min_{i \in Q} \{HE\_Score_i\},
\]

\(HE\_Score\) is calculated as:

\[
HE\_Score_i = (1 - \rho)LB_i + \rho\widehat{LB}_i
\]

\(\widehat{LB}_i\) is the estimated value of the best feasible solution in subtree of node \(i\) and \(\rho\) is a user-defined weight parameter.

2.3 Measuring the diversity of solutions

A number of metrics exist for measuring the diversity of a set of solutions. A good metric needs to be model agnostic and ideally scaled such that diversity scores given by the metric are easy to interpret. Danna and Woodruff (2009) outlined three problem agnostic measures for the diversity of solutions: \(DBin\), defined in more detail below and used in our tests, is scaled by the number of variables and solutions generated and considers just the binary variables; \(DAll\) which considers all variable types; and \(DCV\) which is the scaled version of \(DAll\).

The \(DBin\) metric (defined only on binary variables) is the average scaled Hamming distance between all pairs of solutions in a set \(S\), that is,

\[
DBin(S) = \frac{2}{|S|(|S| - 1)} \sum_{j=1}^{|S|} \sum_{k=j+1}^{|S|} DBin(x^{(j)}, x^{(k)}),
\]

where \(x^{(j)}\) is the \(j^{th}\) solution generated by the oracle, and \(DBin()\) computes the Hamming distance between a pair of solutions, that is,

\[
DBin(x^{(j)}, x^{(k)}) = \frac{1}{|B|} \sum_{i \in B} |x_i^{(j)} - x_i^{(k)}|,
\]

where \(B\) is the set of binary variables and \(|B|\) is the number of binary variables. An advantage of the \(DBin\) metric is that it takes values between 0 and 1 inclusive and does not depend on the size of the solution set or the number of variables.

3 Diversity-Emphasizing Node Selection rules

Within the branch-and-count algorithm (Achterberg et al. 2008), we investigated several variants of the best-first search (BestFS) node selection rule that consider solution set diversity when selecting the next node to evaluate. We focused on BestFS because, as our results in §4 show, it generated the most diverse solution sets when compared with other well-known node selection rules (such as DFS) when diversity was not considered in the node selection task. What follows is a description of each of the custom node selection rules tested in this work.
3.1 Diverse-BFS (D-BFS(α))

The Diverse-BFS (D-BFS α) node selection rule considers both the lower bound of a node as well as the diversity of the node with respect to other solutions already in the near-optimal set. That is, this rule inputs a set of open nodes $O$ and selects the next node $i'$ according to:

$$i' \in \text{arg min}_{i \in O} \{(1 - \alpha) \mathcal{L}_i + \alpha D_i\},$$

where $\alpha \in [0, 1]$ is a parameter that trades off the bound of node $i$ against its diversity score $D_i$ and $\mathcal{L}_i$ is a scaled lower bound of node $i$, that is,

$$\mathcal{L}_i = \frac{LB_i - \min_{j \in O} LB_j}{\max_{j \in O} LB_j - \min_{j \in O} LB_j}.$$

The lower bound is scaled to $[0, 1]$, commensurate with the diversity score $D_i \in [0, 1]$. The value of $D_i$ represents the partial diversity of node $i$ with respect to the current solution set $\bar{S}$. We use the term partial because it is computed based only on the binary variables that have been fixed at a particular node in the branching tree.

3.2 Diverse-BFS with tree depth (D-BFS(α, β))

The D-BFS(α, β) node selection rule considers the lower bound, the diversity and the depth of a node with respect to other solutions in the near-optimal set. This rule inputs a set of open nodes $O$ and selects the next node $i'$ according to:

$$i' \in \text{arg min}_{i \in O} \{(1 - \alpha - \beta) \mathcal{L}_i + \alpha D_i + \beta H_i\},$$

where $(1 - \alpha - \beta), \alpha, \beta$ form a convex combination and are the parameters that control the weight of the scaled lower bound of node $i$, $\mathcal{L}_i$, the diversity score $D_i$, and the scaled depth of node $i$, $H_i$. Like $\mathcal{L}_i$, $H_i$ is scaled as:

$$H_i = \frac{\text{Depth}_i - \text{MinP\,lunge\,Depth}}{\text{MaxP\,lunge\,Depth} - \text{MinP\,lunge\,Depth}},$$

where $\text{MinP\,lunge\,Depth}$ and $\text{MaxP\,lunge\,Depth}$ are set at the beginning of the computation and $\text{Depth}_i$ is the depth of node $i$ in the tree.

3.3 Diverse-BFS with solution cutoff (D-BFS(α, s))

The D-BFS(α, s) rule considers only the lower bound of a node until it has generated a small set of up to $s$ solutions prior to incorporating the diversity of a node with respect to the solutions already in the near-optimal set. This rule selects the next node $i'$ according to:

$$i' \in \begin{cases} \text{arg min}_{i \in O} \{\mathcal{L}_i\} & \text{number of solutions found so far} < s, \\ \text{arg min}_{i \in O} \{(1 - \alpha) \mathcal{L}_i + \alpha D_i\} & \text{otherwise,} \end{cases}$$

where $s$ is the solution cutoff parameter, that is, the number of solutions that must be accumulated before diversity is considered in node selection and $\alpha \in [0, 1]$ is a parameter that trades off the bound of node $i$ against its diversity score $D_i$. 

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3.4 Diverse-BFS with depth cutoff (D-BFS($\alpha, d$))

The D-BFS($\alpha, d$) rule considers only the lower bound of a node until the depth of the active node reaches a depth $d$ prior to also considering the diversity of the node with respect to the solutions already in the near-optimal set. This rule selects the next node $i'$ according to:

$$i' \in \begin{cases} \arg \min_{i \in O} \{L_i\} & \text{depth of nodes in current iteration} < d, \\ \arg \min_{i \in O} \{(1 - \alpha)L_i + \alpha D_i\} & \text{otherwise}, \end{cases}$$

where $d$ is the depth cutoff parameter, that is, the depth that must be reached before diversity is considered in the node selection and $\alpha \in [0, 1]$ is a parameter that trades off the bound of node $i$ against its diversity score $D_i$. Diversity is only triggered upon reaching a depth of $d$ or greater.

3.5 DiversiTREE - Diverse-BFS with solution cutoff and tree depth (D-BFS($\alpha, \beta, s$))

DiversiTREE selects the next node $i'$ according to:

$$i \in \begin{cases} \arg \min_{i \in O} \{L_i\} & \text{number of solutions found so far} < s, \\ \arg \min_{i \in O} \{(1 - \alpha)L_i + \alpha D_i + \beta H_i\} & \text{otherwise}, \end{cases}$$

where $\alpha, \beta, s$ are parameters as defined in previous sections.

3.6 Other Diverse-BFS methods tested

We also tested several other methods for emphasizing solution set diversity. However, these additional methods were not as effective as the methods described in §3.1 - §3.5 above. They are:

1. Using the minimum of diversity and depth, that is, select next node $i'$ according to:

$$i' \in \arg \min_{i \in O} \{(1 - \alpha)L_i + \alpha \min(D_i, H_i)\}.$$

2. Using the maximum of diversity and depth, that is, select next node $i'$ according to:

$$i' \in \arg \min_{i \in O} \{(1 - \alpha)L_i + \alpha \max(D_i, H_i)\}.$$

3. Using the product of diversity and depth, that is, select next node $i'$ according to:

$$i' \in \arg \min_{i \in O} \{(1 - \alpha)L_i + \alpha D_i H_i\}.$$

These node selection rules were also tested with a nonzero solution cutoff parameter $s$, but were still not effective.

4 Computational Experiments.

To measure the effect of using diversity-emphasizing node selection rules on solution set diversity, we ran several sets of experiments on selected problems from MIPLIB (Koch et al. 2011, Bixby et al. 1998, Gleixner et al. 2021) using several different node selection rules, including the customized ones described in §3. We compared our approach with two state-the-art methods: ONE TREE (Danna et al. 2007) and BRANCH-AND-COUNT (Achterberg et al. 2008).

Experiments were run to answer the following questions:
Research Question 1: Among common node selection rules (such as BestFS and DFS), do some produce a more diverse set of near-optimal solutions than others? §4.2

Research Question 2: What are the best parameters to use for the parameterized diversity-emphasizing node selection rules presented in §3? When using the best parameters, do the diversity-emphasizing node selection rules compute solution sets that are more diverse than those computed by competing approaches? §4.3

Research Question 3: What parameters should be used when using diversity-emphasizing node selection rules on a new problem? §4.4

4.1 Experimental Setup

All code was implemented in C++ using SCIP Optimization suite 7.0 (Gamrath et al. 2020) and run on a server running Intel Xeon processors with sixteen cores and thirty two GB of memory. Apart from SCIP currently being one of the fastest non-commercial solvers for mixed integer programming (MIP) and mixed integer nonlinear programming, it provides a convenient way to use custom node selection rules. We evaluated our methods against the state-of-the-art ONETREE method, implemented in GAMS-CPLEX.

4.2 Diversity of common node-selection rules

We first examined the diversity produced by common node selection rules. For this initial set of experiments, we selected seven problems from MIPLIB that had greater than 10,000 solutions within 1% of optimality (see Table 2 in Appendix A).

We used the common node selection rules listed in §2.2 to request the generation of sets with sizes ranging from 50 to 2,000 near-optimal solutions, and computed the diversity. Figure 1 below shows the $\text{DBin}$ diversity scores achieved by these common node selection rules for different solution set sizes ($p_1$). We labeled the different node selection rules with a “BC” prefix to indicate the use of branch-and-count to generate the solution sets. As shown in Figure 1 the best-first search (BCBFS) method finds sets with the greatest diversity in 5 out of 7 test problems. The upper confidence bounds for trees (BCUCT) node selection rule had the best performance in 2 out of the 7 test problems and achieved a similar diversity value to hybrid estimate (BCHE) in all other cases. The depth first search (BCDFS) was outperformed in terms of diversity in all of the instances.

The plots also indicate that diversity (averaged for each problem instance) tends to start low and become incrementally higher as the number of requested solutions increases. We hypothesize that this may be due to a situation where as more solutions are generated, more variables are fixed or modified; increasing the Hamming distance from the first solution found. However, this trend did not hold for all of the individual problem instances.
Figure 1: The final $DBin$ diversity score achieved by common node selection rules (BestFS, DFS, UCT and HE) available on SCIP. We prefix each node selection rule name with “BC” to indicate the use of the “branch-and-count” method. The BestFS node selection rule resulted in greater diversity for a majority of problems.

The superior performance of BestFS over other common rules suggested its continued use for comparison in the remainder of our experiments.

4.3 Parameter optimization for diversity-emphasizing rules: training set

The most general diversity-emphasizing node selection rules have up to three parameters to be tuned: $\alpha$ controls the emphasis on diversity for the selected node, $\beta$ controls the emphasis on depth within the search tree for the selected node, and $S$ controls the emphasis on the number of solutions generated before employing the $\alpha$ and $\beta$ values in the node selection process. We used a grid search to tune the parameters and find the best-performing values. Toward this end, we used several problem instances from MIPLIB (Gleixner et al. 2021, Koch et al. 2011, Bixby et al. 1998) and randomly split the set of problems into a training and testing set using a 75:25 split. We use the training set problems to find the best parameters and then tested the performance of these parameters on the testing set problems. Using a grid-search on a $20 \times 20 \times 20$ grid over $\alpha$, $\beta$, and $S$ on $[0, 1]$ with increment 0.01 on $[0, 0.09]$ and 0.1 on $[0.1, 1]$, we
tested different parameters values across all training set problems shown in Table [2] in Appendix [A] for different numbers (10, 50, 100, 200 and 1000) of requested near optimal solutions $p_1$ and values of $q$ (% near optimal) in the range $[0.01, 0.1]$ with increment 0.01. As a result, we obtained for each instance the best performing values of $\alpha$, $\beta$, and $S$ over every $p_1$ and $q$. It is computationally impractical to run a grid search for every new problem instance prior to applying our node selection rule. We therefore attempted to identify patterns in the mapping between problems and optimal parameter values, so as to allow the identification of a smaller number of parameter settings with good performance. Thus, our next step was to determine whether we could group problems together based on their optimal parameter settings. Toward this end, we ran a standard hierarchical clustering algorithm available in Python’s Scikit-Learn package (Pedregosa et al. 2011) to cluster the problems into groups based on their best parameter settings, that is, the settings that yielded the highest $DBin$ scores for that problem. When the number of requested solutions is small (that is, 10), the clustering algorithm found the following four groups:

1. High $\alpha$, High $S$, Low $\beta$ (HHL): $\alpha \geq 0.9$, $S \geq 0.7$, $\beta \leq 0.2$.
2. High $\alpha$, Low $S$, Low $\beta$ (HLL): $\alpha \geq 0.9$, $S \leq 0.2$, $\beta \leq 0.2$.
3. Low $\alpha$, Low $S$, High $\beta$ (LLH): $\alpha \leq 0.2$, $S \leq 0.2$, $\beta \geq 0.8$.
4. Low $\alpha$, High $S$, High $\beta$ (LHH): $\alpha \leq 0.2$, $S \geq 0.7$, $\beta \geq 0.8$.

In the HHL group, diversity is emphasized heavily ($\alpha \geq 0.90$), but only after a large number of solutions have been accumulated ($S \geq 0.70$). In the HLL group, diversity is also heavily emphasized, but starting after a moderate number of solutions have been found ($S \leq 0.20$). The LLH group tends to select solutions at greater depths in the tree ($\beta \geq 0.80$) after a small number of solutions have been accumulated ($S \leq 0.20$). Finally, the LHH group emphasizes diversity lightly ($\alpha \leq 0.20$) and mostly selects solutions at greater depths in the tree ($\beta \geq 0.80$) after a large number of solutions have been accumulated ($S \geq 0.70$). The structure of these four groups indicates that our method is most effective when we generate a small number of seed solutions and then emphasize diversity at greater depths in the tree.

To assess the efficacy of DIVERSITREE, we then selected a single parameter setting for each of the four groups, as shown in Table [1]. Using the data from the grid search, we took the weighted average of the settings in a group as $G_1$ and the settings that occurred the most frequently in that group as $G_2$. We computed the diversity of the training set problems using $G_1$ and $G_2$ separately and selected either $G_1$ or $G_2$ as the best setting for the group, depending on which of the two produced the best diversity. We found that these parameter settings worked well for different values of $p_1$ and $q$.

Table 1: The $\alpha$, $\beta$ and $S$ parameter settings used in both training and testing.

<table>
<thead>
<tr>
<th>Number of solutions requested</th>
<th>HHL</th>
<th>HLL</th>
<th>LLH</th>
<th>LHH</th>
</tr>
</thead>
<tbody>
<tr>
<td>10, 50, 100, 200, 1000</td>
<td>$\alpha : 0.94$, $\beta : 0.06$, $s : 0.80$</td>
<td>$\alpha : 0.95$, $\beta : 0.06$, $s : 0.20$</td>
<td>$\alpha : 0.01$, $\beta : 0.99$, $s : 0.05$</td>
<td>$\alpha : 0.18$, $\beta : 0.8$, $s : 0.70$</td>
</tr>
</tbody>
</table>

For each problem instance, we then ran DIVERSITREE using the parameters from its assigned group from the clustering algorithm (see Figure 6 in the Appendix). The parameter settings in Table [1] were used for all values of $p_1$ and $q$. Specifically, we use the following two-phase approach. In phase one, we generate a larger solution set $p_1$ with 10, 50, 100, 200, and 1000 solutions. In phase two, we then use a subset selection method (similar to local search algorithm in Danna and Woodruff (2009)) to select $p = 10$ diverse solutions—a number that seems reasonable to present to a decision maker. We ran this process for values of $q$ from 1% to 10% across all the problems in the training set. We
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compare the performance of our method with two state-of-the-art methods: with the BCBFS rule, and with the ONETREE method results reported in [Danna and Woodruff, 2009]. These competing methods were used in phase one of the two-phase approach, with the subset selection method being employed in phase two.

In Figure 2 and 3 we plot the percent improvement of the different groups of DiversiTREE over ONETREE for values of \( q \) from 1% to 10%, and \( p = 10 \) for different \( p_1 \) values. In Figure 2 we show plots for \( p_1 \leq 100 \) and in Figure 3 we show plots for \( p_1 \geq 200 \). As the figure shows, DiversiTREE achieves an improvement in diversity over ONETREE of up to 160% and at least 60%, irrespective of the four parameter settings used. Beyond outperforming ONETREE, all the parameter groups also give similar performance on the average with no more than 10% gap between any group. Among the DiversiTREE results, parameter groups HHL and HLL appear to perform best. Thus, we recommend that when using our method on a new problem either the HHL (\( \alpha = 0.94, \beta = 0.06, s = 0.80 \)) of HLL (\( \alpha = 0.95, \beta = 0.06, s = 0.20 \)) parameter settings should be used. In the next section we test the HHL parameter setting on a set of new problems that were not used for parameter tuning.

![Graphs showing improvement and runtime](image)

Figure 2: This figure shows plots for \( p_1 \leq 100 \). The plots on the left shows the average percent improvement on diversity (\( DBin \)) achieved by different parameter group settings of DiversiTREE over ONETREE aggregated across all problems in the training set. The run times are shown in the plots on the right. The runtime for DiversiTREE were similar for the four different parameter groups, hence this figure shows the average runtime over the four groups.
4.4 Performance of tuned parameter groups on test set of problems

The results of the previous section raise the question of how parameters should be tuned on a new problem. To answer this question, we tested our method using the HHL parameter setting, which was recommended in the previous section. We test our method with the HHL setting on a test set of problems not used in parameter tuning (see Table 3 in Appendix B). We ran the same two-phase approach for diverse, near-optimal solution generation as we did in the training phase. We ran this process for $p_1 \in \{10, 50, 100, 200, 1000\}$ and $q$ from 1% to 10%. We kept the size of the final solution set to $p = 10$. Although the our method performed better than BCBFS\(^1\) and ONE_TREE for all four of the parameter settings, we only present results for the recommend HHL setting.

We use the HHL parameter setting on the test data and the results achieved are shown in Figure 4 (for $p_1 \leq 100$) and 5 (for $p_1 \geq 200$), which displays results similar to those in Figures 2 and 3 for the training set. DIVERSITREE generated solution sets with improvement over ONE_TREE of up to 139% and no worse than 32% irrespective of the four parameter groups used. DIVERSITREE also significantly outperforms BCBFS in terms of diversity for all values of $p_1$, as BCBFS generated solution sets with improvement of up to 36% and no worse than 0%. In terms of runtime, DIVERSITREE achieves similar runtime as BCBFS, although the ONE_TREE method runs significantly faster than both methods, which is unsurprising given that while DIVERSITREE explicitly searches for solution, ONE_TREE only focuses on near-optimality. Unlike the training set data where parameter groups HHL and HLL dominated the DIVERSITREE results, the parameter groups LHH and LLH dominated the diversity results generated in the test set.

\(^1\)In using BCBFS, we found that the default parameters on SCIP (i.e., $MINPLUNGEDEPTH = -1$, $MAXPLUNGEDEPTH = -1$, and $MAXPLUNGEQUOT = 0.25$) performed poorly. Thus, we manually tuned these settings to improve the diversity obtained by BCBFS. These tuned parameter settings were used in the results shown in the remainder of the paper.
In practice, a decision-maker seeking a diverse set of near-optimal solutions would need to define \( p \) (the number of near-optimal solutions), \( q \% \) (a bound on how far these solutions may be from optimality), and select a setting in any of the groups we specified in §4.3 (without need for parameter tuning); \( p \) near-optimal solutions can then be directly generated within \( q \% \) of the optimal, or a two-phase approach can be used to generate the solution set. The result of our tests suggest that the solution set generated would be no worse than BCBFS and would be significantly better than the state-of-the-art ONETree method.

Figure 4: This figure shows plots for \( p_1 \leq 100 \). Plots on the left show the percent improvement on diversity (\( DBin \)) achieved by DiversITree and BCBFS on the problems in the test set using the parameter setting from group HHL shown in Table 1. The plots on the right show the runtime. The runtime for DiversITree were similar for the four different parameter groups, hence this figure shows the average runtime over the four groups.
Figure 5: This figure shows plots for \( p_1 \geq 200 \). Plots on the left show the percent improvement on diversity (\( DBin \)) achieved by DIVERSITREE and BCBFS on the problems in the test set using the parameter setting from group HHL shown in Table II. The plots on the right show the runtime. The runtime for DIVERSITREE were similar for the four different parameter groups, hence this figure shows the average runtime over the four groups.

5 Example: Railway Timetabling Problem

To provide a concrete example, we tested DIVERSITREE on a public transport scheduling problem within the MIPLIB2017 set \(^{[6]}\) (Gleixner et al. 2021). Details about the problem formulation and variables is available in \(^{[7]}\) Liebchen and Möhring (2003). \(^{[8]}\) Liebchen and Peeters (2002) discuss the general problem formulation. The problem models the cyclic railway timetabling problem where we have information about a railway network in a graph representing its infrastructure and traffic line. Each traffic line is operated every \( T \) time units and the goal of the problem is to determine periodic departure times within the interval \([0, T]\) at every stop of every line. The problem has 397 variables; 77 of them are binary variables, 94 integer variables and 226 continuous variables. The final objective is to obtain an arrival/departure timetable with minimal passenger and vehicle waiting times. The problem is represented as a graph \( G = (N, A, l, u) \) with a set of nodes \( N \) representing a set of events, and arcs \( A \) representing set of trains. The weights on the arcs represent the time when event \( v_i \in N \) occurs and \([l, u]\) the allowable time interval for this event. The events are represented as triplets \((\text{train}, \text{node}, \text{arrival})\) or \((\text{train}, \text{node}, \text{departure})\) and the binary variable \( b_{ij} \) is 1 if arc \((i, j)\) is selected. The model is mainly based on periodic constraints, which relate the arrival and departure time variables through the time window \([l, u]\) within which the event \( i \) must occur.

For problems such as these, the solutions provided by the MIP model will be reviewed by a decision maker prior to implementation. Thus, in this context it can be useful to provide the decision maker with a set of near-optimal solutions from which to choose. This will allow the decision maker to consider not only the cost of the solution but also other factors such as variability in estimated demands, crew shortages, behavior of new equipment, or propagated delays, without having to re-solve the problem. For \( q = 1\% \), the problem had 181 near-optimal solutions, and when \( q \) increased to 3\%, the number of near-optimal solutions increased to 6,264.

We ran the DIVERSITREE and ONE TREE algorithms on this problem for \( p_1 = 10, p = 10 \) and \( q = 3\% \). DIVERSITREE computed a solution set with a \( DBin \) value of 0.299, while ONE TREE’s set has a \( DBin \) value of 0.044. A further
A review of the generated solutions shows that of the 77 binary variables, ONETREE gave a solution set in which 68 of the binary variables had the same value in all ten solutions. In addition, ONETREE generated a set of ten solutions of which only six solutions were unique. Among the six unique solutions, five of them had at most two variables with different values indicating very close similarity of the solutions. In contrast, DIVERSITREE's gave a solution set in which only 23 of the variables were the same in all ten solutions, all ten solutions were unique and at least nine variables had different values among the solutions, indicating the diversity of the solutions. This experiment provides further evidence supporting that the DIVERSITREE approach provides a much more diverse set of train schedules from which a decision maker may select.

6 Conclusion

We introduce a novel approach to generate diverse, near-optimal solution sets by emphasizing solution diversity in the node selection step of a branch-and-bound algorithm. Our results reveal that our modified node selection rule yields up to 140% better diversity than known methods for generating diverse solutions. Our methods provide a fast way to generate diverse sets of near-optimal solutions, useful where there is utility in having a diverse set of options for decision making. We presented several methods for emphasizing diversity in node selection rules and optimal parameters that yield the most diverse set of solutions for the problems tested. We identified four groups of optimal parameters for different problems by clustering the parameter groups giving the best diversity (DBin) on the training set. Each group sets an optimal solution cutoff value and also sets how much diversity and depth to consider in determining the next solution added to the set of diverse solutions. When tested on new problems, our method (using the identified optimal parameters) ran in similar time as regular node selection rules and gave solution pools that were significantly more diverse.

A positive result of our study was that the four parameter setting groups identified during the parameter tuning on the training set performed well on a previously unseen set of problems in a test set. Even so, understanding the relationship between parameter settings and different classes of problems such that we can select the best parameter for any problem with a minimal amount of tuning would be beneficial in practice. A second area of interest which is also an extension of this work is diversifying solution pools on select variables (see Voll et al. [2015]). In cases where a cluster of variables represents an attribute that is desirable in a machine learning algorithm (such as fairness or intelligence), it may be useful and informative to generate solutions pools that are diverse on only that attribute or interpret and cluster the generated solutions based on the attribute. Finally, we only reported results using DBin as a diversity metric. It would be useful to understand how the new node selection method performs when using other metrics for computing diversity.

Acknowledgments

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References


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Appendix A  Problems in the training set

Table 2 captures the problems we solved in the training set. They are randomly selected problems from MIPLIB (Gleixner et al. (2021), Koch et al. (2011), Bixby et al. (1998)). We did remove instances that did not complete computation of the objective value within 30 minutes. In total, 27 problem instances are used in this training set. We capture the characteristics of the problem below.

Table 2: The problem instances used for training in §4.2 and §4.3 and their characteristics are shown in this table.

<table>
<thead>
<tr>
<th>Problem Instance</th>
<th>Total variables</th>
<th>Binary variables</th>
<th>General integer variables</th>
<th>Continuous variables</th>
<th>Solutions within 1% of the optimum</th>
</tr>
</thead>
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Appendix B  Problems in the testing set

Table 3 captures the problems we solved in the testing set. They are randomly selected problems from MIPLIB (Gleixner et al. (2021)). We did remove instances that did not complete computation of the objective value within 30 minutes. In total, 9 problem instances are used in this training set. We capture the characteristics of the problem below.

Table 3: The problem instances used for testing in §4.2 and §4.3 and their characteristics are shown in this table.

<table>
<thead>
<tr>
<th>Problem Instance</th>
<th>Total variables</th>
<th>Binary variables</th>
<th>General integer variables</th>
<th>Continuous variables</th>
<th>Solutions within 1% of the optimum</th>
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Appendix C  Parameter groups for diversity-emphasizing rules

Figure 6 shows the clustering of the problem instances into the four groups. As the figure shows, these four groups consolidate to three (HHL, HLL, and LLH) when the number of requested solutions reaches 50 and to two (HHL and HLL) for 200 requested solutions or more. The consolidation to groups HHL and HLL indicate that emphasizing diversity after generating a seed set of solutions results in a higher overall diversity of all generated solutions.

One might suspect that two instances of the same problem (e.g., stein27 and stein45) would typically have the same parameter group. However, surprisingly we found that similar problems like stein27/stein45 and qnet1/qnet1.0 did not always belong to the same group. At $p_1 \geq 50$, some problems took too long to complete all test cases in the grid search and thus were excluded from the parameter groups shown in Figure 6.

Figure 6: The four parameter groups and the problem instances in each group as the number of requested solutions increases from 10 to 1,000.