# Finding Diverse Solutions of High Quality to Binary Integer Programs

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Typical output from an optimization solver is a single optimal solution. At the same time, a set of high-quality and diverse solutions could be beneficial in a variety of contexts, for example problems involving imperfect information, or those for which the structure of high-quality solution vectors can reveal meaningful insights. In view of this, we discuss a new method to obtain multiple high-quality yet diverse solutions to pure binary (0–1) integer programs, employing fractional programming techniques to manage these typically competing goals. Specifically, we develop a general approach that makes use of Dinkelbach's algorithm to sequentially generate solutions that evaluate well with respect to both i) individual performance and, as a whole, ii) mutual variety. Experiments on a number of test instances yield encouraging computational results.

*Key words:* binary (0–1) integer programming; fractional programming; Dinkelbach's algorithm; decision making; multiple solutions; solution diversity; solution quality

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## 1. Introduction

Mathematical programming solvers routinely generate a single optimal solution. While this is essential from the an optimality point of view, there are scenarios where it may be advantageous to consider multiple solutions, and particularly if they are high-quality and diverse. To give a few examples, one could imagine the following scenarios. A project manager wishes to fund several R&D projects subject to a limited budget, and is interested in examining dissimilar solutions with respect to risk exposure. A personnel supervisor has committed to a monthly schedule, and shifting employee availability requires impromptu adjustments. A decision-maker evaluates several attractive options and selects the most appropriate according to their domain expertise. In each of these examples there could be great value in having a readily available set of high-quality and yet diverse solutions.

Mathematical programs are typically abstract representations of real-world problems. Their parameters often include "best-guess" estimates and approximations of uncertain or fluctuating data [1–4], and further may entirely omit factors that are mathematically difficult to express, such

as the quality of work and service [5]. Given this, multiple solutions of high quality may offer more flexibility for the decision maker, especially when they are mutually diverse. Additionally, having several diverse solutions that evaluate well can provide insight into attractive features and inherent tradeoffs in the solution space. This is important, for example, in situations that are time-sensitive or cost-sensitive, or for one-time decisions having significant implications [see, e.g., 6, 7].

Many studies [8–12] discuss the merit of multiple high-quality solutions. While quality is clearly important, solution diversity seems to receive somewhat less exposure, appearing in domains such as mixed integer programming [9, 10, 12], constraint programming [13], heuristic search [14–16] and multiobjective optimization [17].

Although a number of effective approaches exist to generate either diverse or high-quality solutions independently, few can accomplish both simultaneously [11]. Solutions of relatively high quality tend to display strong structural similarities among the variable values. On the other hand, solutions that exhibit higher diversity may well have disparate objective function values given their lack of proximity in the feasible region. Thus, an inherent tension exists when simultaneously considering both quality and diversity.

Even so, the ability to generate multiple solutions of high quality in reasonable time clearly exists given contemporary computational capabilities and industrial-strength solvers. While too many solutions may prove overwhelming to decision makers [9], a handful of such solutions, properly chosen, is of great benefit in the decision-making process [9, 10], and can serve to paint a more complete landscape of the possibilities that a decision maker may consider. This is the topic we address in this paper. Namely, we discuss how to effectively generate a manageable set of diverse yet high-quality solutions for pure binary (0–1) integer programs. This is an important class of mathematical programs, including combinatorial optimization problems such as the knapsack, assignment, bin-packing, traveling salesman, and various scheduling problems, among others [18, 19].

Our contribution is a relatively fast and efficient method to dynamically generate multiple high-quality and diverse solutions to binary integer programs. The method is straightforward to implement and works in conjunction with any integer programming solver. Moreover, our approach, by construction, contains an optimal solution to the original problem – an important consideration in instances that feature exact problem data.

The remainder of the paper is organized as follows. We formally define the problem we solve in Section 2, and propose metrics for solution quality and diversity. In Section 3 we describe our approach for selecting a reasonably-sized set of such solutions. Section 4 highlights our computational experiments and results on test instances from the literature, while Section 5 concludes with

directions for future work.

## 2. Problem Description

Consider the general pure binary integer programming optimization problem:

$$\begin{aligned} \max \quad & \left\{ c^\top x \mid x \in \mathcal{S} \right\}, \\ \text{where} \quad & \mathcal{S} = \{ x \in \{0,1\}^n : Ax \leq b \}. \end{aligned} \tag{BIP}$$

Problem (BIP) consists of a vector $x$ of binary variables of dimension $n$, a right-hand side vector $b \in \mathbb{R}^m$, together with a matrix $A \in \mathbb{R}^{m \times n}$ and a vector $c \in \mathbb{R}^n$. We assume $\mathcal{S} \neq \emptyset$, and note that the feasibility set $\mathcal{S}$ is bounded. Without loss of generality we consider only the maximization case.

Let $x^* \in \mathcal{S}$ be an optimal solution to (BIP) and $z^* = c^\top x^*$ be its optimal objective function value. For the sake of exposition, we assume there exists at least one alternative feasible solution in addition to $x^*$ in $\mathcal{S}$, i.e., $\mathcal{S} \setminus \{x^*\} \neq \emptyset$, so that the discussion on alternate solutions is relevant. With respect to $x^*$ and $z^*$, we next briefly review some common ways to assess diversity as well as quality.

### 2.1 Assessing Diversity, Assessing Quality

Measuring diversity between two binary vectors (e.g., $x^*, x \in \mathcal{S}$) can be accomplished using a variety of metrics, for example the $L_1$ (taxicab) norm and the $L_2$ (Euclidean) norm.

The quality of any $x \in \mathcal{S}$ is measured with objective function $c^\top x$, taking a maximum value at $z^* = c^\top x^*$. The distance from the optimal objective function value $z^*$ can be expressed as:

$$z^* - c^\top x, \tag{1}$$

which is nonnegative for any $x \in \mathcal{S}$ as $z^* = c^\top x^* \geq c^\top x$. The quality of the solution $x$ deteriorates as this difference grows larger.

### 2.2 Simultaneously Addressing Solution Diversity and Quality

While for any $x \in \mathcal{S}$ we can independently assess both diversity and quality, as mentioned in Section 1 solutions that perform well tend to lack diversity due to structural similarities. Likewise, solutions that score rather high in diversity are likely to be from a remote area of the feasible region, and thus may not evaluate well in terms of the objective function. This situation produces tension when both are desirable.

Multiobjective optimization is one approach used to handle the conflicting objectives of achieving diversity while ensuring quality [20, 21]. Metaheuristic approaches are also considered to bring

about diversity in solution sets of multiobjective problems [14, 15, 22], including approaches that aim to improve the distribution of non-dominated solutions [23, 24]. Another common way to resolve two conflicting objectives is by optimizing one of the objectives while constraining the other, for example as in classical portfolio theory [25].

We propose an alternate methodology to achieve balance between solution quality and diversity. Given problem (BIP) and $x^*$, $z^*$, consider the modified objective:

$$\mathcal{R} = \frac{N(x)}{D(x)} = \frac{\text{relative solution diversity}}{\text{relative deterioration in objective function quality}}. \tag{2}$$

With respect to $x^*$ and $z^*$, given any $x \in \mathcal{S}$, objective $\mathcal{R}$ expresses the ratio of relative solution diversity to relative deterioration in the objective function corresponding to $x$. To measure solution diversity, we can consider the $L_1$ norm:

$$\|x - x^*\|_1 = \sum_{i=1}^{n} |x_i - x_i^*|, \tag{3}$$

whereas (1) captures the deterioration of the objective function corresponding to $x$. To eliminate scaling issues, we normalize these diversity and quality measures (discussed in Section 2.4) to create relative measures. However, nonlinearities remain in objective (2) arising from both the diversity measure as well as the objective's fractional nature.

### 2.3 Expressing Diversity in a Linear Fashion

The following involves an optimal solution $x^*$ and any $x \in \{0,1\}^n$ and is a linear expression of diversity [26]:

$$\sum_{i:x_i^*=0} x_i + \sum_{i:x_i^*=1} (1 - x_i). \tag{4}$$

**Proposition 1** *With respect to an optimal solution $x^*$ to* (BIP) *and any $x \in \{0,1\}^n$, expressions* (3) *and* (4) *are equivalent over all $x \in \{0,1\}^n$.*

**Proof.** For any $x_i, i = 1, \ldots, n$, there are four cases to consider; two where $x_i$ and $x_i^*$ are not equal, and two where they are equal. If $x_i \neq x_i^*$, then either i) $x_i = 0$ and $x_i^* = 1$, so that both (3) and (4) evaluate to 1 because $|x_i - x_i^*| = 1$ and $(1 - x_i) = 1$; or else ii) $x_i = 1$ and $x_i^* = 0$, where again both (3) and (4) evaluate to 1 because $|x_i - x_i^*| = 1$ and $x_i = 1$. If $x_i = x_i^*$, then both (3) and (4) evaluate to 0. ■

Metric (4) is linear, and introducing it as the diversity measure in (2) gives an advantage over more conventional but nonlinear norm metrics. We note that this is possible due to the binary nature of the decision variables.

### 2.4 Normalizing Objective Terms

Diversity expression (4) and quality expression (1) may be of widely varying scale, and can thereby introduce a predisposed bias into the ratio $\mathcal{R}$. To offset any disparate magnitudes in these metrics, we normalize both expressions.

For the diversity metric, we use the length of the interval over which diversity can vary from $x^*$ within $\mathcal{S}$ [27]:

$$\text{max diversity} - \text{min diversity} = \max_{x \in \mathcal{S}} \left\{ \sum_{i:x_i^*=0} x_i + \sum_{i:x_i^*=1} (1 - x_i) \right\}, \tag{5}$$

By definition the minimum diversity value is zero, so (5) can be determined by solving a single binary integer program. The relative solution diversity can be found by dividing diversity measure (4) by (5).

To normalize quality, we use the length of the interval over which the solution quality can deteriorate from $x^*$ within $\mathcal{S}$ (as measured by the objective):

$$\text{max deterioration} - \text{min deterioration} = \max_{x \in \mathcal{S}} \left\{ z^* - c^\top x \right\}, \tag{6}$$

As in (5), we solve a single binary integer program, and similarly note that the minimum deterioration value is zero. Thus the relative objective function deterioration can be found by dividing (1) by (6).

We merge normalization factors (5) and (6) into a single factor:

$$\mathcal{F} = \frac{\max\limits_{x \in \mathcal{S}} \left\{ z^* - c^\top x \right\}}{\max\limits_{x \in \mathcal{S}} \left\{ \sum\limits_{i:x_i^*=0} x_i + \sum\limits_{i:x_i^*=1} (1 - x_i) \right\}}. \tag{7}$$

The nonnegativity of (5) and (6) imply that normalization factor $\mathcal{F}$ is nonnegative. Additionally, should the cost of solving two additional binary integer programs be very high for a given problem instance, an approximate value for $\mathcal{F}$ may be computed by relaxing the binary variables and solving the linear programming relaxations.

### 2.5 Putting It All Together

With respect to $x^*$ and $z^*$, the following optimization problem over $\mathcal{S}$ identifies an $x \in \mathcal{S}$ that maximizes the ratio of relative diversity to relative objective function deterioration:

$$\max_{x \in \mathcal{S}} \quad \mathcal{R} = \mathcal{F} \, \frac{N(x)}{D(x)} = \mathcal{F} \, \frac{\left( \sum\limits_{i:x_i^*=0} x_i + \sum\limits_{i:x_i^*=1} (1 - x_i) \right)}{(z^* - c^\top x) + \epsilon}, \tag{8}$$

where $\epsilon$ is a small positive constant that serves to ensure the denominator remains positive, an important consideration given the tendency for some binary integer programs to exhibit multiple optimal solutions [see, e.g., 28].

# 3. Solution Approach: Incorporating Diversity and High Quality

Formulation (8) is a specific type of mathematical program known as a fractional, or hyperbolic, binary programming problem [29], an area that has been studied extensively [30–32, among others]. To establish a convention for the ensuing discussion, we now denote an original optimal solution of (BIP) as $x^{(0)^*}$ in lieu of $x^*$. We first discuss how to obtain a single diverse and high-quality solution, and then elaborate on finding multiple such solutions.

## 3.1 Finding A Single Diverse Solution of High Quality

Dinkelbach's Algorithm [33] can solve the fractional binary program in (8). It does so by solving a sequence of linearized problems that are related to the original nonlinear fractional programming problem. Algorithm 1 details our implementation, with $\mathcal{S}$ as in (BIP), some initial feasible solution $x^0$ (e.g., $x^{(0)^*}$), $\mathcal{F}$ as in (7), and $N(x)$ and $D(x)$ as in (8).

**Algorithm 1** Dinkelbach: Find Diverse, High-Quality Solution via (8)

**Input:** Feasibility set $\mathcal{S}$, $x^0$, normalization factor $\mathcal{F}$, numerator $N(x)$, and denominator $D(x)$.
**Output:** Optimal solution $x^k$.

1: **DINKELBACH**$(\mathcal{S}, x^0, \mathcal{F}, N(x), D(x))$
2: Let $k \leftarrow 0$.
3: **repeat**
4: Compute $\lambda^{(k+1)} \leftarrow \mathcal{F}\frac{N(x^k)}{D(x^k)}$, and let $k \leftarrow k+1$.
5: Determine $x^k \leftarrow \underset{x \in \mathcal{S}}{\operatorname{argmax}} \left\{\mathcal{F}N(x) - \lambda^k D(x)\right\}$.
6: **until** $\mathcal{F}N(x^k) - \lambda^k D(x^k) = 0$.
7: **return** Optimal solution $x^k$.

Algorithm 1 operates by computing the value for parameter $\lambda^k$ with respect to solution $x^k$ in Step 4. It subsequently uses that value to solve the parameterized optimization problem in Step 5, returning $x^k$. When the parameter $\lambda^k$ reaches a value such that the resulting $x^k$ satisfies $\mathcal{F}N(x^k) - \lambda^k D(x^k) = 0$, Algorithm 1 terminates. Upon completion at iteration $k$, it returns an optimal solution $x^k$ that maximizes the ratio of relative solution diversity to relative deterioration in objective function quality. While each subproblem in Step 5 is, in general, an $\mathcal{NP}$-Hard problem, Dinkelbach's algorithm itself has been shown to have superlinear convergence [34].

### 3.2 Finding Multiple Diverse Solutions of High Quality

While Algorithm 1 generates a single high-quality and diverse solution with respect to $x^{(0)^*}$, it may very well be desirable to identify a set $\mathcal{X}$ containing high-quality and diverse solutions. We can construct such a set $\mathcal{X}$ by iteratively calling Algorithm 1 as will be discussed in Algorithm 2, after having addressed some preliminary considerations.

Let us consider constructing $\mathcal{X}$ by successively generating solutions that exhibit both high quality and diversity. Beginning with $\mathcal{X}$ empty, we first add $x^{(0)^*}$ to $\mathcal{X}$, so that $\mathcal{X} = \left\{x^{(0)^*}\right\}$. An initial call to Algorithm 1 generates a solution that is optimal with respect to $\mathcal{S}$ and the fractional objective in (8); however, to repeat this process, two additional considerations must be taken into account.

First, whereas the previous diversity measure (4) measures the distance from a single binary vector, we are now interested in solutions that are diverse – not solely from $x^{(0)^*}$ – but also from all elements presently in $\mathcal{X}$. Consider this process for iteration $\ell > 1$. The diversity measure for each subsequent solution should reflect the relative distance from all elements contained in $\mathcal{X} = \left\{x^{(0)^*}, \ldots, x^{(\ell-1)^*}\right\}$; otherwise maximizing a distance metric such as (4) continues to emphasize movement away from only $x^{(0)^*}$. So we propose the following modified diversity metric that makes use of the centroid $\mathbf{c} = \left(\mathbf{c}_i = \frac{1}{\ell}\sum_{j=0}^{\ell-1} x_i^{(j)^*}, i = 1, \ldots, n\right)$ to capture collective movement away from all elements presently contained in $\mathcal{X}$:

$$\sum_{i=1}^{n} \{(1-\mathbf{c}_i)x_i + \mathbf{c}_i(1-x_i)\} = \sum_{i=1}^{n} \mathbf{c}_i + \sum_{i=1}^{n}(1-2\mathbf{c}_i)x_i. \tag{9}$$

Nonnegative expression (9) generalizes (4), as can be seen in the case of $\mathcal{X} = \left\{x^{(0)^*}\right\}$. It computes the average $L_1$ distance from the elements of $\mathcal{X}$, uniformly measuring diversity away from all elements of $\mathcal{X}$. It can also be seen as a voting scheme that places varying emphasis upon each $x_i$ based upon the cumulative weighting over values of $x_i^{(j)^*}$ from previous iterations.

Second, to construct a set $\mathcal{X}$ of diverse solutions, we need to enforce that a unique solution, if one exists, is returned upon each call to Algorithm 1. That is, we want to ensure that previous solutions are not revisited on subsequent iterations. We can accomplish this by prohibiting previous solutions $x^{(\ell)^*}$ through the following inequality [35]:

$$\sum_{i:x_i^{(\ell)^*}=0} x_i + \sum_{i:x_i^{(\ell)^*}=1} (1-x_i) \geq 1. \tag{10}$$

We use (10) to define an updated feasibility set in Step 3 of Algorithm 2.

For iteration $\ell$, we can also define normalization factor $\mathcal{F}_\ell$ as:

$$\mathcal{F}_\ell = \frac{\max\limits_{x \in \mathcal{S}_\ell} \left\{ z^* - c^\top x \right\}}{\max\limits_{x \in \mathcal{S}_\ell} \left\{ \sum\limits_{i=1}^{n} \mathbf{c}_i + \sum\limits_{i=1}^{n} (1 - 2\mathbf{c}_i) x_i \right\} + \epsilon}, \tag{11}$$

where we introduce some small constant $\epsilon > 0$ to prevent division by zero in the unusual case where there are no additional feasible solutions in $\mathcal{S}_\ell$ distinct from the element(s) of $\mathcal{X}$.

We note that the deterioration in the objective function as expressed in (1) remains a valid measure for every solution $x \in \mathcal{S}_\ell$, and so no adjustment is necessary to account for multiple solutions. Taking $N_\ell(x)$ as in (9), this leads to the following optimization problem:

$$\max_{x \in \mathcal{S}_\ell} \quad \mathcal{R}_\ell = \mathcal{F}_\ell \, \frac{N_\ell(x)}{D(x)} = \mathcal{F}_\ell \, \frac{\left( \sum\limits_{i=1}^{n} \mathbf{c}_i + \sum\limits_{i=1}^{n} (1 - 2\mathbf{c}_i) x_i \right)}{(z^* - c^\top x) + \epsilon}. \tag{12}$$

Given a finite positive integer $\mathcal{K} \geq 2$, Algorithm 2 will return a set $\mathcal{X}$ of the $\mathcal{K}$-best solutions by solving (12) in an iterative manner. Of course, it may occur that fewer than $\mathcal{K}$ solutions are returned, for example if $\mathcal{S}$ contains only a small number of feasible solutions.

We compute the collective diversity of solutions in $\mathcal{X}$ along the lines of [12] and [36], that is:

$$D_{bin}(\mathcal{X}) = \frac{2}{n|\mathcal{X}|(|\mathcal{X}| - 1)} \sum_{i=1}^{n} \sum_{j=1}^{|\mathcal{X}|-1} \sum_{\ell=j+1}^{|\mathcal{X}|} \left| x_i^{(j)^*} - x_i^{(\ell)^*} \right|. \tag{13}$$

We use (13) to evaluate the collective diversity of $\mathcal{X}$ after its return from Algorithm 2.

### 3.3 Additional Algorithmic Considerations

We next discuss two enhancements for our approach. The first reduces the total number of iterations in every call to Algorithm 1, which in turn improves the overall computational performance of Algorithm 2. Second, we highlight the adaptability of our approach by proposing an additional diversity metric that measures the minimum distance from all previously identified solutions in $\mathcal{X}$.

#### 3.3.1 Decreasing The Iteration Count in Dinkelbach's Algorithm

Step 10 of Algorithm 2 requires an initial solution to be passed to Algorithm 1. Some candidates are feasible solutions from previously solved integer programs, such as those arising from the integer programs in (11), as well intermediate solutions from Step 5 of Algorithm 1. We propose to maintain a list $\mathcal{L}$ of such solutions. This choice is important for the overall efficiency of Algorithm 2, because every call to Algorithm 1 results in an integer program being solved in Step 5 for

**Algorithm 2** Finding $\mathcal{K}$-best Solutions via Dinkelbach's Algorithm

**Input:** Feasibility set $\mathcal{S}$, $x^{(0)^*}$, $z^*$, and finite integer $\mathcal{K} \geq 2$.
**Output:** Set $\mathcal{X}$ of $\mathcal{K}$-best solutions (or fewer, if $\mathcal{S}$ contains fewer than $\mathcal{K}$ feasible solutions).

1: Initialize $\mathcal{X} \leftarrow x^{(0)^*}$, let $\ell = 0$, and let $\mathcal{S}_\ell \leftarrow \mathcal{S}$.
2: **repeat**
3: $\quad \mathcal{S}_{\ell+1} \leftarrow \mathcal{S}_\ell \cap \left\{ \sum_{i:x_i^{(\ell)^*}=0} x_i + \sum_{i:x_i^{(\ell)^*}=1} (1 - x_i) \geq 1 \right\}$.
4: $\quad \ell \leftarrow \ell + 1$.
5: $\quad$ **if** $\mathcal{S}_\ell = \emptyset$ **then**
6: $\quad\quad$ **return** Proof of infeasibility and partial set $\mathcal{X}$.
7: $\quad$ **else**
8: $\quad\quad$ Compute current normalization factor $\mathcal{F}_\ell$ based on $\mathcal{X}$ and (11).
9: $\quad\quad$ Derive current numerator $N_\ell(x)$ for (12) based on $\mathcal{X}$ and (9).
10: $\quad\quad$ Identify initial solution $x^0$ to pass into Algorithm 1.
11: $\quad\quad$ $x^{(\ell)^*} \leftarrow$ **DINKELBACH**$(\mathcal{S}_\ell, x^0, \mathcal{F}_\ell, N_\ell(x), D(x))$.
12: $\quad\quad$ Add optimal solution $x^{(\ell)^*}$ to $\mathcal{X}$, i.e., $\mathcal{X} \leftarrow \mathcal{X} \cup \{x^{(\ell)^*}\}$.
13: **until** $|\mathcal{X}| = \mathcal{K}$.
14: **return** $\mathcal{X}$.

each iteration. Thus reducing the overall number of iterations per call to Algorithm 1 can have a significant effect on the performance of Algorithm 2. For each iteration $\ell$, in Step 10 of Algorithm 2 we choose $x^0 \in \underset{x \in \mathcal{L}}{\operatorname{argmax}} \left\{ \mathcal{F}_\ell \frac{N_\ell(x)}{D(x)} \right\}$.

### 3.3.2 Alternative Diversity Metric

There are a variety of ways to evaluate diversity. To illustrate that our approach works with other diversity measures, we consider the following metric that measures the minimum distance from previously identified solutions in $\mathcal{X}$:

$$\min_{j=0,\ldots,\ell-1} \left\{ \sum_{i:x_i^{(j)^*}=0} x_i + \sum_{i:x_i^{(j)^*}=1} (1 - x_i) \right\}. \tag{14}$$

As an alternative to diversity measure (9) in Algorithm 2, metric (14) can also be maximized over all $x \in \mathcal{S}_\ell$ to find a most diverse element:

$$\max_{x \in \mathcal{S}_\ell} \mathcal{R}_\ell = \mathcal{F}_\ell \, \frac{N_\ell(x)}{D(x)} = \mathcal{F}_\ell \, \frac{\left( \min_{j=0,\ldots,\ell-1} \left\{ \sum_{i:x_i^{(j)^*}=0} x_i + \sum_{i:x_i^{(j)^*}=1} (1 - x_i) \right\} \right)}{(z^* - c^\top x) + \epsilon}. \tag{15}$$

While the expression in (14) is nonlinear, it is straightforward to linearize. This can be done by adding a single unrestricted variable $q$ which is maximized over all $x \in \mathcal{S}_\ell$, and lower bounds, for

every element of $\mathcal{X}$, the inner diversity metric in (14) (i.e., expression (4)). Thus, for every iteration of Algorithm 2, a single constraint is added to $\mathcal{S}_\ell$ to ensure this relationship.

# 4. Computational Discussions

We begin this section by comparing and contrasting relevant computational experiments, and subsequently discuss the computational performance of Algorithm 2.

## 4.1 Comparing and Contrasting Related Methods in the Literature

Two of the most relevant studies to our work are [10] and [12]. The main emphasis of [10] is finding high-quality solutions to mixed-integer programs in an efficient manner, although diversity is only tangentially discussed in Algorithm 5. However, diversity is a central focus in [12], where after pre-populating a set $S$ of high-quality solutions, the authors use both exact and heuristic approaches to identify a subset of $p$ solutions that are of maximum collective diversity. Similarly, our approach implements exact approaches to identify a set of several high-quality and diverse solutions. Whereas [10] and [12] operate on mixed-integer programs, at present we concern ourselves with only binary integer programs.

Both aforementioned studies use a proprietary method (namely, the *one-tree* algorithm [37]) to identify a large set $S$ containing solutions within $q\%$ of the optimum. While a threshold of 1% is quite reasonable, it is ultimately subjective, potentially excluding a valuable solution having much higher diversity lying just outside the quality threshold. Our approach, on the other hand, sequentially generates the most attractive high-quality and diverse solutions that maximize ratio $\mathcal{R}_\ell$ in (12) or (15). Further, our approach is free to operate in conjunction with any integer programming solver, and is likewise free of the up-front requirements to pre-identify and store potentially large amounts of information in memory, a significant limitation in the computational findings of [12]. Finally, our approach explicitly includes an actual optimal solution of (BIP). Depending upon the problem context and corresponding data accuracy, this may be of critical importance to decision makers, e.g., some combinatorial optimization problems such as the traveling salesman problem can have precise data.

## 4.2 Computational Setup

In advance of discussing our computational findings, we next detail the test sets and environment used to evaluate our algorithmic approaches.

#### 4.2.1 Computational Test Sets

We considered two test sets. The first was comprised of seven multiple knapsack instances from [38, 39]. The second consisted of more difficult pure binary integer programming instances from MIPLIB 2003 [40] and MIPLIB 2010 [41] having an "easy" categorization and nonempty feasible regions. Twelve of the MIPLIB 2003 instances coincided with those considered in [12].

#### 4.2.2 Computational Environment

We developed our algorithms in C++ and compiled the source code using g++ version 4.4.6 20110731 (Red Hat 4.4.6-3) on a Dell R610 server with 2 Intel Xeon X5690 CPUs each with 6 cores running at 3.47 GHZ and 48GB of RAM. We used the callable library of IBM ILOG CPLEX 12.4 [37] to perform the optimization, and implemented a time limit of one hour for the solution to any binary integer program (e.g., Step 8 of Algorithm 2; Step 5 of Algorithm 1). Given the large potential numerator to denominator ratios for our objective function, we set the CPX_NUMERICAL_EMPHASIS parameter to CPX_ON to prioritize numerical stability. Finally, analogous to [12], we set our algorithm to retrieve $\mathcal{K} = 10$ solutions.

### 4.3 Computational Results

Table 1 displays our computational results on the first test set of seven multiple knapsack instances from [39], while Table 2 displays our results on the MIPLIB test instances. Of the 72 total MIPLIB test instances, it displays the 40 instances for which $|\mathcal{X}| \geq 2$ for at least one of diversity measures (9) and (14). The column entitled "Instance" indicates whether the instance came from MIPLIB 2003 or MIPLIB 2010[†], while the column entitled "$m \times n$" indicates the number of rows and columns. The column entitled "Mean Iterations" reports the average number of iterations for a given call to Algorithm 1 using diversity measures (9) and (14), while the column $D_{bin}(\mathcal{X})$ reports the value of (13) using diversity measures (9) and (14) as well as the diversity reported in [12][‡].

#### 4.3.1 Computational Results: Performance of Algorithm 2

For the first test set, our approach identified $|\mathcal{X}| = 10$ solutions to all seven multiple knapsack instances using each of diversity measures (9) and (14). For (9), the mean number of iterations was 2.5, the mean runtime for the algorithm was 95 seconds, and the mean value of $D_{bin}(\mathcal{X})$ was 25.4%, while for measure (14) these values were 2.9 iterations, 94 seconds, and 27.3%, respectively.

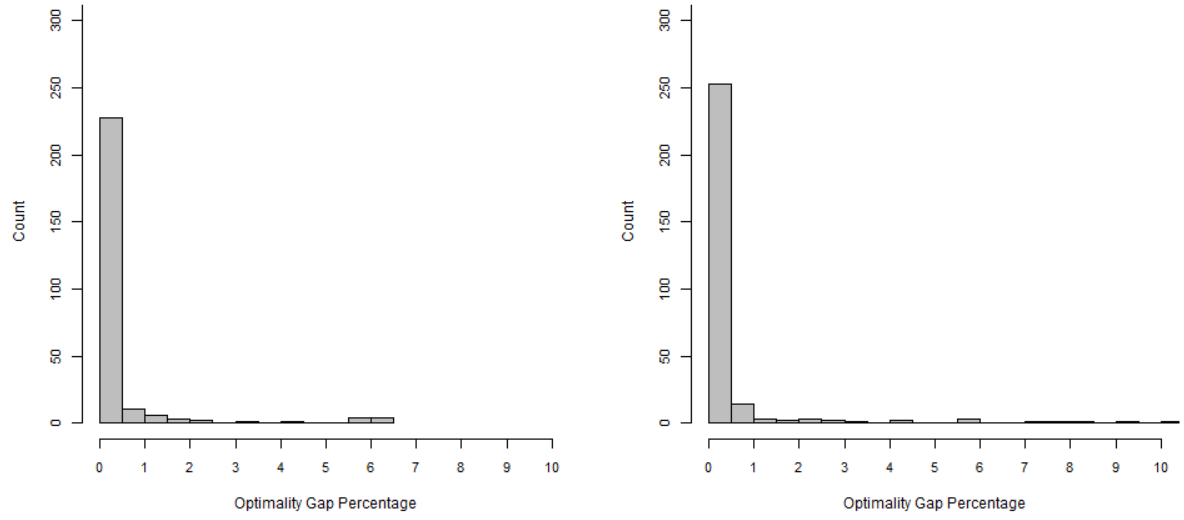
For the second test set, there were 29 MIPLIB instances for which we were able to obtain $|\mathcal{X}| = 10$ solutions using both diversity measures (9) and (14). For (9), the mean number of

Table 1: Algorithm 2 on Multidimensional Knapsack Problems [39]

| | | | $\lvert\mathcal{X}\rvert$ | | Mean Iterations | | Time (seconds) | | $D_{bin}(\mathcal{X})$ | |
|---|---|---|---|---|---|---|---|---|---|---|
| Instance | $m$ | $n$ | (9) | (14) | (9) | (14) | (9) | (14) | (9) | (14) |
| mknap_1 | 10 | 6 | 10 | 10 | 2.3 | 2.7 | <1 | <1 | 0.4556 | 0.4556 |
| mknap_2 | 10 | 10 | 10 | 10 | 2.3 | 2.6 | <1 | 6 | 0.3622 | 0.4044 |
| mknap_3 | 10 | 15 | 10 | 10 | 2.4 | 2.6 | 143 | 26 | 0.2548 | 0.2548 |
| mknap_4 | 10 | 20 | 10 | 10 | 2.6 | 2.8 | 127 | 134 | 0.2456 | 0.2556 |
| mknap_5 | 10 | 28 | 10 | 10 | 2.9 | 2.6 | 169 | 149 | 0.1643 | 0.1579 |
| mknap_6 | 5 | 39 | 10 | 10 | 2.6 | 3.1 | 94 | 145 | 0.1698 | 0.2285 |
| mknap_7 | 5 | 50 | 10 | 10 | 2.3 | 3.7 | 128 | 199 | 0.1249 | 0.1587 |

iterations was 2.3, the mean runtime was 4,995 seconds, and the mean value of $D_{bin}(\mathcal{X})$ was 7.1%, whereas for measure (14) these values were 2.6 iterations, 6,010 seconds, and 7.3%, respectively.

We observe some interesting and consistent behavior from these aggregate results. It appears that diversity measure (9) is able to find the full number of solutions (ten), on average, with slightly fewer iterations and in less overall time (though all of these instances completed in under 12 hours for either of the two metrics). With respect to the overall diversity of the set $|\mathcal{X}|$ using (13), metric (14) slightly outperformed (9) across both test sets. Thus both measures appear to have their respective merits.




(a) 270 Alternate Solutions Using (9)

(b) 270 Alternate Solutions Using (14)

Figure 1: Solution Quality – Highlighting Optimality Gap of 270 Alternate Solutions from 30 MIPLIB Instances for which $|\mathcal{X}| = 10$

Table 2: Algorithm 2 on BIP Instances from MIPLIB [40, 41]

| | | | $\lvert\mathcal{X}\rvert$ | | Mean It. | | Time (sec) | | $D_{bin}(\mathcal{X})$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Instance | $m$ | $n$ | (9) | (14) | (9) | (14) | (9) | (14) | (9) | (14) | DW[‡] |
| acc-tight5[†] | 3,052 | 1,339 | 10 | 10 | 2.0 | 2.0 | 15,065 | 21,616 | 0.1431 | 0.1416 | |
| acc-tight6[†] | 3,047 | 1,335 | 10 | 10 | 1.0 | 1.0 | 10,150 | 11,734 | 0.1512 | 0.1478 | |
| air03 | 124 | 10,757 | 10 | 10 | 2.7 | 3.0 | 67 | 210 | 0.0006 | 0.0009 | |
| air04 | 823 | 8,904 | 10 | 10 | 2.7 | 2.8 | 23,188 | 5,867 | 0.0029 | 0.0028 | |
| air05 | 426 | 7,195 | 10 | 10 | 2.9 | 3.9 | 1,148 | 3,666 | 0.0052 | 0.0070 | |
| bley_xl1[†] | 175,620 | 5,831 | 10 | 10 | 2.3 | 2.7 | 1,136 | 1,381 | 0.0064 | 0.0056 | |
| cap6000 | 2,176 | 6,000 | 10 | 10 | 3.1 | 3.0 | 253 | 452 | 0.0022 | 0.0022 | 0.0088 |
| eil33-2[†] | 32 | 4,516 | 10 | 10 | 2.2 | 2.8 | 1,593 | 4,212 | 0.0018 | 0.0020 | |
| eilB101[†] | 100 | 2,818 | 10 | 10 | 3.1 | 3.6 | 17,863 | 24,637 | 0.0082 | 0.0096 | |
| l152lav | 97 | 1,989 | 10 | 10 | 2.2 | 2.6 | 198 | 426 | 0.0112 | 0.0121 | 0.0225 |
| lseu | 28 | 89 | 10 | 10 | 2.6 | 2.8 | 198 | 373 | 0.1333 | 0.1498 | |
| mine-166-5[†] | 8,429 | 830 | 10 | 10 | 3.0 | 4.1 | 8,202 | 14,522 | 0.0052 | 0.0056 | |
| mitre | 2,054 | 10,724 | 10 | 10 | 2.3 | 2.3 | 24 | 63 | 0.0037 | 0.0037 | |
| mod008 | 6 | 319 | 10 | 10 | 2.3 | 2.7 | 67 | 932 | 0.0145 | 0.0170 | 0.0220 |
| mod010 | 146 | 2,655 | 10 | 10 | 2.3 | 2.3 | 147 | 198 | 0.0059 | 0.0059 | 0.0230 |
| neos-777800[†] | 479 | 6,400 | 10 | 10 | 1.0 | 1.0 | 383 | 88 | 0.0250 | 0.0250 | |
| neos-957389[†] | 5,115 | 6,036 | 10 | 10 | 2.0 | 2.0 | 72 | 89 | 0.0250 | 0.0249 | |
| ns1688347[†] | 4,191 | 2,685 | 10 | 10 | 2.1 | 2.1 | 12,298 | 16,303 | 0.0320 | 0.0294 | |
| nw04 | 36 | 87,482 | 10 | 10 | 2.6 | 3.1 | 171 | 432 | 0.0001 | 0.0001 | 0.0001 |
| opm2-z7-s2[†] | 31,798 | 2,023 | 10 | 10 | 2.6 | 2.9 | 12,952 | 19,398 | 0.0375 | 0.0797 | |
| p0033 | 16 | 33 | 10 | 10 | 2.2 | 2.2 | 74 | 371 | 0.1778 | 0.1758 | 0.2707 |
| p0201 | 133 | 201 | 10 | 10 | 2.3 | 2.6 | 110 | 355 | 0.1612 | 0.1650 | 0.1705 |
| p0282 | 241 | 282 | 10 | 10 | 3.0 | 3.4 | 251 | 1,253 | 0.0072 | 0.0071 | 0.1118 |
| p0548 | 176 | 548 | 10 | 10 | 2.6 | 2.6 | 444 | 966 | 0.0371 | 0.0360 | 0.0587 |
| p2756 | 755 | 2,756 | 10 | 10 | 2.7 | 2.6 | 389 | 1,436 | 0.0627 | 0.0624 | |
| reblock67[†] | 2,523 | 670 | 10 | 10 | 3.6 | 3.6 | 37,656 | 42,174 | 0.0051 | 0.0110 | |
| stein27 | 118 | 27 | 10 | 10 | 1.0 | 1.0 | 35 | 105 | 0.4889 | 0.4840 | 0.4889 |
| stein45 | 331 | 45 | 10 | 10 | 1.6 | 1.9 | 585 | 805 | 0.4840 | 0.4602 | 0.4840 |
| tanglegram2[†] | 8,980 | 4,714 | 10 | 10 | 2.0 | 2.3 | 123 | 239 | 0.0318 | 0.0306 | |
| neos-1440225[†] | 330 | 1,285 | 6 | 10 | 1.0 | 1.0 | 12,802 | 12,115 | 0.0546 | 0.0538 | |
| ex9[†] | 40,962 | 10,404 | 8 | 8 | 1.0 | 1.0 | 89 | 91 | 0.0134 | 0.0134 | |
| tanglegram1[†] | 68,342 | 34,759 | 10 | 5 | 2.2 | 2.8 | 32,073 | 29,161 | 0.0114 | 0.0119 | |
| neos808444[†] | 18,329 | 19,846 | 8 | 3 | 1.0 | 1.0 | 16,571 | 7,354 | 0.0499 | 0.0508 | |
| acc-tight4[†] | 3,285 | 1,620 | 6 | 3 | 1.0 | 1.5 | 12,712 | 5,159 | 0.1686 | 0.1778 | |
| enigma | 21 | 100 | 4 | 4 | 2.0 | 2.0 | 45 | 138 | 0.1133 | 0.1133 | |
| neos18[†] | 11,402 | 3,312 | 3 | 2 | 2.5 | 3.0 | 7,782 | 5,240 | 0.1222 | 0.1437 | |
| neos-1109824[†] | 28,979 | 1,520 | – | – | – | – | – | – | – | – | |
| neos-941313[†] | 13,189 | 167,910 | 2 | – | 3.0 | – | 6,860 | – | 0.0081 | – | |
| ns894788[†] | 2,279 | 3,463 | – | 2 | – | 1.0 | – | 7,317 | – | 0.0684 | |

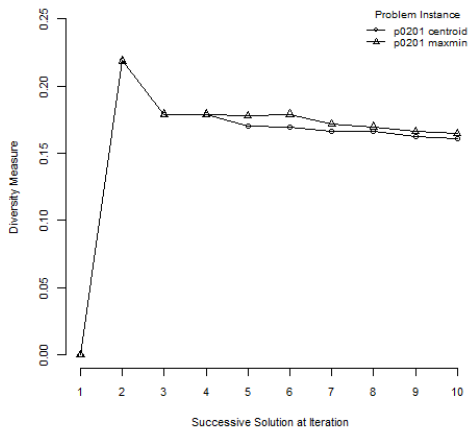
Further investigations into the instances for which we found a full ten solutions yield some intriguing insights. For diversity measure (9), of the 270 total alternative solutions (i.e., not $x^*$) returned from Algorithm 2, over 56% were additional optimal solutions (i.e., no gap in optimality). The distribution of these solutions with respect to their distance from optimality are displayed in Figure 1(a). A similar distribution for measure (14) appears in Figure 1(b) depicting 151 optimal solutions of the 270 total alternate solutions (greater than 55%). From these figures we can see that, while a majority of solutions appear within 1% of optimal, roughly a tenth of all alternative solutions were outside of that range.

Figure 2 illustrates the progression of diversity for metrics (9) and (14) as the set $\mathcal{X}$ is constructed for several instances. For each successive solution on the y-axis, it displays the corresponding values of metric (13). The first, Figure 2(a), exemplifies most instances, in that the diversities obtained with either of metrics (9) or (14) track in a similar manner. However, there are several instances for which this differs. Figures 2(b) and 2(c) demonstrate a few of the instances where metric (9) outperforms (14), while Figure 2(d) illustrates a more exceptional case where (14) outperforms (9). Note that in each of the instances, both diversity measures identify the same first alternate solution (i.e., $x^{(1)^*}$).

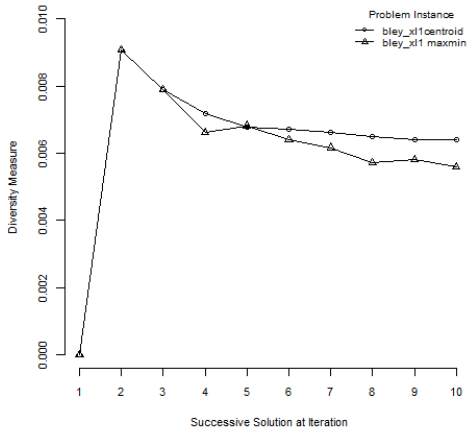
#### 4.3.2 Computational Results: Comparing Related Methods

In our opinion, the computational runtimes reported in Table 2 to generate a small but reasonably-sized set of $\mathcal{K}$ solutions are modest. For most instances we obtained cumulative runtimes in well-under half an hour, while for others (mostly from the more challenging MIPLIB2010) the runtimes were somewhat longer. As depicted in Figure 1, a vast majority of the solutions to individual MIPLIB test instances were very near optimal (i.e. within 0.5%, and included a number of multiple optimal instances). As an example, solving the stein27 instance using (9) took less than a minute to identify a set of ten solutions, all optima, that had a collective diversity value of 0.4889. This diversity value matched that obtained by [12] using a heuristic local search. Only a few instances exhibited solutions with optimality gaps greater than 5%, illustrating that some solutions contribute to the fractional objective by emphasizing diversity.

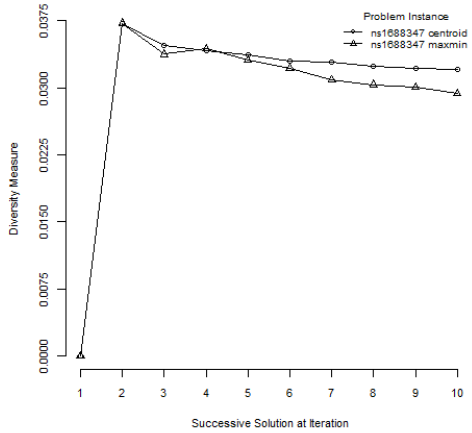
In [12], the task of finding high-quality and diverse solutions is separated into two components: first running the one-tree algorithm for one hour to identify a large set of high-quality solutions (within 1% of optimal), and subsequently finding diverse solutions in this extensive set using either a distinct integer program or via heuristic methods. This contrasts with our approach to simultaneously generate high-quality yet diverse solutions on the fly, and appears to be one of its main



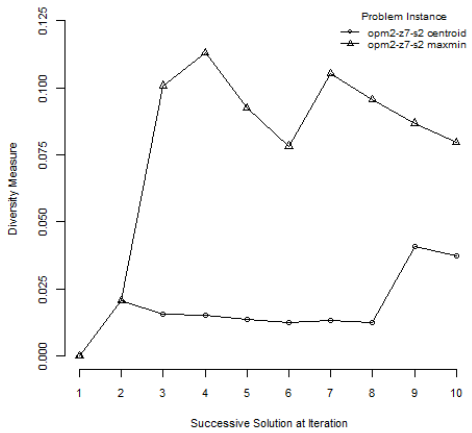

(a) Progression for p0201 instance




(b) Progression for bley_xl1 instance




(c) Progression for ns1688347 instance




(d) Progression for opm2-z7-s2 instance

Figure 2: Progression in Solution Diversity in Successive Iterations of Algorithm 2 Using Metrics (9) and (14)

advantages. Indeed, for eleven of the twelve MIPLIB 2003 instances we had solved in common, we identified ten solutions having competitive values for $D_{bin}(\mathcal{X})$ and averaging just over three minutes in runtime for diversity measure (9), and in just over nine minutes for (14). The longest runtime for these instances was cap6000 using diversity measure (14), lasting almost 30 minutes. In contrast, for each of the cap6000, l152lav, mod010, nw04, p0282, p0548, and stein27 instances, the exact algorithm of [12] did not finish within ten days (although they did obtain superior results in terms of $D_{bin}(\mathcal{X})$ with various heuristic approaches). There was only one instance (disctom) which our approach could not solve that [12] solved.

Thus, while our algorithm takes less time to complete on the eleven solved MIPLIB instances that we had in common, this appears to come at the expense of some solution diversity, a strength of [12] given that they explicitly optimize for diversity over a set $S$ of already identified high-quality solutions. Although on three of these instances (cap6000, mod010, p0282) our approach did not compare well with the heuristic results of [12], we did obtain respectable diversity results in the remaining eight instances. One factor likely contributing to this observation is that, by construction, our approach requires an optimal solution $x^{(0)^*}$ to be included into the solution set $\mathcal{X}$, whereas no such restriction is required in the approaches of [12]. Given these tradeoffs in solution time and overall diversity, it may be best to regard our methodology and that of [12] as complementary.

We should also mention that we tested a rather naïve strategy to find diverse solutions by randomly perturbing objective function coefficients [see, e.g., 42]. However, the approach did not yield a set of solutions that were simultaneously diverse and of high quality. Instead, the sets consistently featured either high-quality solutions with low diversity (corresponding to small perturbations), or solutions with greater diversity but having relatively lower quality (corresponding to higher perturbations).

## 5. Conclusions

We present a new approach to generate multiple high-quality yet diverse solutions to pure binary (0–1) integer programs. Our method simultaneously obtains such solutions to pure binary program (BIP) with a modified, fractional objective over the same feasible region. Given an optimal solution $x^*$ and optimal objective function value $z^*$ to (BIP), we propose two measures of diversity from $x^*$ for the numerator, while the denominator measures the deterioration in objective quality from the optimal value $z^*$. Our algorithmic approach uses an implementation of Dinkelbach's Algorithm [33] to handle the fractional objective and sequentially generates multiple high-quality and

diverse solutions. Computational experiments indicate that the method is efficient given the rather modest runtimes on a variety of test instances from the literature. We also note that our approach is independent of the integer programming solver, and thus could be coupled with, for example, an open source solver such as CBC [43].

It is worth mentioning that certain nonlinear binary integer programs may also be amenable to the proposed methodology, for example if such functions can be represented in a piecewise-linear fashion using binary variables [see, e.g., 44]. Furthermore, our methodology is not limited to calling an IP solver, per se; a call to any blackbox solver or solution approach could be incorporated in Step 5 of Algorithm 1.

Future extensions include allowing weights on the numerator and denominator to promote either greater diversity or quality. Additionally, it may be of interest in the diversification process to weight individual subsets of variables from which subsequent solutions should be particularly far removed, for example, a group of 0–1 variables on which many other model decisions hinge. Still other diversity measures could be incorporated into the numerator of (12). Another avenue is extending the problem setting to integer and mixed integer cases, though as noted in both [10] and [12] expressing diversity involving a set of continuous variables can be challenging.

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