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Variable Neighborhood Descent Branching applied to the Multi-Way Number Partitioning Problem

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Abstract

This paper presents an application of the Variable Neighborhood Descent Branching method to solve the Multi-Way Number Partitioning Problem. This problem consists of distributing the elements of a given sequence into k disjoint subsets such that the sums of each subset elements fit in the shortest interval. It shows a new method to decompose the MWNPP in n-1 subproblems using local branching constraints. This decomposing justifies the neighborhood structure used in the proposed algorithm. The study of parameter settings defines the operation of the proposed algorithm. The results shows that there is no statistically significant difference of objective value between proposed algorithm and mathematical model solved by CPLEX, but the time used by both methods are significantly different.

Keywords: Combinatorial Optimization, Multi-Way Number Partitioning Problem, Variable Neighborhood Descent Branching, Matheuristics.

1 Introduction

A partition of a set X is a collection of mutually disjoint subsets whose union forms X. A k-partition is a partition with exactly k non-empty subsets. In this article, the subsets belonging to the partition are called parts, the set \mathbb{Z}_+ denotes

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the set of strictly positive integers. Furthermore, the notation $I_m = \{y \in \mathbb{Z} : 1 \le y \le m\}$ represents the closed set of integers between 1 and m.

The Two-Way Number Partitioning Problem (TWNPP) consists of finding a 2-partition for the indexes of a given sequence V. The purpose of the problem is to minimize the difference between the sums of elements in distinct parts. A generalization of TWNPP is the Multi-Way Number Partitioning Problem (MWNPP). In this problem, the number of parts k in which the sequence elements V are to be distributed is fixed. Let the weight $g(A_j)$ be given by the sum of the elements whose indexes are contained in the part A_j . Given a numerical sequence V, the goal is to find a k-partition for its indexes, so that the set of weights $\{g(A_j)\}_{j=1}^k$ be contained in the shortest possible interval.

TWNPP is formally listed in [7] as one of the basic NP-complete problems. There are a number of equivalences demonstrated between TWNPP and other NPcomplete problems. On the other hand, MWNPP appears originally in an article about the analysis of a constructive heuristic called Differencing Method, better known as Karmarkar-Karp Heuristic (KKH), proposed in [6]. According to [4], MWNPP is a very difficult problem to solve using general purpose meta-heuristics, such as Genetic Algorithms, Simulated Annealing and others. In many cases, these methods lose in computational time and performance for constructive heuristics such as KKH and even for the Longest Processing Time heuristic (LPT), proposed by [5]. The construction of exact algorithms for the solution of these problems is proposed in [8]. For this, a Backtrack procedure is performed in constructive heuristics. When the LPT heuristic is used during the enumeration, the Complete Greedy Algorithm (CGA) is produced; if KKH is used, the Complete Karmarkar-Karp Algorithm (CKK) is generated. The first improvement to be proposed in these algorithms occurs with the algorithm Recursive Number Partitioning (RNP), proposed by [9]. The second improvement is due to [12], in which a new data structure applied to the CKK algorithm is proposed, speeding up the search in the Karmarkar-Karp Tree. Through successive MWNPP conversions of a (k-1)-partition to a k-partition, [11] proposes an algorithm based on solving smaller subproblems. Currently, the state of the art for MWNPP is the Sequential Number Partitioning algorithm, presented in [10], and the Cached Iterative Weakening algorithm, shown in [14]. A complete and highly relevant analysis of these algorithms is found in [13].

Given a mathematical model for the MWNPP, a branching technique by insertion of Local Branching Constraints is proposed in [3]. These constraints are defined from an initial solution x^s , and determine how close or far a feasible solution can be of x^s . This technique allowed the proposition of many exact and approximate methods for the solution of combinatorial optimization problems. One of these methods is the Variable Neighborhood Descent Branching (VNDB), described in [1], which defines its neighborhoods using Local Branching Constraints.

This article addresses an adaptation of the VNDB method to the MWNPP using the constructive heuristic LPT as an initial solution. The ability to exclude regions already exploited from the search space by simply adding constraints to the mathematical model justifies the application of VNDB to solve this problem. The analysis of the computational time spent and the upper bound for each instance shows that VNDB, with a reasonable number of neighborhoods, finds results as good as the standard CPLEX solver and, in addition, in a shorter run time. The article is organized as follows. Section 2 presents the problem addressed and states a mathematical model for MWNPP. Section 3 introduces an analysis of local branching constraints. Section 4 addresses the proposed VNDB method and evaluates the particularity of its neighborhood in rings. Following, Section 5 presents the computational tests performed for the comparison between the algorithms. Finally, Section 6 concludes the paper, including a critique about the found results and the

proposed scope.

2 Problem Statement

MWNPP treated here is the version originally addressed in [6]. Its input is a sequence V and its output is a k-partition of the indexes of V.

Definition 2.1 Let $V = \{v_1, v_2, \ldots, v_n\}$ be a sequence of positive integers, and k a positive integer. Find a k-partition of the V indexes, in the form $\{A_1, A_2, \ldots, A_k\}$, that minimizes the function:

$$f(\{A_1, A_2, \dots, A_k\}) = \max_{j'} \{g(A_{j'})\} - \min_j \{g(A_j)\}.$$
 (1)

For instance, the sequence $V = \{11, 25, 13, 34, 89, 65, 43, 96, 56, 87\}$ may be partitioned in the ways shown in Table 1 for the values $k \in \{3, 4, 5, 6\}$. The feasible and optimal values of the objective function for these cases are presented in Table 2.

	feasible	optimal			
k = 3	$\underbrace{\{96, 43, 34\}}_{173}, \underbrace{\{89, 56, 25\}}_{170}, \underbrace{\{87, 65, 13, 11\}}_{176}$	$\underbrace{\{89, 87\}}_{176}, \ \underbrace{\{25, 13, 34, 43, 56\}}_{171}, \ \underbrace{\{11, 65, 96\}}_{172}$			
k = 4	$\underbrace{\{96, 25, 13\}}_{134}, \ \underbrace{\{89, 34\}}_{123}, \ \underbrace{\{87, 43\}}_{130}, \ \underbrace{\{65, 56, 11\}}_{132}$	$\underbrace{\{25, 13, 89\}}_{127}, \ \underbrace{\{43, 87\}}_{130}, \ \underbrace{\{34, 96\}}_{130}, \ \underbrace{\{11, 65, 56\}}_{132}$			
k = 5	$\underbrace{\{11, 89, 13\}}_{113}, \ \underbrace{\{25, 87\}}_{112}, \ \underbrace{\{96\}}_{96}, \ \underbrace{\{34, 65\}}_{99}, \ \underbrace{\{43, 56\}}_{99}$	$\underbrace{\{11,89\}}_{100}, \ \underbrace{\{25,87\}}_{112}, \ \underbrace{\{13,96\}}_{109}, \ \underbrace{\{34,65\}}_{99}, \ \underbrace{\{43,56\}}_{99}$			
k = 6	$\underbrace{\{96\}}_{96}, \ \underbrace{\{89\}}_{89}, \ \underbrace{\{87\}}_{87}, \ \underbrace{\{11, 13, 65\}}_{89}, \ \underbrace{\{56, 25\}}_{81}, \ \underbrace{\{43, 34\}}_{77}$	$\underbrace{\{96\}}_{96}, \ \underbrace{\{89\}}_{89}, \ \underbrace{\{87\}}_{87}, \ \underbrace{\{11, 25, 43\}}_{79}, \ \underbrace{\{13, 65\}}_{78}, \ \underbrace{\{34, 56\}}_{90}$			

Table 1 Solutions of MWNPP for $k \in \{3, 4, 5, 6\}$.

	Table 2Objective function values.						
	feasible	optimal					
k = 3	176 - 170 = 6	176 - 171 = 5					
k = 4	134 - 123 = 11	132 - 127 = 5					
k = 5	113 - 96 = 17	112 - 99 = 13					
k = 6	96 - 77 = 19	96 - 78 = 18					

MWNPP can be modeled using binary variables x_{ji} to indicates if the *i*-th term of the sequence V belongs to the part j ($x_{ji} = 1$) or not ($x_{ji} = 0$). Only pairs (j, i) outside the lower right triangle must be set to avoid multiplicities. Using this set of variables, a mixed integer programming (MIP) formulation for MWNPP can be given as:

$$\min t_2 - t_1 \tag{2a}$$

st.
$$t_1 \le \sum_{i=j} v_i x_{ji} \le t_2, \quad \forall j \in I_k$$
 (2b)

$$\sum_{i=1}^{\min\{i,k\}} x_{ji} = 1, \quad \forall i \in I_n$$
(2c)

$$t_1, t_2 \in \mathbb{R}_+ \tag{2d}$$

$$x_{ji} \in \{0, 1\}, \quad \forall (j, i) : i \ge j \tag{2e}$$

The objective function (2a) minimizes the size of the interval containing $\{g(A_j)\}_{j=1}^k$. Constraints (2b) guarantees that each part is non-empty, since $t_1 > 0$, and that the weight associated to each part are contained in the interval $[t_1, t_2]$. Constraints (2c) guarantee that the parts are disjoint and that all elements of V are allocated to some part, since the problem is only well defined when $n \ge k$. Finally, constraints (2d) ensure that the constraints of $\max_j\{g(A_j)\}$ and $\min_j\{g(A_j)\}$ are always positive. This MIP model were first introduced in [2], with a little difference in relation to the variables excluded.

The solution of this model implies the solution of MWNPP, but there is still a surjective correspondence between feasible solutions of the mathematical model and the set of k-partitions.

3 Analysis of Local Branching Constraints

Local Branching constraints define the Hamming distance between a given solution and a feasible solution of the problem by counting the number of variables with different values [3]. Consider an incumbent solution x^s for the mathematical model (2). Let B be the set of pairs of indexes (j, i) such that $x_{ji}^s = 1$. Local Branching constraints are defined by the following expressions:

$$\Delta(x^s, x) := \sum_{ji \in B} (1 - x_{ji}) + \sum_{ji \notin B} x_{ji} \le R$$
(3a)

$$\Delta(x^s, x) := \sum_{ji \in B} (1 - x_{ji}) + \sum_{ji \notin B} x_{ji} = R$$
(3b)

$$\Delta(x^s, x) := \sum_{ji \in B} (1 - x_{ji}) + \sum_{ji \notin B} x_{ji} \ge R$$
(3c)

The constraint (3a) means that a feasible solution must be at a Hamming distance less than or equal to R with respect to the solution x^s . Thus, the neighborhood $\mathcal{N}_R(x^s)$ is a disk of radius R and center x^s . In the constraint (3b), only solutions with Hamming distance exactly equal to R in relation to x^s are allowed. This neighborhood structure is a degenerate ring with center at x^s and internal and external radius equal to R. Finally, the constraint (3c) considers all the space

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outside the radius disk R and center x^s as space of feasible solutions.

It is important to note that Local Branching constraints do not always define the exact neighborhood structure, because its shape will depend on the intersection with the feasible region of the mathematical model of the problem studied.

Let x^1 and x^2 be two distinct feasible solutions of model (2). The first column of the solution matrix always has the values $x_{11}^1 = 1$ and $x_{11}^2 = 1$. Therefore, there are n-1 columns left for the variables to assume different values. From the second column forwards, an increase of at most two units per column at the total Hamming distance can be obtained since, due to the constraints (2c), there is only one j such that $x_{ji} = 1$ for each i column. Thus, the Hamming distance between two feasible solutions of the mathematical model (2) is always an even number. Therefore, it can be concluded that:

$$\forall x^1, x^2 \quad \exists r \in I_{n-1} : \quad \Delta(x^1, x^2) = 2r \tag{4}$$

and, as a consequence of (4), the maximum Hamming distance between two feasible solutions can be given as:

$$\max\{\Delta(x^1, x^2)\} = 2(n-1).$$
(5)

Therefore, there is a decomposition of MWNPP into subproblems with constraints (3b). Using the equation (4), a subproblem $P_r(x^s)$ resulted by adding the constraint $\Delta(x^s, x) = 2r$ to the model (2) is given as:

$$(P_r(x^s)) \quad \min t_2 - t_1 \tag{6a}$$

st.
$$t_1 \le \sum_{i=j}^n v_i x_{ji} \le t_2, \quad \forall j \in I_k$$
 (6b)

$$\sum_{i=1}^{\min\{i,k\}} x_{ji} = 1, \quad \forall i \in I_n$$
(6c)

$$\sum_{ji\in B} (1-x_{ji}) + \sum_{ji\notin B} x_{ji} = 2r$$
(6d)

$$t_1, t_2 \in \mathbb{R}_+ \tag{6e}$$

$$x_{ji} \in \{0, 1\}, \quad \forall (j, i) : i \ge j$$
 (6f)

It is known that the mathematical model (6) only assumes feasible solutions when $1 \leq r \leq n-1$ due to the equation (5). It is also important to note that $P_{r_1}(x^s)$ and $P_{r_2}(x^s)$ have no feasible solution in common whenever $r_1 \neq r_2$, because its distances from solution x^s are distinct in this case. Therefore, the collection of subproblems $\{P_r(x^s)\}_{r=1}^{n-1}$ is a decomposition of the mathematical model (2) and, thus, a decomposition of MWNPP.

4 Proposed Algorithm

The proposed VNDB algorithm works with the insertion and removal of Local Branching Constraints aiming, in addition to the definition of neighborhoods, the memory of the search space already explored using mathematical expressions. Thus, let x^1 be a feasible solution of the problem (2) and x^2 be the solution of the subproblem $P_1(x^1)$. The initial problem of VNDB is $P_1(x^1)$. The next subproblem will be $P_2(x^1)$ or $P_1(x^2) \cap \{\Delta(x^1, x) \ge 2\}$, depending on which is the best solution, or x^1 or x^2 . The same logic applies to each of the possibilities.

In general, method decisions are made as follows. Let M be a set of constraints of type (3c) and $(x^l)_{l=1}^m$ a sequence of solutions found by VNDB. In the iteration t, the solution of the subproblem $P_r(x^l) \cap M$ leads to the solution x^{l+1} . If the solution x^{l+1} is better than x^l , the subproblem is updated by adding the constraint $\Delta(x^l, x) \geq 2(r+1)$ to the set M and yielding the set M'. This step eliminates the feasible region of the $P_r(x^l)$ subproblem. Finally, the constraint $\Delta(x^l, x) = 2r$ is replaced by the constraint $\Delta(x^{l+1}, x) = 2$. This procedure creates a problem in the form $P_1(x^{l+1}) \cap M'$. If the solution x^{l+1} is no better than x^l , the constraint $\Delta(x^l, x) = 2r$ is changed by $\Delta(x^l, x) = 2(r+1)$, generating the subproblem $P_{r+1}(x^l) \cap M$.

The mathematical model (7) shows the structure of the VNDB subproblem after passing through m distinct solutions and performing $t = \sum_{l=1}^{m} r_l$ iterations.

$$\min t_2 - t_1 \tag{7a}$$

s.t.
$$t_1 \le \sum_{i=j}^n v_i x_{ji} \le t_2, \quad \forall j \in I_k$$
 (7b)

$$\sum_{i=1}^{\min\{i,\kappa\}} x_{ji} = 1, \quad \forall i \in I_n \tag{7c}$$

$$\sum_{ji\in B_m} (1-x_{ji}) + \sum_{ji\notin B_m} x_{ji} = 2r_m \tag{7d}$$

$$\sum_{ji\in B_l} (1-x_{ji}) + \sum_{ji\notin B_l} x_{ji} \ge 2r_l, \quad \forall l \in I_{m-1}$$
(7e)

$$t_1, t_2 \in \mathbb{R}_+ \tag{7f}$$

$$x_{ji} \in \{0, 1\}, \quad \forall (j, i) : i \ge j$$
 (7g)

The subproblem (7) has m more constraints than the mathematical model (2). The constraint (7d) represents the current neighborhood of the iteration. The m-1 constraints (7e) make infeasible the search regions of the previous subproblems. The increase of m with the number of iterations depends on the initial solution chosen and the size of the neighborhood structure. The values $r_l \in I_{n-1}$ define by how many neighborhoods each solution passed without being surpassed.

 \boldsymbol{n}

min (i h)

Algorithm 1 VNDB	
1: function VNDB (\dot{x}, N)	▷ Initial solution and number of neighborhoods
2: $r \leftarrow 1$	▷ Initial neighborhood
$3: t \leftarrow 1$	▷ Iteration
4: while $t < Itermax$ and $r \le N$ do	
5: $add \ \Delta(\dot{x}, x) = 2r$	
6: $\ddot{x} \leftarrow solve()$	\triangleright Subproblem solution
7: remove $\Delta(\dot{x}, x) = 2r$	
8: if optimal then	
9: if $f(\ddot{x}) \ge f(\dot{x})$ then	\triangleright Without improved solution
10: $r \leftarrow r+1$	\triangleright Next neighborhood
11: else	\triangleright Improved solution
12: $add \ \Delta(\dot{x}, x) \ge 2(r+1)$	\triangleright Exclusion of explored search space
13: $r \leftarrow 1$	\triangleright Return to the first neighborhood
14: $\dot{x} \leftarrow \ddot{x}$	\triangleright Update solution
15: end if	
16: else if <i>feasible</i> then	\triangleright No search space reduction
17: if $f(\ddot{x}) \ge f(\dot{x})$ then	
18: $r \leftarrow r+1$	
19: else	
20: $r \leftarrow 1$	
21: $\dot{x} \leftarrow \ddot{x}$	
22: end if	
23: else	\triangleright Infeasible or $solve()$ does not find solution
24: r = r + 1	
25: end if	
26: $t \leftarrow t+1$	
27: end while	
28: return \dot{x}	
29: end function	

Algorithm 1 summarizes the above explanations. The stopping criterion is the exhaustion of the N neighborhoods in a given solution or by the maximum number of iterations *Itermax* (or maximum time). In practice, the function *solve()* also has a time limit to resolve the VNDB subproblem. Then there must be conditional deviations for all possible solution status: {*feasible, optimal, infeasible*}.

When the method *solve()* returns a feasible but not optimal improvement solution, it is not possible to exclude the subproblem region because there is some unexploited space that may still contain the optimal solution to the general problem.

5 Computational Experiments

The proposed VNDB algorithm and the mathematical model presented in Section 2 were coded in C++ using the Concert Technology of CPLEX 12.6 in the default configuration. The computational experiments were carried out on an Intel Core i7-3770 CPU 3.4 GHz with 8 cores and 32GB RAM running on a Ubuntu 16.04 64-bit operating system using clang compiler version 3.8. The test instances composed of a set of sequences were randomly generated as follows. Sequences with n integer elements with 12 digits ranging from 0000000000 to 999999999999 are generated by randomly sampling for 12 consecutive times a number between 0 and 9 using a uniform distribution. A.F. Faria et al. / Electronic Notes in Theoretical Computer Science 346 (2019) 437–447

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The computational experiments are performed aiming to compare the quality of the solution ub and the computational time associated to the VNDB and the CPLEX solver applied in the mathematical model 2 considering a time limit of t = 4500 seconds. The measures used to compare the results are based on the relative error measure given by $gap(B, A) = \frac{z(A)-z(B)}{z(A)}100\%$, where z(A) and z(B)corresponds to the objective function value associated to the best solution provided by algorithm A and algorithm B, respectively. This function shows that the solution provide by the algorithm B is better than the solution provided by the algorithm Awhen gap(B, A) > 0. For instance, the gap(B, A) = 90% means that the response of the algorithm A would have to be divided by 10 to match the algorithm B response. The closer to 100% is the result of the function gap(B, A), better the algorithm Bis compared to an algorithm A. The same measure applies to the run time of the algorithms. The order of the algorithms in the function entry is gap(VNDB, MIP). The values of $gap() \ge 100\%$ are due to rounding.

A set of experiments was performed using the generated instances with $n \in \{100, 200, 400, 800\}$ and considering $k \in \{3, 4, 5, 6\}$. Tables A.1 and A.2 present the computational experiments results, i.e., the runtime (in seconds) and the upper bound (ub), for each instance. These results are used to compute the gap() presented in Table A.3. Table A.3 may be observed for a descriptive analysis of the results. First, the VNDB runtime is always shorter since the gap_t values are greater than 60%, indicating a runtime of at least 2.5 times smaller. VNDB finds the optimal solution for 9 instances in the k = 3 column when $gap_{ub} = 100\%$ is observed. Furthermore, the number of times that the ub provided by the VNDB algorithm exceeds the one provided by the mathematical model (2) solved via CPLEX solver, which corresponds to the number of positive gap_{ub} observed, is a total of 39 of the 80 instances tested. In more detail, VNDB presented to be best in 10 instances of column k = 3, 8 instances of column k = 4, 8 instances of column k = 5, and 13 instances of column K = 6.

Finally, a set of statistical tests using objective function values f_{alg} as samples is performed. The tests aim to answer whether it is possible to assert with 95% confidence if the objective function values f_{MIP} , associated to the best solution attained by CPLEX solver when solving the mathematical model (2), are smaller than the *ub* obtained through VNDB, given by f_{VNDB} . The hypothesis test used is:

$$\begin{cases} H_0: f_{MIP} \ge f_{VNDB} \\ H_1: f_{MIP} < f_{VNDB} \end{cases}$$

$$\tag{8}$$

Table 3 shows the p-values of the statistical tests using objective function values f_{alg} as samples. The hypothesis test rejects the null hypothesis only in instances with k = 4. In this case, it is possible to state that there is a difference between the algorithms and this difference is significant, i.e., the *ub* obtained through VNDB is inferior to objective function values f_{MIP} associated to the mathematical model (2). In other cases, there is no difference between the results.

Student test	K=3	K=4	K=5	K=6
p-values	16,66%	3,77%	7,04%	46,12%

Table 3 Results of the paired t-test with 95% confidence using the objective function values.

6 Conclusion

This article presented an adapted VNDB mathematic for solving MWNPP and a comparison with the solution of the mathematical model using the CPLEX solver. Results were obtained using randomly generated instances with uniformly distributed elements.

Computational experiment results show that VNDB never reaches the maximum time available for execution due to neighborhood exhaustion and a large number of solved subproblems with non-optimal status. Despite this, VNDB has statistically as good results as the same MIP running for a shorter time interval. The only exception is its performance in instances where k = 3. A drawback found in the computational experiments is that the CPLEX solver does not seem to set time in a deterministic way on a multi-core processor. This causes some problems to take up to 4500 seconds more in MIP execution.

As future work, a more elaborate parameter analysis can be applied to the proposed VNDB so that it can use all the available time for the experiment. Thus the comparison with the MIP problem can be more fair.

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A Appendix

Wathematical Wodel 2 Tresuits									
	k=3		k=4		k=5			k=6	
n	Time	ub	Time	ub	Time	ub	Time	ub	
100	4063,50	49240	4513,94	249893	4498,00	455322	4495,52	1200561	
100	3980,16	55843	4479,21	209860	$4525,\!60$	1605769	4523,85	5603669	
100	4179,41	32015	4457,30	427940	$4510,\!53$	140990	4532,32	2602217	
100	4120,93	52069	4455,24	93999	4558,21	1182564	4485,31	4725930	
100	3905,11	6408,5	4475,06	80173,5	4542,53	1102740	4553,10	2951999	
200	4371,95	13166,5	4519,97	135307	$4557,\!98$	1123962	4587,85	1590144	
200	4381,11	4431	4537,66	65535	4542,90	739145	4666,52	4826459	
200	4402,95	8819	4524,11	166066	4631,01	638049	4562,95	3675251	
200	4367,34	19287	4448,33	214235	4578,41	1169098	4621,10	1855193	
200	4390,39	45946	4504,69	159946	$4479,\!97$	1656139	4562,59	2524163	
400	4375,50	16053,5	4612,23	253728	$4691,\!69$	194989	4753,60	888856	
400	4532,59	52235	4563,96	358952	4600,64	1119839	4663,89	6310376	
400	4531,44	4809	4611,12	32728	4707,68	1849077	4670,92	3613928	
400	4553,46	24003	4591,07	292372	$4672,\!92$	406028	4690,89	791927	
400	4523,91	22076	4576,98	129955	$4672,\!51$	732207	4705,01	2657192	
800	4805,05	2348	4846,90	121657	4853, 19	490825	4932,21	1054196	
800	4674,52	69290	4877,63	63272	$4874,\!87$	363647	4894,91	4864688,999023	
800	4782,10	19733,5	4851,47	436698	4859,28	646373	4896,03	1937925	
800	4728,13	7854	4829,16	97683	4884,95	515063	4834,07	2996054,999023	
800	4792,19	30999	4844,46	116701	4851,21	533006	4921,96	1044665	

Table A.1 Mathematical Model 2 Results

All resources used for experiments of this paper (including codes, instances, and results) are available in https://github.com/AlexandreFrias/ AlgorithmsLAGOS2019.

	k=3		k=4		k	=5	k=6	
n	Time	ub	Time	ub	Time	ub	Time	ub
100	912,14	39322	744,14	458052	680,49	596504	658,14	596504
100	1558,98	0	985,70	233894	905,41	596225	417,39	2996624
100	878,13	43515	667,90	295726	552,37	1132949	893,61	1379484
100	711,36	0	718,82	585619	$469,\!65$	468677	867, 56	1848561
100	582,89	0	1079,56	229865	875,49	1425028	531,09	3014678
200	1490,28	0	1233,08	128692	1210,58	689690	$1204,\!65$	681721
200	1000,42	33602	1256, 11	59067, 5	800,97	1969700	823,28	2017573
200	1094, 12	86025	1252,33	337142	847,00	642697	831,02	1674668
200	1448,89	46660	876,20	421421	838,17	821353	579,58	4273737
200	1441,05	76803	1135,23	216298	1231,48	747272	427,39	4989050
400	1744,63	0	1732,56	192672	697, 12	1013347	598, 29	560329
400	1000,71	0	1100,20	244158	778,44	877283	473,71	2102136
400	1457,58	0	636,83	103158	742,47	134151	529,31	1154835
400	1014,13	73047	1027,87	72002	1065,58	795390	557,70	740184
400	615,47	0	628,12	153911	399,66	930850	546,27	1298980
800	1534,66	66186	807,00	60500	1224,68	2681189	1148,09	3373820
800	695,73	0	968,98	2234417	1087,70	1456731	1043,90	3383655
800	670,97	91676	892,95	377468	1113,92	586678	1138,06	9116751
800	1179,86	105889	792,00	1757558	1183,25	7326466	1128,57	8909755
800	1407,38	91542	812,39	618097	972,31	9596348	1121,96	4947780

Table A.2 VNDB Results

Table A.3 Comparison between VNDB and Mathematical Model 2 using gap(vndb, mip) on upper bound and runtime.

	k=3		k=4		k=5		k=6	
n	gap_t	gap_{ub}	gap_t	gap_{ub}	gap_t	gap_{ub}	gap_t	gap_{ub}
100	77,55%	$20,\!14\%$	83,51%	-83,30%	$84,\!87\%$	-31,01%	85,36%	50,31%
100	60,83%	100,00%	77,99%	-11,45%	79,99%	62,87%	90,77%	46,52%
100	78,99%	-35,92%	85,02%	30,90%	87,75%	-703,57%	80,28%	46,99%
100	82,74%	100,00%	83,87%	-523,01%	89,70%	60,37%	80,66%	60,88%
100	85,07%	100,00%	75,88%	-186,71%	80,73%	-29,23%	88,34%	-2,12%
200	65,91%	100,00%	72,72%	4,89%	73,44%	$38,\!64\%$	73,74%	$57,\!13\%$
200	77,17%	-658,33%	72,32%	9,87%	82,37%	-166,48%	82,36%	58,20%
200	75,15%	-875,45%	72,32%	-103,02%	81,71%	-0,73%	81,79%	$54,\!43\%$
200	66,82%	-141,93%	80,30%	-96,71%	$81,\!69\%$	29,74%	87,46%	-130,37%
200	67,18%	-67,16%	74,80%	-35,23%	72,51%	54,88%	90,63%	-97,65%
400	60,13%	100,00%	62,44%	24,06%	85,14%	-419,69%	87,41%	36,96%
400	77,92%	100,00%	75,89%	$31,\!98\%$	$83,\!08\%$	21,66%	89,84%	66,69%
400	67,83%	100,00%	86,19%	$-215,\!20\%$	84,23%	92,74%	$88,\!67\%$	68,04%
400	77,73%	-204,32%	77,61%	$75,\!37\%$	77,20%	-95,90%	88,11%	6,53%
400	86,40%	100,00%	86,28%	-18,43%	$91,\!45\%$	-27,13%	88,39%	51,11%
800	68,06%	-2718,82%	83,35%	50,27%	74,77%	-446,26%	76,72%	-220,04%
800	85,12%	100,00%	80,13%	$-3431,\!45\%$	$77,\!69\%$	-300,59%	$78,\!67\%$	30,44%
800	85,97%	-364,57%	81,59%	13,56%	77,08%	9,24%	76,76%	-370,44%
800	75,05%	-1248,22%	83,60%	-1699,25%	75,78%	-1322,44%	$76,\!65\%$	-197,38%
800	70,63%	-195,31%	83,23%	-429,64%	79,96%	-1700,42%	77,21%	-373,62%