VNS with GA-based parameter tuning for solving the k-domination problem

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ABSTRACT

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In this paper we are concerned with solving a generalized version of the well-known minimum dominating set problem, the so-called k-domination problem, $k \in \mathbb{N}$. This problem is about finding a minimal cardinality subset D of vertices of a graph G = (V, E) such that every $v \in V$ belongs to D or has at least k neighbors from D. The k-domination problem has applications in distributed systems, biological networks etc. We propose a variable neighborhood search (VNS) metaheuristic for solving the k-domination problem. The VNS is equipped with an efficient fitness function that allows it to consider both feasible and infeasible solutions, while appropriately penalizing infeasible solutions. The control parameters of the VNS are tuned using a genetic algorithm. The method is compared to the best known heuristic approaches from the literature: the beam search and several greedy approaches. Experimental evaluations are performed on a real-world benchmark set whose instances represent the road networks of different cities. The VNS provided new state-of-the-art results for all considered problem instances with $k \in \{1, 2, 4\}$.

CCS CONCEPTS

• Theory of computation \rightarrow Optimization with randomized search heuristics; *Evolutionary algorithms*.

KEYWORDS

Variable neighborhood search, graph domination, genetic algorithm, parameter tuning

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1 INTRODUCTION

A graph G=(V,E) is an abstract mathematical structure in which V represents a set of elements called vertices (or nodes) and a set of pairs $e=uv=(u,v)\in E\subseteq V\times V$ called edges of G. In this paper, we are concerned with simple undirected graphs that have no loops and where the edges have no directions, i.e., $e=\{u,v\}=uv=vu\in E$. Graphs serve as models for many real-world problems describing relationships among various objects in biology, physics, social networks, etc. [12, 19, 23, 26].

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One of the best known classes of problems studied from theoretical, computational and practical points of view are domination problems on graphs [11]. The basic problem of this class is the minimum dominating set problem. The subset $D \subset V$ is called domi*nating set* if every vertex $v \in V$ belongs to D or there is at least one vertex $w \in D$ such that $uw \in E$. The search for the smallest possible dominating set D of the graph G is called the minimum dominating set problem (MDSP) [10]. This problem has many applications, for example, in biological networks [21], document summarization [27], graph mining [2], etc. From an algorithmic point of view, this problem is NP-hard. It is solved by various exact approaches, such as branch-and-reduce algorithms [28], an approach that uses the fundamental cut-sets of the graph [17], etc. Heuristic approaches are more common in the literature, e.g., a genetic algorithm [13], simulated annealing [14], ant colony optimization [16], to name a few. Several generalizations of MDSP, arising from practical experience, are proposed in the literature: the minimum weight dominating set problem [25], the minimum total dominating set problem [30], the minimum connected dominating set problem [1], etc.

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In this paper, we study the *minimum k-domination problem* (MkDP) [4], for a fixed $k \in \mathbb{N}$. The k-dominating set D of a graph G is such a subset of V that every vertex not belonging to D is adjacent to at least k vertices in D [18]. A minimum k-dominating set represents the optimal solution of MkDP. The NP-completeness of the k-domination decision problem is formally proved for the split graphs, see details in the above citation. (Note that the definition of this problem is not unique in the literature – there is a definition where the goal is to find a minimum cardinality vertex set D such that every vertex of G is within distance k of some vertex in D [3].)

Regarding previous solutions to this problem, several greedy approaches have been proposed by Couture et al. [5], Gagarin et al. [9], and Gagarin and Corcoran [8]. Recently, Corcoran and Gagarin proposed a Beam search approach [4], which is currently the best-performing heuristic approach for small to medium sized real-world instances.

MkDP has applications in distributed systems [29], where a k-dominating set in these systems is a set of processors such that each processor outside the must have at least k neighbors in the set.

We propose a variable neighborhood search (VNS) metaheuristic for solving MkDP. The contributions of our work can be summarized as follows:

- The control parameters of the VNS are tuned with genetic algorithm PyGAD [7].
- VNS for MkDPA significantly improves the state-of-the-art results for all considered problem instances, where k ∈ {1, 2, 4}.
- VNS is able to quickly produce solutions of reasonable quality which is not the case for approaches previously proposed in the literature.

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2 FORMAL PROBLEM DEFINITION

Let G=(V,E) be a simple undirected graph and $k\in\mathbb{N}$ be fixed. For $v\in V$, N(v) is a set of all adjacent vertices of v in the graph G, i.e. $N(v)=\{w\mid vw\in E\}$. A set $D\subseteq V$ is called k-dominating set if for every $v\in V\setminus D$ holds $|N(v)\cap D|\geq k$. The MkDP is an optimization problem whose objective is to find a k-dominating set with minimal cardinality:

$$\arg\min_{D\subseteq V}|D|\tag{1}$$

$$s.t. \ \forall v \in V \setminus D, |N(v) \cap D| \ge k.$$
 (2)

As for the search space of the MkDP, we adapt it to the needs of our VNS. Not only feasible solutions are handled, but also infeasible ones – they are additionally penalized, see Section 3. In other words, every subset of V is a candidate solution in our VNS. Therefore, the size of the search space is $2^{|V|}$.

3 THE PROPOSED ALGORITHM

In this section, we first give an overview of the variable neighborhood search (VNS). Then we introduce the main components of VNS for solving MkDP: the fitness function, the shaking procedure and the efficient local search.

3.1 Variable neighborhood search

Variable neighborhood search is a single-based solution metaheuristic proposed by Mladenović and Hansen [20]. The basic idea of the approach is to systematically exchange neighborhoods of the current best solution (incumbent solution) to avoid getting stuck in a local optimum. VNS has proven to be one of the most powerful metaheuristic, achieving excellent results on diverse classes of problems, such as scheduling problems [6], vehicle routing problems [24], median problems [15], etc.

The VNS for solving the MkDP is given in Algorithm 1.

VNS generally requires at least two control parameters $d_{min}, d_{max} \in \mathbb{N}$, which define the increasing sizes of the neighborhood structures $\mathcal{N}_{d_{min}}(D), \ldots, \mathcal{N}_{d_{max}}(D)$ around given solution D. A solution D' belongs to the neighborhood $\mathcal{N}_{d}(D)$ of the solution D if it can be obtained from D by removing $\min(d, |D|)$ vertices from D and then adding d vertices from $V \setminus D$ into D.

The third parameter commonly used in VNS is $p_{move} \in [0,1]$. This parameter corresponds to the probability of moving to a new solution if it has the same quality (fitness) as the incumbent solution. Finally, the fourth control parameter penalty is specific to MkDP. It is real-valued and is used to define the relative influence of solution feasibility and solution quality (size of k-dominating set) on the overall value of the fitness function (more details are given in Section 3.2). The return value of VNS is called D_{best} – it is the incumbent solution.

At the beginning, the neighborhood size d is set to the smallest, i.e. to d_{min} . The initial incumbent solution D_{best} is generated by performing local search on an empty set (local search is explained in Section 3.3). Then the algorithm enters the main loop (lines 5-18). The loop is run until at least one of the termination criteria is met. At each iteration of the loop, the following steps are executed:

Algorithm 1 VNS scheme for solving MkDP

```
1: Input: d_{\min}, d_{\max}, p_{move}, penalty
2: Output: best found solution D_{best}
3: d \leftarrow d_{\min}, d_{\max\_init} \leftarrow d_{\max}
4: D_{best} \leftarrow \mathsf{LocalSearch}(\emptyset)
 5: while TerminationCriteriaNotMet() do
       D' \leftarrow \texttt{Shaking}(\mathcal{N}_d(D_{best}))
       D'' \leftarrow \mathsf{LocalSearch}(D')
       if fitness(D'') < fitness(D_{best}) \lor (fitness(D'') =
       fitness(D_{best}) \land r \in U_{[0,1]} < p_{move}) then
          D_{best} \leftarrow D^{\prime\prime}
           d \leftarrow d_{\min}
10:
           d_{max} \leftarrow \min(d_{\max\_init}, |D_{best}|/2)
11:
        else
12:
           d \leftarrow d + 1 // try with next neighborhood
13:
           if d > d_{max} then
14:
              d \leftarrow d_{min}
15:
           end if
16:
       end if
17:
18: end while
19: return D_{best}
```

- Shaking($\mathcal{N}_d(D_{best})$) a solution D' is selected randomly from the set of solutions belonging to the d-th neighborhood structure around the solution D_{best} .
- LocalSearch the selected solution D' may be improved by a local search procedure, as explained in Section 3.3.
- The solution D' becomes new incumbent if it has better fitness than the previous incumbent. Alternatively, it may become new incumbent with probability p_{move} if its fitness is the same. In both cases, d is reset to d_{\min} . The parameter d_{max} is dynamically set to $\min(d_{\max_init}, |D_{best}|/2)$ to prevent neighborhoods that are too large, i.e., neighborhoods larger than half the incumbent size.
- If the solution D' does not become new incumbent, d is increased – this further increases diversification. If this increase leads to d > d_{max}, d is circularly reset to d_{min}.

3.2 Fitness function

To evaluate the solution D, the following nonlinear fitness function is used:

$$fitness(D) = (1 + violations(D)) \cdot (1 + penalty \cdot |D|)$$
 (3)

where

$$violations(D) = \sum_{v \in V \setminus D} k - C(D, v)$$
 (4)

and

$$C(D, v) = \min(k, |N(v) \cap D|). \tag{5}$$

It can be seen that violations(D) quantifies the overall degree of solution D inadmissibility, i.e., for each vertex v that does not belong to a candidate dominating set D, k-C(D,v) measures how strongly vertex v locally violates the k-domination condition. Thus, C(D,v) quantifies the opposite – how strongly the vertex v satisfies the k-domination condition. In particular, when vertex v has k or

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more vertex neighbors in D, the value of $k - \min(k, |N(v) \cap D|)$ is zero. Otherwise, C(D, v) is positive and at most k.

Therefore, the proposed fitness function evaluates both feasible and infeasible solutions. Since the fitness function is to be minimized, the following three observations can be made about the values of the fitness function:

- For sufficiently small values of the parameter penalty, the feasibility of the solution is relatively preferred over the cardinality of the solution. This means that when comparing feasible and infeasible solutions, the feasible solution is favored.
- When comparing two infeasible solutions of the same cardinality, the *less infeasible* solution is preferred, i.e. the one with the lower *violations*(·) value.
- When comparing two feasible solutions, the one with the lower cardinality is preferred.

3.3 Local search

The goal of local search (LS) is to improve the solution D' obtained in the shaking phase by applying multiple local improvements to the structure of the solution. The LS tailored to MkDP is described in Algorithm 2.

Our LS procedure consists of two phases. In the first phase, the vertices are added to achieve feasibility – when the solution is not feasible. In the second phase, the vertices are removed to improve the objective function. The removal is done in a way that does not affect the feasibility previously achieved. In both phases, the best improvement strategy is used. This means that all eligible vertices are checked for inclusion/exclusion and then the best vertex is included/excluded. Each phase ends with the first iteration where no improvement in fitness is found.

Fast fitness evaluation. Computing the fitness function (3) takes O(|E|) time – the most time consuming part is computing the $violations(\cdot)$ function. For dense graphs, this complexity can go up to $O(|V|^2)$. Since local search makes many fitness function calls it is too costly to compute the fitness function from scratch every time. In order to execute LocalSearch procedure efficiently, fast calculations of the fitness function are applied. Before LS enters the first while loop, $C(D_{best}, v), \forall v \in V$ for given solution D_{best} are computed and saved. During vertex addition, that is $D' = D_{best} \cup \{v\}$, violations(D') is calculated in the following way:

$$violations(D') = violations(D_{best})$$

$$- (k - C(D_{best}, v)) I_{(C(D_{best}, v) < k)}$$

$$- \sum_{w \in N(v) \setminus D_{best}} I_{(C(D_{best}, w) < k)}$$
 (6)

where I stands for the indicator function

The part $-(k-C(D_{best},v))\mathbb{I}_{(C(D_{best},v)< k)}$ adjusts for the effect of the added vertex v, i.e., if v was previously satisfied before (satisfied the k-domination condition), then this indicator function takes the value zero, so nothing changes. This is true because v remains satisfied – it is now part of k-dominating set. Otherwise, if vertex v has previously violated the k-domination condition, the total violations are reduced by the previous degree of vertex v violation, i.e. $(k-C(D_{best},v))$.

Algorithm 2 Local Search

```
1: Input: a solution D
 2: Output: a (possibly) improved solution D_{best}
 3: D_{best} \leftarrow D
4: best_{fit} \leftarrow fitness(D_{best})
    // first, achieve feasibility by adding vertices
 5: improved ← True
6: while improved do
       improved \leftarrow False
       best_v \leftarrow None
       for v \in V \setminus D_{best} do
           D' \leftarrow D_{best} \cup \{v\}
10:
           if new_{fit} = fitness_{fast}(D') < best_{fit} then
11:
              best_v \leftarrow v
12:
              best_{fit} \leftarrow new_{fit}
13:
              improved \leftarrow True
14:
15:
           end if
       end for
16:
       if improved then
17:
           D_{best} \leftarrow D_{best} \cup \{best_v\}
18:
       end if
19:
20: end while
    // second, remove vertices, but keep the feasibility
21: improved \leftarrow True
    while improved do
       improved \leftarrow False
23
       best_v \leftarrow None
24:
       for v \in D_{best} do
25:
26:
           D' \leftarrow D_{best} \setminus \{v\}
           if new_{fit} = fitness_{fast}(D') < best_{fit} then
27:
              best_v \leftarrow v
28:
              best_{fit} \leftarrow new_{fit}
29:
              improved \leftarrow True
30:
          end if
31:
           if improved then
32:
              D_{best} \leftarrow D_{best} \setminus \{best_v\}
33:
34:
       end for
35:
36: end while
37: return D_{best}
```

The part $-\sum_{w \in N(v) \setminus D_{best}} \mathbb{I}_{(C(D_{best}, w) < k)}$ adjust for the effect on the vertex v neighbors, which were not in the k-dominating set D_{best} , i.e. $W = N(v) \setminus D_{best}$. If some of these vertices $w \in W$ violated k-domination condition, adding the adjacent vertex v to the solution reduces the total violations. Otherwise, if a vertex w was satisfied, adding v to the solution does not change anything.

In case of a vertex removal, the similar idea is used.

4 EXPERIMENTAL EVALUATION

In this section we analyze the quality of the proposed VNS method. ¹ For this purpose, we include the competing heuristic approaches

 $^{^1}$ All instances, source codes of the VNS and GA tuning algorithms, and detailed experimental results are available on the GitHub page for this work: anonymousURL.

Table 1: Large-sized instance characteristics.

City	V	E
Belgrade	19,586	7,561,185
Berlin	29,461	9,944,851
Boston	44,797	28,164,740
Dublin	37,982	21,630,466
Minsk	10,487	1,375,618

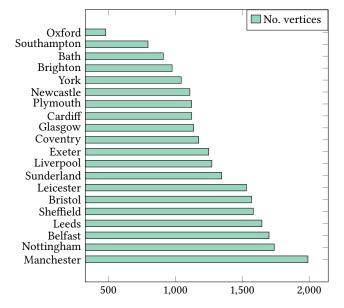


Figure 1: The number of vertices in the small to medium sized instances.

from the literature. The following four methods for MkDP are compared:

- The standard greedy method from [9, 22], denoted by SG;
- Greedy method from [8], denoted by PG;
- Beam search approach from [4], denoted by BS;
- VNS approach, as described in Section 3, denoted by VNS.

Benchmark instances. For comparison, we consider the benchmark introduced in [4]. It consists of 20 small to medium sized instances, where all instances represent road networks of different cities modeled as reachability graphs. In addition to these, the authors have provided the program that generate road networks for five large cities: Belgrade, Berlin, Boston, Dublin, and Minsk. Since the road networks change over time, the obtained graphs do not fully match those used in the [4], so their properties are given in Table 1.

The characteristics of 20 small to medium sized instances can be found in [4]. Unlike the five large networks, these 20 instances are exactly the same as in [4] – we obtained them directly from the authors. Figures 1–2 show the number of vertices and edges of these instances.

Testing environment. Experiments were performed on a computer running Intel Core i9-9900KF CPU @3.6GHz with 64GB RAM, under Microsoft Windows 10 Pro OS. VNS is implemented in Python 3.9.

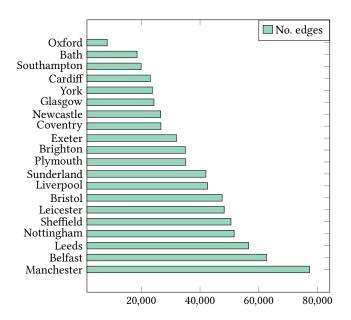


Figure 2: The number of edges in the small to medium sized instances.

The results of SG, PG and BS for small to medium sized instances are taken from [4] as reported in their experimental section. The results for the five large instances were obtained by running the original implementation of PG (obtained from the authors). According to the same authors, BS was inefficient for the large instances due to its high computational complexity. Therefore, we did not include this algorithm in the large instance comparison. PG and VNS algorithms are run ten times (using different random seeds) per each problem instance.

The termination criteria of the VNS are: (i) the maximum running time of 30 minutes, and (ii) the maximum number of 2000 iterations. The time limit of 30 minutes is not checked during initialization (line 4 in Algorithm 1). This means that VNS can take more than 30 minutes to finish for some very large instances, such as Dublin and Boston.

4.1 Parameters tuning

As mentioned earlier, VNS for MkDPA involves four control parameters: d_{min} , d_{max} , p_{move} and penalty. The range of parameters used for tuning are given in Table 2.

Table 2: VNS parameter ranges.

Parameter	Domain	Step
d_{min}	[1, 10]	1
d_{max}	[2, 100]	1
p_{move}	[0, 1]	0.05
penalty	[0.001, 0.02]	0.001

As for the tuning tool, we have decided to use genetic algorithm called PyGAD. This implementation, proposed in [7], is available as

an open-source Python library. All (20) small to medium sized problem instances were tuned separately for each $k \in \{1, 2, 4\}$, resulting in a total of 60 control parameter configurations. PyGAD was used as an outer optimizer calling the inner VNS method in a multiprocessing manner – each PyGAD chromosome (solution) encodes a single VNS control parameter configuration and corresponds to a separate process. VNS was limited to 100 iterations. The PyGAD parameters were as follows:

- *num_generations* = 50 number of generations;
- num_parents_mating = 5 number of chromosomes selected as parents for the mating pool;
- sol_per_pop = 10 number of chromosomes in the population:
- *mutation_probability* = 0.1 the mutation probability;
- *num_genes* = 4 number of genes in the chromosome, the same as the number of control parameters of VNS.

Parameter tuning for large instances was too inefficient. Therefore, we used reasonable manually configured parameters for these instances: $d_{min}=1, d_{max}=+\infty, p_{move}=0.5, penalty=0.01$. (Note that d_{max} has implicit upper bound – it is set in line 11 of Algorithm 1.)

4.2 Experimental results

Tables 3-5 contain the experimental results for $k \in \{1, 2, 4\}$, respectively. The first column gives the name of the instance (city) for which the results are reported. The next block contains the results of VNS – the best result and the average solution quality over ten runs. The third block reports the results of the best approach from the literature for each instance – the name of the approach, the best obtained result and average solution quality over ten runs. Note that the labels BS1, BS2 or BS4 correspond to BS approach with beam widths of 1,2 and 4, respectively.

The following conclusions can be drawn from these results.

- For k = 1, VNS outperformed all competing approaches for small to medium sized instances. VNS also outperformed the PG approach for the large-sized instances.
- Concerning the results for k=2, VNS outperformed all competing approaches by nearly 15% in terms of the average solution quality. Similar conclusions hold for the large instances: VNS produces $\approx 5-15\%$ improvement rate over the second best PG approach.
- The situation is similar for k=4. VNS outperforms the second-best algorithm by more than 15% in some cases (see, for example, the instance Nottingham where VNS achieved a score 165 over BS4 which achieved a score 193). For the large instances, VNS again outperforms PG in all cases.

The average times (in seconds) for reaching the best solution in VNS are shown as stacked bar graphs in Figures 3-4. The smaller the size of an instance, the less time VNS takes on average to reach the best solution. Figures 3-4 clearly show that as k increases, the average times to reach the best solutions increase rapidly. In case of the large instances, it can be seen from Figure 4 that the most time consuming instances in terms of reaching the best solution are Boston and Dublin. These two instances are indeed the largest in terms of number of vertices/edges (see Table 1).

Table 3: Results for k=1.

	VNS		Literature		
City	Best	Avg.	Alg.	Best	Avg.
Bath	38	38	BS4	43	44.6
Belfast	39	39	BS4	48	50.2
Brighton	21	21	BS4	28	28.2
Bristol	37	37	BS2	46	47.4
Cardiff	39	39	BS4	48	50.6
Coventry	38	38.2	BS4	44	44.8
Exeter	38	38	BS4	50	50.6
Glasgow	50	50.2	BS4	58	59.2
Leeds	40	40	BS4	51	52.4
Leicester	38	38	BS4	51	51.5
Liverpool	28	28	BS4	38	38.4
Manchester	38	38.8	BS4	45	45.9
Newcastle	44	44	BS4	51	52.6
Nottingham	44	44	BS4	55	56.6
Oxford	24	24	BS4	27	27.9
Plymouth	31	31	BS4	39	40.3
Sheffield	42	42	BS4	51	52.5
Southampton	25	25	BS4	28	29.6
Sunderland	36	36	BS4	46	46.3
York	32	32	BS4	39	39.1
Belgrade	85	88.4	PG	103	103.4
Berlin	102	104.5	PG	125	125.9
Boston	99	101.2	PG	101	102.7
Dublin	93	99	PG	112	113.8
Minsk	100	102	PG	125	126

5 CONCLUSIONS AND FUTURE WORK

In this paper we have studied the k-domination problem, $k \in \mathbb{N}$, a generalized version of the prominent minimum dominating set problem. This problem has been solved so far by several constructive and incremental approaches. We proposed the variable neighborhood search (VNS) metaheuristic to solve this problem. It is equipped with an effective fitness function that evaluates both feasible and infeasible solutions. Moreover, an efficient local search procedure with best-improvement strategy and fast fitness function evaluation plays an important role in obtaining high-quality solutions. The efficiency of our VNS has been validated on the real-world benchmark, where it has been shown that VNS outperform all existing heuristic state-of-the-art approaches.

For future work, one could consider improving the VNS to work more efficiently with very large graphs, such as social networks. Also, VNS could be compared to exact approaches such as integer linear programming models, solved by state-of-the art solvers, such as Cplex or Gurobi.

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 A new heuristic for the minimum connected dominating set problem on ad hoc

Table 4: Results for k = 2.

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	VNS		Literature		
City	Best	Avg.	Alg.	Best	Avg.
Bath	71	71.8	BS1	86	89
Belfast	76	76.2	BS4	96	97.6
Brighton	40	41.1	BS4	49	49.4
Bristol	73	73.7	BS4	91	94
Cardiff	79	79.4	BS4	92	95.6
Coventry	73	73.2	BS4	84	85.1
Exeter	77	77.3	BS4	94	95.7
Glasgow	93	94.2	BS4	108	110.6
Leeds	79	80.5	BS4	98	99.6
Leicester	75	75.2	BS4	93	94.1
Liverpool	57	57	BS4	71	72
Manchester	77	78.4	BS4	90	91.5
Newcastle	83	84.3	BS4	94	95.4
Nottingham	84	85.3	BS4	102	103.3
Oxford	47	47	BS4	54	54.9
Plymouth	62	62.1	BS4	73	75
Sheffield	84	84.7	BS4	97	98.9
Southampton	50	50.1	BS4	60	61.1
Sunderland	73	73.7	BS4	87	89.1
York	68	68	BS4	77	77.6
Belgrade	169	172.3	PG	196	197.3
Berlin	206	207.1	PG	239	240.1
Boston	181	194.6	PG	190	191.6
Dublin	181	184.4	PG	209	211.3
Minsk	197	201.1	PG	238	240.4

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Table 5: Results for k = 4.

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	VNS		Literature		
City	Best	Avg.	Alg.	Best	Avg.
Bath	139	140.4	BS4	159	160
Belfast	147	148.5	BS4	177	179.6
Brighton	78	79.3	BS4	92	94.8
Bristol	145	146.7	BS4	175	176.4
Cardiff	160	161.9	BS4	181	183.2
Coventry	150	150.6	BS4	170	172.6
Exeter	157	158.3	BS4	181	182.3
Glasgow	174	175.4	BS4	197	199.8
Leeds	152	152.4	BS4	186	187.1
Leicester	151	152.6	BS4	175	177.7
Liverpool	112	114	BS4	132	133
Manchester	154	156.4	BS4	177	178.5
Newcastle	153	154.8	BS2	169	171.5
Nottingham	165	166.6	BS4	193	195.2
Oxford	89	89.2	BS2	99	100.8
Plymouth	115	116	BS4	135	137
Sheffield	160	161.6	BS4	180	182.2
Southampton	97	97.8	BS4	112	113.2
Sunderland	142	142.5	BS4	162	163.6
York	129	130.1	BS4	144	145.8
Belgrade	344	346.3	PG	372	374.5
Berlin	408	409.2	PG	444	446.2
Boston	341	341	PG	367	368.7
Dublin	363	363	PG	388	390.2
Minsk	387	391.5	PG	454	457.6

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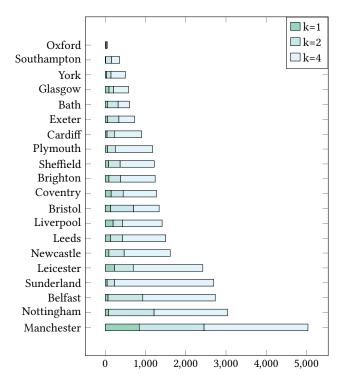


Figure 3: Average times (in seconds) of finding the best solution for small to medium sized instances.

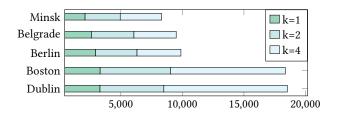


Figure 4: Average times (in seconds) of finding the best solution for large instances.

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