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A sampling-based exact algorithm for the solution of the minimax diameter clustering problem

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Abstract We consider the problem of clustering a set of points so as to minimize the maximum intra-cluster dissimilarity, which is strongly NP-hard. Exact algorithms for this problem can handle datasets containing up to a few thousand observations, largely insufficient for the nowadays needs. The most popular heuristic for this problem, the complete-linkage hierarchical algorithm, provides feasible solutions that are usually far from optimal. We introduce a sampling-based exact algorithm aimed at solving large-sized datasets. The algorithm alternates between the solution of an exact procedure on a small sample of points, and a heuristic procedure to prove the optimality of the current solution. Our computational experience shows that our algorithm is capable of solving to optimality problems containing more than 500,000 observations within moderate time limits, this is two orders of magnitude larger than the limits of previous exact methods.

Keywords clustering · diameter · large-scale optimization

1 Introduction

Clustering is one of the most essential tasks in data mining and machine learning (Anderberg 1973; Kaufman and Rousseeuw 1990). It involves the reading and treatment of unlabeled observations so as to identify hidden and non-obvious patterns that could otherwise not be found by simple inspection

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of the data. It is often used at the first stages of mining procedures with the objective of labeling the data for further mining using more sophisticated models and algorithms.

In its simplest form, a clustering problem can be formally defined as follows. We are given a positive integer $K > 1$ representing the number of sought clusters. We are also given a set V of observations, and we denote by $\mathcal{P}(V)$ the set of K-partitions of V, this is partitions composed of exactly K subsets each. Let $f : \mathcal{P}(V) \longrightarrow \mathbb{R}$ be a real-valued function. The objective is to find a K-partition $P^* = \{P_i^*\}_{i=1}^K \in \mathcal{P}(V)$ such that $P^* \in \arg\min\{f(P) : P \in \mathcal{P}(V)\}$.

The function f is usually described by means of a symmetric dissimilarity matrix $d : V \times V \longrightarrow \mathbb{R}_+$. The dissimilarity d_{uv} of two observations $u, v \in V$ indicates the degree of discrepancy between them. For a partition $P = \{P_i\}_{i=1}^K$, the *maximum diameter* is defined as $Dmax(P) = \max\{\max\{d_{uv} : u, v \in P_k\} : 1 \leq k \leq K\}$. The minimax diameter clustering problem (MMDCP) is the problem of finding a partition $P^* \in \arg\min\{Dmax(P) : P \in \mathcal{P}(V)\}$.

The classic book of Garey and Johnson (1979) refers to the MMDCP as *the clustering problem*, to prove that the associated decision problem is strongly NP-complete. This highlights the historical importance of the MMDCP which is perhaps the most intuitive among clustering criteria.

Existing exact algorithms for the MMDCP have little practical use as they can only handle problems containing up to a few thousand observations. The state-of-the-art algorithm for this problem based on constraint programming is capable of solving problems containing up to 5,000 observations (Dao et al 2017).

In this article we present an exact method for the MMDCP that typically runs in a time that is comparable to the time needed to compute the associated dissimilarity matrix and that, moreover, consumes only a limited amount of memory resources. The algorithm iterates between the execution of an exact clustering routine performed on a sampling of the objects, and that of a heuristic routine used to enlarge that sampling if deemed necessary.

The remainder of this article is organized as follows. In Section 2 we provide a literature review on exact and heuristic algorithms for the MMDCP and related problems, as well as on uses of sampling-based algorithms within exact frameworks. In Section 3 we present our algorithmic framework and provide guarantees on the quality of the solutions obtained by the method. In Section 4 we present in detail the algorithm used in the exact subroutine of the method. In Section 5 we present the heuristic subroutine used to prove the optimality of the current sample, or to enlarge it. In Section 6 we mention some acceleration techniques used. In Section 7 we present some computational evidence of the usefulness of our method. In Section 8 we briefly discuss the limitations encountered during the testing phase of our method. Section 9 concludes our paper and provides insights on potential avenues for future research.

2 Literature review

The MMDCP is traditionally handled using an agglomerative hierarchical algorithm, namely the *complete-linkage algorithm.* This algorithm begins with every point in V belonging to a single cluster, and then iteratively merges the two nodes u, v of minimum dissimilarity. Each time that a merge occurs, the dissimilarity matrix is updated by removing one column and one row associated with one of the two nodes merged. The remaining row and column corresponds to a merged node $z = \{u, v\}$. The dissimilarity between a point w and the merged node z is set to $d_{wz} \leftarrow \max\{d_{wu}, d_{wv}\}$. A naïve implementation of this algorithm runs in $O(n^3)$ time and uses $O(n^2)$ space (Johnson 1967). A specialized implementation of the algorithm runs in $O(n^2)$ time and uses $O(n)$ space (Sibson 1973; Defays 1977). The complete-linkage algorithm is a heuristic for the MMDCP and seldom finds optimal solutions as reported by Alpert and Kahng (1997); Hansen and Delattre (1978).

The FPF (*Furthest Point First*) method introduced in Gonzalez (1985) for the solutions of the MMDCP works with the idea of *head* objects for each cluster of the partition to which each object is assigned. In the first iteration, an object is chosen at random as the head of the first cluster and all objects assigned to it. In the next iteration, the furthest object from the first head is chosen as the head of the second cluster. Then, any object which is closer to the second head than to the first one is assigned to the second cluster. The algorithm continues for K iterations, choosing the object which is the furthest to its head as the head of the new cluster. The FPF heuristic is guaranteed to find a partition with diameter at most two times larger than the diameter of the optimal partition.

Regarding exact methods for the MMDCP, Hansen and Delattre (1978) explore the relationship between diameter minimization and graph-coloring to devise a branch-and-bound method to solve problems of non-trivial size. Brusco and Stahl (2006) proposes a backtracking algorithm, denoted Repetitive Branch-and-Bound Algorithm (RBBA), that branches by assigning each object to one of the possible K clusters. Pruning is performed whenever: (i) the number of unassigned objects is smaller than the number of empty clusters; (ii) the assignment of an object to a particular cluster yields a partition with a diameter larger than the diameter of the best current branch-and-bound solution; and (iii) there is an unassigned object that cannot be assigned to any of the clusters of the partial solution. Recently, Dao et al (2017) proposed a constraint programming approach for the MMDCP whose computational performance outranked the previous exact approaches found in the literature. In particular, the method obtained the optimal partitions for many benchmark instances, the largest of which with 5,000 objects grouped in three clusters.

Iterative sampling is a method that ignores parts of the problem and solves a restricted master problem (RMP) of usually much smaller size. It then executes a subproblem (SP) that either proves the optimality of the solution associated with the RMP, or enlarges it by adding the parts that were wrongly ignored. Lozano and Smith (2017) used this idea to solve a shortest path interdiction problem. The algorithm samples paths that are likely to be attacked by an attacker. The paths that are not identified as such are ignored and thus the associated restricted problem (a MIP) contains much fewer binary variables than the original problem. The optimality of the solution is validated by solving a shortest path problem. The algorithm showed very good results as it was capable to scale and solve problems several orders of magnitude larger than earlier methods.

Our algorithm is inspired form the need of handling large datasets. We are not the first to elaborate upon the need of developing a scalable algorithm able to handle large datasets while avoiding as much as possible the scanning of the whole data. Zhang et al (1997) use a tree structure to estimate and store the distribution of the dissimilarities. Their algorithm then relies on this estimator to proceed to cluster the data. In Bradley et al (1998), the authors introduce an algorithm for the k-means clustering problem that uses compression and discarding of data to reduce the number of observations. Fraley et al (2005) introduce a sampling-based algorithm to solve problems containing large amounts of data in a sequential fashion. At every iteration of their algorithm, typically much smaller datasets are considered. Unlike our method, all these algorithms are heuristic in nature.

3 Iterative sampling

The iterative sampling method uses an exact and a heuristic procedure interchangeably to find a small sample whose optimal solution is that of the original problem, and to build an optimal solution from enlarging that sample. Let us denote by (Q) the problem

$$\omega^* = \min\{Dmax(P) : P \in \mathcal{P}(V)\}. \tag{1}$$

For a given sample $U \subseteq V$, we let $Q(U)$ the problem Q restricted to the sample U, $\omega^*(U)$ be its optimal value and $P^*(U)$ its optimal solution.

For a given initial sample U_0 (that might be empty, but is indeed initialized to contain $K+1$ nodes as explained in detail in Section 6), we set $U \leftarrow U_0$ and $t \leftarrow 0$. At iteration t, one solves problem $Q(U)$ to optimality. A heuristic procedure iteratively enlarges the partition $P^*(U)$ and tries to build a feasible solution for problem Q of cost $\omega^*(U)$. If all nodes in $V \setminus U$ can be inserted into one cluster of $P^*(U)$ without entailing an increase of the objective, the resulting partition is returned. Otherwise the set U is enlarged, we let $t \leftarrow t+1$ and the same process is applied again on the enlarged sample. The following pseudo-code illustrates the method:

Algorithm 1 Iterative sampling

```
Require: $V, K$
Ensure: Optimal $K$-partition $P^* = \{P_i^* : i = 1 \dots K\}$ of $V$
  $U \leftarrow U_0$
  $\omega^*(U), \omega^* \leftarrow \infty$
  $P^*(U), P^* \leftarrow \emptyset$
  $W \leftarrow \emptyset$
  repeat
    $U \leftarrow U \cup W$
    $(\omega^*(U), P^*(U)) \leftarrow$ ExactClustering($U$)
    $(\omega^*, P^*, W) \leftarrow$ HeuristicClustering($P^*(U), V \setminus U$)
  until $W = \emptyset$
  return $P^*$
```

In this algorithm, procedure `ExactClustering(U)` solves problem $Q(U)$ to optimality for a given sample U of V. It returns the optimal solution $P^*(U)$ and its objective value $\omega^*(U)$. The function `HeuristicClustering(`$P^*(U)$`,` $V \setminus U$`)` completes the solution found by `ExactClustering(U)` and returns the resulting partition P^* (not necessarily an optimal one), its value ω^* and a set W containing the nodes that could not be inserted into $P^*(U)$ without increasing its maximum diameter ($\emptyset$ if no such node exists). The next two results support the exactness and finiteness of our approach:

Lemma 1 *For any sample $U \subseteq V$, $\omega^*(U) \leq \omega^*$.*

Proof Let $P^* = (P_i^*)_{i=1}^K$ be an optimal clustering of V. Then the clustering $R = (U \cap P_i^*)_{i=1}^K$ is a clustering of U of smaller diameter or equivalent diameter ω^*. It follows that $\omega^*(U) \leq \omega^*$. □

Proposition 1 *The iterative sampling method ends in a finite number of iterations and returns an optimal clustering of V.*

Proof At every iteration, procedure `HeuristicClustering(`$P^*(U)$`,` $V \setminus U$`)` either proves the optimality of the current subproblem (if it returns $W = \emptyset$), or the set U is augmented. In the worst case, U will grow up to become equal to V, in which case procedure `ExactClustering(U)` is guaranteed to return an optimal solution of the problem. □

Remark 1 A simple worst-case time analysis of our method would suggest that it is indeed theoretically slower than solving the complete problem at once. In practice, one would expect the iterative sampling method to exploit the high degeneracy of the MMDCP to prove optimality after a few iterations. In this case, procedure `ExactClustering(U)` solves problems several orders of magnitude smaller than the original one.

4 Sub-routine `ExactClustering(U)`: Branch-and-price

In this section we describe an exact algorithm for the MMDCP used as the exact subroutine within the iterative sampling framework. The algorithm is based on the solution of a set-covering formulation of the MMDCP by branch-and-price. We first include a high-level description of our branch-and-price algorithm. Second, we introduce the set-covering formulation of the problem. In the following subsections we describe the different parts of the method, namely the pricing and branching schemes.

4.1 High-level description of column generation

A branch-and-price algorithm is a LP-based branch-and-bound algorithm in which lower bounds are computed by solving a LP by column generation (CG). In CG, one solves iteratively a restricted master problem (RMP) and a pricing subproblem (PS). Usually, the RMP is associated to an integer-linear program (ILP) for which the integrality constraints are relaxed, and for which only a subset of variables is considered. In our case, the ILP corresponds to a set-covering problem $SC(U, K)$ which, if solved explicitly for the whole set of variables, would return an optimal K-clustering of the nodes in U. Let $\mathcal{C}$ denote the set all possible covers of U, and let $\mathcal{C}' \subseteq \mathcal{C}$ denote a subset of those covers. Let $RMP(U, K, \mathcal{C}')$ denote the RMP associated to the covers defined in $\mathcal{C}'$. Let $(\overline{x}, \overline{\mu})$ denote the fractional primal and dual solutions associated with $RMP(U, K, \mathcal{C}')$. Let $PS(\mu)$ denote the pricing subproblem constructed from using the dual variables μ to build covers of negative reduced cost. Let X denote the set of columns of negative reduced cost as found by $PS(\mu)$. The following pseudo-code is a high-level description of a column generation algorithm:

Algorithm 2 Column generation

```
**Require:** $U, K$
**Ensure:** Optimal solution $x$ of $RMP(U, K, \mathcal{C})$
  $\mathcal{C}' \longleftarrow \mathcal{C}_0$
  $X \longleftarrow \emptyset$
  **repeat**
    $\mathcal{C}' \leftarrow \mathcal{C}' \cup X$
    $(\overline{x}, \overline{\mu}) \longleftarrow RMP(U, \mathcal{C}')$
    $X \longleftarrow PS(\mu)$
  **until** $X = \emptyset$
  $(x, \mu) \longleftarrow RMP(U, \mathcal{C}')$
  **return** $x$
```

This CG is then embedded into a branch-and-bound algorithm, for which is necessary to define proper branching rules. In our case, this part is explained in detail in Section 4.5.

4.2 Set-covering formulation of the MMDCP

We are given a sample U of V. We denote by E the set of undirected edges linking any two nodes in U. A cluster can either be equal to a singleton $\{u\}$ or to a pair $(S, e) \in \mathcal{P}(U) \times E$, where e represents one possible edge of maximum diameter within the nodes in S. The set of all feasible clusters containing two or more nodes is denoted by $\mathcal{C}$. For a cluster $t = (S, e) \in \mathcal{C}$ we denote $S_t = S, e_t = e$.

For every $u \in U$, we let s_u be a binary variable equal to 1 iff node u is clustered alone, and we let d_u be its diameter (as we will explain in Section 4.5, a node can have a strictly positive diameter following a branching decision). For a given edge $e = \{u, v\} \in E$, d_e denotes the dissimilarity between nodes u and v. For every $t \in \mathcal{C}$ we consider a binary variable z_t that will take the value 1 iff the cluster t is retained. For every node $u \in U$ we let a_{ut} be a binary constant that takes the value 1 iff $u \in S_t$. Also, for every edge $e \in E$ we let b_{et} be a binary constant that takes the value 1 iff $e = e_t$. We finally define a continuous variable ω equal to the maximum diameter among the chosen clusters. The MMDCP restricted to the sample U (or equivalently problem $Q(U)$, as defined in Section 3) can thus be formulated as follows:

$$\min_{s,\omega,z} \quad \omega \tag{2}$$

subject to

$$\omega - \sum_{t \in \mathcal{C}} b_{et} d_e z_t \geq 0 \qquad e \in E \tag{3}$$

$$\omega - d_u s_u \geq 0 \qquad u \in U \tag{4}$$

$$\sum_{t \in \mathcal{C}} a_{ut} z_t + s_u = 1 \qquad u \in U \tag{5}$$

$$\sum_{t \in \mathcal{C}} z_t + \sum_{u \in U} s_u = K \tag{6}$$

$$z_t \geq 0 \qquad t \in \mathcal{C} \tag{7}$$

$$z_t \text{ is integer} \qquad t \in \mathcal{C} \tag{8}$$

Constraints 3 state that the maximum diameter is greater or equal to the edge of maximum diameter in cluster t. Constraints 4 ensure that the maximum diameter is also larger than the diameter of node u if it is clustered alone. The set of constraints 5 state that each node belongs to one cluster, and the constraints 6 express that the optimal partition contains exactly K clusters. Without loss of generality, they can be replaced by

$$\sum_{t\in\mathcal{C}} a_{ut} z_t + s_u \geq 1 \quad u \in U,$$

and

$$\sum_{t\in\mathcal{C}} z_t + \sum_{u\in U} s_u \leq K,$$

since a covering of the nodes which is not a partition cannot be optimal, and any partition with less than K clusters has objective value greater or equal to the optimal partition with K clusters. By replacing the equality constraint by inequalities, the dual variables associated do never change sign, which results on more stable optimization algorithms.

We solve this problem by means of branch-and-price. The linear relaxation of problem (2)-(8) is solved by column generation, whereas the integrality constraints are imposed through branching.

4.3 Pricing subproblem

Let us assume that the linear relaxation of problem (2)-(8) has been solved restricted to a subset $\mathcal{C}' \subset \mathcal{C}$ of feasible clusters. We can extract dual variables $(\sigma_e)_{e\in E}, (\alpha_u)_{u\in U}, (\lambda_u)_{u\in U}$ and γ for constraints (3), (4), (5) and (6), respectively. The reduced cost of variables s_u, z_t are denoted as $\overline{c_u}, \overline{c_t}$, respectively, and are equal to

$$\overline{c_u} = d_u \alpha_u - \lambda_u - \gamma \tag{9}$$

$$\overline{c_t} = d_{e_t} \sigma_{e_t} - \sum_{u\in U} a_{ut} \lambda_u - \gamma \tag{10}$$

The pricing subproblem is performed in two steps. In the first step, we search for single-node clusters of negative reduced cost. This can be done by simple inspection by evaluating expression (9) for every possible $u \in U$.

If no such cluster exists, the second step of the pricing subproblem searches for a feasible cluster t of minimum reduced cost, this is such that expression (10) is minimized. We formulate this problem as an integer program, as follows. For every $u \in U$, we let x_u be a binary variable equal to 1 iff $u \in S_t$. For every edge $e \in E$ we let y_e be a binary variable equal to 1 iff $e = e_t$. We consider the following integer program:

$$\min_{x,y} \quad \phi \quad = \quad \sum_{e\in E} \sigma_e d_e y_e - \sum_{u\in U} \lambda_u x_u \tag{11}$$

subject to

$$\sum_{f\in E} d_f y_f - d_e(x_u + x_v - 1) \geq 0 \qquad e = \{u,v\} \in E \qquad (12)$$

$$2y_e - x_u - x_v \leq 0 \qquad e = \{u,v\} \in E \qquad (13)$$

$$\sum_{e\in E} y_e = 1 \qquad (14)$$

$$x_u \in \{0,1\} \qquad u \in U \qquad (15)$$

$$y_e \in \{0,1\} \qquad e \in E \qquad (16)$$

Now, this pricing subproblem will select one edge $e \in E$ (associated to a variable $y_e = 1$) and construct a node subset accordingly (associated to the set $\{u \in U : x_u = 1\}$). We would like to highlight that, if the edge $e_t = \{u_t, v_t\}$ is chosen in advance (meaning that $y_{e_t} = 1$), one can *a priori* fix to zero all variables x_u such that $\max\{d_{uu_t}, d_{uv_t}\} > d_{e_t}$ and to one variables x_{u_t}, x_{v_t}. Let us denote then $U^t = \{u \in U \setminus \{u_t, v_t\} : \max\{d_{uu_t}, d_{uv_t}\} \leq d_{e_t}\}$. The optimal set of nodes for a fixed e_t can be found by solving the following integer program:

$$\max_x \quad \phi'(e_t) \quad = \quad \sum_{u\in U^t} \lambda_u x_u \qquad (17)$$

subject to

$$x_u + x_v \leq 1 \qquad u, v \in U^t, u < v, d_{uv} > d_{e_t} \qquad (18)$$

$$x_u \in \{0,1\} \qquad u \in U^t \qquad (19)$$

The relationship between ϕ and $\phi'(u_t, v_t)$ is as follows:

$$\phi = \min\{\sigma_e d_e - (\phi'(e) + \lambda_u + \lambda_v) : e = \{u,v\} \in E\} \qquad (20)$$

4.4 Solution of the pricing subproblem

The solution of the pricing subproblem exploits the aforementioned property to derive an efficient heuristic and exact method. It relies on the sorting of the edges in E in increasing order with respect to the quantity $\sigma_e d_e - \lambda_u - \lambda_v$, with $e = \{u,v\} \in E$. The greedy heuristic is several orders of magnitude faster than the exact procedure and is always executed first. The exact princing method is thus only executed when the heuristic fails at finding columns of negative reduced cost.

4.4.1 Greedy heuristic

Our greedy heuristic starts, for every edge $e = \{u,v\} \in E$, with a cluster containing the nodes u and v, and expanding it while possible.

Set $k \leftarrow 1$, and let $e_k = \{u_k, v_k\}$ be the k-th element of E. We let $C = \{u_k, v_k\}$, $S \leftarrow U^k$. Let us set $j \leftarrow 1$. At any iteration $j \geq 1$, C represents the current cluster and S the set of nodes that can be inserted into C without exceeding the diameter given by d_{e_k}. At iteration $j+1$, we will set $v^* \leftarrow \arg\max\{\lambda_v : v \in S\}$. We then update C and S as follows: the new cluster becomes $C \leftarrow C \cup \{v^*\}$; the new set S becomes $S \leftarrow S \setminus \{v \in S : d_{vv^*} > d_{e_k}\}$. If S is empty, we check if the reduced cost associated to cluster (C, e_k) is negative. If so, stop and return (C, e_k). Otherwise, set $k \leftarrow k+1$ and restart unless $k > |E|$, in which case the algorithm is stopped and no column is returned.

4.4.2 Exact algorithm

Let $\overline{\omega}$ be the linear relaxation value associated with the current set of columns. Let ω^* be the current upper bound of the problem. We define the absolute gap as the difference $\omega^* - \overline{\omega}$ and denote it by `gap`.

Let $k \leftarrow 1$ and let $e_k = \{u_k, v_k\}$ be the next edge to inspect. Our exact algorithm computes a maximum weighted clique on the graph $G^k = (U^k, E^k)$, with $E^k = \{e = \{u,v\} : e \in E, u, v \in U^k, d_e \leq d_{e_k}\}$. Each node $u \in U$ has a weight equal to λ_u. We compute $\phi'(e_k)$ using CLIQUER (Östergård 2002). Let us denote $\overline{c_k} \leftarrow \sigma_{e_k} d_{e_k} - (\phi'(e_k) + \lambda_{u_k} + \lambda_{v_k}) - \gamma$. Depending in the value of $\overline{c_k}$, three possible cases arise:

1. If $\overline{c_k} < 0$, then a column (a feasible cluster) of negative reduced cost has been detected. Stop and return the associated cluster.
2. Else if $0 \leq \overline{c_k} <$ `gap`, then do nothing.
3. Else (i.e. if $\overline{c_k} \geq$ `gap`), then no column $t \in \mathcal{C}$ such that $e_t = e_k$ can be part of an optimal solution improving upon the incumbent. Therefore, edge e_k can be removed from the computation of ϕ in (20) without compromising the exactness of the algorithm.

In cases 2 and 3, we set $k \leftarrow k+1$ and restart the procedure with the next available edge. If none, we abort the algorithm and return *nil*.

4.5 Branch-and-bound

Let $((\overline{s_u})_{u \in U}, (\overline{z_t})_{t \in \mathcal{C}})$ be the optimal solution at the end of the column generation process. Let us define, for every $e \in E$, $\overline{y_e} = \sum_{t \in \mathcal{C}} b_{et} \overline{z_t}$. We also define, for every edge $e = \{u, v\} \in E$, $\overline{x_e} = \sum_{t \in \mathcal{C}} a_{ut} a_{bt} \overline{z_t}$. In addition, we define, for every node $u \in U$, $\overline{r_u} = \sum_{e = \{u,v\} | v \in U \setminus \{u\}} \overline{y_e}$. The solution might be declared unfeasible if $\overline{s_u}, \overline{y_e}, \overline{x_e}$ or $\overline{r_u}$ are fractional for some edge e or node u. Depending on the branching decision chosen, the two children problems are built as follows:

1. If $\overline{s_u} \in]0,1[$ is the chosen branch: We create two children nodes, namely $s_u = 0$ and $s_u \geq 1$. For $s_u = 0$ we remove the variable s_u from the child master and from the computation of the reduced costs. For the branch $s_u \geq 1$, we simply add the inequality to the child node. As the variable is already in the current node master, there is no need to remove it and

therefore no need to consider its dual in the computation of the reduced costs when using expression (9).
2. If $\overline{y_e} \in]0,1[$ is the chosen branch: We create two children nodes, namely $y_e = 0$ and $y_e \geq 1$. For $y_e = 0$ we remove the edge e from the computation of ϕ in (20) and also remove all clusters $\{(S,e) \in \mathcal{C}'\}$ from the master problem. For the branch $y_e \geq 1$, we simply add the following inequality to the child node: $\sum_{t \in \mathcal{C}} b_{et} z_t \geq 1$. Its dual must be taken into account for the computation of the reduced costs.
3. If $\overline{x_e} \in]0,1[$ is the chosen branch, with $e = \{u,v\}$: We create two children nodes, namely $x_e = 0$ and $x_e = 1$. For $x_e = 0$, we need to assure that u and v will never be on the same cluster. Thus, we remove from the master problem all clusters containing both nodes. In addition, we modify their dissimilarity to be $d_{uv} \leftarrow +\infty$. For the branch $x_e = 1$, we need to assure that every cluster containing u will also contain v. We proceed to *shrink* these two nodes into a single node $\{uv\}$, and update its diameter to $d_{\{uv\}} \leftarrow d_u + d_v$. Also, for every $w \in V \setminus \{u,v\}$, we let $d_{\{u,v\}w} \leftarrow \max\{d_{uw}, d_{vw}, d_{\{uv\}}\}$. We also remove from the master problem all clusters containing one of the nodes but not both.
4. If $\overline{r_u} \in]0,1[$ is the chosen branch: We create two children nodes, namely $r_u = 0$ and $r_u \geq 1$. For $r_u = 0$, we remove from the master all clusters $(S,e) \in \mathcal{C}'$ such that one of the endpoints of e is equal to u. All edges $\{e = \{v,w\} \in E : v = u \text{ or } w = u\}$ are removed from the computation of ϕ in (20). For the branch $r_u \geq 1$, we simply add the following inequality to the child node: $\sum_{t \in \mathcal{C}} \sum_{\{e=\{u,v\} \in E : v \in S\}} b_{et} z_t \geq 1$.

We have implemented a hybrid branching strategy that performs strong branching for the first 1000 node separations, and pseudo-cost branching afterwards.

5 Sub-routine `HeuristicClustering(`$P^*(U)$`, `$V \setminus U$`)`: Completion heuristic

To prove the optimality of the solution associated to the current set U or that another iteration of the algorithm is necessary, we have implemented the following completion heuristic. For every subset $S \subseteq V$, we let $diam(S) = \max\{d_{uv} : u,v \in S\}$ be the diameter of set S. We also let $P^*(U) = \{P_i^*(U) : i = 1 \dots K\}, \omega^*(U)$ be the associated optimal clustering of those nodes and the optimal solution value, respectively. For every node $u \in V \setminus U$ and for every cluster $P_i^*(U) \in P^*(U)$, we let $\nu(u,i) = \max\{d_{uv} : v \in P_i^*(U)\}$. For each $u \in V \setminus U$, the clusters are sorted in non-decreasing order of $\nu(u,i)$, this is $\nu(u,i_1) \leq \nu(u,i_2) \leq \dots \leq \nu(u,i_K)$. In case of a tie among two or more clusters, we proceed to sort them in non-decreasing order of diameter. Following ties are broken arbitrarily. For every $1 \leq i \leq K$, we denote by $P_i^*(U,u)$ the i-th cluster according to this ordering. Note that this means that for two different observations u and v, $P_i^*(U,u)$ may represent a different cluster than $P_i^*(U,v)$ (as the clusters are sorted, for each node in $V \setminus U$, differently).

The next problem is to define an ordering of the nodes in $V \setminus U$. The intuition behind our approach is to sort the nodes so as to favor the detection of insertions that would necessarily entail an increase of the maximum diameter in the early stages of the completion process. For every $u \in V \setminus U$, we consider the following quantities:

$$l_1(u) = \max\{0, diam(P_1^*(U,u) \cup \{u\}) - \omega^*(U)\} \tag{21}$$
$$l_2(u) = diam(P_1^*(U,u) \cup \{u\}) - diam(P_1^*(U,u)) \tag{22}$$
$$l_3(u) = diam(P_1^*(U,u) \cup \{u\}) \tag{23}$$
$$l_4(u) = diam(P_1^*(U,u)) \tag{24}$$

The nodes are sorted in non-increasing order of l_1. Ties are broken by considering l_2, l_3 and l_4, in that order. Following ties are broken by considering the same reasoning with $P_2^*(U,\cdot)$, $P_3^*(U,\cdot)$, and so on.

Let us denote $V \setminus U \leftarrow \{u_1, \ldots, u_s\}$ the nodes in $V \setminus U$ sorted according to the aforementioned ordering of nodes. Let $j \leftarrow 1$. Each cluster is inspected according to the ordering defined by the quantities $\nu(u_j, \cdot)$. Node u_j is thus inserted in the first cluster where it fits if its addition does not entail an increase in the maximum diameter given by $\omega^*(U)$. If no such cluster exists, the algorithm stops. We check whether the insertion of node u_j was not possible because of another previously inserted node $u_l, l < j$. If no such u_l exists, we return $W = \{u_j\}$, otherwise we return $W = \{u_l, u_j\}$. If the insertion is, however, possible, we update the diameter of the cluster involved, let $j \leftarrow j+1$ and restart, unless j reaches $s+1$ in which case the algorithm stops and the global optimal clustering is returned.

6 Acceleration techniques

To accelerate the whole procedure, some remarks are in order.

First, a preprocessing of the nodes allows a reduction in the number of items. Indeed, it is possible to discard duplicates (an item is said to be a duplicate of another if they share the exact same attributes). While for some problems this procedure did not help to reduce the number of points, for others the reduction reached a 70% of the nodes (*KDD cup 10%*, from 494,020 to only 145,583 nodes). In addition, we perform dimension reduction by removing dimensions whose standard deviations are equal to 0. This happens for a particular dimension only when the same value is given for all items in the dataset. Therefore, removing that dimension does not change the optimal solution value.

Second, the set U may be initialized to contain zero or more nodes from the set V. Indeed, for the MMDCP, it is always preferable to begin with a set U containing at least $K+1$ nodes. Any set smaller than that will always have cost 0 (it suffices to cluster all nodes apart). In our implementation we have performed the following procedure to initialize the set U.

1. Compute the centroid $\overline{u}$ of the points in V. If the i-th dimension of the problem is a numerical variable, we let $\overline{u}_i$ be $\frac{1}{|V|}\sum_{u\in V} u_i$. On the contrary, if it is a categorical variable, we let $\overline{u}_i$ to be the mode of the values $(u_i)_{u\in V}$.
2. Let then T be the set containing the $\rho = \min\{5000, |V|\}$ farthest points in V from $\overline{u}$. For each $p \in T$, we let T_p be built iteratively as follows: in step 1, $T_p = \{p\}$. From step 2 to $K+1$, we insert into T_p the node $v \in V \setminus T_p$ whose closest distance to a node in T_p is maximum.
3. The best possible K-clustering for T_p can be obtained by clustering together the two nodes $u, v \in T_p$ whose dissimilarity is the smallest, and then all the other $K-1$ nodes apart. The dissimilarity d_{uv} is then the value of the optimal clustering for T_p.

This algorithm if executed ρ times would turn to be excessively time consuming, even for a small number of clusters. Indeed, after each execution of the heuristic, we retain the value ν of the largest clustering diameter found so far. We abort the execution of this algorithm as soon as the constructive heuristic has been executed 100 times without generating a solution of value larger than ν.

Third, we always warm-start the branch-and-price procedure by computing lower and upper bounds for the problem, as follows: An upper bound can be obtained by executing the constructive heuristic introduced in Section 5. Moreover, we have implemented an *iterated local search* method to improve this solution that uses the LS presented in Fioruci et al (2012), with a perturbation based on the random selection of diameter nodes (two nodes that have maximum intra-cluster distance) and the reassignment of those nodes to randomly selected clusters. The value achieved by the ILS is then used as a cut-off value for the branch-and-price algorithm. Also, the optimal solution from the previous iteration of the branch-and-price provides a lower bound on the value of the optimal solution at the current iteration (thanks to the monotonicity of the MMDCP). Let ω' be that lower bound. We enforce it by adding to the master problem the inequality

$$\sum_{t\in\mathcal{C}} \sum_{e\in E'} b_{et} z_t \geq 1, \tag{25}$$

where $E' = \{e \in E : d_e \geq \omega'\}$. Certainly, one needs to consider its dual variable in the computation of the reduced costs for the column generation process.

7 Computational results

The proposed algorithm was programmed in C++ using the GNU g++ compiler v5.2. The general purpose linear programming solver used by CG was CPLEX 12.6. Maximum weighted cliques necessary to the exact solution of the auxiliary problem are computed using CLIQUER (Östergård 2002). The algorithm was compiled and executed in a single core on a machine powered by an Intel Xeon E5-2637 CPU 3.5 GHz x 16 with 128GB of RAM, running the Oracle Linux OS.

In our experimental analysis, we consider some classical problems from clustering, classification and regression tasks. The summary information of these problems is reported in Table 1. In this table we report the name of the problem (under column labeled *Problem*), the number of objects to be clustered (under column labeled n), the number of sought clusters (under column labeled K), the number of dimensions (under column labeled s), and the reference (under column labeled *Ref.*). The only problems for which a dimensionality reduction could be applied (as explained in Section 6) are: *Census* (from 41 to 39), *Image segm* (from 19 to 18), *Ionosphere* (from 34 to 33), *KDD cup 10%* (from 41 to 39), and *Segmentation* (from 19 to 18).

It is important to compare clustering algorithms using classical or well documented benchmark datasets since the hardness of a clustering problem depends not only on the number of objects (n), but also on the number of sought clusters (K) and on how the objects are spread in the space. For example, if objects are embedded in an Euclidean space and located in very separated clusters, any reasonable exact method should find the optimal solution regardless of the number of objects, which would bias any conclusions regarding the performance of the algorithm.

The selected problems contain mixed numerical and categorical data. The dissimilarity between two objects $u = (u_i)_{i=1}^s, v = (v_i)_{i=1}^s$ is computed as:

$$d_{uv} = \sqrt{\sum_{i=1}^{s} g(u_i, v_i)}, \tag{26}$$

where $g(x, y)$ is equal to $(x - y)^2$ if x and y are two numerical values, equal to 1 if x and y are two categorical values whose string representations differ, and equal to 0 if x and y are two categorical values whose string representations are the same. The number of categorical dimensions are reported in parenthesis (whenever > 0) under column s of Table 1.

Remark that storing the whole dissimilarity matrix for dataset *Cover type* would require approximately 10 TB of memory. Our method does not require such large amount of resources.

To assess the efficiency of our method, thereafter labeled IS, we have designed three experiments. In the first experiment, summarized in Table 2, we consider a sequential implementation of our algorithm and compare it against the results of three algorithms: the CP algorithm of Dao et al (2017), the $RBBA$ of Brusco and Stahl (2006) and the BB of Delattre and Hansen (1980) We restrict our analysis to the problems used in the experimental analysis of Dao et al (2017) with no dimensionality reduction. The algorithms were executed on a 3.4 GHz Intel Core i5 processor with 8G Ram running Ubuntu. As one can see from this table, our algorithm takes less than two seconds to solve all the problems, including problem *Waveform (v2)* that passed from being solved in almost a minute, to only 1.9 seconds.

Table 1 Problems details

Problem	n	K	s	*Ref.*
Iris	150	3	4	Lichman (2013)
Wine	178	3	13	Lichman (2013)
Glass	214	7	9	Lichman (2013)
Ionosphere	351	2	34	Lichman (2013)
User knowledge	403	4	5	Kahraman et al (2013)
Breast cancer	569	2	30	Lichman (2013)
Synthetic control	600	6	60	Alcock and Manolopoulos (1999)
Vehicle	946	4	18	Siebert (1987)
Yeast	1,484	10	8	Lichman (2013)
Mfeat (morph)	2,000	10	6	Dao et al (2017)
Multiple features	2,000	10	649	Lichman (2013)
Segmentation	2,000	7	19	Dao et al (2017)
Image segm	2,310	7	19	Lichman (2013)
Waveform (v1)	5,000	3	21	Lichman (2013)
Waveform (v2)	5,000	3	40	Lichman (2013)
Ailerons	13,750	10	41	Torgo (2009)
Magic	19,020	2	10	Lichman (2013)
Krkopt	28,056	17	6 (3)	Lichman (2013)
Shuttle	58,000	7	9	Lichman (2013)
Connect-4	67,557	3	42 (42)	Lichman (2013)
SensIt (acoustic)	96,080	3	50	Duarte and Hu (2004)
Twitter	140,707	2	77	Lichman (2013)
Census	142,521	3	41 (28)	Lichman (2013)
HAR	165,633	5	18	Ugulino et al (2012)
IJCNN1	191,681	2	22	Prokhorov (2001)
Cod-Rna	488,565	2	8	Uzilov et al (2006)
KDD cup 10%	494,090	23	41 (7)	Lichman (2013)
Cover type	581,012	7	54	Blackard (1998)

Our second experiment, summarized in Table 3, aims at analyzing the scalability of our algorithm for large datasets. We restrict our analysis to problems containing 5,000 objects or more. In this table, label *it* represents the number of main iterations of our algorithm, this is the number of times that the completion heuristic needs to be executed. Label n' represents the number of objects in the last iteration of the algorithm right before the final completion heuristic takes place. The time (in minutes) spent in the last completion heuristic execution is reported under column labeled lch(min). Under column labeled p we report the percentage of objects that are successfully inserted in their closest cluster according to the ordering described in Section 5. This provides a measure of the efficiency of that ordering in the case that the last completion heuristic were aborted prematurely in a heuristic setting. The total running time spent by our algorithm (in minutes) is shown under column

Table 2 Running times (in seconds) on small datasets

Problem	*Opt*	*RBBA*	*BB*	*CP*	*IS*
Iris	2.6	1.4	1.8	< 0.1	< 0.1
Wine	458.1	2.0	2.3	< 0.1	< 0.1
Glass	5.0	8.1	42.0	0.2	0.2
Ionosphere	8.6		0.6	0.3	0.2
User knowledge	1.2		3.7	0.2	1.1
Breast cancer	2,378.0		1.8	0.5	0.2
Synthetic control	109.4			1.6	0.4
Vehicle	264.8			0.9	0.2
Yeast	0.7			5.2	1.6
Mfeat (morph)	1,595.0			8.59	0.6
Segmentation	436.4			5.7	0.6
Waveform (v2)	15.6			50.1	1.9

Table 3 Detailed results of the iterative sampling method for the MMDCP

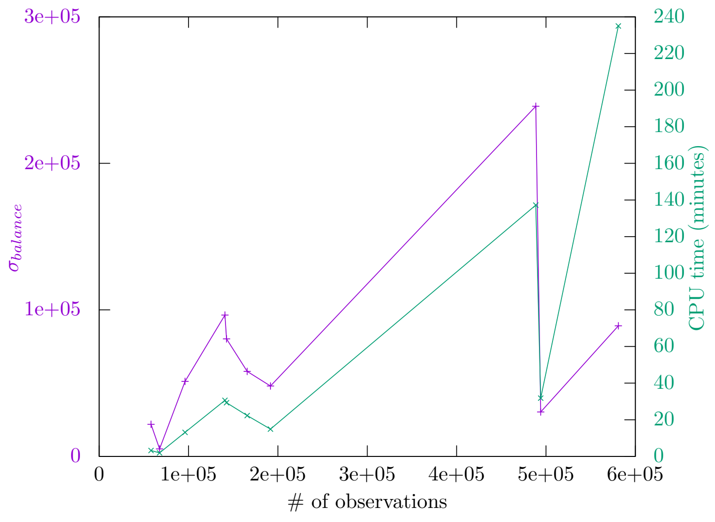
Problem	*opt*	*it*	n'	lch(min)	p	t(min)	$\sigma_{balance}$
Waveform (v1)	13.74	10	21	< 0.1	99.7	< 0.1	35.02
Waveform (v2)	15.58	9	22	< 0.1	99.8	< 0.1	192.89
Ailerons	230.71	33	47	< 0.1	99.7	0.2	1368.06
Magic	692.44	3	12	0.4	100.0	0.4	12445.79
Krkopt	2.00	64	81	< 0.1	82.8	0.4	1438.73
Shuttle	6,157.44	5	14	3.0	99.9	3.2	21884.03
Connect-4	3.87	8	17	1.6	98.2	1.9	5110.38
SensIt (acoustic)	4.47	6	15	12.7	99.9	13.1	51191.90
Twitter	80,734	2	11	30.2	100.0	30.6	96446.54
Census	100,056	3	13	28.8	99.9	29.3	80207.60
HAR	1,078.73	8	18	21.8	99.9	22.3	57993.89
IJCNN1	3.97	5	14	14.5	99.9	14.9	48023.16
Cod-Rna	934.68	3	12	136.4	100.0	137.2	238954.72
KDD cup 10%	144,165	26	53	29.7	99.9	31.8	30290.33
Cover type	3,557.3	153	166	149.8	99.9	235.0	89122.85

labeled t(min). Finally, column $\sigma_{balance}$ reports the standard deviation on the cardinality of the optimal clusters.

As shown in this table, our method is capable of solving all these problems within reasonable time limits. Typically, only very small subsets of V need to be handled by the `ExactClustering(U)` subroutine at every iteration of the algorithm. In addition, if the last completion heuristic were aborted prematurely and the remaining objects added into their closest cluster —according to the ordering defined in Section 5—, the resulting heuristic would effectively find the right clustering for a 98.6% of the objects on average.

Yet, Figure 1 illustrates the correlation between the time spent by our method and the balance among the different clusters in the optimal solutions.

Fig. 1 Computimes times and balance deviations for different problems



We restricted our analysis to problems solved by our method in more than one minute. Indeed, the time spent by the completion heuristic is quadratic on the size of the largest cluster, and consequently, balanced clusters are the best case for proving optimality.

It is important to highlight that our algorithm's running time for a given dataset is comparable to the time needed to compute its dissimilarity matrix, which is $O(n^2)$ time. Moreover, on some very large datasets, it proves even faster as shown in Figure 2. This demonstrates that it is possible to devise exact methods for the MMDCP that to not need to rely on a pre-computation and storage of the dissimilarity matrix.

Besides establishing new paradigms for the performance of algorithms for the MMDCP, our method also plays an important role on providing benchmark results for heuristics. In the following experiment, we compare the performance of our algorithm against the complete-linkage heuristic (Johnson 1967; Sørensen 1948; Defays 1977). It is well-known that the method seldom finds optimal solutions as reported by Alpert and Kahng (1997); Hansen and Delattre (1978). But how far are its heuristic solutions from optimality? Our third experiment, reported in Table 4, aims at answering this question by contrasting minimum diameter results obtained by complete-linkage (*C-L*) and *IS* on small datasets —those that could be handled by the `hclust()` routine in R given the available RAM memory. We can notice that minimum diameter partitions provided by the complete-linkage algorithm can be up to $\approx 45\%$ far from optimality, being $\approx 17\%$ worse in average. This is a clear indication of the ineffectiveness of *C-L* on finding near-optimal solutions for the MMDCP.

Fig. 2 Dissimilarity matrix computation (DMC) vs iterative sampling (IS)

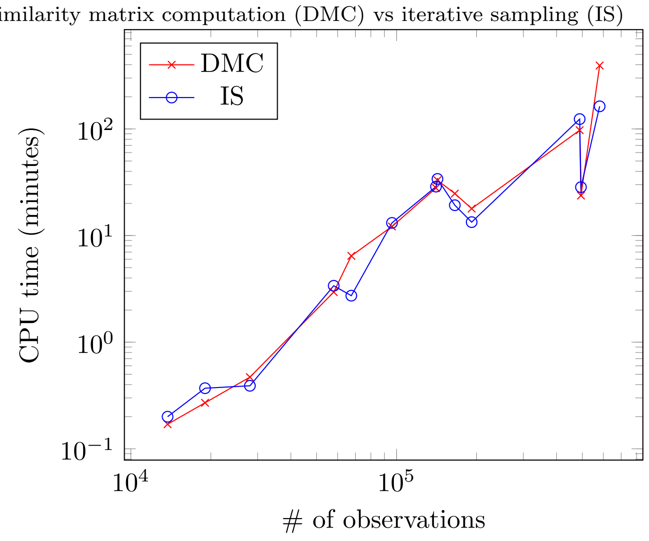


Table 4 *C-L* and *IS* on small datasets.

Problem	*C-L*	*IS*	*rel.diff.*(%)
Iris	3.21	2.58	24.42
Wine	665.15	458.13	45.19
Glass	5.69	4.97	14.49
Ionosphere	9.27	8.6	7.79
User knowledge	1.31	1.17	11.97
Breast cancer	2455	2377.96	3.24
Synthetic control	119.82	109.36	9.56
Vehicle	332.28	264.83	25.47
Yeast	0.77	0.67	14.93
Mfeat (morph)	2124.04	1594.96	33.17
Segmentation	442.57	436.4	1.41
Waveform (v1)	15.30	13.74	11.35
Waveform (v2)	17.29	15.58	10.98
Ailerons	295.47	230.71	28.07
Magic	829.69	692.44	19.82
Average			17.46

8 Hard instances

We have encountered difficulties in using our method when trying to solve the MMDCP on problems *Pendigits*, *Letter*, *Birch1*, *Birch2* and *Birch3* (all of which can be downloaded freely from the UCI benchmark database). Our algorithm stalled after a sufficiently large number of iterations that made the

Table 5 Hard Problems details

Problem	n	K	s	*Ref.*
Pendigits	10,992	10	16	Lichman (2013)
Letter	20,000	26	16	Lichman (2013)
Birch1	100,000	100	2	Zhang et al (1997)
Birch2	100,000	100	2	Zhang et al (1997)
Birch3	100,000	100	2	Zhang et al (1997)

Table 6 Detailed results of the iterative sampling method for the hard instances

Problem	*gap*	*it*	n'	*lch*(min)	p	t(min)	$\sigma_{balance}$
Pendigits	16.17	87	97	< 0.1	88.5	196.7	704.59
Letter	32.98	98	124	< 0.1	67.8	60.1	766.19
Birch1	77.25	150	250	0.4	30.1	52.9	193.07
Birch2	47.64	202	307	0.1	89.1	145.6	341.83
Birch3	74.97	167	267	0.4	37.7	74.8	1800.00

exact subroutine prohibitively too costly. Table 5 presents the main parameters of these problems.

To be able to execute our algorithm on these datasets and report its results, we performed the following modification to the method (it does not modify in any way the behavior of our algorithm for the already solved instances). We added a limit of 1000 nodes in queue in the branching tree of the branch-and-price method. This is not the number of nodes inspected so far, but the number of nodes that remain in queue for separation. When this limit is reached for the first time, the completion heuristic is performed fully on the optimal solution obtained for the previous sampling. The optimal solution of `ExactClustering(U)` on the previous sampling provides a valid lower bound for the problem. The completion heuristic provides an upper bound.

Table 6 reports our results. It contains the same information provided in Table 3, except for column *opt* which is replaced by column *gap* referring to the relative difference (in %) between the upper and lower bounds obtained by the algorithm.

All these problems have in common the existence of a large number of alternate solutions for values of the maximum diameter that are close to the optimal value. When this happens, a set W that might induce an increase in the diameter for a given solution might be clustered perfectly fine for some alternate one. In the next iteration, the optimal clustering subroutine will necessarily find an optimal solution of the same value. Moreover, the existence of many such solutions will also harm the resolution process because of the symmetries involved, which is a known weakness of LP-based branch-and-bound methods. We believe that, as a matter of future research, one may implement an alternative algorithm for `ExactClustering(U)` as, for instance, the *CP* of Dao et al (2017).

9 Concluding remarks

We have presented an iterative sampling algorithm for the solution of the minimax diameter clustering problem (MMDCP), which is strongly NP-hard. Our implementation of the method outperforms the state-of-the-art algorithm for this problem by solving datasets that are two orders of magnitude larger than those handled by previous schemes. We can identify three potential avenues for future research: first, to find other uses for the sampling method, either in classification or other areas where set-partitioning problems with high degrees of degeneracy arise frequently; second, in what concerns specifically the MMDCP, to work on the robustness of the method to allow the solution of problems with noise; third, to build a heuristic implementation of the method to allow the solution of arbitrarily large datasets, either applied to the MMDCP or to another partitioning problem.

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