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Accelerating Benders decomposition for the *p*-median problem through variable aggregation

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Abstract : The *p*-median problem is a classical location problem where the goal is to select *p* facilities while minimizing the sum of distances from each location to its nearest facility. Recent advancements in solving the *p*-median and related problems have successfully leveraged Benders decomposition methods. The current bottleneck is the large number of variables and Benders cuts that are needed. We consider variable aggregation to reduce the size of these models. We propose to partially aggregate the variables in the model based on a start solution; aggregation occurs only when the corresponding locations are assigned to the same facility in the initial solution. In addition, we propose a set of valid inequalities tailored to these aggregated variables. Our computational experiments indicate that our model, post-initialization, provides a stronger lower bound, thereby accelerating the resolution of the root node. Furthermore, this approach seems to positively impact the branching procedure, leading to an overall faster Benders decomposition method.

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1 Introduction

The *p*-median problem is one of the fundamental problems in location science (Laporte et al., 2019), where the aim is to select *p* facilities while minimizing the sum of distances from each location to its nearest facility. The *p*-median problem was introduced by Hakimi (1964) and is known to be NP-hard (Kariv and Hakimi, 1979). It has numerous practical applications (Rahmaniani et al., 2017; Laporte et al., 2019). Particularly, in the data mining and machine learning literature, the problem is referred to as the *k*-medoids problem (see e.g. Pinheiro et al. (2020)).

Benders decomposition is one of the most well-known solution methods to solve difficult combinatorial problems (Benders, 1962). Benders decomposition formulations for the *p*-median problem date back to Cornuejols et al. (1980) and Magnanti and Wong (1981). Benders decomposition has shown to be successful on a multitude of location problems (Fischetti et al., 2016b,a; Cordeau et al., 2019; Coniglio et al., 2022; Gaar and Sinnl, 2022; Ramírez-Pico et al., 2023; Ljubić et al., 2024). In particular, Duran-Mateluna et al. (2023) use a Benders decomposition method to solve the *p*-median problem for instances up to 238,000 locations.

The goal in the *p*-median problem is to cover N locations by opening p out of M possible facilities, while minimizing the sum of distances from each location to its nearest facility. To simplify notation and without loss of generality, we assume that N = M. Let d_{ij} denote the distance from location ito a facility j and let $N_i \leq N$ be the number of unique distances from i to any facility; the sorted distances are denoted by $D_i^0 \leq D_i^1 \leq D_i^2 \leq \cdots \leq D_i^{N_i}$, where $D_i^0 = -\infty$ is the distance to an artificial facility. The binary variable y_j is equal to 1 if facility j is selected, and 0 otherwise. The continuous variable θ_i represents the distance from location i to the closest selected facility. Let [N] be the set $\{1, 2, \ldots, N\}$ and [0, N] be the set $\{0, 1, \ldots, N\}$. A compact Benders reformulation (Duran-Mateluna et al., 2023) can be written as

$$\min\sum_{i=1}^{N} \theta_i,\tag{1}$$

s.t.
$$\sum_{j=1}^{N} y_j = p,$$
(2)

$$\theta_i \ge D_i^{n_i+1} - \sum_{j:d_{ij} \le D_i^{n_i}} (D_i^{n_i+1} - d_{ij}) y_j, \qquad i \in [N], n_i \in [0, N_i - 1],$$
(3)

$$y_j \in \{0, 1\}, \qquad j \in [N].$$
 (4)

In (1) we minimize the sum of the distances from location i to the nearest facility. Exactly p facilities are selected due to (2), while the so-called Benders cuts are given in (3). In a Benders decomposition approach the method starts with a subset of Benders cuts. Afterwards, violated Benders cuts are identified and added to the model until no more violations can be identified.

The current bottleneck of a Benders decomposition approach for the *p*-median problem is that the mathematical model becomes too large, since the number of variables and Benders cuts is proportional to the number of locations N. In the worst case, N Benders cuts are added in every iteration of the Benders decomposition. Instead of solving the *disaggregated* model, one potential solution is to define an *aggregate* variable $\bar{\theta} = \sum_{i=1}^{N} \theta_i$ and aggregated Benders cuts

$$\bar{\theta} \ge \sum_{i=1}^{N} [D_i^{n_i+1} - \sum_{j:d_{ij} \le D_i^{n_i}} (D_i^{n_i+1} - d_{ij})y_j], \qquad \forall (n_1, n_2, \dots, n_N) : l \in [N], n_l \in [0, N_l - 1],$$

which leads to a so-called fully aggregated mathematical formulation.

A fully aggregated Benders formulation has been investigated in location problems. For instance, by Fischetti et al. (2016b) and Ljubić et al. (2024), for the uncapacitated facility location problem and

the discrete ordered median problem, respectively. They present both disaggregated (multicut) and fully aggregated (single cut) formulations that are solved using Benders decomposition. An aggregated model may be preferred since the reduced formulation can be solved faster. However, such a model tends to converge more slowly, as the aggregate constraints are less restrictive. For several related location problems, effective aggregation strategies have been developed by leveraging problem-specific structures. For the uncapacitated hub location problem, Contreras et al. (2011) design cuts tailored to the structure involving hubs. Ramírez-Pico et al. (2023) examined the so-called adaptive Benders cuts for two-stage stochastic programming. Their approach starts with a limited set of scenarios, where each Benders cut corresponds to one scenario. These cuts are then dynamically disaggregated, generating additional scenarios (and more Benders cuts).

In this paper, we propose a *partially* aggregated Benders decomposition method for the *p*-median problem, meaning that some locations may be aggregated. We propose three key steps. First, during initialization, we partially aggregate locations based on a start solution, such that location that are likely to be assigned to the same facility are in the same aggregate variable and aggregate cut. Second, to accelerate the Benders decomposition, we propose a set of valid inequalities to strengthen the formulation in initial iterations. Third, if branching is required to obtain an integer solution, we introduce aggregated binary decision variables to branch on.

Our contribution can be summarized as follows. First, we propose a partially aggregated Benders decomposition framework for the *p*-median problem, which contains both disaggregate and fully aggregated Benders decomposition as special cases. Second, we show how to adjust the state-of-theart Benders decomposition method in order to solve the partially aggregated Benders decomposition. Last, we demonstrate the effectiveness of our method on both benchmark instances and newly introduced instances. In particular, our model, post-initialization, has a stronger lower bound compared to the disaggregate formulation, enabling faster resolution of the root node. Additionally, our proposed solution approach seems to positively impact the performance during the branch-and-cut phase.

The remainder of this paper is organized as follows. Related work is discussed in Section 2. In Section 3 we present a disaggregated Benders decomposition and a framework for the aggregated variant. Section 4 outlines our solution approach for the aggregated Benders decomposition. Our computational experiments are presented in Section 5. Finally, conclusions are drawn in Section 6.

2 Related work

Several mixed-integer programming formulations have been developed to model the *p*-median problem (ReVelle and Swain, 1970; Cornuejols et al., 1980; Magnanti and Wong, 1981; Elloumi, 2010) and connections between these formulations are still being investigated (Duran-Mateluna et al., 2023; Agra and Requejo, 2024). Numerous methods have been proposed to solve these *p*-median formulations to optimality. Senne et al. (2005) introduced a branch-and-price algorithm that incorporates stabilized column generation and Lagrangian relaxation, enabling them to solve instances up to 900 locations. Avella et al. (2007) propose a branch-and-cut-and-price algorithm with delayed column and row generation, allowing for the resolution of instances with nearly 3800 locations. García et al. (2011) consider a column generation approach that is embedded in a branch-and-bound framework, successfully solving instances up to 85,900 locations and p = 70,000 facilities. Ren et al. (2022) implement a (parallel) branch-and-bound method integrated with Langrangian relaxation, achieving a 0.1% optimality gap for instances with up to 100,000 locations on a single core and instances with up to 1 million locations when using 6000 cores.

Due to the large number of locations and facilities, heuristics have been designed to aggregate locations, such that optimization models remain applicable (Irawan and Salhi, 2015a). The *p*-median problem can be partitioned into smaller subproblems that can be solved within a reasonable amount of time. However, this results in a loss of information, as the model no longer utilizes the original location data. The difference between the optimal objective value and the one obtained using an aggregation heuristic is known as the aggregation error. Hillsman and Rhoda (1978) formally defined the aggregation error for the *p*-median (and related) problems. Current and Schilling (1987) were the first to study the elimination of aggregation errors, while Goodchild (1979) demonstrated that aggregation errors have a large impact on the results, potentially leading to inaccurate objective values. For Euclidean *p*-median problems in the plane, smaller error bounds have been proven (Qi and Shen, 2010). Aggregation techniques have been used to enhance heuristics for solving large scale *p*-median problems, e.g., Avella et al. (2012), Irawan et al. (2014), Irawan and Salhi (2015b) and Salhi and Irawan (2015). Although aggregation is typically done at the location level, it can also be applied at the facility level (Avella et al., 2012). Further details can be found in Irawan and Salhi (2015a).

In this paper, we show how to apply aggregation in the current state-of-the-art Benders decomposition method from Duran-Mateluna et al. (2023), without any aggregation error.

3 Benders decomposition framework

In this section, we present a disaggregated Benders decomposition formulation, which is used by the current state-of-the art Benders decomposition method to solve the p-median problem. Afterwards, we introduce an aggregated Benders decomposition framework, which contains as special cases the disaggregated and fully aggregated Benders decomposition.

3.1 Disaggregated Benders decomposition

Due to the large number of Benders cuts of the form (3), Duran-Mateluna et al. (2023) propose to solve (1)–(4) using Benders decomposition. The main idea of Benders decomposition is to iteratively solve a restricted master problem (RMP) on a subset of Benders cuts of the form (3), denoted by \mathcal{B}_i for each location *i*. A solution to the RMP may violate a Benders cut not yet in \mathcal{B}_i . In this case, we apply a separation algorithm to identify violated Benders cuts, which are subsequently added to the RMP. This iterative process continues until a feasible, possibly fractional, solution is obtained. We apply branch-and-Benders cut (Rahmaniani et al., 2017) to obtain an optimal solution, so we keep track of one set of cuts throughout the branching tree. The RMP can be formulated as

$$\min\sum_{i=1}^{N} \theta_i,\tag{5}$$

s.t.
$$\sum_{j=1}^{N} y_j = p,$$
(6)

$$\theta_i \text{ satisfies } \mathcal{B}_i, \qquad i \in [N],$$
(7)

$$y_j \ge 0, \qquad \qquad j \in [N], \tag{8}$$

Note that (5) and (6) are equal to (1) and (2), respectively. The integrality constraints on y_i are relaxed in (8).

Let $(\mathbf{y}, \boldsymbol{\theta})$ be a feasible, possibly fractional, solution to the RMP. We must verify whether there exists Benders cuts that are not yet in the RMP and violate the given solution. For a fixed solution, we can consider a separation problem for each location in [N]. For an efficient implementation to identify violated Benders cuts we refer to Algorithm 1 in Duran-Mateluna et al. (2023), which runs in $\mathcal{O}(N)$ for each location in [N].

3.2 Aggregated Benders decomposition

In this section we present a (partially) aggregated Benders decomposition framework. A priori we define which distance variables θ_i are aggregated. Let $P = \{Q_1, \ldots, Q_R\}$ be a partition of the set of

locations into R disjoint subsets, satisfying $Q = \bigcup_{r=1,...,R} Q_r = [N]$ and $Q_r \cap Q_s = \emptyset, \forall r \neq s$. We denote the aggregated variables by $\bar{\theta}_{Q_r}$, such that $\bar{\theta}_{Q_r} = \sum_{i \in Q_r} \theta_i$. When R = N we obtain the disaggregated Benders decomposition, whereas setting R = 1 leads to a fully aggregated Benders decomposition. For each set Q_r we define *aggregated* Benders cuts

$$\bar{\theta}_{Q_r} \ge \sum_{i \in Q_r} [D_i^{n_i+1} - \sum_{j: d_{ij} \le D_i^{n_i}} (D_i^{n_i+1} - d_{ij})y_j], \quad \forall (n_1, n_2, \dots, n_N) : l \in Q_r, n_l \in [0, N_l - 1].$$
(9)

This leads to the following Aggregated Restricted Master Problem (ARMP)

l

$$\min\sum_{r=1}^{R} \bar{\theta}_{Q_r},\tag{10}$$

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s.t.
$$\sum_{i=1}^{N} y_i = p,$$
(11)

$$\bar{\mathcal{B}}_{Q_r}$$
 satisfies $\bar{\mathcal{B}}_r$, $r \in [R]$, (12)

$$i \ge 0, \qquad \qquad i \in [N]. \tag{13}$$

In (10) we minimize the aggregated distance variables. As before, (11) ensures that we select exactly p facilities, while (12) enforces the feasibility of the current set of aggregated Benders cuts $(\bar{\mathcal{B}}_r)$ for each set Q_r .

4 Aggregated Benders decomposition for Euclidean distances

In the remainder of this paper we assume that the locations lie in a k-dimensional Euclidean space. To solve the aggregated Benders decomposition we propose to add three additional steps to the existing disaggregated Benders decomposition from Duran-Mateluna et al. (2023). First, based on a start solution we partially aggregate the distance variables. Second, we introduce a set of valid inequalities for the aggregate distance variables in order to strengthen the lower bound in the initial iterations of the Benders decomposition. Third, we add aggregate binary variables before starting the branching procedure.

4.1 Constructing a partition

Suppose we have a feasible start solution, represented by a partition $P = \{Q_1, \ldots, Q_p\}$. Each set Q_r contains one selected facility $m_r \in Q_r$. We define the set of locations outside Q_r as $Q_r^o = Q \setminus Q_r$, which we refer to as outside locations. The distance between a location *i* and a set of locations *Q* is defined as $d(i, Q) = \min_{j \in Q} d_{ij}$. The shortest distance from Q_r^o to the selected facility m_r is $\rho_r = d(m_r, Q_r^o)$, which we call the *radius* of set Q_r . Based on the radius, we split each Q_r into a group of central locations Q_r^c and remaining locations Q_r^e , which are defined below.

Definition 4.1 (Central locations). Given a set Q_r and a radius ρ_r the central locations are in the set $Q_r^c = \{i \in Q_r : d_{im_r} < \frac{1}{3}\rho_r\}$.

Definition 4.2 (Remaining locations). The remaining locations are given by the set $Q_r^e = Q_r \setminus Q_r^c$.

The concepts of central and remaining locations are visualized in Figure 1. In this figure, the yellow locations represent set Q_r , where we assume that $m_r = 1$ is the selected facility. The locations in Q_r are partitioned into a set of central locations Q_r^c and a set of remaining locations Q_r^e , based on radius ρ_r . The radius ρ_r is calculated as the shortest distance from the selected facility $m_r = 1$ to the nearest location outside the cluster, which is in this case a location in $Q_{r'}$ (represented by blue dots).



Figure 1: An example of a set $Q_r = \{1, 2, 3, 4, 5\}$ (corresponding to yellow dots) which is divided into two groups $Q_r^c = \{1, 2\}$ and $Q_r^e = \{3, 4, 5\}$ based on a radius ρ_r , determined by the distance from $m_r = 1$ to the closest location from another cluster $Q_{r'} = \{6, 7, 8\}$ (corresponding to blue dots).

For each set Q_r we have one aggregated variable $\theta_{Q_r^c}$ corresponding to set Q_r^c and several nonaggregated variables θ_i for each location $i \in Q_r^e$. Thus, when constructing the ARMP in (10)–(13), the model contains both aggregated and disaggregated Benders cuts.

The motivation behind the division into two groups Q_r^c and Q_r^e is as follows. Consider a good initial solution with m_r as the selected facility and suppose that in an optimal solution, m_r is not selected as facility. If another location from the set Q_r^c is selected as a facility, we can construct (strong) lower bounds for the partial objective $\bar{\theta}_{Q_r^c}$. Similarly, when a location from the set Q_r^e or Q_r^o is selected as facility we derive (weaker) lower bounds on $\bar{\theta}_{Q_r^c}$. These bounds can be added to the formulation through valid inequalities.

4.2 Valid inequalities

The main idea of the valid inequalities is to impose, for each $r \in [R]$, a lower bound on the (partial) objectives $\bar{\theta}_{Q_r^c}$ and $\theta_s, \forall s \in Q_r^e$. We propose three types of valid inequalities, which are added for each set Q_r .

4.2.1 Valid inequalities 1

We introduce three types of constants. First, for each central location $q \in Q_r^c$ let us define

$$\delta_{rq}^c = \sum_{i \in Q_r^c} d_{iq},$$

i.e., δ_{rq}^c is the 1-median objective for the central locations $i \in Q_r^c$ when $q \in Q_r^c$ is selected as the unique facility in Q_r . Second, for each remaining location $q \in Q_r^e$, we define

$$\delta^e_{rq} = \sum_{i \in Q^e_r} \min\{d_{iq}, d(i, Q^o_r)\}$$

The term δ_{rq}^e is a lower bound on the partial objective for the central locations $i \in Q_r^c$ when $q \in Q_r^e$ is selected as the unique facility in Q_r . Since outside locations in set Q_r^o may also be selected as a facility we take the minimum between distance d_{iq} and the distance from i to its nearest outside location, represented by $d(i, Q_r^o)$. Third, let D_r^c be the sum of distances from each location $i \in Q_r^c$ to its closest outside location, i.e.

$$D_r^c = \sum_{i \in Q_r^c} d(i, Q_r^o)$$

Consider the following valid inequality

$$\bar{\theta}_{Q_r^c} \ge D_r^c - \sum_{q \in Q_r^c} (D_r^c - \delta_{rq}^c) y_q - \sum_{q \in Q_r^e} (D_r^c - \delta_{rq}^e) y_q.$$
(14)

The valid inequality has a similar interpretation to a disaggregated Benders cut (3). When exactly one facility q is selected, the terms D_r^c cancel out and the remaining terms δ_{rq}^c and δ_{rq}^e represent a lower bound on the partial objective $\bar{\theta}_{Q_r^c}$. When no facility is selected in Q_r , a lower bound of D_r^c remains. By construction it holds that $D_r^c \ge \delta_{rq}^c$ and $D_r^c \ge \delta_{rq}^e$. For some locations $q \in Q_r^e$ it holds that $D_r^c = \delta_{rq}^e$, meaning that selecting these locations as facility does not change the lower bound in the valid inequality.

In Lemma 4.3 we prove that when exactly one location $q \in Q_r$ is selected as facility and this location belongs to the central locations Q_r^c , then the bound is tight: $\bar{\theta}_{Q_r^c} = \delta_{rq}^c$.

Lemma 4.3. Assume without loss of generality that $y_q = 1$ for some $q \in Q_r^c$. If $\sum_{i \in Q_r^c} y_i = \sum_{i \in Q_r} y_i = y_q = 1$, then $\bar{\theta}_{Q_r^c}$ is equal to δ_{rq}^c .

Proof. The distance d_{ij} between any two central locations $i, j \in Q_r^c$ is at most $\frac{2}{3}\rho_r$. Similarly, the distance d_{ij} from a central location $i \in Q_r^c$ to an outside location $j \in Q_r^o$ is at least $\frac{2}{3}\rho_r$. Since $y_q = 1$ and no other location is selected, it must hold that all locations in Q_r^c are assigned to the same facility q. Thus, given that q is selected as facility in an optimal solution the partial objective $\overline{\theta}_{Q_r^c}$ is equal to δ_{rq}^c , which is the 1-median objective of set Q_r^c with q as facility.

In the next theorem, we prove the validity of (14).

Theorem 4.4. Given a feasible solution $(\boldsymbol{\theta}, \mathbf{y})$, where the elements of vector \mathbf{y} are integral, the valid inequalities (14) are correct.

Proof.

We convert the solution vector \mathbf{y} to a matrix \mathbf{X} , where x_{iq} takes the value 1 when location i is assigned to q and 0 otherwise. Note that $y_q \ge x_{iq}$. If q is selected as facility, $y_q = 1$, this does not always imply that i is assigned to q. Conversely, $y_q = 0$ implies that $x_{iq} = 0$ for all locations i.

We aim to prove the correctness of valid inequality (14), which is rewritten as

$$\bar{\theta}_{Q_r^c} + \sum_{q \in Q_r^c} (D_r^c - \delta_{rq}^c) y_q + \sum_{q \in Q_r^e} (D_r^c - \delta_{rq}^e) y_q - D_r^c \ge 0.$$
(15)

The realized partial objective can be expressed in terms of x_{iq} variables as

$$\bar{\theta}_{Q_r^c} = \sum_{q \in (Q_r^c \cup Q_r^e) \cup Q_r^o)} \sum_{i \in Q_r^o} d_{iq} x_{iq},$$

$$\geq \sum_{q \in Q_r^o} \sum_{i \in Q_r^c} d(i, Q_r^o) x_{iq} + \sum_{q \in (Q_r^c \cup Q_r^e)} \sum_{i \in Q_r^c} d_{iq} x_{iq}$$

Using the definitions of D_r^c and δ_{rq}^c we bound the first summation in the left-hand side of (15) as

$$\sum_{q \in Q_r^c} (D_r^c - \delta_{rq}^c) y_q$$

$$\begin{split} &= \sum_{q \in Q_r^c} (\sum_{i \in Q_r^c} d(i, Q_r^o) - \sum_{i \in Q_r^c} d_{iq}) y_q, \\ &= \sum_{q \in Q_r^c} \sum_{i \in Q_r^c} (d(i, Q_r^o) - d_{iq}) y_q, \\ &\geq \sum_{q \in Q_r^c} \sum_{i \in Q_r^c} (d(i, Q_r^o) - d_{iq}) x_{iq}, \end{split}$$

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where the inequality holds because $y_q \ge x_{iq}$. Similarly, the second summation in the left-hand side of (15) can be bounded as well

$$\begin{split} &\sum_{q \in Q_r^e} (D_r^c - \delta_{rq}^e) y_q, \\ &= \sum_{q \in Q_r^e} [\sum_{i \in Q_r^c} d(i, Q_r^o) - \sum_{i \in Q_r^c} \min\{d_{iq}, d(i, Q_r^o)\}] y_q, \\ &= \sum_{q \in Q_r^e} \sum_{i \in Q_r^c} [d(i, Q_r^o) - \min\{d_{iq}, d(i, Q_r^o)\}] y_q, \\ &\geq \sum_{q \in Q_r^e} \sum_{i \in Q_r^c} [d(i, Q_r^o) - \min\{d_{iq}, d(i, Q_r^o)\}] x_{iq}, \\ &\geq \sum_{q \in Q_r^e} \sum_{i \in Q_r^e} [d(i, Q_r^o) - d_{iq}] x_{iq}. \end{split}$$

The first inequality holds because $y_q \ge x_{iq}$. When leaving out the minimization we obtain the second inequality.

Using the results above, the left hand side of (15) can be written as

$$\begin{split} \bar{\theta}_{Q_{r}^{c}} + &\sum_{q \in Q_{r}^{c}} (D_{r}^{c} - \delta_{rq}^{c}) y_{q} + \sum_{q \in Q_{r}^{e}} (D_{r}^{c} - \delta_{rq}^{e}) y_{q} - D_{r}^{c} \\ \geq &\sum_{q \in Q_{r}^{o}} \sum_{i \in Q_{r}^{c}} d(i, Q_{r}^{o}) x_{iq} + \sum_{q \in (Q_{r}^{c} \cup Q_{r}^{e})} \sum_{i \in Q_{r}^{c}} d_{iq} x_{iq} + \sum_{q \in Q_{r}^{c}} \sum_{i \in Q_{r}^{c}} [d(i, Q_{r}^{o}) - d_{iq}] x_{iq} + \sum_{q \in Q_{r}^{c}} \sum_{i \in Q_{r}^{c}} [d(i, Q_{r}^{o}) - d_{iq}] x_{iq} - D_{r}^{c} \\ = &\sum_{q \in Q_{r}^{o}} \sum_{i \in Q_{r}^{c}} d(i, Q_{r}^{o}) x_{iq} + \sum_{q \in Q_{r}^{c}} \sum_{i \in Q_{r}^{c}} d(i, Q_{r}^{o}) x_{iq} + \sum_{q \in Q_{r}^{c}} \sum_{i \in Q_{r}^{c}} d(i, Q_{r}^{o}) x_{iq} - D_{r}^{c} \\ = &\sum_{i \in Q_{r}^{c}} \sum_{q \in (Q_{r}^{c} \cup Q_{r}^{e} \cup Q_{r}^{o})} d(i, Q_{r}^{o}) x_{iq} - D_{r}^{c} \\ = &\sum_{i \in Q_{r}^{c}} d(i, Q_{r}^{o})[\sum_{q \in (Q_{r}^{c} \cup Q_{r}^{e} \cup Q_{r}^{o})} x_{iq}] - D_{r}^{c} \\ = &D_{r}^{c} - D_{r}^{c} \\ = &0 \end{split}$$

To conclude, valid inequality (14) is correct.

4.2.2 Valid inequalities 2

We add valid inequalities for the disaggregated distance variables corresponding to each location $s \in Q_r^e$. Let D_s^0 be equal to the distance from s to its closest central location $q \in Q_r^c$, i.e., $D_s^0 = d(s, Q_r^c)$. In addition, we can calculate D_s^1 as follows

$$D_s^1 = \min_{q \in Q: d_{sq} > D_s^0} d_{sq}$$

This leads to the second valid inequality

$$\theta_s \ge D_s^1 - \sum_{q \in Q: d_{sq} \le D_s^0} (D_s^1 - d_{sq}) y_q, \qquad \forall s \in Q_r^e, \tag{16}$$

which is a Benders cut up to distance D_s^0 .

4.2.3 Valid inequalities 3

We add the following two types of valid inequalities

$$\bar{\theta}_{Q_r^c} \ge \sum_{q \in Q_r^c} d(q, Q \setminus \{q\})(1 - y_q), \tag{17}$$

$$\theta_s \ge d(s, Q \setminus \{s\})(1 - y_s), \qquad \forall s \in Q_r^e.$$
(18)

Valid inequality (17) states that when y_q is not selected as a facility, the partial objective $\theta_{Q_r^c}$ must at least include the distance from q to its nearest neighbor. Similarly, (18) enforces that when y_s is not selected, the distance θ_s must be at least equal to the distance from s to its nearest neighbor.

4.3 Solution approach

We solve the ARMP using a similar approach to Duran-Mateluna et al. (2023), where we make use of their separation algorithm to identify violated Benders cuts. They propose to solve the root node using Algorithm 1. A start solution, represented by the vector \mathbf{y}^h , is fixed and the separation algorithm is executed in order to generate initial Benders cuts. The LP relaxation and the separation algorithm are iteratively run until no more violated Benders cuts are found. Note that in each iteration the lower bound is updated and an upper bound can be obtained by using a simple rounding heuristic.

| Algo | writhm 1 Solving the root node. |
|------------|--|
| Inp Out | ut: Start solution \mathbf{y}^h sput: Best lower and upper bound LB^* and UB^* |
| 1: | Run the separation algorithm with \mathbf{v}^h |
| 2: | while a violated cut has been identified do |
| 3: | Add the violated cuts to the ARMP |
| 4: | Solve the ARMP to obtain a solution \mathbf{y} and a lower bound LB |
| 5: | Run the separation algorithm with \mathbf{y} |
| 6: | Update $LB^* \leftarrow LB$ |
| 7: | Calculate UB using a rounding heuristic on y |
| 8: | Update $UB^* = \min\{UB^*, UB\}$ |
| ٩٠ | end while |

Our proposed solution approach is summarized in Algorithm 2. Based on a start solution, represented by a partition P, we partially aggregate the distance variables θ and add a set of valid inequalities (14), (16)–(18), to strengthen the formulation. The root node is solved as described in Algorithm 1. When a fractional solution is obtained, we perform two improvement procedures outlined by Duran-Mateluna et al. (2023) to decrease the size of the model, namely constraint reduction and reduced cost fixing. Also, we add integrality constraints to the **y** variables. While we keep the original y_i variables, we also add aggregate integer $\bar{y}_{Q_r^c}$ variables, for the central locations in a set $Q_r^c \subseteq Q_r$. When the start solution is close to an optimal solution, it is likely that exactly one y_i variable is selected in the set Q_r^c . We expect that the inclusion of the aggregate variables $\bar{y}_{Q_r^c}$ helps the branching process. In summary, we propose Algorithm 2, which incorporates steps 1, 2 and 7 into a disaggregate Benders decomposition approach for the p-median problem.

Algorithm 2 Aggregated Benders decomposition.

Inputs:

Sorted distances $D_i^0 \leq D_i^1 \leq D_i^2 \leq \cdots \leq D_i^{N_i}$ A start solution, represented by $P = \{Q_1, \dots, Q_p\}$

- 1: Partially aggregate the distance variables $\boldsymbol{\theta}$ based on P (see Section 4.1)
- 2: Add valid inequalities (14), (16)–(18) based on P (see Section 4.2)
- 3: Solve the root node using Benders decomposition (see Algorithm 1)
- 4: Stop if the solution is integral
- 5: Perform the improvement procedure of Duran-Mateluna et al. (2023)
- 6: Add integrality constraints to the y variables in (13)
- 7: Partially aggregate the decision variables $\bar{y}_{Q_r^c} := \sum_{q \in Q_r^c} y_q \in \mathbb{N}, \forall r \in [p]$
- 8: Apply branch-and-cut

4.4 Solving Benders decomposition with kd-tree

The separation algorithm requires the indices corresponding to the sorted distances, $D_i^0 \leq D_i^1 \leq D_i^2 \leq \cdots \leq D_i^{N_i}$. Duran-Mateluna et al. (2023) store these indices in a matrix **S** with a space complexity of $\mathcal{O}(N^2)$. In practice storing the entire **S** may be unnecessary, as only the first K_i indices from **S** are typically utilized for each location *i*. To improve memory efficiency, we propose to store the *N* locations in a tree-based data structure to dynamically compute the required indices. Tree-based structures have been successfully applied to heuristic methods for Euclidean location problems (Salhi and Irawan, 2015). We utilize a kd-tree, which is a binary search tree with a space complexity of $\mathcal{O}(N)$. A kd-tree enables efficient retrieval of the nearest location in $\mathcal{O}(\log N)$ time. Additionally, it can be augmented with an efficient K-nearest neighbors algorithm.

In our approach, we dynamically identify the relevant indices during the separation algorithm. Specifically, for location i, we use a kd-tree to find its K_i -nearest neighbors. The process terminates when the separation algorithm can be solved with these K_i indices, otherwise we increase K_i (see Appendix A.3 for implementation details) and reattempt to solve the separation algorithm.

5 Computational results

In this section we present a computation study on several types of instances. First, we outline the instance types and parameters settings that are used. Next, we compare the disaggregated Benders decomposition with our aggregated one on a wide range of instances. We then investigate the impact of varying the quality of the start solution and assess the contribution of each proposed step and valid inequality in the aggregated Benders decomposition. Last, we show that using a kd-tree data structure can improve the performance of both the disaggregated and aggregated Benders decomposition.

5.1 Experimental setup

5.1.1 Overview of the instances

We evaluate our methods on the same Euclidean instances as Duran-Mateluna et al. (2023), namely TSP instances (Reinelt, 1991; Beasley, 1990) and BIRCH instances. We follow the notation of Duran-Mateluna et al. (2023) to categorize TSP instances as 'medium' and 'huge'. Additionally, we introduce three new sets of instances. First, we consider a set of huge TSP instances with low values of p, named TSP-huge-low-p. Second, we introduce a new category of even larger TSP instances, called TSP*. To the best of our knowledge, it is the first time in the literature that p-median instances of such magnitude are considered using an exact solver without massive parallelization. Third, we include a new set of CIRCLE instances, generated following the procedure described by Irawan et al. (2014). The instance categories that we consider are detailed in Table 1. For all instances, the locations are given by two-dimensional coordinates in Euclidean space.

The CIRCLE instances, introduced by Irawan et al. (2014), are constructed to ensure well-separated clusters, enabling a geometric argument to provide a proof of optimality for these *p*-median instances. These instances represent an ideal scenario for our algorithm, as the valid inequalities (14), (16)-(18) also provide bounds. If these valid inequalities are sufficiently strong, we expect our algorithm to identify an optimal solution within a few Benders iterations.

For the TSP instances, the distance between locations is calculated as the Euclidean distance rounded down to the nearest integer as done in García et al. (2011) and Duran-Mateluna et al. (2023). The maximum rounding error between the actual and rounded distance is given by $\epsilon_{rounding} \ge |d_{true} - d_{rounded}|$. We modify Definition 4.1 such that locations $q \in Q_r$ satisfying $d(q, m_r) < \frac{1}{3}\rho_r - \epsilon_{rounding}$ belong to Q_r^c . Since distances are rounded down to the nearest integer, the maximum rounding error is $\epsilon_{rounding} = 1$. For the BIRCH and CIRCLE instances we set $\epsilon_{rounding} = 10^{-6}$.

Table 1: Overview of the instances, including the number of observations (N), number of facilities (p), the rounding error $(\epsilon_{rounding})$ and whether the instances are considered for the first time in the literature.

| instance category | 1 | V | | p | $\epsilon_{rounding}$ | new instances |
|-------------------|--------|--------|--------|--------|-----------------------|---------------|
| | min | max | min | max | | |
| TSP-medium | 2103 | 5934 | 10 | 500 | 1 | |
| TSP-huge | 71009 | 238025 | 10000 | 200000 | 1 | |
| TSP-huge-low- p | 71009 | 238025 | 5 | 100 | 1 | yes |
| TSP^* | 498378 | 744710 | 350000 | 700000 | 1 | yes |
| BIRCH | 25000 | 89600 | 25 | 64 | 10^{-6} | |
| CIRCLE | 20000 | 80000 | 10 | 40000 | 10^{-6} | yes |

5.1.2 Technical specifications

The experiments are carried out on an AMD Rome 7H12 processor 3.2 GHz with 1 TB RAM, although we limit the memory to 120 or 500 GB depending on the instance size. The MIP problems are solved using the commercial solver CPLEX 20.1. We use the same parameter settings for CPLEX as Duran-Mateluna et al. (2023), which are summarized in Table B1. The separation algorithm is implemented within the GenericCallback of CPLEX and gets called when a feasible integral solution is found, similar to Duran-Mateluna et al. (2023). Additionally, we apply the callback when a fractional solution is identified, which offers a slight improvement (see Table C1).

5.1.3 Computation times

We impose a time limit of 10 hours on the Benders decomposition method as described in Algorithm 2. This is stricter than the limit used in Duran-Mateluna et al. (2023), where a 10 hour time limit for the branch-and-cut phase is applied only after solving the root node.

Similar to Duran-Mateluna et al. (2023) we assume the instance data structure, e.g. matrix \mathbf{S} , and a start solution are given as input to the Benders decomposition method. These computation times are not included in the time limit. However, it is important to note that in some cases the calculation of the sorted distances needed to construct matrix \mathbf{S} may be longer than the running time of the Benders decomposition method. Let T^{init} , T^{root} and $T^{B\&C}$ be, respectively, the time to initialize the aggregate model, the time to solve the root node, and the entire time of the branch-and-cut procedure (including the initialization and root node solving time). See Figure A1 for more details on the relation between the reported computation times.

Instances provably solved to optimality within the time limit are highlighted in bold, while instances from existing benchmark datasets that are solved to optimality for the first time in the literature are marked with a \dagger .

5.1.4 Start heuristic

Start solutions are usually generated using a metaheuristic named PopStar (Resende and Werneck, 2004) or a k-means++ algorithm (see Appendix A.1 and A.2). In the k-means++(*iter*₁, *iter*₂) algorithm, the parameters *iter*₁ and *iter*₂ specify the maximum number of restarts for the entire method and the number of inner iterations, respectively. As noted by Duran-Mateluna et al. (2023), the popStar heuristic becomes computationally expensive for large instances. To address this, we replace the popStar heuristic with k-means++(10,10) algorithm for large instances. Furthermore, due to the high memory requirements to store the matrix **S** we allocate up to 500 GB RAM to some instances. These settings are summarized in Table 2. Setting A of the Benders decomposition is applied to TSP-medium instances, while setting B is used for most other instances. Setting C is specifically applied when solving a Benders decomposition with a kd-tree.

Table 2: Overview of the different settings of the Benders decomposition for the distance data structure, memory limit and start heuristic.

| setting | distance data structure | memory limit (in GB) | start heuristic |
|---------|---|----------------------|---|
| A B | $\begin{array}{c} \text{matrix } \mathbf{S} \\ \text{matrix } \mathbf{S} \end{array}$ | 120 500 | $\begin{array}{c} \text{popStar} \\ k\text{-means} + +(10, 10) \end{array}$ |
| С | kd-tree | 120 | k-means++(10, 10) |

5.2 TSP instances

5.2.1 Comparison between disaggregated and aggregated Benders decomposition

Table 3 shows the results of the disaggregated and aggregated Benders decomposition with setting A on TSP-medium instances. While initializing the aggregated Benders decomposition takes on average 3 seconds, it reduces the average time required to solve the root node from 124 to 66 seconds. In addition, aggregation seems to reduce the time spent on the branch-and-cut, since the average computation time decreases from around 6200 to 4000 seconds. The disaggregated Benders is not able to solve five instances, compared to two when using the aggregated Benders.

The results with setting B for the TSP-huge instances are shown in Table 4. On average 220 seconds are spent on the initialization step of the aggregated Benders decomposition, which reduces the root node solving time from around 6200 seconds to 2000 seconds. Aggregation seems to have less impact on the branch-and-cut procedure compared to the TSP-medium instances.

In the literature, we were unable to find experiments that consider TSP-huge instances with low values of p. Table 5 presents the results on TSP-huge instances with values of p ranging from 5 to 100. The disaggregated Benders fails to complete a single Benders iteration for any of these instances. In contrast, the aggregated Benders decomposition successfully solves several Benders iterations, such that a gap can be calculated. Additionally, one instance with p = 10 is solved to optimality using branch-and-cut within the time limit.

5.2.2 Changing the start heuristic

We investigate the impact of the quality of the start solution on the solution time. The solutions obtained from k-means++(1,1) serve as a baseline, representing random start solutions. The solutions from k-means++(1,10) and k-means++(10,10) represent improved start solutions. We also evaluate popStar, a state-of-the-art heuristic that expected to outperform the k-means++ heuristics. Finally, we analyze an ideal scenario where the aggregated Benders decomposition is initialized with optimal solutions.

Table 6 shows the computation times for various start solutions. Changing the start solution has minimal impact on the time required to solve the root node, which averages between 63 and 74 seconds.

| ins | tance | | disa | ıggregat | ed Bend | ers | | | aggr | egated 1 | Benders | | | |
|---------|-------|-----|------|------------|------------|------|------------------|------|------------|------------|------------|------|------|-------|
| name | N | p | gap | T^{root} | $T^{B\&C}$ | iter | UB | gap | T^{init} | T^{root} | $T^{B\&C}$ | iter | vars | cons |
| d2103 | 2103 | 10 | 0.00 | 15 | 33 | 8 | 687321 | 0.00 | 3 | 4 | 11 | 6 | 179 | 3868 |
| d2103 | 2103 | 20 | 0.00 | 21 | 37 | 10 | 482926 | 0.00 | 3 | 12 | 29 | 9 | 206 | 3834 |
| d2103 | 2103 | 50 | 0.03 | 36 | TL | 12 | 302190^\dagger | 0.00 | 2 | 22 | 12726 | 18 | 335 | 3636 |
| d2103 | 2103 | 100 | 0.00 | 24 | 3728 | 12 | 194664 | 0.00 | 1 | 17 | 3057 | 17 | 395 | 3616 |
| d2103 | 2103 | 200 | 0.00 | 4 | 7 | 11 | 117753 | 0.00 | 1 | 2 | 6 | 11 | 494 | 3616 |
| d2103 | 2103 | 300 | 0.00 | 5 | 8 | 15 | 90471 | 0.00 | 0 | 2 | 3 | 17 | 360 | 4084 |
| d2103 | 2103 | 400 | 0.00 | 2 | 10 | 10 | 75324 | 0.00 | 1 | 1 | 4 | 7 | 439 | 4118 |
| d2103 | 2103 | 500 | 0.00 | 2 | 5 | 13 | 64006 | 0.00 | 1 | 1 | 5 | 14 | 524 | 4144 |
| pcb3038 | 3038 | 10 | 0.00 | 68 | 68 | 8 | 1211704 | 0.00 | 2 | 15 | 17 | 6 | 301 | 5494 |
| pcb3038 | 3038 | 20 | 0.00 | 84 | 498 | 10 | 839494 | 0.00 | 3 | 62 | 373 | 10 | 304 | 5508 |
| pcb3038 | 3038 | 50 | 0.00 | 60 | 390 | 10 | 506339 | 0.00 | 4 | 32 | 249 | 10 | 346 | 5484 |
| pcb3038 | 3038 | 100 | 0.00 | 55 | 236 | 11 | 351500 | 0.00 | 1 | 32 | 335 | 8 | 395 | 5486 |
| pcb3038 | 3038 | 200 | 0.00 | 22 | 117 | 9 | 237399 | 0.00 | 1 | 12 | 109 | 9 | 416 | 5644 |
| pcb3038 | 3038 | 300 | 0.00 | 12 | 23 | 11 | 186833 | 0.00 | 2 | 5 | 18 | 15 | 450 | 5776 |
| pcb3038 | 3038 | 400 | 0.00 | 6 | 9 | 8 | 156276 | 0.00 | 2 | 2 | 6 | 10 | 489 | 5898 |
| pcb3038 | 3038 | 500 | 0.00 | 4 | 6 | 11 | 134798 | 0.00 | 1 | 2 | 3 | 10 | 563 | 5948 |
| fl3795 | 3795 | 10 | 0.00 | 13 | 13 | 7 | 520940 | 0.00 | 7 | 5 | 12 | 7 | 1678 | 4254 |
| fl3795 | 3795 | 20 | 0.00 | 10 | 10 | 10 | 319722 | 0.00 | 5 | 2 | 7 | 7 | 1295 | 5040 |
| fl3795 | 3795 | 50 | 0.00 | 8 | 8 | 12 | 150940 | 0.00 | 5 | 4 | 8 | 8 | 988 | 5714 |
| fl3795 | 3795 | 100 | 0.00 | 9 | 9 | 12 | 88299 | 0.00 | 5 | 5 | 9 | 9 | 858 | 6074 |
| fl3795 | 3795 | 200 | 0.00 | 14 | 1067 | 14 | 53928 | 0.00 | 2 | 11 | 843 | 25 | 871 | 6238 |
| fl3795 | 3795 | 300 | 0.00 | 8 | TL | 17 | 39586 | 0.00 | 1 | 11 | 1575 | 35 | 940 | 6300 |
| fl3795 | 3795 | 400 | 0.00 | 9 | 496 | 18 | 31354 | 0.00 | 1 | 8 | 274 | 23 | 1095 | 6190 |
| fl3795 | 3795 | 500 | 0.00 | 7 | 7 | 15 | 25976 | 0.00 | 1 | 6 | 7 | 17 | 1116 | 6348 |
| rl5934 | 5934 | 10 | 0.00 | 1203 | 10901 | 10 | 9792218 | 0.00 | 10 | 545 | 2665 | 10 | 517 | 10854 |
| rl5934 | 5934 | 20 | 0.00 | 906 | TL | 11 | 6716215 | 0.00 | 5 | 596 | TL | 16 | 602 | 10704 |
| rl5934 | 5934 | 50 | 0.00 | 631 | TL | 13 | 4030771 | 0.00 | 6 | 341 | TL | 17 | 678 | 10612 |
| rl5934 | 5934 | 100 | 0.03 | 377 | TL | 12 | 2722527 | 0.00 | 7 | 219 | 30553 | 16 | 805 | 10458 |
| rl5934 | 5934 | 200 | 0.00 | 139 | 747 | 9 | 1805530 | 0.00 | 4 | 83 | 1516 | 14 | 1066 | 10136 |
| rl5934 | 5934 | 300 | 0.00 | 94 | 140 | 10 | 1392419 | 0.00 | 5 | 29 | 79 | 11 | 1346 | 9776 |
| rl5934 | 5934 | 400 | 0.00 | 62 | 332 | 10 | 1143940 | 0.00 | 3 | 14 | 191 | 10 | 1536 | 9596 |
| r15934 | 5934 | 500 | 0.00 | 53 | 77 | 13 | 972799 | 0.00 | 2 | 11 | 26 | 13 | 1745 | 9378 |
| avg | | | 0.00 | 124 | 6218 | | | 0.00 | 3 | 66 | 3960 | | | |

Table 3: Time (in s) and gap (in %) using disaggregated and aggregated Benders decomposition with setting A on TSP-medium instances. The number of iterations, number of aggregated variables and number of valid inequalities are denoted by iter, vars and cons, respectively. TL=36000 seconds.

However, the branch-and-cut procedure exhibits greater variability in computation time. Initializing the aggregated Benders decomposition with an optimal solution results in an average computation time of 3700 seconds. The best performing method, popStar, achieves computation times comparable to those obtained when initializing with an optimal solution. This is because popStar produces start solutions with objective values close to the optimal solutions.

5.2.3 Contribution of each step in the aggregated Benders decomposition

Recall that our approach adds three steps to the disaggregated Benders decomposition, namely partially aggregating the distance variables, adding valid inequalities and partially aggregating the decision variables. Table 7 reports the time spent when incrementally adding these steps with setting A on TSP-medium instances. We first analyze the time spent solving the root node. Activating the first step, which aggregates the θ variables, reduces the average time from 124 to 99 seconds. Incorporating the second step, adding valid inequalities, further reduces the time to an average of 66 seconds. A similar trend is observed in the branch-and-cut procedure. The average computation time decreases from around 6200 seconds to 5000 seconds with the first step, and further to 3900 seconds when activating the second step. The third step, adding the aggregate y variables, seems to have minimal impact on

usa115475 115475

usa115475 115475

ara238025 238025

ara238025 238025

ara238025 238025

ara238025 238025

ara238025 238025

238025

238025

238025

238025

ara238025 238025 100000

ara238025 238025 150000

ara238025 238025 200000

ara238025

ara238025

ara238025

ara238025

avg

| ir | stance | | disag | ggregat | ed Bend | ers | | | aggr | egated | Benders | 3 | | |
|-----------|--------|-------|-------|------------|------------|------|--------------------|------|------------|------------|------------|------|-------|--------|
| name | N | p | gap | T^{root} | $T^{B\&C}$ | iter | UB | gap | T^{init} | T^{root} | $T^{B\&C}$ | iter | vars | cons |
| ch71009 | 71009 | 10000 | 0.04 | 11455 | TL | 12 | 4275352 | 0.02 | 46 | 2396 | TL | 11 | 14298 | 131800 |
| ch71009 | 71009 | 20000 | 0.00 | 970 | TL | 17 | 2377850 | 0.00 | 39 | 551 | TL | 13 | 24164 | 124908 |
| ch71009 | 71009 | 30000 | 0.00 | 524 | 632 | 19 | 1464151 | 0.00 | 45 | 414 | 612 | 14 | 33985 | 111266 |
| ch71009 | 71009 | 40000 | 0.00 | 237 | 338 | 21 | 879336 | 0.00 | 32 | 377 | 526 | 12 | 43522 | 91274 |
| ch71009 | 71009 | 50000 | 0.00 | 114 | 227 | 16 | 463553 | 0.00 | 20 | 115 | 251 | 12 | 53010 | 65656 |
| ch71009 | 71009 | 60000 | 0.00 | 54 | 184 | 18 | 167565 | 0.00 | 13 | 32 | 177 | 14 | 62307 | 35330 |
| pla85900 | 85900 | 10000 | 9.10 | TL | TL | 5 | 178470093 | 0.00 | 66 | 3506 | TL | 16 | 11924 | 167918 |
| pla85900 | 85900 | 20000 | 0.00 | 12950 | TL | 15 | 118414166 | 0.00 | 63 | 4361 | TL | 11 | 21284 | 167692 |
| pla85900 | 85900 | 30000 | 5.16 | TL | TL | 80 | 86944715^\dagger | 0.00 | 65 | 210 | 1582 | 9 | 30640 | 159818 |
| pla85900 | 85900 | 40000 | 0.00 | 46 | 168 | 27 | 69944715 | 0.00 | 49 | 204 | 677 | 9 | 40364 | 141964 |
| pla85900 | 85900 | 50000 | 0.00 | 36 | 181 | 15 | 52944715 | 0.00 | 52 | 163 | 487 | 8 | 50194 | 117922 |
| pla85900 | 85900 | 60000 | 0.00 | 79 | 239 | 21 | 35944715 | 0.00 | 41 | 129 | 406 | 9 | 60132 | 89418 |
| pla85900 | 85900 | 70000 | 0.00 | 39 | 130 | 14 | 18977475 | 0.00 | 29 | 44 | 169 | 15 | 70086 | 57936 |
| pla85900 | 85900 | 80000 | 0.00 | 12 | 114 | 26 | 4512752 | 0.00 | 17 | 14 | 150 | 24 | 80047 | 22796 |
| usa115475 | 115475 | 10000 | 27.80 | TL | TL | 3 | 8765753 | 3.48 | 181 | 12097 | TL | 13 | 18743 | 213244 |
| usa115475 | 115475 | 20000 | 0.01 | 6764 | TL | 13 | 5287528 | 0.01 | 155 | 2314 | TL | 13 | 27387 | 213600 |
| usa115475 | 115475 | 30000 | 0.00 | 2642 | TL | 13 | 3815715 | 0.00 | 131 | 1481 | TL | 16 | 36006 | 210336 |
| usa115475 | 115475 | 40000 | 0.00 | 1706 | 2114 | 17 | 2876909 | 0.00 | 125 | 1119 | 2565 | 13 | 44847 | 201514 |
| usa115475 | 115475 | 50000 | 0.00 | 1109 | 1391 | 17 | 2189144 | 0.00 | 81 | 999 | 1555 | 16 | 53749 | 188094 |
| usa115475 | 115475 | 60000 | 0.00 | 781 | 1061 | 14 | 1651400 | 0.00 | 69 | 990 | 1439 | 13 | 62897 | 169688 |
| usa115475 | 115475 | 70000 | 0.00 | 629 | 943 | 16 | 1214299 | 0.00 | 77 | 878 | 1364 | 15 | 72168 | 146742 |

24

15

15

13

14

22

18

12

12

13

851481 0.00

548097 0.00

3.69

0.00

0.00

0.00

0.00

0.00

0.00

0.00

0.00

0.01

0.21

1397282

857548

630983

494842

401835

334279

283627

244233

214233

184241

88025 0.00

38025 0.00

73

53

665

854

699

629

627

541

510

421

411

369

307

146

220

385

197

6007

6100

3320

2520

1915

2073

2142

2888

3004

3843

3609

738

2032

889 12

703 11

TL12

TL 13

TL12

11

13

11

13

16

4560

4283

4733

4510

5768

8293

8116

3805

12961

TL

690

54116

TL12

TL 17

28560

5529

5224

5859

5128

5423

7648

7081

3785 283

2497

12734

Table 4: Time (in s) and gap (in %) using disaggregated and aggregated Benders decomposition with setting B on TSPhuge instances. The number of iterations, number of aggregated variables and number of valid inequalities are denoted by iter, vars and cons, respectively. TL=36000 seconds

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the computation time. In Appendix C.2 we also provide a detailed comparison of the performance of each individual type of valid inequalities.

5.2.4 Lower bound in the first iteration

80000

90000

10000

20000

30000

40000

50000

60000

70000

80000

90000

0.00

0.00

0.32

0.01

0.00

0.00

0.00

0.00

0.00

0.00

0.00

0.00

0.00

0.00

1.21

348

202

9199

10280

6812

4630

4183

4722

3800

3827

3985

3795

2091

750

6223

Figure 2 visualizes the lower bound in the first iteration of the Benders decomposition with setting B for different values of p on TSP-huge instances. The root node lower bound (red line) indicates the optimal objective value when solving the LP relaxation. Ideally, we would like to be as close as possible to this objective value. The figure shows that the objective value in the first iteration when using aggregated Benders (blue line) is equal to or higher compared to disaggregated Benders (black line).

This leads to the question whether the objective value in subsequent Benders iterations is also higher for aggregated Benders compared to disaggregated Benders. Figure 3 shows the objective value per iteration of the Benders decomposition for two selected instances (the other instances exhibit similar behaviors). For the instances with p = 10000 we notice that the objective value of the aggregated

90436

404188

391192

389844

81534 120476

34524 426868

50455 414808

78632 396704

88883 393260

109809 388040

22 115810 382198

11 121186 375986

9 156729 291012

13 201882 140130

91034

65516

97436

104098

| ins | tance | | disa | iggrega | ted Ben | ders | | | aggre | gated E | Benders | | | |
|------------|--------|-----|------|------------|------------|------|------------|-------|------------|------------|------------|------|-------|--------|
| name | N | p | gap | T^{root} | $T^{B\&C}$ | iter | UB | gap | T^{init} | T^{root} | $T^{B\&C}$ | iter | vars | cons |
| ch71009 | 71009 | 5 | - | TL | TL | 0 | 279898768 | 2.49 | 26107 | TL | TL | 5 | 7643 | 126742 |
| ch71009 | 71009 | 10 | - | TL | TL | 0 | 184135561 | 0.00 | 13962 | 7255 | 24698 | 10 | 7184 | 127670 |
| ch71009 | 71009 | 50 | - | TL | TL | 0 | 82188868 | 7.49 | 2692 | TL | TL | 4 | 6666 | 128786 |
| ch71009 | 71009 | 100 | - | TL | TL | 0 | 58002900 | 10.69 | 1627 | TL | TL | 4 | 6785 | 128648 |
| pla85900 | 85900 | 5 | - | TL | TL | 0 | 9852614013 | - | TL | TL | TL | 0 | 6687 | 158436 |
| pla85900 | 85900 | 10 | - | TL | TL | 0 | 7067159042 | 4.96 | 17240 | TL | TL | 3 | 6646 | 158528 |
| pla85900 | 85900 | 50 | - | TL | TL | 0 | 3282348405 | 7.05 | 3441 | TL | TL | 3 | 7093 | 157714 |
| pla85900 | 85900 | 100 | - | TL | TL | 0 | 2330305935 | 8.06 | 1712 | TL | TL | 3 | 6984 | 158032 |
| usa115475 | 115475 | 5 | - | TL | TL | 0 | 514450906 | - | TL | TL | TL | 0 | - | - |
| usa115475 | 115475 | 10 | - | TL | TL | 0 | 361392225 | - | TL | TL | TL | 0 | - | - |
| usa115475 | 115475 | 50 | - | TL | TL | 0 | 152557601 | 7.97 | 20182 | TL | TL | 3 | 11410 | 208230 |
| usa115475 | 115475 | 100 | - | TL | TL | 0 | 107188213 | 10.76 | 5158 | TL | TL | 3 | 10788 | 209574 |
| ara238025 | 238025 | 5 | - | TL | TL | 0 | 80129403 | - | TL | TL | TL | 0 | - | - |
| ara 238025 | 238025 | 10 | - | TL | TL | 0 | 56557295 | - | TL | TL | TL | 0 | - | - |
| ara 238025 | 238025 | 50 | - | TL | TL | 0 | 24926972 | - | TL | TL | TL | 0 | - | - |
| ara238025 | 238025 | 100 | - | TL | TL | 0 | 17482258 | 14.01 | 14955 | TL | TL | 2 | 19785 | 436680 |

Table 5: Time (in s) and gap (in %) using disaggregated and aggregated Benders decomposition with setting B on TSP-huge-low-p instances. The number of iterations, number of aggregated variables and number of valid inequalities are denoted by iter, vars and cons, respectively, for TL=36000 seconds.

Table 6: Average time (in s) when using different start solutions for aggregated Benders decomposition on TSP-medium instances. Times are averaged over each instance with the same name. We also report the average gap between the start solution and optimal (or best-known) solution. TL=36000 seconds.

| instar | ice | disagg Ber | regated iders | | | | ag | gregated | l Bender | s | | | |
|---------|---------------|---------------|------------------|------------|------------|-------------|------------|-------------|------------|------------|------------|------------|------------|
| | | pop | Star | kmea (1 | (ns++, 1) | kmea (1, | ns++ 10) | kmea (10 | ns++, 10) | pop | Star | opt | imal |
| name | N | T^{root} | $T^{B\&C}$ | T^{root} | $T^{B\&C}$ | T^{root} | $T^{B\&C}$ | T^{root} | $T^{B\&C}$ | T^{root} | $T^{B\&C}$ | T^{root} | $T^{B\&C}$ |
| d2103 | 2103 | 14 | 4979 | 8 | 3663 | 9 | 4927 | 9 | 3452 | 8 | 1978 | 8 | 1694 |
| pcb3038 | 3038 | 39 | 168 | 24 | 209 | 20 | 241 | 20 | 241 | 20 | 136 | 19 | 116 |
| fl3795 | 3795 | 10 | 4701 | 10 | 4667 | 8 | 774 | 8 | 515 | 6 | 339 | 7 | 694 |
| rl5934 | 5934 | 433 | 15025 | 254 | 18185 | 243 | 18226 | 214 | 15405 | 230 | 13375 | 235 | 12321 |
| avg | | 124 | 6218 | 74 | 6681 | 70 | 6042 | 63 | 4903 | 66 | 3957 | 67 | 3706 |
| avg gap | gap 0.1% 9.0% | | 0% | 5. | 8% | 4. | 7% | 0. | 1% | 0.0% | | | |

Table 7: Average time (in s) while adding more steps to the aggregated Benders decomposition with setting A on TSPmedium instances. Times are averaged over each instance with the same name. TL=36000 seconds.

| instar | nce | disaggrega | ted Benders | aggre | gate θ | add ine | qualities | aggre | gate y |
|---------|------|------------|-------------|------------|---------------|------------|------------|------------|------------|
| name | N | T^{root} | $T^{B\&C}$ | T^{root} | $T^{B\&C}$ | T^{root} | $T^{B\&C}$ | T^{root} | $T^{B\&C}$ |
| d2103 | 2103 | 14 | 4979 | 15 | 4889 | 8 | 1996 | 8 | 1978 |
| pcb3038 | 3038 | 39 | 168 | 31 | 170 | 20 | 135 | 20 | 136 |
| fl3795 | 3795 | 10 | 4701 | 9 | 1235 | 6 | 340 | 6 | 339 |
| rl5934 | 5934 | 433 | 15025 | 341 | 13936 | 229 | 13291 | 230 | 13375 |
| avg | | 124 | 6218 | 99 | 5057 | 66 | 3940 | 66 | 3957 |

Benders is higher for around 5 iterations. For the other instance with p = 200000 we notice that both lines start with an objective of 0, but the aggregated Benders jumps earlier to a non-negative objective value compared to disaggregated Benders.



Figure 2: Lower bound in the first iteration for TSP-huge instances.



Figure 3: Lower bound in each iteration for two TSP-huge instances.

5.3 BIRCH instances

In Table 8 we compare the disaggregated and aggregated Benders decomposition with setting B on the BIRCH instances. The time to solve the branch-and-cut procedure for aggregated Benders is on average 5100 seconds compared to 2700 seconds for disaggregated Benders. This can be explained by the observation that for the aggregated Benders most time is spent on initializing the aggregate model. This shows that adding all possible valid inequalities might not be a good idea. A possible improvement would be to add a limited number of valid inequalities.

| inst | ance | | disa | ggregat | ed Bend | ers | | | aggi | regated | Benders | | | |
|---------|-------|----|------|------------|------------|------|----------|------|------------|------------|------------|----------------|-------|--------|
| name | N | p | gap | T^{root} | $T^{B\&C}$ | iter | UB | gap | T^{init} | T^{root} | $T^{B\&C}$ | iter | vars | cons |
| BIRCH1 | 25000 | 25 | 0.00 | 143 | 144 | 5 | 31229.3 | 0.00 | 515 | 30 | 546 | 3 | 9251 | 31548 |
| BIRCH2 | 36000 | 36 | 0.00 | 2975 | 2977 | 6 | 45115.6 | 0.00 | 662 | 50 | 714 | 5 | 12144 | 47784 |
| BIRCH3 | 49000 | 49 | 0.00 | 380 | 383 | 5 | 61384.1 | 0.00 | 1540 | 70 | 1612 | $\overline{7}$ | 16736 | 64626 |
| BIRCH4 | 64000 | 64 | 0.00 | 786 | 790 | 6 | 80053.9 | 0.00 | 3097 | 94 | 3195 | 6 | 21229 | 85670 |
| BIRCH5 | 30000 | 25 | 0.00 | 191 | 193 | 6 | 37563.6 | 0.00 | 1502 | 61 | 1564 | 4 | 10974 | 38102 |
| BIRCH6 | 43200 | 36 | 0.00 | 4612 | 4616 | 7 | 54191.4 | 0.00 | 1546 | 105 | 1654 | 6 | 13151 | 60170 |
| BIRCH7 | 58800 | 49 | 0.00 | 18860 | 18864 | 6 | 73626.8 | 0.00 | 2361 | 123 | 2487 | 7 | 20113 | 77472 |
| BIRCH8 | 76800 | 64 | 0.00 | 1301 | 1307 | 7 | 96039.4 | 0.00 | 4978 | 160 | 5142 | 7 | 23995 | 105738 |
| BIRCH9 | 35000 | 25 | 0.00 | 511 | 514 | 6 | 43902.1 | 0.00 | 1377 | 84 | 1462 | 4 | 12802 | 44446 |
| BIRCH10 | 50400 | 36 | 0.00 | 9741 | 9745 | 6 | 63169.2 | 0.00 | 1586 | 123 | 1713 | 5 | 16707 | 67458 |
| BIRCH11 | 68600 | 49 | 0.00 | 752 | 758 | 6 | 85833.5 | 0.00 | 4727 | 193 | 4925 | 8 | 21725 | 93848 |
| BIRCH12 | 89600 | 64 | 0.00 | 1612 | 1619 | 6 | 112059.2 | 0.00 | 15120 | 289 | 15415 | 6 | 28116 | 123096 |
| BIRCH21 | 25000 | 25 | 0.00 | 272 | 273 | 6 | 17696.2 | 0.00 | 920 | 198 | 1119 | 20 | 10223 | 29604 |
| BIRCH22 | 36000 | 36 | 0.00 | 371 | 373 | 8 | 27423.0 | 0.00 | 989 | 1047 | 2037 | 24 | 14343 | 43386 |
| BIRCH23 | 49000 | 49 | 0.00 | 688 | 692 | 10 | 44149.0 | 0.00 | 1894 | 916 | 2813 | 33 | 16259 | 65580 |
| BIRCH24 | 64000 | 64 | 0.00 | 834 | 839 | 11 | 58832.6 | 0.00 | 3002 | 1348 | 4353 | 29 | 24925 | 78278 |
| BIRCH25 | 30000 | 25 | 0.00 | 402 | 405 | 8 | 21829.9 | 0.00 | 1042 | 460 | 1504 | 22 | 10984 | 38082 |
| BIRCH26 | 43200 | 36 | 0.00 | 530 | 535 | 12 | 32339.4 | 0.00 | 2341 | 594 | 2938 | 11 | 15211 | 56050 |
| BIRCH27 | 58800 | 49 | 0.00 | 1033 | 1038 | 9 | 50857.9 | 0.00 | 3549 | 837 | 4390 | 14 | 18498 | 80702 |
| BIRCH28 | 76800 | 64 | 0.00 | 1842 | 14981 | 15 | 66562.4 | 0.00 | 3843 | 8397 | 14355 | 49 | 35007 | 83714 |
| BIRCH29 | 35000 | 25 | 0.00 | 507 | 510 | 11 | 24810.9 | 0.00 | 1368 | 675 | 2045 | 26 | 13700 | 42650 |
| BIRCH30 | 50400 | 36 | 0.00 | 687 | 691 | 13 | 38102.6 | 0.00 | 2826 | 6739 | 9568 | 36 | 19658 | 61556 |
| BIRCH31 | 68600 | 49 | 0.00 | 1378 | 1385 | 14 | 61850.6 | 0.00 | 4421 | 2544 | 6969 | 33 | 24432 | 88434 |
| BIRCH32 | 89600 | 64 | 0.00 | 2486 | 2496 | 20 | 78777.0 | 0.00 | 18731 | 12229 | 30967 | 53 | 38790 | 101748 |
| avg | | | 0.00 | 2204 | 2755 | | | 0.00 | 3497 | 1557 | 5145 | | | |

Table 8: Time (in s) and gap (in %) using disaggregated and aggregated Benders decomposition with setting B on BIRCH instances. The number of iterations, number of aggregated variables and number of valid inequalities are denoted by iter, vars and cons, respectively. TL=36000 seconds.

On average the disaggregated method needs 2200 seconds for solving the root node and around 500 seconds for the branch-and-cut, leading to a total running time of 2700 seconds. In contrast, the aggregated Benders requires on average 3500 seconds to add the valid inequalities, 1500 seconds to solve the root node and 100 seconds for the branch-and-cut, leading to a total computation time of 5100 seconds. Although the aggregated Benders speeds up the root node and branch-and-cut phases, the time spent adding inequalities is too high.

5.4 CIRCLE instances

The CIRCLE instances are designed to ensure that the clusters are well-separated, which facilitates the process of obtaining high-quality initial solutions. Note that this is the first time these instances have been addressed using an exact method in the literature. The main idea of our introduced valid inequalities is to calculate a lower bound that holds for several solutions close to the provided start solution. Thus, we expect our aggregation to perform well for the CIRCLE instances.

This expectation seems to be confirmed in Table 9, where we compare disaggregated and aggregated Benders decomposition with setting B. The time to initialize the model is on average 3300 seconds, this reduces the time to solve the root node from on average 8300 seconds for the disaggregated to 280 seconds for the aggregated Benders decomposition, representing an improvement of nearly a factor of 30. The total time spent on the branch-and-cut phase is reduced from on average 8300 seconds for the disaggregated to 3600 seconds for the aggregated Benders decomposition, reducing the computation time by more than half.

| insta | ince | | disag | ggregat | ed Bend | lers | | | aggre | gated E | Benders | | | |
|-------------------|-------|-------|-------|------------|------------|------|-------------|------|------------|------------|------------|------|-------|--------|
| name | N | p | gap | T^{root} | $T^{B\&C}$ | iter | UB | gap | T^{init} | T^{root} | $T^{B\&C}$ | iter | vars | cons |
| C20000_10 | 20000 | 10 | 0.00 | 3604 | 3606 | 4 | 15749249.9 | 0.00 | 921 | 53 | 973 | 2 | 11000 | 18020 |
| $C20000_{-}50$ | 20000 | 50 | 0.00 | 188 | 188 | 4 | 3298500.2 | 0.00 | 145 | 4 | 149 | 3 | 9442 | 21216 |
| $C20000_{-}100$ | 20000 | 100 | 0.00 | 159 | 159 | 6 | 1797000.1 | 0.00 | 74 | 3 | 77 | 4 | 7191 | 25818 |
| $C20000_{-}500$ | 20000 | 500 | 0.00 | 177 | 177 | 7 | 442500.2 | 0.00 | 28 | 2 | 30 | 4 | 7890 | 25220 |
| C20000_1000 | 20000 | 1000 | 0.00 | 104 | 105 | 7 | 217499.9 | 0.00 | 18 | 2 | 20 | 5 | 7465 | 27070 |
| $C20000_{-}5000$ | 20000 | 5000 | 0.00 | 24 | 26 | 6 | 45000.0 | 0.00 | 13 | 12 | 26 | 6 | 5001 | 39738 |
| $C20000_{-}10000$ | 20000 | 10000 | 0.00 | 16 | 20 | 43 | 15000.0 | 0.00 | 17 | 7 | 24 | 5 | 10000 | 36534 |
| C80000_10 | 80000 | 10 | - | TL | TL | 0 | 245998500.1 | 0.00 | 32801 | 3199 | TL | 3 | 44000 | 72020 |
| C80000_50 | 80000 | 50 | - | TL | TL | 0 | 50396999.9 | 0.00 | 8987 | 232 | 9219 | 3 | 38874 | 82352 |
| C80000_100 | 80000 | 100 | - | TL | TL | 0 | 26393999.9 | 0.00 | 4528 | 65 | 4593 | 4 | 34362 | 91476 |
| C80000_500 | 80000 | 500 | 0.00 | 6524 | 6526 | 8 | 5985000.1 | 0.00 | 893 | 20 | 913 | 4 | 32715 | 95570 |
| C80000_1000 | 80000 | 1000 | 0.00 | 3491 | 3493 | 8 | 2985000.0 | 0.00 | 501 | 10 | 512 | 5 | 32279 | 97442 |
| C80000_5000 | 80000 | 5000 | 0.00 | 1409 | 1417 | 7 | 689999.7 | 0.00 | 231 | 27 | 258 | 4 | 30191 | 109618 |
| C80000_10000 | 80000 | 10000 | 0.00 | 971 | 986 | 7 | 330000.0 | 0.00 | 199 | 234 | 432 | 5 | 29209 | 121558 |
| $C80000_{-40000}$ | 80000 | 40000 | 0.00 | 381 | 436 | 57 | 60000.0 | 0.00 | 166 | 347 | 513 | 6 | 40000 | 146200 |
| avg | | | 0.00 | 8337 | 8343 | | | 0.00 | 3302 | 281 | 3583 | | | |

Table 9: Time (in s) and gap (in %) using disaggregated and aggregated Benders decomposition with setting B on CIRCLE instances. The number of iterations, number of aggregated variables and number of valid inequalities are denoted by iter, vars and cons, respectively. TL=36000 seconds.

5.5 Solving Benders decomposition with kd-tree

5.5.1 TSP-huge instances

The computational results for solving Benders decomposition using a kd-tree on TSP-huge instances are presented in Table 10, comparing both disaggregated and aggregated Benders decompositions. Column T^{read} shows the time required to read the data and constructing the distance data structure, which is either the **S** matrix or a kd-tree. Column T^{heur} reports the time taken by the k-means++(10,10) heuristic.

Introducing a kd-tree increases the time needed for the branch-and-cut procedure, $T^{B\&C}$. This is due to the additional time taken by the separation algorithm, while the time to solve the master problem remains unchanged, as can be observed in Table C4. However, utilizing a kd-tree decreases the total computation time, consisting of T^{read} , T^{heur} and $T^{B\&C}$. The use of a kd-tree reduces T^{read} from approximately 1300 to 2 seconds. A similar effect is observed on T^{heur} , which decreases from around 2800 to 60 seconds.

In summary, applying a kd-tree eliminates the need to compute and store the sorted matrix \mathbf{S} , making Benders decomposition with a kd-tree both time and memory efficient.

Table 10: Average time (in s) and gap (in %) using disaggregated and aggregated Benders decomposition with the matrix S or a kd-tree on TSP-huge instances. Times are averaged over each instance with the same name. TL=36000 seconds.

| instar | instance disaggregated Benders | | | | | | | | | | aggregated Benders | | | | | | | | |
|-----------|--------------------------------|------|---------------|------------|------------|------|------------|-----------------|------------|------|--------------------|------------|------------|--------------------|-----------------|------------|------------|--|--|
| | | ma | trix S | (settir | ıg B) | ko | dtree (s | etting | ; C) | ma | trix \mathbf{S} | (settir | ng B) | kdtree (setting C) | | | | | |
| name | N | gap | T^{read} | T^{heur} | $T^{B\&C}$ | gap | T^{read} | Γ^{heur} | $T^{B\&C}$ | gap | T^{read} | T^{heur} | $T^{B\&C}$ | gap 2 | Γ^{read} | T^{heur} | $T^{B\&C}$ | | |
| ch71009 | 71009 | 0.01 | 318 | 745 | 12230 | 0.08 | 1 | 17 | 12387 | 0.01 | 318 | 744 | 12261 | 0.01 | 1 | 17 | 8835 | | |
| pla85900 | 85900 | 0.00 | 405 | 1022 | 13604 | 0.00 | 2 | 27 | 13648 | 0.00 | 408 | 1026 | 9434 | 0.00 | 1 | 27 | 9459 | | |
| usa115475 | 115475 | 0.00 | 768 | 1726 | 12749 | 0.01 | 1 | 40 | 16556 | 0.39 | 768 | 1719 | 12946 | 0.00 | 1 | 39 | 13101 | | |
| ara238025 | 238025 | 0.03 | 2924 | 5806 | 12395 | 0.41 | 5 | 119 | 16171 | 0.31 | 2897 | 5921 | 15673 | 0.34 | 4 | 118 | 16770 | | |
| avg | | 0.01 | 1347 | 2796 | 12734 | 0.16 | 2 | 60 | 15045 | 0.21 | 1338 | 2834 | 12961 | 0.12 | 2 | 59 | 12795 | | |

5.5.2 TSP* instances

Table 11 presents results for both disaggregated and aggregated Benders decomposition with a kdtree (setting C) on TSP^{*} instances. Instance lrb744710 would theoretically require 2 TB of RAM to store matrix **S** when using the start-of-the-art Benders decomposition. In contrast, we solve several instances to optimality on a node with 120 GB of RAM (in practice even less memory is used). The disaggregated and aggregated Benders decomposition have similar computation times.

Table 11: Time (in s) and gap (in %) using disaggregated and aggregated Benders decomposition with a kd-tree (setting C) on TSP* instances. The number of iterations, number of aggregated variables and number of valid inequalities are denoted by iter, vars and cons, respectively. TL=36000 seconds.

| in | nstance | | disa | ggregat | ed Bend | lers | | | ag | gregate | d Bende | Benders | | | | | |
|-------------------------------------|--|------------------------------|------------------------------------|-------------------------|---------------------|------------------|---|--------------------------------------|----------------------|-------------------------|---------------------|----------------|---|--|--|--|--|
| name | N | p | gap | T^{root} | $T^{B\&C}$ | iter | UB | gap | T^{init} | T^{root} | $T^{B\&C}$ | iter | vars | cons | | | |
| lra498378 lra498378 lra498378 | 498378 498378 498378 | $350000 \\ 400000 \\ 450000$ | 0.91 0.00 0.00 | $14195 \\ 8659 \\ 3870$ | TL 9109 4004 | $19 \\ 44 \\ 19$ | 170044 98378 48379 | 0.18 0.00 0.00 | $1401 \\ 961 \\ 545$ | $11735 \\ 9201 \\ 4467$ | TL 13729 6215 | 14 13 16 | 378838 419166 460110 | $\begin{array}{r} 467188\\ 326004\\ 166738\end{array}$ | | | |
| lrb744710 lrb744710 lrb744710 | $744710 \\ 744710 \\ 744710 \\ 744710$ | 600000 650000 700000 | 7.63 0.00 0.00 | TL 15615 8448 | TL 15615 8448 | 7 13 20 | 151951 94710 44 710 | 100.63 0.00 0.00 | 2413 1624 877 | TL 15871 8737 | TL 17495 9614 | $5\\14\\20$ | $\begin{array}{c} 604540 \\ 652888 \\ 701366 \end{array}$ | 535604 359412 173186 | | | |
| avg | | | 1.42 | 14465 | 18196 | | | 16.80 | 1303 | 14335 | 19842 | | | | | | |

6 Conclusion & discussion

We consider the p-median problem, where the goal is to select p facilities such that the sum of distances between each location and its nearest facility is minimized. The bottleneck in the current state-of-theart Benders decomposition is the large number of variables in the formulation.

We propose a partially aggregated Benders decomposition framework, which contains no and full aggregation as a special case. In our solution approach, we partially aggregate the variables based on a start solution. We aggregate variables for a group of so-called central locations, which are locations that we expect to be assigned to the same facility. We develop valid inequalities for the central locations and the remaining locations.

In our numerical experiments, we show that these valid inequalities strengthen the initial Benders iterations. Specifically, after initializing the model we often obtain an improved lower bound, resulting in a faster resolution of the root node. Across all types of instances, incorporating the valid inequalities reduces the average time required to solve the root node, in some cases by nearly a factor 30. Additionally, for certain instances, these valid inequalities positively influence the branch-and-cut phase, reducing the computation time by more than half.

However, for some instances, we observe that identifying a large number of valid inequalities can slow down the overall method. The additional time required to add these valid inequalities may offset the speedup gained from having stronger valid inequalities in the first Benders iterations. For further research, it may be interesting to strike a balance between the number of valid inequalities and the obtained speed up.

The approach we present may be generalized to instances with asymmetric distances. However, it may be challenging to define a group of central locations, particularly because the distance from a location to itself may be non-zero. Further research is required to develop a procedure for determining such a group of central locations and corresponding valid inequalities.

Appendix

A Details on the algorithms

A.1 The *k*-means++ algorithm

The k-means++ algorithm, also known as Lloyd's algorithm, is summarized in Algorithm 3. The method is initialized with a random selection of centroids, followed by an iterative assignment and recalculation of centroids. The maximum number of restarts and internal iterations are $iter_1$ and $iter_2$, respectively.

Algorithm 3 The *k*-means++ algorithm

```
1: Choose initial centroids
```

```
2: while objective has not converged or iteration limit, iter<sub>2</sub>, has not been reached do
```

3: Assignment step: assign points to closest centroid

A.2 Solving *k*-means++ with kd-tree

The assignment step usually has a complexity of $\mathcal{O}(kN)$, which can be reduced by using a kd-tree data structure to $\mathcal{O}(k \log N)$. We construct a kd-tree containing the coordinates of all the centroids and assign each location $i \in [N]$ to its nearest centroid by performing a nearest neighbor look up.

After obtaining the centroid solution using the k-means++ algorithm, we convert it to a p-median solution. We construct a kd-tree containing all N locations. For each centroid, we efficiently identify the nearest location which is labeled as a facility. These facilities are inserted into a new kd-tree. Finally, we assign each location $i \in [N]$ to the nearest facility.

A.3 Solving the separation algorithm with kd-tree

When solving the separation algorithm with a kd-tree we initially limit our search to the first K_i indices, for each location in [N]. We initialize $K_i = 5$ for all locations. If the separation algorithm cannot be solved because the current K_i indices are insufficient, we perform the following update on K_i :

$$K_i = K_i + \max\{10, \lfloor 0.1 \cdot \max_{j \in [N]} \{K_j\} \rfloor\}.$$

This update increments K_i by 10 or by 10% of the current maximum K_i value across all locations, whichever is larger.

B Parameters

Table B1: Values of the CPLEX parameters as suggested by Duran-Mateluna et al. (2023).

| parameter name | value | description |
|---|--|--|
| RelGap AbsGap MIP Emphasis BRDIR | $10^{-10} \\ 0.9999 \\ BestBound \\ 1$ | the relative tolerance to the best integer objective the absolute tolerance to the best integer objective focus on proving optimality branch up first |

^{4:} Update step: recalculate the centroids based on the assignment

^{5:} end while



Figure A1: Overview of the notation for the reported computation times and how they relate to each other.

C Computational results

C.1 Different callback settings

Table C1: Time (in s) using disaggregated Benders decomposition with setting B on TSP-medium instances. The GeneralCallback in CPLEX gets called either when a candidate solution is found or additionally when a relaxation solution is identified. TL=36000 seconds.

| ins | stance | | candidate only | candidate and relaxation | | | | |
|---------|--------|-----|-----------------------|--------------------------|--|--|--|--|
| name | N | p | $\overline{T^{B\&C}}$ | $T^{B\&C}$ | | | | |
| d2103 | 2103 | 10 | 32.9 | 32.6 | | | | |
| d2103 | 2103 | 20 | 63.8 | 37.1 | | | | |
| d2103 | 2103 | 50 | TL | TL | | | | |
| d2103 | 2103 | 100 | TL | 3728.5 | | | | |
| d2103 | 2103 | 200 | 7.3 | 7.2 | | | | |
| d2103 | 2103 | 300 | 7.7 | 7.9 | | | | |
| d2103 | 2103 | 400 | 5.1 | 10.0 | | | | |
| d2103 | 2103 | 500 | 9.6 | 4.5 | | | | |
| pcb3038 | 3038 | 10 | 67.3 | 68.4 | | | | |
| pcb3038 | 3038 | 20 | 780.3 | 498.1 | | | | |
| pcb3038 | 3038 | 50 | 270.7 | 390.5 | | | | |
| pcb3038 | 3038 | 100 | 327.1 | 235.7 | | | | |
| pcb3038 | 3038 | 200 | 140.3 | 116.8 | | | | |
| pcb3038 | 3038 | 300 | 32.3 | 23.4 | | | | |
| pcb3038 | 3038 | 400 | 14.1 | 8.7 | | | | |
| pcb3038 | 3038 | 500 | 6.4 | 6.4 | | | | |
| fl3795 | 3795 | 10 | 13.5 | 13.4 | | | | |
| fl3795 | 3795 | 20 | 9.9 | 10.0 | | | | |
| fl3795 | 3795 | 50 | 7.8 | 7.8 | | | | |
| fl3795 | 3795 | 100 | 9.0 | 9.0 | | | | |
| fl3795 | 3795 | 200 | 5648.9 | 1066.7 | | | | |
| fl3795 | 3795 | 300 | 9060.8 | TL | | | | |
| fl3795 | 3795 | 400 | 1186.1 | 495.9 | | | | |
| fl3795 | 3795 | 500 | 7.5 | 7.5 | | | | |
| rl5934 | 5934 | 10 | 9446.6 | 10901.4 | | | | |
| rl5934 | 5934 | 20 | TL | TL | | | | |
| rl5934 | 5934 | 50 | TL | TL | | | | |
| rl5934 | 5934 | 100 | TL | TL | | | | |
| rl5934 | 5934 | 200 | 1927.4 | 746.7 | | | | |
| rl5934 | 5934 | 300 | 151.6 | 140.1 | | | | |
| rl5934 | 5934 | 400 | 485.9 | 331.6 | | | | |
| rl5934 | 5934 | 500 | 95.6 | 76.6 | | | | |
| | | | 6556.7 | 6218.2 | | | | |

C.2 Contribution of each type of valid inequality

We evaluate the effectiveness of the three types of proposed valid inequalities, namely (14), (16) and (17)–(18). Specifically, we examine the reduction in solving time at the root node and the branchand-cut procedure. Additionally, we assess the quality of the lower bound (the objective value of the RMP) obtained in the first iteration of the Benders decomposition. The percentage improvement in the lower bound is calculated relative to the one obtained from the disaggregated Benders decomposition.

In Table C2 we compare the effectiveness of the individual valid inequalities for TSP-medium instances. Valid inequalities (14) are the strongest, improving the lower bound during the first iteration of the Benders decomposition by on average 25%, compared to the disaggregated Benders, while valid inequalities (16) result in the fastest computation times. Interestingly, these running times seem to suggest that adding valid inequalities (16) is sufficient, even though they have a smaller impact on the initial lower bound.

Table C2: Average time (in s) when adding one type of valid inequality to the aggregated Benders decomposition with setting A on TSP-medium instances. Times are averaged over each instance with the same name. We also report the number of valid inequalities added and the improvement (in %) in the lower bound achieved during the first iteration, compared to disaggregated Benders. The last column reports the improvement (in %) when adding all valid inequalities. TL=36000 seconds.

| instar | nce | va | lid ineq | ualities | (14) | va | lid ineq | ualities | (16) | valid | inequa | lities (17) | 7)–(18) | all |
|---------|------|------------|------------|----------|--------|------------|------------|----------|--------|------------|------------|---------------|---------|--------|
| name | N | T^{root} | $T^{B\&C}$ | # cuts | improv | T^{root} | $T^{B\&C}$ | # cuts | improv | T^{root} | $T^{B\&C}$ | # cuts | improv | improv |
| d2103 | 2103 | 16 | 7185 | 196 | 28.7 | 8 | 2393 | 1737 | 16.4 | 13 | 4329 | 1932 | 17.7 | 46.0 |
| pcb3038 | 3038 | 36 | 253 | 197 | 19.2 | 17 | 161 | 2630 | 14.3 | 33 | 211 | 2827 | 8.9 | 35.5 |
| fl3795 | 3795 | 11 | 860 | 195 | 31.8 | 7 | 396 | 2690 | 15.8 | 12 | 881 | 2885 | 6.6 | 48.7 |
| rl5934 | 5934 | 330 | 13398 | 198 | 21.9 | 185 | 12363 | 4897 | 15.3 | 358 | 15754 | 5095 | 1.9 | 33.1 |
| avg | | 98 | 5424 | 196 | 25.4 | 54 | 3828 | 2988 | 15.4 | 104 | 5274 | 3185 | 8.8 | 40.8 |

The performance of TSP-huge instances differs noticeably from that of TSP-medium instances, as can be seen in Table C3. For larger instances, valid inequalities (14) and (17)–(18) improve the initial lower bound by 92% and 111%, respectively. In contrast, valid inequalities (16) decrease the initial lower bound, caused by the aggregation of variables.

Each individual type of valid inequality improves the solving time of the root node. Additionally, only valid inequalities (14) improve the solving time of the branch-and-cut procedure, suggesting that these valid inequalities are sufficient.

Table C3: Average time (in s) when adding one type of valid inequality to the aggregated Benders decomposition with setting A on TSP-huge instances. Times are averaged over each instance with the same name. We also report the number of valid inequalities added and the improvement (in %) in the lower bound achieved during the first iteration, compared to disaggregated Benders. The last column reports the improvement (in %) when adding all valid inequalities. TL=36000 seconds.

| instar | instance | | | valid inequalities (14) | | | | ualities | (16) | valid | all | | | |
|------------|----------|------------|------------|---------------------------|--------|------------|------------|----------|--------|------------|------------|--------|--------|--------|
| name | N | T^{root} | $T^{B\&C}$ | # cuts | improv | T^{root} | $T^{B\&C}$ | # cuts | improv | T^{root} | $T^{B\&C}$ | # cuts | improv | improv |
| ch71009 | 71009 | 1472 | 6475 | 14225 | 101.4 | 803 | 12221 | 32461 | -3.3 | 1282 | 12165 | 46686 | 132.2 | 170.6 |
| pla85900 | 85900 | 6688 | 9624 | 17525 | 153.6 | 1243 | 9364 | 40316 | -14.7 | 1992 | 9370 | 57842 | 174.1 | 195.4 |
| usa115475 | 115475 | 5313 | 12842 | 25128 | 72.6 | 4911 | 15960 | 61212 | 3.0 | 5375 | 12608 | 74494 | 79.4 | 119.2 |
| ara 238025 | 238025 | 3604 | 13778 | 47148 | 60.5 | 2828 | 14025 | 135945 | 0.8 | 5223 | 17235 | 183093 | 82.6 | 121.3 |
| avg | | 4383 | 11336 | 29071 | 91.9 | 2654 | 13148 | 77130 | -2.9 | 3848 | 13378 | 103154 | 111.2 | 146.2 |

C.3 Detailed computational results when solving the root node

Table C4: Time (in s) of solving the root node using disaggregated and aggregated Benders decomposition with the matrix S or a kd-tree on TSP-huge instances. The time to spent on the master problem and separation algorithm are denoted by T^{MP} and T^{SP} , respectively. TL=36000 seconds.

| in | stance | | disaggregated Benders | | | | | | | aggregated Benders | | | | | |
|------------|--------|--------|-----------------------|----------------|------------|---------------------|----------|------------|---------------------|--------------------|------------|---------------------|----------|------------|--|
| | | | matrix | κ S (se | etting B) | kdtree | e (sett | ing C) | matrix | s S (se | tting B) | kdtree (setting | | | |
| name | N | p | $\overline{T^{MP}}$ | T^{SP} | T^{root} | $\overline{T^{MP}}$ | T^{SP} | T^{root} | $\overline{T^{MP}}$ | T^{SP} | T^{root} | $\overline{T^{MP}}$ | T^{SP} | T^{root} | |
| ch71009 | 71009 | 10000 | 11453 | 1 | 11455 | 12939 | 135 | 13074 | 2394 | 1 | 2396 | 1620 | 102 | 1721 | |
| ch71009 | 71009 | 20000 | 969 | 1 | 970 | 1021 | 140 | 1162 | 549 | 1 | 550 | 538 | 100 | 638 | |
| ch71009 | 71009 | 30000 | 523 | 1 | 524 | 498 | 124 | 622 | 413 | 1 | 414 | 388 | 77 | 465 | |
| ch71009 | 71009 | 40000 | 235 | 1 | 237 | 232 | 92 | 325 | 376 | 1 | 377 | 383 | 56 | 439 | |
| ch71009 | 71009 | 50000 | 114 | 1 | 114 | 140 | 109 | 250 | 113 | 1 | 114 | 114 | 51 | 165 | |
| ch71009 | 71009 | 60000 | 53 | 1 | 54 | 36 | 108 | 144 | 31 | 1 | 31 | 30 | 56 | 87 | |
| pla85900 | 85900 | 10000 | TL | 1 | TL | TL | 25 | TL | 3503 | 2 | 3505 | 3285 | 67 | 3352 | |
| pla85900 | 85900 | 20000 | 12949 | 1 | 12950 | 13134 | 68 | 13202 | 4359 | 1 | 4360 | 3213 | 38 | 3251 | |
| pla85900 | 85900 | 30000 | TL | 3 | TL | 35715 | 305 | TL | 209 | 1 | 210 | 265 | 24 | 289 | |
| pla85900 | 85900 | 40000 | 45 | 1 | 46 | 39 | 73 | 113 | 203 | 1 | 204 | 198 | 21 | 219 | |
| pla85900 | 85900 | 50000 | 35 | 1 | 36 | 40 | 46 | 87 | 162 | 1 | 162 | 199 | 27 | 226 | |
| pla85900 | 85900 | 60000 | 77 | 1 | 79 | 46 | 60 | 107 | 128 | 1 | 129 | 82 | 29 | 111 | |
| pla85900 | 85900 | 70000 | 38 | 1 | 39 | 26 | 37 | 64 | 42 | 1 | 43 | 42 | 35 | 76 | |
| pla85900 | 85900 | 80000 | 10 | 1 | 12 | 12 | 77 | 89 | 11 | 1 | 12 | 13 | 51 | 64 | |
| usa115475 | 115475 | 10000 | TL | 1 | TL | TL | 15 | TL | 12091 | 4 | 12095 | 33004 | 69 | 33073 | |
| usa115475 | 115475 | 20000 | 6762 | 2 | 6764 | 8348 | 51 | 8399 | 2309 | 3 | 2312 | 2134 | 47 | 2181 | |
| usa115475 | 115475 | 30000 | 2640 | 1 | 2642 | 2594 | 45 | 2640 | 1476 | 3 | 1479 | 1555 | 44 | 1599 | |
| usa115475 | 115475 | 40000 | 1704 | 1 | 1706 | 1654 | 40 | 1694 | 1115 | 2 | 1117 | 1370 | 29 | 1399 | |
| usa115475 | 115475 | 50000 | 1107 | 1 | 1109 | 1138 | 36 | 1175 | 995 | 2 | 997 | 1005 | 27 | 1032 | |
| usa115475 | 115475 | 60000 | 779 | 1 | 781 | 790 | 32 | 823 | 986 | 2 | 988 | 1038 | 22 | 1060 | |
| usa115475 | 115475 | 70000 | 627 | 1 | 629 | 505 | 37 | 543 | 874 | 2 | 876 | 883 | 27 | 909 | |
| usa115475 | 115475 | 80000 | 346 | 1 | 348 | 336 | 44 | 381 | 382 | 2 | 384 | 337 | 16 | 353 | |
| usa115475 | 115475 | 90000 | 201 | 1 | 202 | 206 | 35 | 242 | 193 | 2 | 195 | 203 | 18 | 221 | |
| ara 238025 | 238025 | 10000 | 9190 | 8 | 9199 | 8116 | 1039 | 9157 | 5995 | 9 | 6004 | 5576 | 1582 | 7158 | |
| ara 238025 | 238025 | 20000 | 10272 | 6 | 10280 | 9140 | 623 | 9765 | 6091 | 6 | 6097 | 5235 | 755 | 5990 | |
| ara 238025 | 238025 | 30000 | 6806 | 5 | 6812 | 6153 | 453 | 6608 | 3312 | 4 | 3317 | 2539 | 538 | 3077 | |
| ara 238025 | 238025 | 40000 | 4624 | 4 | 4630 | 4083 | 414 | 4498 | 2513 | 4 | 2517 | 1592 | 428 | 2019 | |
| ara238025 | 238025 | 50000 | 4178 | 4 | 4183 | 3837 | 370 | 4208 | 1907 | 4 | 1911 | 1852 | 373 | 2226 | |
| ara238025 | 238025 | 60000 | 4717 | 4 | 4722 | 3412 | 306 | 3719 | 2067 | 3 | 2071 | 2073 | 514 | 2586 | |
| ara238025 | 238025 | 70000 | 3794 | 5 | 3800 | 3573 | 544 | 4120 | 2135 | 4 | 2139 | 2223 | 188 | 2411 | |
| ara238025 | 238025 | 80000 | 3821 | 4 | 3827 | 3446 | 342 | 3789 | 2879 | 4 | 2884 | 2750 | 239 | 2989 | |
| ara238025 | 238025 | 90000 | 3980 | 3 | 3985 | 3676 | 247 | 3924 | 2993 | 5 | 2999 | 2777 | 189 | 2966 | |
| ara 238025 | 238025 | 100000 | 3791 | 3 | 3795 | 3467 | 226 | 3694 | 3836 | 3 | 3840 | 3331 | 191 | 3522 | |
| ara 238025 | 238025 | 150000 | 2031 | 31 | 2091 | 2030 | 4254 | 6307 | 3603 | 3 | 3606 | 3298 | 160 | 3458 | |
| ara238025 | 238025 | 200000 | 747 | 2 | 750 | 785 | 222 | 1007 | 730 | 4 | 733 | 712 | 242 | 954 | |
| avg | | | 5903 | 3 | 5908 | 5805 | 308 | 6112 | 2028 | 2 | 2030 | 2453 | 184 | 2637 | |

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