Analyzing Spatial Data with Heuristics Methods and Ensemble: A Case Study of Vehicle Routing Problem

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Abstract: The vehicle routing problem presents an intricate challenge within logistics and cargo transport. The primary objective is to determine the most efficient vehicle routes to visit a designated set of clients while minimizing overall transportation costs. The capacitated vehicle routing problem represents a specific variation of this challenge, introducing constraints such as routes commencing and concluding at the same depot, assigning each client to a single vehicle, and ensuring that the total demand for a route does not exceed the vehicle's capacity. This paper explores the hypothesis that optimal optimization strategy is contingent on spatial data density. Thereby, we evaluate various routing strategies using heuristic methods and ensemble techniques applied to spatial data. The goal is to identify the most effective strategy tailored to a specific spatial data pattern. To accomplish this, we employ two clustering methods – K-means and DBSCAN – to group clients based on their geographical locations. Additionally, we utilize the nearest neighbor heuristic to generate initial solutions, which are subsequently refined through the implementation of the 2-Opt method. Through experiments, we demonstrate the impact of each approach on the resulting routes, taking into account the spatial data distribution.

1 INTRODUCTION

The logistics costs in Brazil, as highlighted in the report by ILOS[1], present a significant challenge, accounting for a larger portion of the country's *Gross Domestic Product* (GDP) compared to many others. The *"Logistics Costs in Brazil"* report from ILOS indicates that logistics costs make up 12.2% of Brazil's GDP, a higher percentage than the 7.8% observed in the United States. A substantial portion of these costs is attributed to transportation, representing 6.8% of Brazil's GDP. Additionally, distribution costs, ranging from 10% to 15% of the product's value, play a crucial role in the overall cost calculation.

The *Vehicle Routing Problem* (VRP) emerges as a key optimization challenge in this context. This combinatorial optimization problem focuses on determining the optimal configuration of routes for a fleet of vehicles tasked with delivering products from a specified depot to a set of destinations (or clients). Given the complexity of logistics and cargo operations, finding efficient solutions to the VRP becomes crucial for reducing costs and enhancing the overall quality of transportation services (Borowski et al., 2020).

The *Capacitated Vehicle Routing Problem* (CVRP) is essential to determine the routes for a set of vehicles to deliver goods to clients, taking into consideration the vehicles' capacities and the demands of each client. Broadly, the CVRP aims to efficiently manage a vehicle's feet to cater to a specific number of clients with varying demands. The goal is to devise a set of routes with the lowest travel cost, all commencing and concluding at the depot. The total demand of clients on any given route must be at most the vehicle's capacity, and each client is visited only once (Jiang et al., 2022).

In this study, two clustering algorithms – K-means and *Density-Based Spatial Clustering of Applications with Noise* (DBSCAN) – are employed for grouping delivery points. The K-means method involves dividing delivery points into groups, initiating with random centers, and iteratively adjusting these centers based on point proximity. Conversely, DBSCAN identifies dense areas amid less dense regions, expanding groups from central points according to prox-

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imity. Building upon these algorithms, two distinct strategies are formulated, each leveraging one of the aforementioned clustering algorithms. Additionally, heuristics such as the nearest neighbor, utilized for generating an initial solution, and the 2-Opt, employed for refining the initially obtained solution, are incorporated. Finally, the algebraic combiner rule is applied to the ensemble technique to join the results, culminating in a final solution.

The literature reveals numerous studies addressing the VRP (Li et al., 2019; Bruni et al., 2014; Santos, 2022; Lima, 2015). However, the application of ensemble techniques to optimize vehicle routing is a relatively less explored area. Therefore, this research intends to contribute to the field of logistics and cargo distribution by aiming to develop more effective solutions for the VRP through the utilization of ensemble techniques.

2 RELATED WORKS

In the past decade, the VRP has been the focus of extensive research, especially in logistics and cargo transportation. Several studies have highlighted its potential as an alternative for reducing logistics costs. In a recent study by (Kangah et al., 2021), an ensemble method is introduced that combines *Particle Swarm Optimization* (PSO) and *Genetic Algorithm* (GA) operators, such as crossover and mutation. The original algorithmic structure of PSO is modified, and selected GA operators are incorporated to create a hybrid algorithm for solving the vehicle routing problem.

In (Lu et al., 2020), the authors used machine learning techniques to solve the CVRP. The L2I algorithm is a learning-based solution for CVRP that has a faster resolution speed than traditional operational research algorithms. The researchers developed a learning-based algorithm for CVRP that categorizes heuristic operators into two groups, which helps improve operations and guides reinforcement learning toward the identified improvement operators. They also presented an ensemble technique where reinforcement learning rules are taught simultaneously, resulting in improved outcomes with the same computational cost.

In their work, (Wang et al., 2021) tackle the VRP as a classical combinatorial optimization challenge that has undergone extensive research. The authors construct a multi-objective optimization model for *Dynamic Vehicle Routing Problem with Time Windows* (DVRPTW) and introduce a new algorithm named EL-DMOEA, where an ensemble learning method is explored to enhance the algorithm's performance.

A hybrid approach for addressing the *Multiple Traveling Salesman Problem* (mTSP) has been introduced by (Silva, 2020), with a specific focus on its application to route scheduling for autonomous vehicles. The approach begins with using K-means as a preprocessing step to generate routes that effectively distribute delivery locations among the vehicles. Subsequently, these routes serve as the initial population for bio-inspired algorithms, namely the GA and *Ant Colony System* (ACS). These algorithms undergo an evolutionary process to discover routes that minimize the overall distance while ensuring balance in the individual routes for each vehicle. The results indicate that the hybrid approaches outperform their classical versions and PSO with increased vehicles and visit locations.

3 BACKGROUND

The **Ensemble Method** is a learning paradigm in which alternative solution proposals for a problem, referred to as components, have their outputs combined to obtain a final solution. In statistics and computer science, ensemble methods constitute a set of techniques that combine multiple learning algorithms to achieve predictive performance superior to individual algorithms (Opitz and Maclin, 1999). Generally, the formation of a group of classifiers, where the final prediction is obtained by combining their predictions, assumes that the diverse opinions, when unified, tend to generate a better decision than those generated by a single component. The success of an ensemble system – that is, its ability to correct errors from some of its members – directly relies on the diversity of the classifiers within the ensemble. The intuition is that if each classifier makes different errors, a strategic combination of these classifiers can reduce the overall error (Polikar, 2009).

According to (Vieira, 2013), the **VRP** involves determining a route to be followed by a fleet of vehicles, ensuring that the demand of all clients is satisfied and each vehicle returns to the initial depot at the end of the route. The objective is to minimize the total cost, travel time, or total route distance. Vehicle routing problems are among the most complex in the combinatorial optimization field (Golbarg and Luna, 2000).

In the **CVRP** the task is to determine the routes that a set of vehicles must take to deliver goods to clients, considering the vehicle's capacities and the demands of each client. The goal is to minimize the overall transportation cost, which may encompass factors such as distance traveled by vehicles, time needed for deliveries, number of required vehicles, and other relevant considerations. Similar to the VRP, the CVRP is classified as an NP-hard problem. The CVRP is formally formulated by (Laporte, 1992) as follows:

Given a graph G = (V, E), where V = $\{v_1, v_2, v_3, ..., v_n\}$ corresponds to the demand points and $E = \{(v_i, v_j) : v_i, v_j \in V, i \neq j\}$ is the set of edges between the demand points. For each client $v_i \in V$ there is an associated demand $q_i \in Q$ that must be supplied by some vehicle. The set E is associated with a non-negative symmetric cost matrix C that represents the cost required to travel between two nodes i and j, where $c_{ij} = c_{ji}$. The following constraints must be respected: (i) each city $v \in V - 1$ must be visited exactly once; (ii) all routes must start and end at the depot; (iii) meet the capacity constraints of the vehicles.

4 METHODOLOGY

In this Section, the strategies employed in constructing heuristics to address the proposed problem are presented.

4.1 Clustering

Clustering entails the application of computational techniques to partition a dataset into distinct groups based on their similarities. As defined by (Priy, 2013), clustering is the process of dividing the population or data points into multiple groups. The objective is to ensure that data points within the same group exhibit greater similarity to each other than to those in other groups. Diverse clustering methods exist, differing primarily in their approach and strategy for group formation. In this study, two distinct methods were employed. The first method utilizes the concept of centroids and is implemented through the K-means algorithm. The second method relies on point density and is executed using the DBSCAN algorithm.

K-means – described initially by (MacQueen, 1967), K-means algorithm aims to partition observations into k groups, where k represents the number of groups. This partitioning of data is done in such a way that different groups are more separated from each other, while observations within each group are closer to each other. To achieve this, it uses the *Sum of Squared Errors*, denoted as (SSE), which seeks to minimize the distance between points and their centroid. Once the model is created, the K-means algorithm calculates the mean of each group, also referred to as centroids, and thereby identifies the centroid closest to each new data point. The centroid serves as the center of the group (Bramer, 2007).

The K-means algorithm aims to classify information based on the inherent structure of the data. This classification relies on the analysis and comparisons of numerical values within the data. Consequently, the algorithm automatically generates an unsupervised classification, requiring no human supervision or pre-existing classification. Due to this characteristic, K-means is considered an unsupervised data mining algorithm.

It is important to note that the K-means method does not guarantee convergence to the global optimum, and the solution obtained often represents a local optimum. The results are influenced by the initial (random) selection of group centers. Additionally, it is necessary to determine the number of groups in advance. In practice, to enhance results, it is common to run the K-means algorithm multiple times with different initial centroids (Chen and Tan, 2021).

DBSCAN – *Density-Based Spatial Clustering of Application with Noise* is a non-parametric density-based clustering method proposed by (Ester et al., 1996). It is effective in identifying groups of arbitrary shapes and sizes, separating noise from data, and detecting natural groups and their arrangements within the data space, without any prior information about the groups. The method requires only one input parameter but supports determining an appropriate value for it. The main idea of the DBSCAN method is that, for each point in a group, the neighborhood for a given radius must contain at least a certain number of points, meaning that the density in the neighborhood must exceed a threshold.

4.2 Elbow Method

This method plays a crucial role in determining the ideal number of clusters, denoted as K, which is an essential parameter for the initial configuration of the K-means algorithm. According to (Sammouda et al., 2021), the elbow criterion technique is a heuristic method applied to determine the number of clusters for data points in a dataset. The elbow technique is used to obtain the optimal number of clusters for a set of data points because it is an empirical, simple, and easy-to-implement method. Applying the K-means clustering algorithm, the elbow method plots the explained variations against the number of clusters and chooses the elbow curve to determine the number of clusters. It relies on calculating the sum of squared errors within the cluster of all data points to represent the quality of aggregation within the same cluster and separation between clusters.

4.3 Initial Solution Generation

Generating an initial solution is a crucial step in many routing algorithms to identify the optimal solution for a given problem. This phase involves the creation of an initial solution that acts as the starting point for the routing algorithm. Initially proposed by (Cover and Hart, 1967), the **Nearest Neighbor Algorithm** consists of composing the route based on the sequential insertion of points through an initial point according to the shortest distance between this point and its other points (neighbors). After determining all distances between the initial point and the other points in the cluster, the remaining points are sorted in decreasing order to enable the choice and determination of the nearest node that will be assigned to the route. According to (Santos and Leal, 2006), this method is usually used to find an initial solution to the problem, which is then gradually improved by other techniques and models. It has a simple and fast application and can be used for highly complex problems.

4.4 Initial Solution Improvement

Heuristics for route improvement are designed to enhance the efficiency of a route by refining a previously obtained solution. They initiate the process with a comprehensive initial solution, acquired through constructive or random methods, and then aim to discover a higher-quality solution within its neighborhood (Siqueira, 2017). If a superior solution is identified, it replaces the current one. This process of seeking route improvement persists until a stopping criterion is met or no further improvements are found (Fraga, 2006). The most well-known category of algorithms for this purpose is the k-opt arc exchange heuristic.

K-Opt Heuristic – initially proposed by (Lin, 1965) for the *Traveling Salesman Problem* (TSP), has found natural applicability to the VRP. This approach represents a classic local search algorithm for the TSP, relying on the exchange of arcs in solutions initially created through constructive heuristics. The number of arcs to be exchanged is determined by the parameter k. Notably, as the parameter k increases, the procedure gradually approximates the total enumeration of neighboring solutions (Goldbarg and Luna, 2005; Bispo, 2018). According to (Croes, 1958), the 2-Opt heuristic exchanges two edges to find an improvement in the current solution. If an improvement is detected in any of these exchanges, it is assumed as the current solution. This process ends when it is no longer possible to make exchanges that improve the solution or a stopping limit is reached.

5 PROPOSED STRATEGIES

The main structures of the proposed strategies are composed of six steps, as presented in the flowchart in Figure 1.

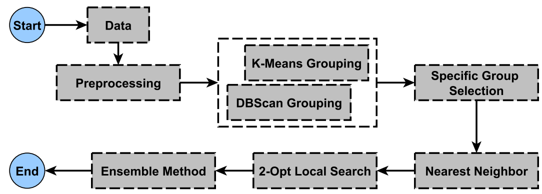


Figure 1: Model general flowchart.

In the initial step, several **preprocessing** operations are performed to ready the data for clustering. Specifically, the latitude and longitude columns contain geographical coordinates represented as strings with commas. To facilitate numerical processing, these commas are substituted with dots in both columns. Subsequently, the columns are converted to the numeric data type.

The second step is related to the **clustering** of clients according to their geographical locations. As mentioned earlier, two strategies have been proposed, each employing a specific clustering method to group the delivery points.

The first strategy (based on the K-means algorithm) utilizes the K-means clustering algorithm, which groups observations into k clusters, where k is the desired number of groups. In clustering algorithms like K-means, it is necessary to determine the appropriate number of clusters for a given dataset. This ensures that the data is divided appropriately and efficiently. An appropriate value of k (i.e., the number of clusters) helps ensure the proper granularity of the groups and maintain a good balance between compressibility and accuracy. To determine the ideal value of k in the instances worked on, the elbow method is used, which assists in defining the optimal number of groups. This value of k should be passed as a parameter at the beginning of the K-means algorithm execution.

In the strategy based on DBSCAN, the clustering of customers into groups is performed using the DBSCAN algorithm. This algorithm is used to group a set of spatial data based on two main parameters: the physical distance of each point and the minimum size of the cluster. DBSCAN identifies dense regions of points in space, considering points that are close enough to each other as part of the same cluster. The parameter ε (epsilon) represents the maximum distance that defines the neighborhood of each point, while the *min_samples* parameter defines the minimum number of points within that neighborhood for the point to be considered the core of a cluster.

In the third step, a **specific group** is selected from those created by the clustering algorithm. The chosen group is stored in a variable, and its total demand is calculated. This means that routes are created in a way that the sum of demands does not exceed the vehicle capacity, which, in this case, is 180. [2]

Following the creation of the routes, an initial route is generated by applying the **nearest neighbor algorithm** to find an initial path that visits all points in the specific group in order of proximity, starting and ending at an initial point (depot), respecting the vehicle capacity constraint and visiting a client only once per vehicle. This is the fourth step of the process.

In the fifth step, the **2-Opt** improvement algorithm is applied to enhance the initial solution obtained through the nearest neighbor algorithm.

In the sixth and final step, the routes are combined to obtain the final solution. This is done through the ***ensemble*** combination rule, using an algebraic combiner approach. This type of combiner is non-trainable and operates on the continuous outputs of classifiers or, in this context, routes.

6 ANALYSIS AND RESULTS

The reference database utilized in this study is the Loggi *Benchmark for Urban Deliveries* (BUD), comprising a collection of data for large-scale problems obtained from the LoggiBUD repository. This dataset simulates the challenges associated with deliveries in the final stage of the logistics chain. The data in this database are structured as JSON data dictionaries, organized by cities. Each JSON file includes information such as the city's name, the served region, the coordinates of the origin point (latitude and longitude), the capacities of the vehicles, and the delivery points (identifier and address coordinates).

The LoggiBUD repository provides two types of instances: *delivery-instances* and *cvrp-instances*. This study uses the *cvrp-instances*, which represent a CVRP. These instances include details such as the depot location, the vehicle capacity, the locations of each delivery, and the associated demands for each delivery. The initial version of LoggiBUD offers a total of 90 training and 30 evaluation instances for the city/state: Rio de Janeiro/Rio de Janeiro (RJ), Brasília/Distrito Federal (DF), and Belém/Pará (PA). Each instance varies in the quantity of packages (deliveries). In the experiments, three samples were generated – one from RJ, other from DF, and the last one from PA. Concerning the deliveries number, RJ has the highest, totaling 4,273 deliveries; DF follows with 987 deliveries; and PA has the lowest, with 297 deliveries.

Tests were conducted using the strategies described in this work and were applied to instances obtained from the LoggiBUD repository[3]. The instances contain information about the depot's location, the fleet vehicle capabilities (180 units of load), the locations of each delivery, and the demands of each delivery, ranging from 1 to 10 weight units. To assess the quality of the solutions obtained by the strategies, two main objectives were considered: minimizing the total distance traveled by trucks and achieving a balance in the distribution of vehicle distances.

In this work, a lower standard deviation in the traveled distances is desirable as it indicates a more balanced distribution of distances among vehicles. The strategies were evaluated through computational experiments involving a set of instances from three Brazilian states (RJ, DF, and PA), in terms of vehicle fleet, a homogeneous fleet was considered, where all vehicles have the same capacity.

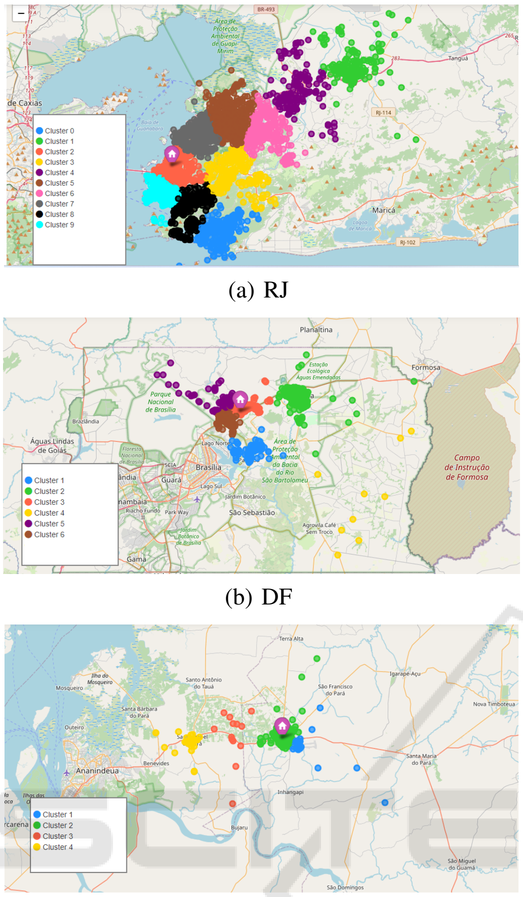
6.1 Strategy Using K-means

The strategy in this approach involves utilizing the K-means algorithm. Determining the appropriate number of clusters for a given dataset is a crucial step in this algorithm. The elbow point on the curve – representing the sum of variances within the cluster concerning the number of clusters – is employed to select the optimal number of clusters. Thus, by applying the elbow method, we observe the ideal value of k is 10 for RJ, 6 for DF, and 4 for PA. Thereupon, these numbers of clusters are utilized in the K-means algorithm to perform clustering.

Figures 2(a), 2(b), and 2(c) display different clusters identified by a distinct color. These clusters are formed based on three dataset attributes: coordinates (latitude and longitude) and each client demand. As observed in Table 1(b), for DF with 986 deliveries, 31 vehicles were utilized, covering a distance of 4,294 kilometers. In Table 1(c), it is evident that in PA was completed 297 deliveries to different points using 12 vehicles, throughout the deliveries, vehicles traveled a total of 1,849 kilometers. In RJ, the delivery number was higher, totaling 4,273, as shown in Table 1(a). To satisfy this demand, 137 vehicles were employed, covering a total distance of 14,632 km.

[2]Pre-established value by the LoggiBUD.

[3]https://loggibud.s3.amazonaws.com/dataset.zip

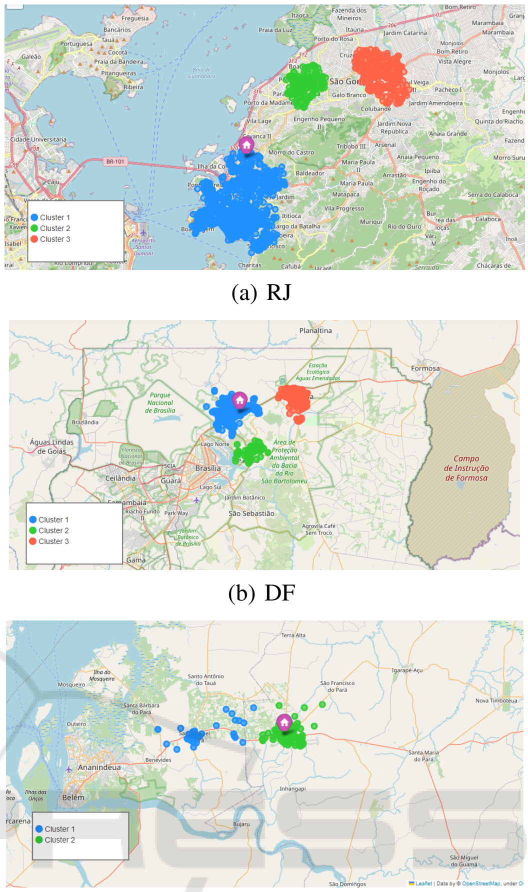


(a) RJ

(b) DF

(c) PA

Figure 2: K-Means clustering in RJ, DF, and PA.



(a) RJ

(b) DF

(c) PA

Figure 3: DBSCAN clustering in RJ, DF, and PA.

6.2 Strategy Using DBSCAN

This strategy utilizes the DBSCAN algorithm where ε is a parameter that sets the maximum distance between two points for them to be considered neighbors. In this scenario, individual ε values are calculated: 1 km for RJ, 3 km for DF, and 3.50 km for PA. These values are the required proximity between points to be considered part of the same cluster.

The second parameter is *min_samples*, defining the minimum number of points necessary to form a valid cluster. Any points failing to meet this criterion are categorized as noise. The chosen *min_samples* values vary according to the geographical context: 10 for RJ, 5 for DF, and 5 for PA. This differentiation considers the anticipated density of points in each region. Unlike K-means, DBSCAN does not necessitate specifying the number of clusters in advance; it automatically determines them based on the ε and *min_samples* parameters.

Figures 3(a), 3(b), and 3(c) provide insight into the geographical distribution of clusters. Notably, only points within the distance defined by ε are selected to form clusters, while those not meeting this criterion are discarded. For RJ, out of the total 4,273 scheduled deliveries, the algorithm selected 3,285 for inclusion in the clusters, while 988 points were discarded for not meeting the criteria. In DF, where initially 986 deliveries were planned, 960 were grouped, and 26 points were considered noise and excluded. In PA, out of the planned 297 points, 27 were identified as noise and not included in the grouping.

The results for instances of RJ, DF, and PA are presented in Tables 1(a), 1(b), and 1(c), respectively. In RJ (Table 1(a)), we can see 3,285 deliveries in total, and 78 trucks were used, covering a distance of 10,264 kilometers. In DF (Table 1(b)), trucks covered 4,454 kilometers to complete 960 deliveries. In PA (Table 1(c)), there were 270 delivery points with a total distance traveled of 2,101 kilometers.

Table 1 consolidated results for the strategies presented. When considering criteria such as solution

Table 1: Results for instances in RJ, DF, and PA.

(a) RJ

Items	K-means	DBSCAN	Loggi
Trucks	137	78	145
Demand	23531	13860	23531
Distance	14632	10264	16985
Delivery Pts	4273	3285	4273
Std Dev (σ)	627.735	3263.221	755.367

(b) DF

Items	K-means	DBSCAN	Loggi
Trucks	31	30	32
Demand	5353	5040	5353
Distance	4294	4454	4902
Delivery Pts	986	960	986
Std Dev (σ)	363.493	843.085	536.415

(c) PA

Items	K-means	DBSCAN	Loggi
Trucks	12	10	10
Demand	1634	1453	1634
Distance	1849	2101	1520
Delivery Pts	297	270	297
Std Dev (σ)	315.981	58.689	457.570

quality concerning the preconized objectives, it is evident that both strategies based on K-means and DBSCAN algorithms provide high-quality solutions.

Analyzing RJ instances (Table 1(a)), it can be observed that the strategy based on the DBSCAN algorithm demonstrated superior performance in terms of number of trucks used and the total distance traveled. However, the DBSCAN strategy did not use the same number of instances as K-means strategy and Loggi approach. The strategy based on K-means algorithm, has benefits in both the number of trucks and the total distance traveled when compared to the Loggi approach.

In the results for DF instances (Table 1(b)), the strategy based on K-means algorithm achieved superior performance in terms of the number of trucks and the total distance traveled when compared to the Loggi approach. Regarding, the strategy based on the DBSCAN algorithm, it is important to highlight that delivery points were different, which may have influenced the comparison of results. In the results for PA (Table 1(c)), the Loggi approach showed better performance in both the number of trucks and the distance traveled compared to the proposed strategies.

Table 1 shows a comparison between solutions obtained by each strategy – K-means and DBSCAN – and Loggi's approach in tests conducted for the three instances under analysis. The K-means algorithm strategy presents the lowest standard deviations for the instances of RJ and DF, being more consistent and predictable in results for these instances. Table 1(c) highlights that the DBSCAN algorithm strategy presents a lower standard deviation, indicating a more consistent and predictable distribution of results for the PA instances. It is important to reiterate that the lower the standard deviation value, the more efficient the deliveries were, pointing to a more effective distribution.

The ensemble combiner rule, based on algebraic sum combination, is used to unify individual results from each optimized route, aiming to obtain an overall measure of route efficiency. This rule acts as the central mechanism to combine individual values of distance traveled on all routes, resulting in a total distance that reflects the overall performance of the adopted strategies, presented in Tables 1(a), 1(b) e 1(c). The process of applying this rule can be described as follows: (i) after the optimization step, the individual distances of each route are obtained, representing the distances traveled by each vehicle; (ii) the ensemble combiner rule comes into action, where the individual distances of all routes are summed through an algebraic expression; (iii) the total distance obtained by summing the individual distances becomes a unified performance measure; (iv) a lower total distance value indicates more efficient routes in terms of minimizing the distance traveled.

7 CONCLUSIONS

This study aimed to develop and apply an approach for spatial data analysis using heuristic methods and ensemble techniques to optimize the vehicle routing process. To achieve this goal, two distinct strategies were proposed, each employing a clustering model to group delivery points (clients) into clusters. The application of the K-means and DBSCAN clustering algorithms allowed for efficient grouping of clients, providing essential information for the creation of routing strategies. The implementation of two distinct strategies, each centered on a specific clustering model, demonstrated the flexibility of the proposed methodology.

Based on the conducted experiments, it can be concluded that both the strategy based on the K-means algorithm and the strategy based on the DBSCAN algorithm produced good results for the CVRP. They demonstrated satisfactory performance in minimizing the total distance traveled by trucks, balancing the distribution of distances traveled, and minimizing the standard deviation. This study provides valuable insights into fleet routing through the analysis of spatial data and heuristic methods. By addressing current challenges and offering guidance for future research, it is anticipated that this work will make a meaningful contribution to the enhancement of logistics and transportation operations.

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