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BinR-LRP: A divide and conquer heuristic for large scale LRP with integrated microscopic agent-based transport simulation

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ABSTRACT

The holistic optimisation of transportation systems is one of the key challenges in transportation science, because it requires the simultaneous consideration of the numerous interactions between the strategic planning level (e.g., the Facility Location Problem [FLP]) and the tactical and operational planning levels (e.g., Vehicle Fleet and Vehicle Routing Problem [VRP]). Traditional methods for solving the Location Routing Problem (LRP) often focus on the fixed constraints and ignore the variable vehicle characteristics, dynamic operations, different modes or underlying infrastructure. This paper proposes an integrated approach for modular and intuitive metaheuristic for LRP. The route planning phase is incorporated by means of agent-based transport simulation, which provides additional flexibility with respect to the vehicle fleet, demand characteristics, or the use of external problem constraints. Therefore, this approach can be easily applied to practical problems and used to optimise transport networks in a flexible and modular manner. Moreover, the algorithm developed here can independently converge to the near-optimal number and location of logistics sites. We also demonstrate the effectiveness and the performance of our approach by performing several simulation experiments in the context of a sensitivity analysis and comparing the results with well-known benchmark solutions. The results indicate that the Binary-Partition LRP heuristic (BinR-LRP) is able to identify better solutions than the benchmark heuristics in most cases. This emphasises its suitability as a scalable and robust optimisation framework, even for oversized LRP instances.

Motivation

Strategic decisions regarding the geographical location of distribution centres in combination with the minimisation of transport costs are the key factors for the successful operation of transport networks. Especially in urban areas, the pressure on the logistics network is growing due to the increased freight demand (Bundesverband Paket & Express Logistik [BIEK], 2021). One of the biggest influencing factors for reducing the negative impact of freight transport is the optimal choice of logistics locations. The optimisation of depot locations can be divided into four subproblems, which are also strongly interrelated: (i) number of warehouses, (ii) location of sites, (iii) customer allocation, and (iv) warehouse level (Friedrich, 2010). Strategic planning of transport networks should also consider the operational decisions of logistics actors, such as route planning (Salhi & Rand, 1989). In addition, other constraints such as delivery time windows, the choice of vehicle type and certain vehicle characteristics on the operational decision level have an impact on route planning and consequently on the overall network design. They must therefore also be taken into account as part of a holistic optimisation approach. A modular, easily implementable metaheuristic that can be integrated into the transportation simulation environment is thus necessary to model and optimise the entire transportation system in a consistent manner.

However, many approaches presented in the literature address the problem of combinatorial network optimisation using encapsulated Mixed Integer Programming (MIP) techniques. As a result, such approaches usually attempt to solve concrete problems or benchmark instances formulated for particular experiments and have limited scalability and reproducibility due to numerous limitations. The development of a modular, flexible heuristic for solving large-scale Location Routing Problem (LRP) is also necessary for several reasons: Traditional Operations Research (OR) heuristics tend to focus mostly on network optimisation with respect to synthetic demand and Euclidean distances. Instead, in the optimisation and practical application of such methods, a

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large number of other individual logistics decisions, occurring on different time scales, play a crucial role. For example, modal split and vehicle choice must be considered with a different consolidation factor depending on region size and demand properties. The size and the cost of a logistics facility in each catchment area have to be also considered individually and examined in each individual decision step. Thus, the actual decision sequence of the logistics actors during the network planning does not occur in the solution space with complete information and cannot be optimised in plain space but rather represent a deep decision tree, where the previous decision of the logistics actors in time step t influences the next unknow decision in $t+1$.

The proposed approach utilises this idea by formulating the LRP as a binary decision tree combining several efficient heuristics into one modular framework. The problem of location optimisation and allocation of customers for Facility Location Problem (FLP) is applied using a divide-and-conquer heuristic with non-hierarchical group clustering. Such an approach reflects the actual decision making in a location planning process achieving the cost minimisation by adding a new facility to the system and comparing the new state with the previous one. Furthermore, we use the route optimisation framework Jsprit to dynamically optimise route planning in each decision step (Schröder et al., 2012). This methodology provides an integrable infrastructure-level route heuristic with freely adjustable problem constraints in each decision step, making it suitable for different scenarios.

In the following, section 2 will provide an overview of the State of the Art in logistics network optimisation, focusing on FLP, VRP and integrated optimisation approaches, i.e. LRP. Section 3 will give a more in-depth description of our methodology, Binary-Partition LRP Heuristic [BinR-LRP], including the general problem formulation and an introduction to the proposed algorithm used for solving large-scale LRP problems with rich constraints. In section 4, the approach will be validated through a series of simulation experiments that include sensitivity analysis conducted on synthetic instances. The methodology will be further validated on small and medium LRP benchmark instances in section 5, demonstrating its feasibility and effectiveness. In the last section, we will discuss the limitations and advantages of the proposed metaheuristic and provide an outlook on scenarios for its further application.

State of the Art in logistics network optimisation

Strategic location planning in freight transport involves many interlinked combinatorial problems on different time scales that ideally need to be optimised simultaneously, e.g., determining the number and size of the opening facilities, the size of the vehicle fleet, routing choices, delivery region properties, and demand properties. Their combinations lead to overcomplex problems, which in most cases can only be solved by means of simplified, aggregated heuristics (Klincewicz, 1991; Campbell, 1994; Min et al., 1997; Guerra et al., 2007; Melo et al., 2006; Campbell & O'Kelly, 2012).

The FLP is one of the most studied combinatorial problems and can be treated from different perspectives. Economic and analytical approaches aim at finding the best locations by either comparing economic decisions qualitatively (Millstein & Campbell, 2018; Liedtke & Murillo, 2012, 2015a) or selecting the best network design e.g. by means of a multi-criteria analysis (Mihajlović et al., 2019; Karaşan et al., 2020). The mathematical models address the FLP by investigating spatial and transportation relationships under the assumption of uniformly distributed demand (Daganzo, 1984, 1985, 1986, 2005; Campbell, 2017; Carlsson & Jia, 2013; Carlsson & Song, 2018). These methods provide a good approximation for large instances where many causalities are unknown and the discrete optimisation is not feasible. OR is mostly concerned with location and network planning by means of discrete optimisation where distances from customers to facilities are minimised either on graphs or in Euclidean space (Akinc et al. 1977; Alumur 2008; Campbell, 2009; Alumur et al.,2012; Guemri et al., 2016). The research conducted in this field mainly focuses on finding a central place in the delivery region and is often treated by means of static and dynamic mixed integer programming models (Guerra et al., 2007; Thanh et al., 2008; Özceylan & Paksoy, 2013; Singh & Goh, 2019; Rostami et al., 2021), clustering (Nadizadeh et al., 2011; Duong et al., 2021), p-median and Hub-Location Models (Tansel et al., 1983; Church & Sorensen, 1994; An et al., 2014). However, these optimisation techniques incorporate numerous constraints and result in the mathematical cost functions with numerous variables, which is hard to solve in practice. Thus, these approaches often experience a lack of transferability since each problem has to be formulated exclusively.

Salhi and Rand (1989) prove that achieving optimal facility location is not possible without considering vehicle routing. Over the past decades, LRP has been extensively studied in the field of OR (Wasner & Zäpfel, 2004; Prins et al., 2007; Barreto et al., 2007; Schneider & Drexl, 2017). Because integrated optimisation problems suffer from high computational complexity, practitioners seek to simplify their metaheuristics with single decomposition or aggregation phases, such as sampling or clustering (Nadizadeh et al., 2011; Alvim et al. 2013; Oudouar et al., 2020). Arnold and Sörensen (2018) address this issue by developing a light-weighted metaheuristic where VRPs are iteratively applied by means of Clark and Wright heuristic for each selected location. Nguyen et al. (2012) combine four heuristics (extended Clark and Wright, nearest neighbour, subtours building, and giant tour solution) to solve a two-echelon location routing problem. A Greedy Randomized Adaptive Search with Learning (GRASP-LP) method has been developed, in which tours for random depots on different echelon layers are created in the first construction phase and these solutions are improved by neighbourhood search in the second phase. Due to computational efficiency numerous GRASP modifications have been developed with respect to the large-scale LRP (Prins et al., 2006; García-Archilla et al., 2013; Contardo et al., 2014). Duhamel et al. (2010) propose a route first-location second metaheuristic based on extended GRASP heuristic. The authors relax the complexity by introducing a Taboo list for opened depots during the giant tour splitting phase. Schmidt et al. (2018) extend a location-routing optimisation algorithm with discrete travel times in the routing phase. Using real road traffic data from Quebec City, Canada, the authors validate their approach minimising the total driving time from multiple depots. Chao et al. (2019) present a two-stage location-routing-inventory heuristic with integrated clustering to improve the search performance. The referred heuristic apply distance-based clustering with customer allocation. In the second stage, ant-colony optimisation for location permutation is adopted for food delivery LRP with time windows. Wang et al. (2018) utilise k-Means clustering and genetic algorithm for routing while Wang et al. (2020) apply Gaussian mixture clustering and improved Clark and Wright savings heuristic to optimise Two-Echelon LRP with Time Windows. Moreno et al. (2020) integrate the TSP tour approximation into the clustering phase proposing an LRP metaheuristic for large instances that combines continuous approximation for routing and clustering for FLP.

The route optimisation is the second optimisation element within the LRP, which takes place on the operational level, and is additionally subject to numerous operational and tactical logistics decisions (time window planning, packing problem, route optimisation, vehicle fleet optimisation). To address all these constraints for route optimisation in a holistic manner, microscopic transport simulations and multi-agent systems (MAS) are widely used in State of the Art. Schröder et al. (2012) use the Multi-Agent Transport Simulation MATSim (Balmer et al., 2009) and integrate the logistics behaviour model Jsprit to represent and simulate agents in urban freight transport. Due to its flexibility and efficiency, the MATSim Freight framework has been successfully extended and recently applied to a wide range of case studies such as food retail and the parcel market. (Liedtke et al., 2013, 2015b; Liedtke, 2014; Matteis et al., 2016, 2019; Schröder & Liedtke, 2017; Thaller et al., 2016; Zhang et al., 2018; Thaller et al., 2017; Thaller, 2018; Thaller, 2019). Llorca and Moeckel (2020) investigate the routes of cargo-bikes using MATSim and Jsprit in different scenarios which are subjects of variable vehicle properties and demand density. However, the application of microscopic transport simulation in LRP faces many complications, especially because agent-based simulation is computationally expensive. Recently, Deineko et al. (2022) present an LRP metaheuristic for large instances that combines Continuous Approximation (CA) for routing and clustering of FLP. In the second phase, after the solution is found, the agent-based transport simulation MATSim and the integrated VRP solver Jsprit are used to investigate the economic and environmental impacts of autonomous trucks in the food retail sector in Germany.

Juan et al. (2015) introduce the term Simheuristics to describe hybrid approaches, where the simulation tools are integrated within or alongside optimisation metaheuristics to handle real-life decisions and uncertainties. Reviewing 222 publications on LRP between 2014 and 2022, Mara et al. (2021) advocate for the rising interest in combined techniques and highlight the importance of the hybrid methods, where the simulation can be integrated into the solution search: "It is presumed that this hybrid technique should be more popular in the future, due to the simplicity and applicability of simheuristics for handling the uncertain value of variables." (Mara et al., 2021, p. 2966).

In general, there is a strong need for the lightweight application of agent-based transport models within LRP heuristics due to the high system complexity and dynamics involved. This enables different levels of location to be optimised in a flexible manner, not only in terms of direct transport routes, but also taking into account different transport modes and demand characteristics. However, the application of MAS models in LRPs is associated with many complications, particularly because both FLP and VRP are NP-hard and cannot be applied iteratively to large LRP. Furthermore, many of the problem formulations presented in the literature remain difficult to reproduce and have limited applicability to case studies, as they often focus on limited mathematical problem formulations. To the best of the authors' knowledge, no method reported in the field of LRP provides the ability to simulate vehicle routing with respect to transport infrastructure and real road traffic conditions. The method presented in this study leverages a modular, recursive divide-and-conquer algorithm with integrated agent-based transport simulation to perform facility selection based on real-world transport planning settings.

Methodology

In the following, the mathematical formalisation of the metaheuristic algorithm as well as the functionalities of the MATSim and Jsprit frameworks are explained in more detail. The integrated methodology presented here is able to converge at the minimum number of facilities and approach their near-optimal locations even under variable logistic constraints such as multiple time windows, traffic conditions, vehicle speed, heterogeneous fleet and other problem-dependent constraints. The framework can easily be extended and flexibly adapted according to the formulated scenario, such as Two-Echelon Logistics Network optimisation and different facilities levels in each customer region (see Deineko et al., 2024).

Formulation and description

The proposed network optimisation algorithm consists of four general stages: (i) clustering stage, (ii) assignment, (iii) costs calculation and (iv) evaluation and recursion step. We further denote variables and sets, such as:

- P as a problem encompassing all customers I
- $P^{'}$ problem partition with a subset of customer $I^{'} \subset I$
- $C(l_{p'}, I^{'})$ is transportation costs function calculated in each partition $P^{'}$ for a potential location l and customer subset $I^{'}$
- L as a set of potential locations defined for this P, where $l_{p'} \in L$
- S is a set with locations added to this solution set $S = \{l_{p'}\}$
- $V \leq \max T$ is a set of heterogeneous vehicle fleet with a given maximal number of all possible vehicles T parametrised for all P.

Let $P = \{I, V\}$ be a problem characterised by a set of customers with defined constraints and demand for all $i \in I$ and vehicle fleet V of the given size T.

In the first stage, the clustering algorithm is applied to partition the problem $P \rightarrow P_i^{'} and P_j^{'}$, where $P_i^{'} and P_j^{'}$ are the subsets such that $P_i^{'} \cap P_j^{'} = P$. We further denote P' as a subproblem of P.

Next, in the assignment stage (ii) a potential location $l_{p'}$ with minimum distance is selected for each P' from a fixed set of all potential locations $l \in L$ such that $P(l_{p'})$ where$l_{p'} = \min_{p' \in P} \overline{d}(l, centre(P'))$.

In (iii) the transportation costs $C(l_{p^{'}}, I_{p^{'}}, V)$ are calculated for all customers in P'. Finally, comparing the costs in this partition $C(P')$ and the sum in the next partitioning $C(P_{i+1}^{'}) + C(P_{j+1}^{'})$, the solution with the minimum costs is then added to the set of the problem solution such that: $C(l_{p^{'}}, I_{p^{'}}, V) < C(l_{p_i^{'}}, I_{p_i^{'}}, V) + C(l_{p_j^{'}}, I_{p_j^{'}}, V) \rightarrow S(l_{p'})$, otherwise proceed to the next iteration $P' \rightarrow P_{i+1}^{'} and P_{j+1}^{'}$. The search is then terminated when all P' exhibit minimum transportation costs or the clusters reach minimum number of customers $N_t \leq N_{min}$, where N_t is the number of customers in partition P' and N_{min} is the maximum allowable number of customers in this partition.

Agent-based transport simulation MATSim and the VRP solver Jsprit

Central part in this methodology is a realistic simulation of passenger and freight transport by means of the microscopic, agent-based transport simulation MATSim (Horni et al., 2016) and the integrated logistics module for freight route optimisation Jsprit (Schröder et al., 2012). The approach is characterised by a high degree of disaggregation. By integrating the simulation of the behaviour of the logistics carriers, the location of the potential facilities can be found with respect to numerous real-world constraints. The optimisation framework is based on the ruin-and-recreate heuristic capable of solving numerous freight transport problem types such as Pickup-and-Delivery VRP, Multi-Depot VRP, VRP with Time Windows, VRP with heterogeneous fleet as well as its combinations (Matteis et al., 2016; Thaller et al., 2016; Zhang et al., 2018). The transport costs optimisation function is subject to the following constraints: (i) both customers and carriers can be parametrised with respected time windows, (ii) a heterogeneous vehicle fleet can be assigned to each carrier, (iii) the vehicle types differ in terms of capacity and costs. Figure 1 shows the model structure of MATSim and Jsprit. Here, three modelling steps have to be carried out. The model is prepared in the first step, i.e. the initial world of MATSim is built up. For this purpose, the infrastructure network as well as the geo-referenced locations and characteristics of the carriers and customers are parametrised. In the second step, the simulation is carried out. Here, the initial plans of the agents are first generated and the tour planning is executed. In a further step, the executed tour plans are evaluated according to standard cost-benefit functions and, if necessary, rescheduled in a further iteration. These three steps, Execution, Scoring and Re-Planning, are executed iteratively until a system optimum is reached.

For a detailed description of the functionality and limitations of this simulation framework, we refer to Schröder et al. (2012).

Metaheuristic algorithm

The initial search starts with a non-hierarchical clustering that consistently distributes two k-centroids in a 2D space. Thereby, the method of choice is K-Means++ Clustering since it has an efficient computational complexity of $(O(log(k))$ and can be considered as a

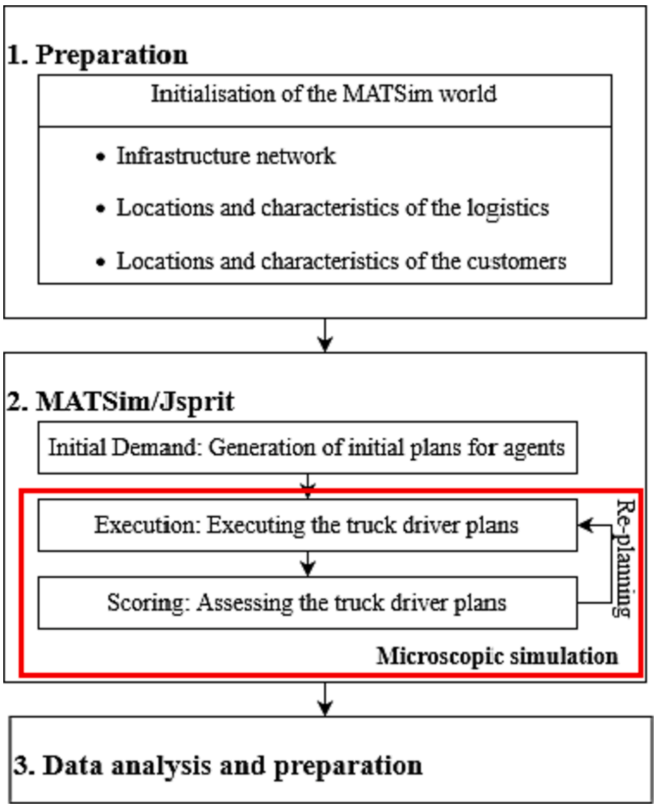

Fig. 1. A schematic representation of the MATSim module with the integrated route planning module Jsprit. Used as an Operational Planning Module in the BinR-LRP heuristic search (Source: Thaller et al. 2018).

suitable choice for combined heuristics (Arthur & Vassilvitskii 2007). Using this algorithm, all customers are first divided into two groups $P_i^{'}$ and $P_j^{'}$. The operational route optimisation and transport costs calculation in each sub-step (each individual cluster) is carried out by means of ruin-and-recreate heuristics utilised in Jsprit which enables finding the minimum transport costs even under complex constraints (limited/unlimited vehicle fleet, customer demand and vehicle specific constraints, etc.). In the last step, the depot costs are calculated by means of a cluster-dependent cost function $C_d(G, K, V)$ where G is the function of the delivery area (e.g. land prices), K is the demand-specific function and V is the fixed costs for opening a facility and deploying the vehicle fleet. It should be noted that the stepwise partitioning and solution search in this framework allows to conditionally adjust facility costs in each cluster e.g. with respect to the land price, storing capacity cost in the facility and the utilised vehicle fleet. Figure 2 shows the feedback between the different methods, as well as to optimised components.

The application of microscopic agent-based transport simulation is a key component for the flexible behaviour-based modelling of different scenarios. In this context, further description of the architecture and the main implementation of the transport optimisation framework Jsprit applied in this study is provided. The pseudocode for code implementation of the proposed algorithm will be presented in the following.

The pseudocode in Table 1 specifies the binary-tree search for proposed metaheuristic. To avoid recursion, which is not feasible for large search trees, the recursive search is replaced by a deep-first search algorithm (i.e. using array deque as a data structure), making the approach suitable for large problem instances. We additionally specify the maximum number of potentially deployed vehicles $V \leq maxT$ in order to constrain the solution space in the initial division steps. By doing so, we skip the instance $P^{'}$ of infeasible size typically at the beginning, since the transport cost calculation framework Jsprit assigns

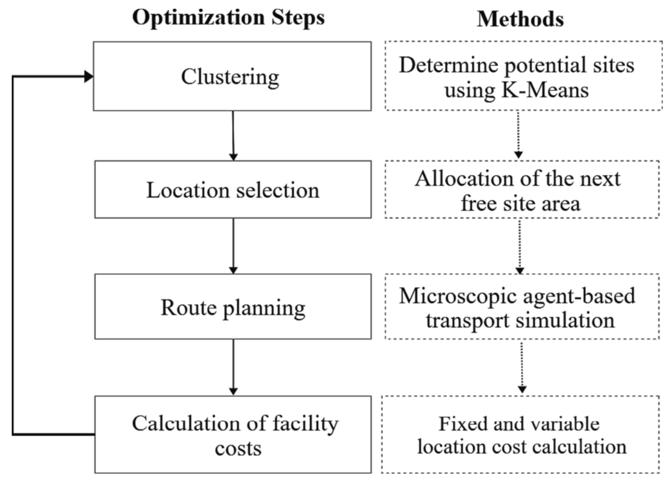

Fig. 2. Overview of the optimisation steps and the corresponding methods.

the penalty cost to unassigned customers and bypasses the intensive computation in large clusters. This constraint allows us to immediately assign $C \rightarrow +\infty$ to $P^{'}$ when the customer demand exceeds the general fleet capacity. It is worth mentioning that the final, optimal number of vehicles in each $P^{'}$ is a subject of general optimisation heuristic within the Jsprit transport cost calculation framework.

Sensitivity analysis

The performance and solution quality of heuristics can vary depending on the characteristics of the problem instance (cf. Srivastava, 1993). To study the behaviour and performance of the search procedure, in this section BinR-LRP will be first applied to the synthetically generated instances.

Overall, the performance of the LRP heuristic is most affected by two factors: the number of customers and the spatial distribution of customers. In the following series of experiments, we first assume 1,000 fixed number of customers distributed in a Euclidean space R of 10,000x10,000. Each customer is assigned with the random uniformly distributed demand in the range $0 < d < 20$. The spatial distribution of customers is then controlled by a so-called "cluster factor" ck where $0 < ck < 1$ and the number of groups k. In this way, the $ck - > 0$ indicates a homogeneous distribution of customers in k regions in R. The factor $ck - > 1$ indicates that the customers are highly clustered in Euclidean space and that the groups k are highly separable. For each generated instance, an additional silhouette coefficient (S_i) was calculated to measure the goodness of clustering (see Rousseeuw, 1987). The silhouette coefficient (S_i) is a measure of the clustering quality and measures the structure of the spatial distribution in the limits $0 < S_i < 1$ in R. Thus, for this set of experiments, we generate the following three types of instances.

- Weakly clustered instances with $S_i \approx 0.3$ (see Table 2: Instances d11133 and d11134). The clients are distributed homogeneously (see Fig. 3).
- Medium clustered instances with $S_i \approx 0.5$ (see Table 2: Instances d11135 and d11136). The neighboring clusters can be distinguished but they are located in proximity to each other.
- Strongly clustered instances with $S_i \approx 0.9$ (see Table 2: Instances d11137 and d11138). The distance between the individual centroids is extreme and the individual groups of customers are far apart (see Fig. 4).

For each of these instances, we run 1,000 iterations to study the behaviour and convergence of the BinR-LRP heuristic. Moreover, in this set of experiments, we declare each centroid found by clustering

Table 1
Main algorithm in BinR-LRP search.

A ← initialise new ArrayDeque for a Deep-first search where:
  key: $C\rightarrow$ max double as an initial cost
  value: $P^{'}$ problem instance with customers and location $l_p{}'$
L ← solution list with optimal locations $l_p{}'$
While A is not empty do:
  $x\rightarrow$ remove entry from A, where $x = P^{'}$ and $C\rightarrow$ costs for this P'
  If x. GroupSize < threshold value $N \leq N_{min}$:
    add $l_p{}'$ to L
    continue
  If x has unassigned customers:
    Set $C\rightarrow maxCosts$
  Split x in $P1$ and $P2$ and calculate the total costs in each partition:$C^{'} = c1 + c2$
  If $C^{'} > C$
    Put x in L
  Else
    add new node to queue $A\rightarrow P1$
    add new node to queue $A\rightarrow P2$
end

Table 2
Sensitivity analysis for the three types of instances: homogeneous ($S_i = 0.3$), medium ($S_i = 0.5$) and highly ($S_i = 0.9$) clustered for the two types of clustering methods: K-Means++ and Fuzzy-K Means. Different clustering methods control the division step in the BinR-LRP heuristic.

Instances	K-Means++ Search					
	S_i	Average no. of depots	Min. no. of depots	Max. no. of depots	Average cost	Rel. standard deviation
d11134	0.3	41	36	44	372,619.10	1.25
d11136	0.5	47	44	51	259,811.28	1.14
d11138	0.9	42	37	46	36,884.20	1.12
Instances	**Fuzzy K-Means Search**					
	S_i	Average no. of depots	Min. no. of depots	Max. no. of depots	Average cost	Rel. standard deviation
d11133	0.3	40	33	45	398,789.07	1.67
d11135	0.5	43	37	49	316,894.45	5.16
d11137	0.9	40	9	46	43,996.83	90.25

algorithm to be a depot location. The underlying hypothesis is that, if the BinR-LRP heuristic is influenced by the clustering in each splitting step, then the final solution must also be subject to significant variation. In order to test the limitations of our heuristic, we additionally implement the Fuzzy K-Means Clustering to reinforce the variation in the final solution (see Table 2: Instances d11133, d11135, d11137). Similar to K-Means++, Fuzzy K-Means allocates a certain number of centroids in the search space with the main difference: the degree of fuzziness of each cluster can also be controlled by a fuzzy parameter (Cebeci & Yildiz, 2015). Consequently, in Fuzzy K-Means, each customer is allocated to a cluster based on a certain probability, and the random formation of customer groups in each iteration is achieved by varying the fuzziness parameter. The objective in this series of experiments is to create a highly unstable and fluctuating solution by utilising additional stochastic components. Overall, the primary objective here is to verify that the BinR-LRP heuristic can consistently converge to an optimal number of locations even under an infeasible initial clustering strategy, while evaluating the degree of variation in the solution quality.

Table 2 shows the results from 1,000 iterations for three generated instances with 1,000 customers, classified according to the silhouette index S_i. Hereby, each instance is solved using both a BinR-LRP heuristic with standard K-Means algorithm and Fuzzy K-Means with variable fuzzy parameters. As expected, the BinR-LRP heuristic with built-in K-Means clustering generally demonstrates lower coefficients of variation (relative standard deviation with respect to the total cost) compared to the heuristic with the integrated Fuzzy K-Means clustering. In this respect, our results reveal that in the instances with homogeneously distributed customers, the BinR-LRP heuristic with K-Means and Fuzzy

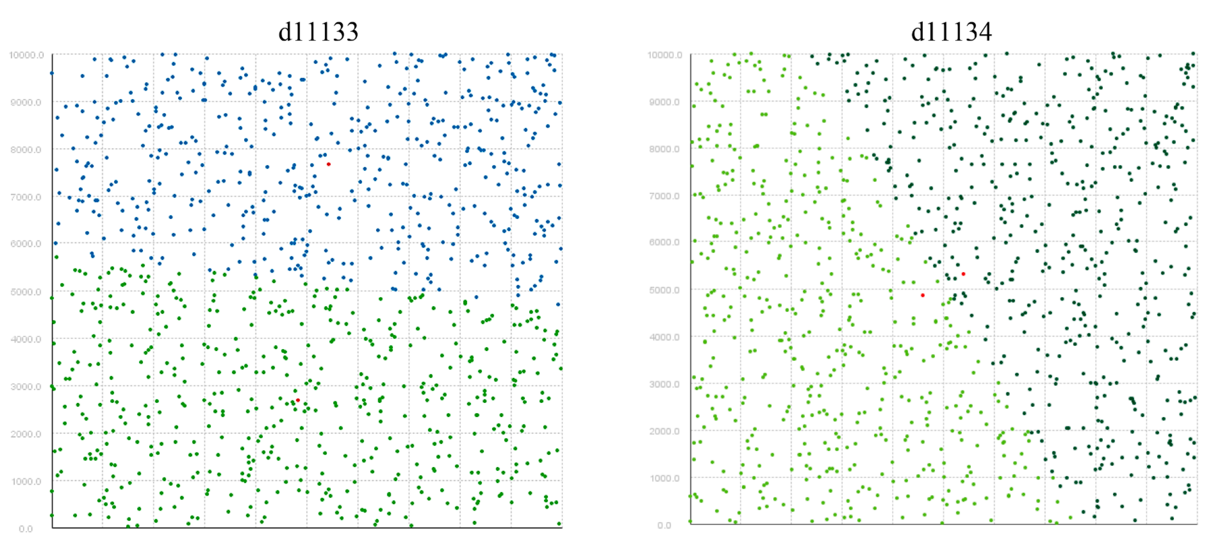

Fig. 3. Initial solution with K-Means and Fuzzy K-Means. The two initial splitting steps for instances d11133 and d11134.

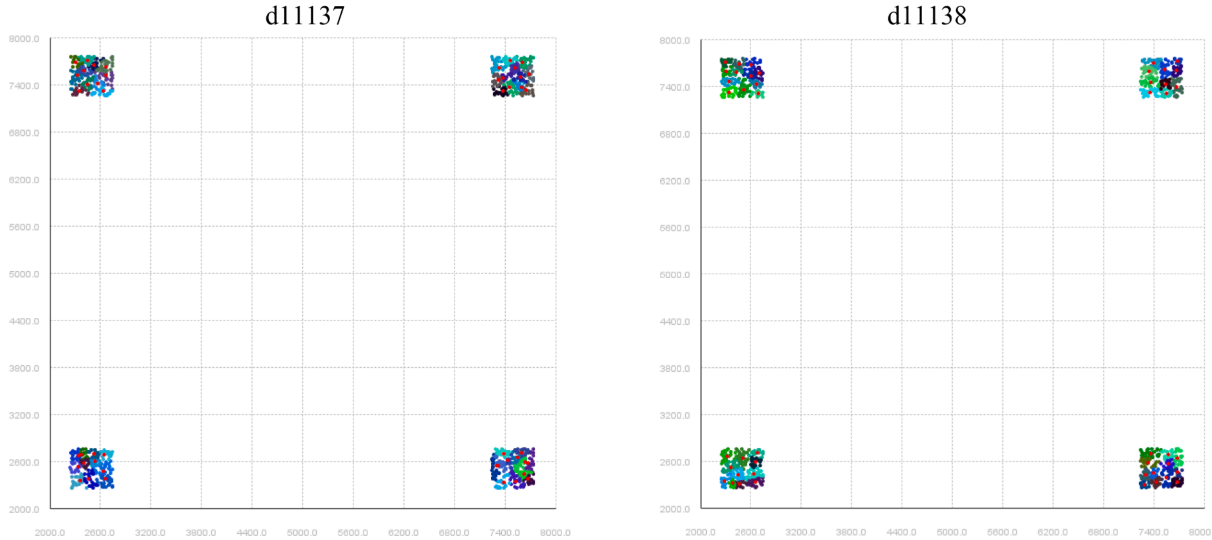

Fig. 4. Instances d11137 (left) and d11138(right); final, best possible solution (solution with the minimal total cost) from 1,000 iterations with 46 depots in d11137 and 45 depots in d11138.

K-Means have similar variations with regard to the total costs (d11134: 1.25 and d11135: 1.67). Thus, in cases where customers are uniformly distributed, the formation of clusters at each division stage is not critical for the final solution. In this case, the algorithm is able to continuously converge to an optimum and this optimum varied only slightly during 1,000 iterations, regardless of the splitting step in each iteration (see also Fig. 5). Furthermore, both K-Means++ and Fuzzy K-Means converge to a similar number of locations: 40 and 41 on average for a homogeneous customer distribution. Thereby, the number of optimal depot locations varies between 36 and 44 for the default K-Means as well as 33 and 45 for Fuzzy K-Means. It is worth noting that the variation of the solution quality decreases with the increasing S_i index in K-Means++ and can reach 90 % in an extreme case (see instance d11137, Fig. 5).

Figure 5 illustrates the behaviour of BinR-LRP heuristic with Fuzzy K-Means and K-Means++ for extremely clustered instances regarding the total transport costs in each solution. With K-Means++, the heuristic shows a low variance with respect to the optimal total costs. In contrast, by using Fuzzy K-Means the total solution costs reach a magnitude up to 15 times higher. However, with the exception of these few outliers, the majority of the solutions vary only slightly (within a standard range between 35,000–45,000).

Figure 6 indicates how the proposed BinR-LRP heuristic reflects the trade-off between the fixed costs for opening a new facility and the increasing variable transport costs per m in each simulation run. In this experiment, we use a test instance with 1,000 customers and the silhouette index $S_i \approx 0.5$ with integrated K-Means++ clustering (Instance d11136). In general, as opening costs increase, the number of optimal facilities in the system decreases for fixed transport costs. The blue line in Figure 6 reflects this behaviour. In contrast, the variable transport costs positively influence the number of depots. Since the opening costs are fixed and the transport costs increase, the total cost of the system can be minimised only by adding additional depots. Figure 6 demonstrates this behaviour using BinR-LRP heuristic.

Validation on benchmark instances

In this section, the performance and accuracy of our heuristic will be tested by first applying it to the benchmark instances proposed by Tuzun and Burke (1999) and comparing it to three classical LRP

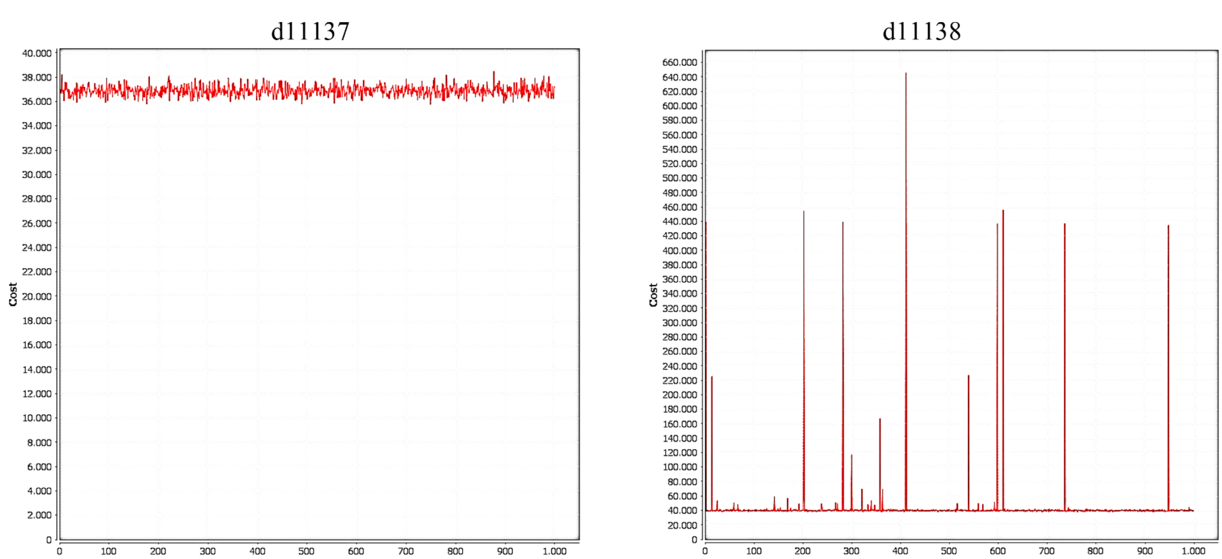

Fig. 5. Total costs from 1,000 iterations for K-Means++ (left) and Fuzzy K-Means (right) for high clustered instances with $S_i = 0.9$ (d11137 and d11138).

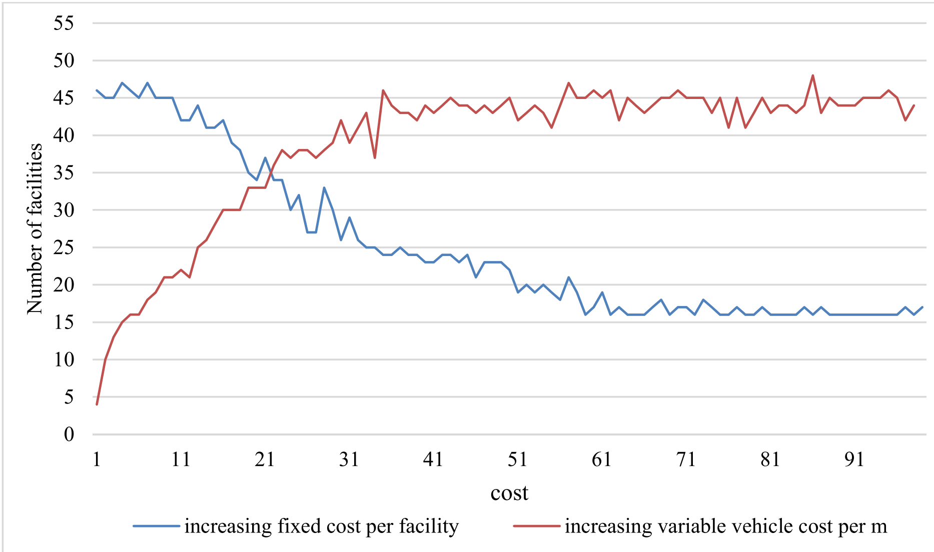

Fig. 6. The trade-off between the increasing fixed cost for opening new facilities and the variable transport cost with respect to the number of facilities in instance d11136.

metaheuristics: (i) Greedy Randomized Adaptive Search [GRASP] (Prins et al., 2006), (ii) Memetic Algorithm with Population Management [MAPM] (Boudia et al., 2006) and (iii) Lagrangean relaxation with Granular Tabu Search [LRGTS] (Prins et al., 2007).

The test dataset consists of 36 synthesised instances each with the following characteristics.

- Variable number of customers: 100, 150 or 200
- Variable number of potential depot locations: 10 or 20
- Uniformly distributed customer demand in the range: [10, 20].
- Variable customer distribution
- Fixed vehicle capacity: 150
- Fixed depot costs and fixed transport costs:100 and 1 respectively

Table 3
Classical LRP instances and comparison of three benchmark heuristics against *BinR-LRP*.

Instances	*Customers*	*Potential sites*	*GRASP*		*MAPM*		*LRGTS*		*BinR-LRP*		
index	*points*	*depot*	*costs*	*depot*	*costs*	*depot*	*costs*	*depot*	*costs*	*depot*	*CPU (sec)*
111,112	100	10	1,525.25	3	1,493,92	3	1,490.82	3	**1,430,77**	3	2.442
111,122	100	20	1,526.9	3	1,471,36	2	1,471,76	3	**1,421,74**	2	0.557
111,212	100	10	1,423.54	2	1,418.83	3	1,412.04	3	**1,317.58**	3	0.607
111,222	100	20	1,482.29	2	1,492.46	2	**1,443.06**	2	1,453.05	2	0.323
112,112	100	10	1,200.24	2	1,173.22	2	1,187.63	2	**1,095.66**	3	0.476
112,122	100	20	1,123.64	3	1,115.37	3	1,115.95	3	**1,058.40**	3	0.425
112,212	100	10	814	3	793.97	2	813.28	3	**702.92**	3	0.438
112,222	100	20	747.84	3	730.51	2	742.96	3	**673.19**	2	0.342
113,112	100	10	1,273.1	3	1,262.32	3	1,267.93	3	**1,193.57**	3	0.455
113,122	100	20	1,272.94	2	1,251.32	3	1,256.12	3	**1,222.54**	3	0.456
113,212	100	10	912.19	3	**903.82**	3	913.06	3	950.95	4	0.603
113,222	100	20	1,022.51	3	1,022.93	4	1,025.51	3	**975.67**	3	0.407
121,112	200	10	2,384.01	3	2,293.99	3	2,296.52	3	**2,153.70**	5	1.081
121,122	200	20	2,288.09	4	2,277.39	3	2,207.5	4	**2,059.25**	5	1.024
121,212	200	10	2,273.19	3	2,274.57	3	2,260.87	4	**2,112.97**	4	0.928
121,222	200	20	2,345.1	3	2,376.25	3	2,259.52	3	**2,072.94**	4	0.94
122,112	200	10	2,137.08	3	2,106.26	3	2,120.76	3	**2,002.91**	2	0.751
122,122	200	20	1,807.29	4	1,771.53	2	1,737.81	3	**1,270.46**	3	0.977
122,212	200	10	1,496.75	2	1,467.54	2	1,488.55	2	**1,342.52**	2	0.789
122,222	200	20	1,095.92	3	1,088	3	1,090.59	3	**885.62**	3	1.029
123,112	200	10	2,044.66	4	1,973.28	4	1,984.06	4	**1,822.66**	4	1.004
123,122	200	20	2,090.95	4	1,979.05	5	1,986.49	4	**1,801.93**	4	1.081
123,212	200	10	1,788.7	2	1,782.23	3	1,786.79	3	**1,593.08**	3	0.969
123,222	200	20	1,408.63	5	1,396.24	5	1,401.16	5	**1,386.08**	4	1.159
131,112	150	10	2,006.7	3	1,959.39	3	1,946.01	3	**1,849.86**	3	0.583
131,122	150	20	1,888.9	4	1,881.67	3	1,875.79	3	**1,724.50**	3	0.574
131,212	150	10	2,033.93	3	1,984.25	3	2,010.53	3	**1,779.01**	4	0.637
131,222	150	20	1,856.07	4	1,855.25	3	1,819.89	3	**1,743.36**	4	0.921
132,112	150	10	1,508.33	3	1,448.27	2	1,448.65	2	**1,249.42**	3	0.994
132,122	150	20	1,456.82	2	1,459.83	2	1,492.86	3	**1,372.44**	2	0.525
132,212	150	10	1,240.4	2	1,207.41	3	1,211.07	3	**1,057.23**	3	0.68
132,222	150	20	940.8	3	934.79	3	936.93	3	**808.94**	3	0.676
133,112	150	10	1,736.9	3	1,720.3	3	1,729.31	3	**1,447.65**	4	0.722
133,122	150	20	1,425.74	3	1,429.34	4	1,424.59	3	**1,248.83**	5	0.841
133,212	150	10	1,223.7	3	1,203.44	3	1,216.32	3	**970.34**	3	0.583
133,222	150	20	1,231.33	4	**1,158.54**	3	1,162.16	3	1,166.32	3	0.609

In the framework of this computational experiment, the problem formulation is carried out with the following constraints.

- Each demand must be served by a single vehicle
- Each route must start and end at the same depot
- The total freight demand must not exceed the vehicle capacity.

For the benchmark instances and their solutions, we refer to the open source dataset of Prodhon (2010). Table 3 shows the instances of Tuzun and Burke (1999) used in this study with the respective results from the three referenced algorithms. The numerical results provided are the total costs, the number of optimal locations, and the computation time. The algorithm introduced in Methodology is implemented in JAVA and tested on CPU Intel(R) i7-8665U CPU, 2112 MHz, 4 Kern(e), 16 GB RAM. To solve the VRP in each partition, the routing framework Jsprit is applied. In these validation tests, the route planning framework Jsprit is used with default control parameters: (i) standard ruin-and-recreate heuristic with "Fast and Regret", (ii) 100 iterations and (iii) unrestricted vehicle fleet.

As a result of the numerical experiments performed, solutions with minimum total costs were found in 33 out of 36 instances. The largest relative deviation is found in instance 122122 with a +26% improvement and instance 133212 with almost a 20% improvement over the best-known solution. It is also worth mentioning that the results presented in Table 3 are derived from only one numerical experiment. Due to the fact that both K-Means++ and Jsprit are subject to stochasticity, multiple iterations of BinR-LRP may result in a superior optimum for all instances. It is noteworthy that in the majority of cases the final solution in this study is consistent with the solutions obtained in the referenced cases in terms of the optimal number of sites. This result is remarkable, as no initial solution is provided at the beginning of the search in the heuristic employed and the algorithm converges independently towards the near-optimal number of locations. Moreover, concerning computational time, a convergence time was measured that can be considered as adequate for practical application. With the exception of instance 111112, convergence time was under 1 second in the majority of cases.

Conclusion and outlook

In the framework of this study, a scalable and easy-to-follow methodology with adjustable constraints was proposed for solving large-scale LRP. This approach consists of several well-known heuristics and a multi-agent transport simulation module combined in one general framework tied by the principles of divide-and-conquer heuristic. In most cases, the classical LRP approaches from the field of OR do not consider agent behaviour on the infrastructure level. Using vehicle routing framework Jsprit integrated in the microscopic agent-based transport simulation MATSim in each decision step the proposed approach can optimise the logistics network considering the underlying infrastructure and reach problem constraints. In several numerical experiments, the developed simheuristic was validated in the framework of a sensitivity analysis on synthetic instances as well as on benchmark instances. Compared to the three classical algorithms GRASP, MAPM and LRGTS, our framework improved the best-known solutions in 92 % of cases. The sensitivity analysis also revealed the stable convergence of the BinR-LRP heuristic for different spatial customer distributions and clustering settings. Only for highly clustered instances the solution was affected when Fuzzy K-Means was applied as an initial clustering method. However, in the majority of cases, the solution yielded from BinR-LRP heuristic varied only slightly for different clustering settings. In the course of this, we suggest either to study the spatial distribution of customers (e.g. using the silhouette coefficient) before applying the BinR-LRP heuristic, or to apply our approach iteratively and then select the solution with the minimum costs. Due to the modular design of the framework and considering the computational efficiency, BinR-LRP is suitable for large scale location optimisation tasks. Numerical experiments demonstrate that the optimal or near-optimal solution can be achieved within a reasonable time, even for instances with 1,000 customers (less than 1 min). Furthermore, we investigated the behaviour of our method with respect to both increasing fixed costs of placing a facility and variable transport costs within the Jsprit model. This result indicates the adequate behaviour of the proposed heuristic, since the trade-off between both cost components, increasing fixed costs and increasing variable transport costs, could be represented. In our future research, we plan to operationalise and apply this methodology within a real-world case study focusing on the optimisation of the micro-depot and parcel station location network for Berlin, Germany.

CRediT authorship contribution statement

Elija Deineko: Conceptualization, Methodology, Writing – original draft. **Carina Kehrt:** Writing – review & editing, Supervision, Project administration. **Gernot Liedtke:** Supervision, Project administration.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: There is no conflict of interest behind this work.

Data availability

Data will be made available on request.

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