Machine Learning-Guided Metaheuristics for Solving Facility Location Problems

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Abstract. Facility Location Problems (FLPs) are critical for optimizing logistics, telecommunications, and emergency networks. However, their $\mathcal{NP}$-hard nature limits the scalability of exact resolution methods. While traditional metaheuristics provide effective approximate solutions, they rely on manual expert design. This doctoral thesis addresses this limitation by proposing the integration of Machine Learning (ML) techniques into metaheuristic frameworks to efficiently solve FLPs. The main objective of this thesis is to develop a comprehensive Neural Combinatorial Optimization (NCO) framework based on ML methods to solve optimization problems. By enabling algorithms to autonomously learn resolution strategies directly from network topologies and self-generated data, this work seeks to generate high-quality solutions in reduced computational times. Furthermore, the project aims to evaluate the real-world applicability of these hybrid models, promoting transparent, efficient, and sustainable optimization practices.

Keywords: Metaheuristics · Machine Learning · Neural Combinatorial Optimization · Facility Location Problems.

- **Proposed title:** Machine Learning-Guided Metaheuristics for Solving Facility Location Problems.
- **Supervisors:** Abraham Duarte Muñoz and Isaac Lozano Osorio.
- **Department (University):** Informática y Estadística, Universidad Rey Juan Carlos (URJC).
- **Start date:** October 2025.
- **Funding:** This doctoral thesis is funded by the FPU grant from the Ministerio de Ciencia, Innovación y Universidades (ref. FPU24/01134).

1 Introduction

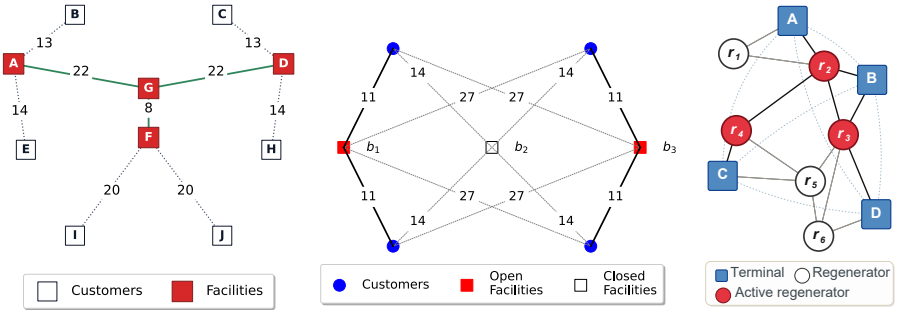
In the field of operations research, Facility Location Problems (FLPs) represent a fundamental optimization challenge. These problems have direct relevance in a wide range of real-world applications, such as the optimization of logistics and distribution networks, the design of telecommunication infrastructure, and the placement of critical resources in emergency scenarios [9,32].

While there are optimization problems that can be solved efficiently using deterministic and exact techniques, the facility location problems addressed in this doctoral thesis belong to the $\mathcal{NP}$-hard complexity class, which significantly limits the scalability of exact methods. When applied to large instances that represent real-world situations, the time and computational resources required to obtain an optimal solution become unfeasible in practice. Given this limitation, there is a clear need to design alternative methods capable of solving these problems efficiently. The goal of these approximate methods is to generate feasible, high-quality solutions that are as close as possible to the optimal solution. To achieve this, heuristic algorithms are typically implemented to construct valid solutions in short computation times [21]. These are guided using metaheuristic frameworks, which have proven effective in exploring the search space, refining initial solutions, and avoiding local optima [13].

Since its introduction, the approach to solving facility location problems has evolved significantly. Early research focused on exact algorithms, establishing a strong formal basis [1,10]. However, these exact methods were limited to instances of moderate size due to scalability issues. To overcome this limitation, the field shifted towards heuristic and metaheuristic methods. Relevant metaheuristic frameworks widely used in combinatorial optimization are the Variable Neighborhood Search (VNS) [24] and the Greedy Randomized Adaptive Search Procedure (GRASP) [11]. VNS systematically explores multiple neighborhood structures and uses random perturbations to escape local optima, proving highly efficient for median and location problems [8,20]. Meanwhile, GRASP combines a randomized greedy construction phase with a local search improvement phase, showing strong performance in complex network design problems [6,28].

Within the FLP family, this doctoral thesis highlights three specific variants as the starting point for the research, where an example of an instance with its optimal solution for each of them is illustrated in Figure 1. First, the Ordered Median Tree Location Problem (OMT) [26] involves selecting exactly p facilities from a set of potential locations (represented as squares in Figure 1a). These active facilities (filled red squares) are connected via a tree structure (solid green lines) to serve the remaining customers, minimizing both tree design and customer assignment costs. Second, the Uncapacitated Facility Location Problem (UFLP) [34] determines an unconstrained number of facilities to open (filled red squares in Figure 1b) from a set of candidate locations (empty squares) to serve all given customers (circles), minimizing the sum of facility opening and customer assignment costs. Finally, the Generalized Regenerator Location Problem (GRLP) [27] models a communication network where terminal nodes (squares in Figure 1c) must be interconnected by activating the minimum possible number of candidate regenerators (filled red circles) to ensure global communication.

A prominent trend in recent years has been the integration of Machine Learning (ML) techniques with metaheuristics to solve combinatorial optimization problems [18]. This aims to create a more intelligent search process, improving performance in terms of solution quality, convergence rate, robustness and efficiency, by extracting useful knowledge from data generated during the search.



(a) OMT. (b) UFLP. (c) GRLP.

Fig. 1: Optimal solutions for the UFLP, OMT, and GRLP problem instances.

For example, Reinforcement Learning (RL) has been used within VNS to select neighborhood operators [17]. Separately, ML has been applied to learn from historical data to predict how solutions should be modified in response to parameter perturbations [19].

Taking this integration a step further, Neural Combinatorial Optimization (NCO) has gained relevance as a powerful data-driven paradigm [4]. In NCO, Deep Learning (DL) models, particularly Graph Neural Networks (GNNs) [29], are trained, typically via RL, to act as solving heuristics [7]. Early NCO approaches focused on incrementally constructing solutions, efficiently solving classic problems such as the Minimum Vertex Cover, Maximum Cut, and the Traveling Salesman Problem [5,7]. Recent research has expanded NCO to other domains like scheduling [15] and Neural Improvement models that guide local search techniques [12]. Despite these advancements, the application of NCO to the facility location family remains largely unexplored [5]. This significant research gap, combined with the rapid and unprecedented advancements in deep learning architectures motivates the present work.

The purpose of this doctoral thesis is to explore and develop efficient metaheuristic techniques for solving facility location problems by directly integrating ML methods to guide the solution space search, analyzing the impact that ML algorithms have on solving these problems [32]. The goal is to obtain high-quality solutions in reduced computational time for $\mathcal{NP}$-hard problems, which are highly relevant in real-world applications. The integration of ML enables optimization methods to extract knowledge from both the network topology and accumulated experience to guide the decision-making during execution.

In this context, the initial hypothesis of this thesis establishes that the use of heuristic and metaheuristic techniques, guided by ML methods, will generate high-quality solutions in reduced computational times for complex facility location problems, while identifying structural patterns applicable to related problems. The main original contribution of this research lies in the exploration and integration of ML within heuristic and metaheuristic frameworks, devel-

oping algorithms capable of learning resolution strategies autonomously rather than relying exclusively on manual expert designs. To validate this hypothesis, the research focuses on the objectives described in Section 2.

2 Objectives

The main objective of this doctoral thesis is to design, develop, and validate hybrid algorithmic approaches that combine metaheuristics with ML to efficiently solve complex Facility Location Problems. To achieve this goal, the research is divided into the following specific objectives:

1. **Literature review and baseline methodology analysis.** As previously stated, the core objective of this research is to integrate ML into metaheuristic algorithms to efficiently obtain high-quality solutions for optimization problems. To achieve this, it is essential to first analyze the methodologies that currently achieve the best performance across the FLP family. The literature demonstrates, for instance, the use of exact models for the OMT [26], evolutionary and genetic algorithms for the UFLP [34], and VNS techniques for the Generalized Regenerator Location Problem GRLP [25]. Additionally, GRASP implementations have proven highly efficient for other variants, such as the Obnoxious p-Median problem [6]. Beyond these traditional methods, the review explores the NCO paradigm [4] and its recent successes in other optimization domains, such as routing [7] and scheduling [15]. Consequently, this objective consists of understanding the state of the art to enable the design of ML-enhanced metaheuristics based on the most recent and highest-performing approaches in the literature.
2. **Exploiting problem structure through advanced optimization techniques.** Before integrating ML, it is necessary to evaluate the fundamental components of modern optimization algorithms. This involves analyzing the most promising metaheuristics currently applied to combinatorial optimization and FLPs [13], as well as the underlying search methodologies, constructive heuristics and search space reduction methods, among other algorithmic techniques [21]. This evaluation requires identifying the computational difficulties inherent to $\mathcal{NP}$-hard optimization problems to determine how these algorithmic strategies adapt best to the FLP family. For example, addressing the OMT [26] demonstrates how exploiting the mathematical structure of a specific problem enables search space reduction and the efficient evaluation of solutions. Similarly, analyzing the UFLP illustrates the importance of tailored constructive methods and advanced local search exploration to accelerate algorithmic convergence [22]. Therefore, the primary goal of this objective is to identify the structural difficulties of $\mathcal{NP}$-hard optimization problems and determine the most effective heuristics, metaheuristics, and search methods for FLPs, establishing the computational baseline required to integrate ML techniques.
3. **Hybridizing metaheuristics with ML techniques.** This objective focuses on designing hybrid algorithms where ML directly guides metaheuristic

components, including solution construction, search space exploration, and neighborhood move selection [18]. Building upon successful approaches, such as using an RL algorithm to automate operator selection [17] or leveraging historical data to predict parameter adjustments [19], this stage aims to apply these data-driven methodologies specifically to the FLP family. This integration evaluates the practical advantages, limitations, and computational challenges of hybridization, establishing a robust baseline for ML-guided frameworks tailored to improve solution quality and accelerate algorithmic convergence.

4. **Design of ML and metaheuristic frameworks for Neural Combinatorial Optimization.** Advancing the hybridization process, the primary goal is to design a unified framework integrating the learning capabilities of ML with the structural advantages of metaheuristics. While DL architectures, such as GNNs [29] trained via RL [33], extract problem properties to generate resolution strategies without the need for hand-crafted heuristics, traditional algorithms provide computational efficiency, algorithmic explainability, and robust search mechanisms [21]. Fusing these paradigms is the core of NCO [4,7]. Consequently, this stage aims to develop a data-driven framework to directly solve optimization tasks by combining both approaches. This framework will be applied to the FLP family to validate its practical applicability, evaluating the performance of learned NCO policies compared to traditional algorithmic methods.
5. **Evaluation of real-world applicability, explainability, and sustainability of the hybrid framework.** The final objective assesses the practical impact of the proposed hybridization by applying them to FLP variants with real-world applications. To quantify the benefits of the ML hybridization, the developed methods will be benchmarked against state-of-the-art traditional algorithms. Beyond standard performance metrics, this evaluation analyzes the computational cost, energy consumption, and overall environmental efficiency [30], promoting green computing practices aligned with the Sustainable Development Goals (SDGs). Additionally, Explainable AI (XAI) techniques [3] will be applied to interpret the underlying decision-making mechanisms of the hybrid models, providing a deeper understanding of their advantages, limitations, and operational behavior. Finally, to ensure reproducibility and foster open science, all implemented code, datasets, and experimental results will be made publicly available.

3 Methodology and work plan

This section outlines the methodology and work plan designed to achieve the proposed objectives. Throughout the development of this doctoral thesis, the main strategy is to document the advancements and findings through articles submitted to high-impact journals indexed in the Journal Citation Reports (JCR). In parallel, the work plan emphasizes writing conference papers and attending international conferences to communicate the progress, obtain valuable feedback

from the scientific community, and ensure continuous information dissemination. Notably, as will be detailed in the subsequent sections, some of the initial objectives have already been addressed, resulting in several conference contributions that are either published or currently under review.

This research follows the scientific method, specifically adopting the three fundamental phases for evaluating heuristic algorithms proposed by Talbi [31]: experimental design, execution, and documentation. The first phase involves defining the experimental objectives and carefully selecting the problem instances to ensure an unbiased and proper algorithmic configuration [23]. The second phase focuses on algorithmic execution within a controlled environment, evaluating key performance indicators beyond computational speed and solution quality, such as algorithmic robustness [2,14]. Finally, the third phase encompasses the exhaustive analysis of the results, incorporating visualization tools to complement the data interpretation and comparing the outcomes against state-of-the-art methods. This rigorous documentation guarantees the reproducibility of the computational experiments while maintaining a flexible approach that adapts to the research progress.

To apply this methodology, the work plan is structured into specific tasks and milestones, grouped according to the previously established objectives:

1. **Literature review and baseline methodology analysis.**
   (a) Conduct a comprehensive literature review on exact, heuristic, and metaheuristic approaches applied to the FLP family.
   (b) Analyze the mathematical formulations and state-of-the-art exact models to understand their computational and scalability limitations.
   (c) Review the recent advancements in ML applied to combinatorial optimization, with a specific focus on the NCO paradigm.
   (d) Identify the methodological gaps in the literature where ML techniques can successfully guide metaheuristic search within the FLP domain.
   (e) Document the theoretical findings to establish the baseline framework that will support the algorithmic design and experimental setup in subsequent stages.
2. **Exploiting problem structure through advanced optimization techniques.**
   (a) Explore the FLP family to analyze its structural difficulties, and select a promising subset of variants (e.g., OMT, UFLP, GRLP) alongside standard benchmark datasets to evaluate the implemented algorithms.
   (b) Design and implement constructive heuristics and neighborhood structures explicitly formulated to exploit the properties of the selected FLPs.
   (c) Evaluate search space reduction methods and objective function factorizations to optimize the efficiency of the algorithmic evaluations.
   (d) Implement traditional metaheuristic frameworks, such as VNS or GRASP, using the previously designed components to establish a robust and highly optimized computational baseline.
   (e) Analyze the performance metrics and structural difficulties encountered by these traditional methods to identify clear integration points for ML.

   (f) Disseminate the baseline methodologies and findings through submissions to high-impact journals and international conferences, showcasing the obtained results and the initial algorithmic evolution.
3. **Hybridizing metaheuristics with ML techniques.**
   (a) Define the specific integration points where ML can assist the metaheuristics, such as operator selection, parameter tuning, or initial solution generation.
   (b) Design data and feature engineering strategies to extract relevant information from both the problem topology and the historical search process.
   (c) Develop hybrid algorithms that incorporate ML models to dynamically guide the metaheuristic search based on the extracted data.
   (d) Conduct extensive computational experiments in a controlled environment to compare the hybrid methods against the metaheuristic baselines.
   (e) Analyze the convergence, solution quality, and robustness of the hybrid approaches to evaluate the impact and advantages of ML integration.
   (f) Disseminate the advancements and findings through submissions to high-impact journals and international conferences, showing the obtained results and the methodological evolution of the hybrid frameworks.
4. **Design of ML and metaheuristic frameworks for Neural Combinatorial Optimization.**
   (a) Design DL architectures using GNNs [29] capable of processing the underlying graph structure and constraints of FLP instances.
   (b) Formulate the optimization process as a sequential decision-making problem to enable the training of these networks via RL algorithms [33].
   (c) Develop a unified framework that integrates the autonomous learning capabilities of NCO models with the robust techniques of metaheuristics.
   (d) Train the NCO models on diverse FLP datasets, evaluating their capacity to generalize and scale to larger, unseen instances without relying on manual expert design.
   (e) Perform a comparative analysis between the NCO-based framework and the previously developed hybrid and traditional algorithmic methods.
   (f) Disseminate the advancements and findings through submissions to high-impact journals and international conferences, showing the obtained results and the methodological evolution of data-driven optimization.
5. **Evaluation of real-world applicability, explainability, and sustainability of the hybrid framework.**
   (a) Apply the hybrid and NCO frameworks to complex FLP instances obtained from real-world scenarios, such as logistics distribution or telecommunications network design.
   (b) Define and measure sustainability metrics, analyzing the computational cost, energy consumption, and overall environmental efficiency.
   (c) Integrate Explainable AI (XAI) techniques to understand the underlying decision-making mechanisms of the ML models, allowing for a deeper understanding of its advantages and limitations.
   (d) Prepare and structure the codebase, datasets, and configuration parameters for public release to ensure reproducibility and foster open science.

(e) Disseminate the advancements and findings through submissions to high-impact journals and international conferences, showing the obtained results, the practical applicability, and the final methodological evolution of the thesis.

4 Relevance

The unprecedented recent success of DL architectures in domains such as Natural Language Processing and Computer Vision has driven significant investments and rapid technological advancements in Artificial Intelligence. This overwhelming growth presents a strong motivation to apply modern ML techniques to other complex and highly relevant fields, notably Combinatorial Optimization (CO). Given the performance of data-driven models in these areas, integrating these architectures into CO shows great potential for significant improvements.

CO plays a critical role in global operations, directly impacting industrial efficiency, resource management, and economic growth. Within this field, the FLP family represents a fundamental area for strategic decision-making [9]. In the context of global logistics, where millions of packages are processed and shipped daily, optimizing the distribution network between facilities and customers is crucial. Even marginal improvements in facility location translate into significant cost savings by reducing delivery times, minimizing the use of material resources, and improving overall efficiency. By optimizing routes, facility placements and customer assignments, companies can drastically reduce fuel consumption and greenhouse gas emissions. Consequently, the algorithms developed in this thesis directly promote environmental sustainability. Furthermore, these methods are important in emergency scenarios, where the optimal location of ambulances, healthcare centers, or critical resources requires advanced metaheuristic and NCO techniques to ensure fast and efficient response times.

The problems addressed in this thesis have highly relevant real-world applications. For instance, the UFLP is one of the most widely studied models in the FLP family, used for designing logistics networks and optimally placing distribution centers. In practice, it has been successfully applied to optimize railway networks, significantly improving efficiency and reducing operational costs [16]. Additionally, the OMT [26] models the equitable distribution of emergency resources or healthcare facilities. Finally, the GRLP [27] is crucial for designing modern telecommunications and optical networks, ensuring global connectivity with minimal infrastructure costs.

From a scientific perspective, this research addresses a significant gap in the current literature. While the NCO paradigm has demonstrated remarkable performance in routing and scheduling tasks [4,15], its application to the FLP family remains largely unexplored. Since facility location environments are inherently structured as customer-facility network graphs, they are well-suited for GNNs. By applying NCO to these unexplored domains, this work will expand the theoretical and practical boundaries of ML-guided optimization, providing the scientific community with new insights into how graph-based neural models can extract structural patterns from location problems.

Scientifically, this research addresses a clear gap in the literature. While the NCO paradigm has proven highly effective in routing and scheduling tasks [4,15], its application to the FLP family remains largely unexplored. Since facility location environments are naturally structured as customer-facility network graphs, they are highly suitable for GNNs. Applying NCO to these problems will extend the scope of ML-guided optimization, providing new insights into how graph-based models extract structural patterns from location networks.

Finally, a major practical advantage of the proposed NCO framework is the democratization of complex optimization. While traditional metaheuristics rely heavily on specialized experts to hand-craft problem-specific heuristics, the NCO approach autonomously learns these resolution strategies directly from data via RL. To ensure this accessibility, the developed framework will be packaged and released as an open-source tool. Consequently, any company, researcher, or individual facing similar optimization challenges can use it to obtain highly competitive solutions, without the need for extensive expertise in operations research or heuristic design.

5 Publications and other results

The work plan and the proposed objectives of this doctoral thesis are being addressed through several research contributions. To date, this progress has resulted in three main articles corresponding to different stages of the research, which have been published, accepted, or submitted to international conferences.

The first contribution addresses the OMT [26] and has been accepted at the 16th Metaheuristics International Conference (MIC) 2026, for publication in the the Lecture Notes in Computer Science (LNCS) series. Addressing Objective 1, this work analyzes state-of-the-art Mixed Integer Linear Programming (MILP) formulations to identify their structural difficulties and computational limitations. To fulfill Objective 2, we designed a GRASP metaheuristic combined with a swap-based local search. This approach explicitly exploits the problem structure, reducing the search space by isolating facility selection as the main combinatorial challenge. Results show that the algorithm significantly outperforms exact formulations, finding the best-known solutions for all benchmark instances at a low computational cost, identifying the structural properties of the FLP family to integrate ML techniques.

The second contribution focuses on the UFLP [34] and was published in the LNCS series at the 11th International Conference on Variable Neighborhood Search (ICVNS) 2025 [22]. Building upon the baseline established in Objective 2, this work implements a Variable Neighborhood Search (VNS) to directly address Objective 3: hybridizing metaheuristics with ML techniques. Specifically, we proposed a RL mechanism to guide the constructive phase of the VNS. The learning algorithm uses information gathered from previous search iterations on the same instance to generate progressively better initial solutions. Extensive computational experiments confirmed that this ML-enhanced hybrid algorithm

obtains highly competitive results, achieving near-zero gaps and outperforming traditional evolutionary algorithms in a fraction of the computational time.

The third contribution explores the GRLP [27] and has been submitted to the Conference of the Spanish Association for Artificial Intelligence (CAEPIA'26) for publication in the Lecture Notes in Artificial Intelligence (LNAI) series. Addressing Objectives 1 and 4, this work analyzes the problem literature and implements an NCO framework. Specifically, we designed a DL architecture including GNNs to process the problem's underlying graph structure, using the open-source library NCOLib[1]. By formulating the optimization as a sequential decision-making process, the GNN is trained via RL to autonomously construct solutions directly from data, without the need for manual heuristics or expert knowledge. These neural constructions are subsequently refined using a local search phase highlithing the hybridization advantages. Results confirm that the autonomously learned neural policy generates better solutions than a highly specific, hand-crafted GRASP constructive heuristic from the literature [27].

Additionally, the progress and preliminary results of this thesis have been presented at relevant academic events. Specifically, these contributions were shared at the V Winter School on Heuristic Optimization of the Red HEUR in collaboration with the Spanish Society of Statistics and Operations Research (SEIO), held at the Universidad de La Laguna (Tenerife) in January 2026, and at the 6th Congress of the International Doctoral School of the Universidad Rey Juan Carlos, held in May 2026. These events provided the opportunity to disseminate the current advancements, receive valuable feedback from the research community, and engage with other presentations closely related to the topics of this doctoral work.

Regarding future work, the research will continue to address Objective 1 by exploring other facility location problems and new techniques to integrate ML and metaheuristics. To further disseminate the findings of Objectives 2 and 3, an extended article addressing the UFLP has been submitted to a JCR-indexed journal of the area and is currently under review, while another paper detailing the OMT algorithmic approach and the new advancements is in preparation for submission. Regarding Objective 4, the developed NCO framework will be refined and tested on other combinatorial problems to validate its generalization capabilities. Finally, to address Objective 5, the NCO framework will be applied to real-world instances to evaluate their practical impact. This concluding phase will assess the proposed methods in terms of explainability (XAI), computational efficiency, and green computing principles, ensuring the development of sustainable and interpretable optimization solutions.

Acknowledgments. This work was made possible through the support of the Ministerio de Economía y Competitividad (grant ref. PID2024-156045NB-I00), Ministerio para la Transformación Digital y de la Función Pública (Cátedra ENIA AI4DDS, ref. TSI-100930-2023-3), Ministerio de Ciencia, Innovación y Universidades (grant ref. FPU24/01134), and Comunidad Autónoma de Madrid (grant ref. TEC-2024/COM-404).

[1] `https://github.com/TheLeprechaun25/NCOLib`

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