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Mathematical optimization and learning models to address uncertainties and sustainability of supply chain management

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Chapter 1

Introduction

As concerns about climate change, biodiversity loss, and pollution have become more widespread, new worldwide challenges deal with the protection of the environment and the conservation of natural resources. Thus, in order to empower sustainability and circular economy ambitions, the world has shifted to embrace sustainable practices and policies. This is carried out, primarily, through the implementation of sustainable business practices and increased investments in green technology. Advanced information systems, digital technologies and mathematical models are required to respond to the demanding targets of the sustainability paradigm. This trend is expanding with the growing interest in production and services sustainability in order to achieve economic growth and development while preventing their negative impact on the environment. A significant step forward in this direction is enabled by Supply Chain Management (SCM) practices that exploit mathematical and statistical modeling to better support decisions affecting both profitability and sustainability targets. Indeed, these targets should not be approached as competing goals, but rather addressed simultaneously within a comprehensive vision that responds adequately to both of them. Accordingly, Green Supply Chain Management (GSCM) can achieve its goals through innovative management approaches that consider sustainable efficiency and profitability to be clearly linked by the savings that result from applying optimization techniques. Savings can be measured according to both sustainability metrics regarding energy, emissions, climate, water or labor, and business metrics regarding all operational and strategic costs. To confirm the above, there is a growing trend of applying mathematical optimization models for enhancing decision-making in pursuit of both environmental and profit performance. Indeed, GSCM takes into account many decision problems, such as facility location, capacity allocation, production planning and vehicle routing.

Besides sustainability, uncertainty is another critical issue in Supply Chain Management (SCM). Different sources of uncertainty may affect several stages of the supply chain, including yields, prices, lead times, production or service demand and all resource supplies, such as physical components or energy from renewables. Considering a deterministic approach would definitely fail to provide concrete decision support when modeling those kinds of scenarios. According to various hypothesis and strategies, uncertainties can be addressed by exploiting several modeling approaches arising from statistics, statistical learning and mathematical programming. While statistical and learning models accounts variability by definition, Robust Optimization (RO) is a particular modeling approach that is commonly applied in solving mathematical programming problems where a certain set of parameters are subject to uncertainty.

In this dissertation, mathematical and learning models are exploited according to different approaches and models combinations, providing new formulations and frameworks to address strategic and operational problems of GSCM under uncertainty. All models and frameworks presented in this dissertation are tested and validated on real-case instances. In particular, all instances concern reverse logistics scenarios from closed-loop supply chains. A closed-loop supply chain combines the traditional supply chain (forward logistics) with reverse logistics, in charge of collecting and processing returned products in order to ensure a socioeconomically and ecologically sustainable recovery. Indeed, one of all accepted definition for Sustainable Supply Chain Management (SSCM) would be one where all products are created, used, and recycled or disposed of in a closed loop method.

This dissertation is structured as follows. Generalities on Supply Chain Management and its variations, along with the main decision problems in GSCM, are introduced in Chapter 2. The chapter also discusses the primary causes of uncertainty in GSCM, gathers the research prospects in this subject, and provides a brief introduction to robust optimization.

Chapter 3 presents a two-stage model to design and operate a waste management (WM) network. In this setting, a regional authority designs the network according to a first strategic stage of the model, while a second operational stage refers to the routing decisions of carriers in charge of the network usage. In particular, the regional authority aims to determine an optimal location for waste disposal facilities, allocate to each facility a proper capacity, cluster waste producing locations, then assign facilities to these clusters without generating overlaps. In doing so, the authority attempts to *i)* assign waste quantities to each facility by considering a safety stock within its capacity in order to avoid shortages during the network operational usage, *ii)* minimize greenhouse gases emissions, *iii)* be as compliant as possible with the solution found by the second stage problem. The latter is a multi-depot routing problem concerning the vehicles in charge of collecting and delivery waste to the network facilities. After properly modeling the problem, a matheuristic solution algorithm is proposed. Validation of the approach is achieved, and computational analysis is presented to highlight how the matheuristic is able to improve upon the first shortsighted solution. This chapter is based on a paper submitted by the author for publication and co-authored by Massimiliano Caramia, Giuseppe Stecca and Emanuele Pizzari.

Chapter 4 investigates the operations of sorting facilities, where materials are collected by a fleet of trucks and then sorted to be converted to secondary raw materials. The activity is characterized by low margins, difficulties to track flows and uncertainties in supplies. Indeed, streams processes of reverse logistics are affected by several uncertainties, such as the stochastic processes regarding material arrivals to sorting facilities. The author proposed in [83] a deterministic formulation to optimally plan and schedule the sorting operations. Then, in this dissertation, the model in [83] is extended by introducing robustness to data uncertainties related to the stochastic nature of reverse logistics streams. Through a specific robust approach, constraints are guaranteed to be satisfied both deterministically and probabilistically. On instances drawn from a real case scenario, experiments are performed and comparisons are made with various planning strategies. The contents of this chapter are also published in [82], a paper co-authored by the author, Claudio Gentile and Giuseppe Stecca.

Chapter 5 presents a procedure to address the main drawback of robust optimization, this is the chance of producing over-conservative solutions with respect to the real occurrences of the stochastic parameters. Indeed, the level of conservatism of robust solutions can be such to constitute a significant cost in terms of optimality reduction, also known as price of robustness. This chapter investigates how demand forecasting can be used in conjunction with robust optimization in order to achieve robust solutions that better control the extra-cost resulting from considering the demand variability. The contents of this chapter are also published in [49], a paper co-authored by the author, Claudio Gentile and Giuseppe Stecca.

Chapter 6 presents a framework that integrates an operational research (OR) model providing optimal capacity allocation with a machine learning (ML) model performing customer cost estimation. This framework is presented as a general approach for every OR model allocating either capacity or resources across multiple non-cooperative customers. The main objective of this framework is investigating the impact of all customer characteristics over the cost that results from the optimization of the process/service concerning that customer. Therefore, the idea behind this framework is considering a set of customer features and their inherent variability in order to evaluate their explanatory power within a customer cost regression task. Accordingly, the purpose of the ML model is providing cost forecasts for a new production/service request. Explainable Artificial Intelligence (XAI) techniques are used at the very end of the framework to validate the information contribution of each considered feature. Validation of the approach is done with real case instances of a pick-up and delivery routing model dealing with reverse logistics operations. The author proposes a new formulation of the considered routing problem and shows the effectiveness of the proposed method. This chapter is based on a paper submitted by the author for publication and co-authored by Marco Boresta and Giuseppe Stecca.

Chapter 2

Green Supply Chain Management under Uncertainty

This chapter introduces some generalities on Green Supply Chain Management (GSCM), presents the main decision problems addressed by GSCM, discusses uncertainty in GSCM, and reports a brief introduction to robust optimization (RO).

This chapter is structured as follows: Section 2.1 introduces the main definitions and concepts of Supply Chain Management (SCM) and its variations, including GSCM and Sustainable Supply Chain Management (SSCM). Section 2.2 reports the most common applications of mathematical programming in GSCM, with a special focus on Closed Loop Supply Chain Management (CLSCM) and Reverse Logistics (RL). Section 2.3 debates about uncertainty issues in GSCM, and Section 2.4 reports some of the research opportunities in GSCM under uncertainty. Finally, Section 2.5 introduces some well known concepts about robust optimization (RO) approaches to solve linear optimization problems with uncertain data. Additional knowledge regarding the probabilistic robust approach presented in [15] is also reported.

The reader interested in additional details and analysis of the reported concepts can refer to the literature references of this chapter.

2.1 Generalities

The Supply Chain (SC) is an organizational system of individuals, undertakings, information and funds that are involved in transferring of goods and services from dealers or sellers to consumers. SC operations are the conversion of natural resources and raw materials into the final product distributed to the end users. A large business network that produces value through products and services delivered to the end user, by means of several upstream and downstream contacts and relations, across numerous procedures and activities [60]. The above is one of the multiple definitions that can explain and bound the concept of SC. Considering the academic literature, the same variety applies to all statements outlining the concept of SCM and its variations, such as Sustainable SCM and Green SCM. The Council of

Supply Chain Management Professionals (CSCMP) define SCM and its related terminology in [80]. The CSCMP asserts that SCM encompasses the planning and management of all activities involved in sourcing and procurement, conversion, and all logistics management activities. Importantly, it also includes coordination and collaboration with channel partners, which can be suppliers, intermediaries, third-party service providers, and customers. In essence, SCM integrates supply and demand management within and across companies. SCM is an integrating function with primary responsibility for linking major business functions and business processes within and across companies into a cohesive and high-performing business model. It includes all the logistics management activities, as well as manufacturing operations, and it drives coordination of processes and activities with and across marketing, sales, product design, finance and information technology.

Nevertheless, as stated in [59] and in Section 1 of this dissertation, the rationale for SCM is also the opportunity for cost savings and better customer service. Indeed, even though all definitions could be satisfactory, only some emphasize the importance of effectiveness and efficiency in SCM. Thus, for the aim of this dissertation, the following definition given in [66] is used as the foundation for developing the models for assessing supply chains effectiveness and efficiency. The authors of [66] refer to SCM as a set of methods used to effectively coordinate suppliers, producers, depots, and stores, so that commodity is produced and distributed in the correct quantities, to the correct locations, and at the correct time, in order to reduce system costs while satisfying service level requirements. The fundamental notion of this definition is that a supply chain must be regulated in order to be fast and reliable, cost-effective, and adaptable enough to satisfy consumer needs.

The reader can refer to [59, 87] for a comprehensive review of statements outlining the concept of SC and SCM.

Another non-trivial exercise would be agreeing on a common definition for green and sustainable supply chains. A review paper focusing purely on definitions for green and sustainable supply chains found a total of 22 definitions for green and 12 definitions for sustainable supply chain management [3]. According to this review, the definitions listed below have received the most Scopus citations for the publication that contains them.

Green Supply Chain Management (GSCM) is about integrating environmental thinking into supply-chain management, including product design, material sourcing and selection, manufacturing processes, delivery of the final product to the consumers as well as end-of-life management of the product after its useful life [103].

Sustainable Supply Chain Management (SSCM) is the management of material, information and capital flows as well as cooperation among companies along the supply chain while taking goals from all three dimensions of sustainable development, i.e., economic, environmental and social, into account which are derived from customer and stakeholder requirements [95].

Corresponding to a global trend, the concept of green and sustainable supply chain management has received more attention in the past decade and garnered emerging clusters of research in this area [46]. All of these research clusters, according to each specific area of interest, are fostering and empowering the ambitions of the sustainability paradigm. Remarkable importance is given to the research area concerning the integration of the closed loop method in SCM, namely Closed Loop Supply Chain Management (CLSCM). These types of supply chains deal with the streams of Reverse Logistics (RL). Logistics is defined by the Council of Logistics Management as the process of planning, implementing, and controlling the efficient, cost-effective flow of raw materials, in-process inventory, finished goods and related information from the point of origin to the point of consumption for the purpose of conforming to customer requirements. RL includes all the activities that are mentioned in the definition above. The difference is that RL encompasses all of these activities as they operate in reverse. Therefore, reverse logistics is the process of planning, implementing, and controlling the efficient, cost-effective flow of raw materials, in-process inventory, finished goods and related information from the point of consumption to the point of origin for the purpose of recapturing value or proper disposal [113]. A closed-loop supply chain is the result of considering forward and reverse supply chains simultaneously. Figure 2.1 illustrates both forward and reverse logistics for a generic supply chain.

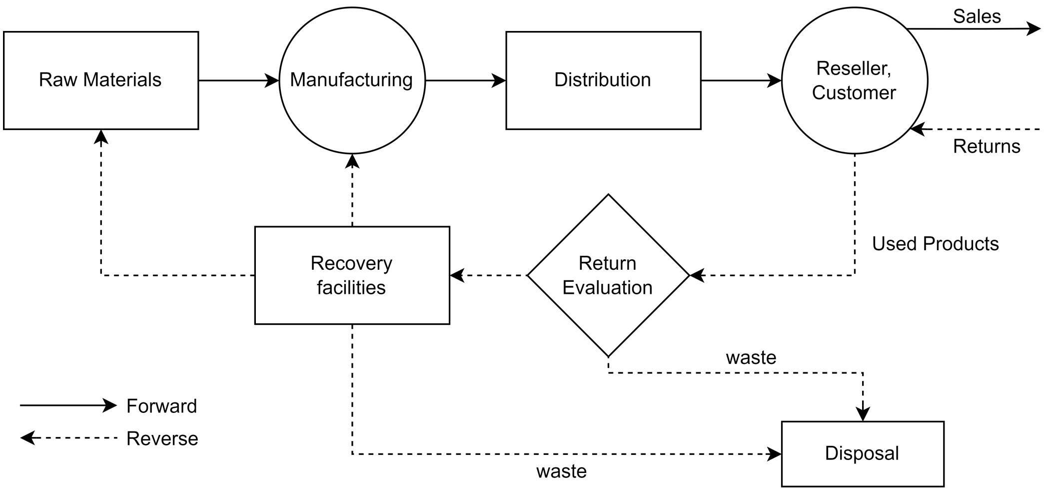


Figure 2.1. A generic form of forward/reverse logistics

Given the incorporation of the closed loop approach in a supply chain, a reverse logistics network faces a variety of decision-making challenges. These challenges, the resulting decision problems and their relevant classifications, are briefly described in the following Section 2.2.

2.2 Decision problems

There are many decision problems addressed by GSCM. That is why optimization models emerged as part of helping practitioners solving real-life problems related to supply chain network, and it has become an integral part of GSCM literature [114]. This section holds a list of these problems, with a particular focus on those arising in CLSCM and RL. For a comprehensive review on optimization in GSCM, SSCM and RL, the reader is referred to [55, 78] and the references therein.

Each decision problem has a different level of planning horizon, which can be categorized into the following three levels.

i) strategic decisions

ii) tactical decisions

iii) operational decisions

In terms of relationships, operational plans lead to the achievement of tactical plans, which in turn lead to the attainment of strategic plans. In terms of timeline, strategic plans are based on longest-term planning horizon, operational plans shortest planning horizon, and tactical plans, in between. Operational plans can even refer to day-to-day decisions. Decision planning can be integrated either "horizontal integration" or "vertical integration". Horizontal integration means by integration the same decision level of optimization problems while vertical integration combines two different levels of decision [84], such as strategic-tactical, strategic-operational or tactical-operational. This dissertation addresses a strategic-tactical problem in Chapter 3, a tactical one in Chapter 4, while chapters 5 and 6 propose planning and learning models integration that are tested with a tactical and an operational problem, respectively.

Besides the level of planning horizon, a literature review can consider some other features for classifying a paper that deal with mathematical programming in this research field. Some of these features are the ones describing the modeling approach, such as deterministic assumption or uncertainty for parameters, decision variables and solution methodologies.

Considering the addressed problem only, there are several types of study subjects in GSCM, RL and CLSC. This dissertation acknowledges to the authors of [55] the following classification of problems in RL and CLSC.

Designing. The main subjects of research are assigned to RL and CLSC network design. The aim of designing is to determine strategic (long-term) decision variables like locations and the capacity of all facilities.

Planning. In a planning problem, the most important decision variables are the quantities of flows between supply-chain network entities, known as midterm decision variables. Some studies regard designing and planning stages simultaneously, and some concentrate on one of them in depth.

Price and coordination. Important discussions between two entities of a supply chain network (for instance, a remanufacturer and a retailer of second market) determine the price of products and coordinate win–win strategies to balance profit margins. Usually, in such problems, optimum price and coordination strategies are determined.

Production planning and inventory management. Some researches in supply chain networks are related to operational decision variables, which play a vital role in supply chain cost efficiencies. Scheduling of products and return products (manufacturing and remanufacturing) simultaneously, and inventory control policies of such production systems, are main subjects of these studies. There are some studies that concentrate on production planning and lot sizing decisions without regarding inventory issues. Such studies are categorized in a different class as ***production planning***. Conversely, there are some studies which concentrate on the inventory management issues such as finding reorder point, base stock, and economic order quantity without regarding production planning subjects. These studies arranged in the category of ***inventory management***.

Vehicle routing. As distribution systems and the related strategies are one of the most effective parts of the network and the total costs are closely dependent on the transportation costs, Vehicle Routing Problem (VRP) is an effective issue in RL and CLSC. There are some studies which directly consider this problem, mostly in proposing efficient solution algorithms.

It must be highlighted that in the review of the literature, some papers do not focus on a particular decision problem, rather propose ***conceptual and analytical frameworks***. These studies analyze some theoretical or practical factors to find a framework for different aspects of RL/CLSC [55].

Considering the classification above, this dissertation addresses a designing and planning problem in Chapter 2, a production planning and scheduling problem in Chapter 3, while chapters 5 and 6 propose conceptual and analytical frameworks that are tested with a production planning problem and a vehicle routing problem, respectively.

The GSCM research domain also incorporate studies that draw attention to several sources of uncertainty in the green supply chains, including the investigation of the resulting risks and the possible uncertainty management methods. The following Section 2.3 reports the main concepts and topics of addressing uncertainty in GSCM.

2.3 Uncertainty in Green Supply Chain Management

Uncertainty is an uncomfortable position.
But certainty is an absurd one.

- Voltaire, philosopher

Uncertainty is an inherent and inevitable feature in the process of green supply chain management[64]. Furthermore, the green supply chain contains more green behaviors than the traditional supply chain, which would face more uncertainty [37]. A comprehensive review in this area is that in [100], which provide a list of 14 sources of uncertainty and 21 uncertainty management strategies. These lists are recently adapted in [37] and presented in the following Table 2.1 and Table 2.2, respectively. As shown in Table 2.1, uncertainties are classified according to three types of sources, such as internal uncertainties which originate inside the specific company, uncertainties which emerge within the organization's supply chain (SC), and external uncertainties from factors outside the SC.

Table 2.1. Sources of uncertainty in GSCM

Internal organization uncertainties	Internal SC uncertainties	External SC uncertainties
Product characteristics	End-customer demand	Environment
Process/manufacturing	Demand amplification	Disruption, natural uncertainties
Control/chaos uncertainties	Customer as a supplier	
Organization structure and human behavior	Parallel interaction	
Information technology/ systems complexity	Order forecast horizon/lead-time gap	
	Chain configuration, infrastructure and facilities	

Instead, as shown in the following Table 2.2, uncertainty management is categorized in reducing uncertainty strategies that enable organizations to reduce uncertainty at its source, and coping with uncertainty strategies, which are not aimed to alter the source of uncertainty, rather look for ways to adapt to uncertainty in order to minimize its impact.

By adopting an uncertainty management approach, it is necessary to consider its links with sustainability performance [101]. The rationale underlying this observation is that an organization's sustainability performance is strongly related to the

Table 2.2. Uncertainty management strategies in GSCM

Reducing uncertainty strategies	Coping with uncertainty strategies
Lean operations	Postponement
Product design	Volume/delivery flexibility
Process performance measurement	Process flexibility
Good decision support system	Customer flexibility
Collaboration	Multiple suppliers
Shorter planning period	Strategic stocks
Decision policy and procedures	Collaboration
Information and communication technology (ICT) system	ICT system
Pricing strategy	Lead-time management
Redesign of chain configuration or infrastructure	Financial risk management
	Quantitative techniques

alignment between uncertainties and the choice of uncertainty management strategies [100]. This provides an intelligent perspective to examine the overall impacts of uncertainty management strategies, which may alter the complexity of managing a company or a supply chain. Indeed, these issues may generate inefficiencies that increase operational costs, resource consumption, and environmental pollution [41]. Consequently, it is important to understand how these strategies, that are intended to alleviate the effects of uncertainty, may lead to new problems that need to be addressed. This is the case, for instance, of robust optimization, a quantitative technique for coping with uncertainty that could induce over-conservative solutions that raise operating costs, resource consumption, and the resulting environmental pollution. In Chapter 5 this drawback of robust optimization is addressed by a framework that integrates a learning model to achieve robust solutions that better control the extra-cost resulting from considering uncertainty. Section 2.5 presents an introduction to the main concepts of robust optimization.

2.4 Research opportunities in GSCM

In terms of research opportunities, literature and content analyses in GSCM under uncertainty [28, 55, 114] reveal that this dissertation explores some of the research gaps in this research area.

In terms of stochastic ways of handling uncertainties in GSCM, literature analyses in [55] assert that researchers should consider two-stage stochastic approaches and robust optimization techniques as future directions of research, instead of regular stochastic programming. Robust optimization is indeed exploited in Chapter 4 as a valid uncertainty management strategy. In addition, the same analysis highlight how the other missing subject in uncertainty issues of GSCM is forecasting parameters approaches. Only a few papers (mostly conceptual) discussed and analyzed forecasting parameters. Accordingly, Chapter 5 investigates how demand forecasting can be used in conjunction with robust optimization in order to achieve a robust optimal planning that mitigates the risk of producing over-conservative solutions.

In addition to price, demand, and costs, GSCM research also considers additional features to be nondeterministic. Some of them are mentioned in [55], such as used products' rate of return, time of receipt of return products, and customer willingness to return them. These are the types of uncertainties that affect most reverse logistics networks, as the use-case of the research work presented in Chapter 6. Actually, those types of uncertainties regard any business engaging multiple customers that make production/service requests in such an unpredictable way that forecasting methods are ineffective. In this scenario, the framework in Chapter 6 investigates how the operative costs are altered by the variability of the customers characteristics and their unpredictable and non-cooperative production/service requests.

In terms of addressing real situations in GSCM, refining the problem based on typical scenarios in reality can increase the functional and practical importance of the research [28]. In agreement with the latter statement, each model and framework described in this dissertation was refined considering real-world applications and verified with real-world data. Particularly, the research work of the following chapters has been supported by two funds from EU POR-FESR program of Lazio region, Italy [Grant No. B86H18000160002] and [Grant No. A0375202036611, CUP B85F21001480002]. The last-mentioned grant refers to a research proposal conceived and detailed by the author.

In terms of research opportunities in solution methodologies, there are different discussions between analytical or exact solution methods and heuristics or meta-heuristics approaches. In many instances, different methods could be effective to some extent. For example, using heuristic and meta-heuristic algorithms to solve large, complex problems is necessary, even if the quality of solutions remains unknown. On the other hand, analytical and exact methods beside general exact solvers are rarely applicable to real-sized instances of a problem or nonlinear problems, so there is still a huge gap between theoretical solution methodologies and successful practical methods [55]. As a result, there is still a significant gap between theoretical solution methodologies and effective practical solutions. Perhaps hybrid algorithms or approximation algorithms might offer a different acceptable approach to theoretically and practically solving complex problems. Chapter 3 presents a meta-heuristic solution algorithm that combines a Local search with a Tabu search logic, and embeds exact methods in some phases of its algorithmic framework. The analyses in [55] illustrate that simulation studies, heuristic methods, and meta-heuristic algorithms are more applicable in practical situations in comparison with analytical or exact solutions.

2.5 Introduction to Robust Optimization

An effective, efficient, and robust supply chain gives countries and businesses a long-term competitive edge and enables them to manage the escalating environmental instability and competitive demands. Indeed, today's supply chains operate in complex environments that are characterized with high uncertainty, frequent disruption, and great variability [53]. These issues are more significant in reverse supply chain networks than in forward supply chains because the quantity and quality of returned goods or waste are more unpredictable in reverse networks [85]. Since decisions in green supply chain management are frequently made in the face of uncertainty, robust optimization and stochastic programming are useful tools to assist in reaching reliable decisions.

Based on the definition of different decision-making environments by [91] and [92], uncertain environments in accordance with [54] can be categorized in three main groups as follows.

1) Decision-making environments with random parameters in which their probability distributions are known for the decision maker. Here, these parameters are called stochastic parameters. Stochastic programming approaches including two-stage stochastic programming, multi-stage stochastic programming, and chance-constrained programming approach belong to this group.

2) Decision-making environments with random parameters in which the decision maker has no information about their probability distributions. Robust optimization (RO) models belong to this group. Several studies considered continuous uncertain parameters within pre-specified intervals, named as interval-uncertainty modelling, in this area.

3) Fuzzy decision-making environments. Flexible and possibilistic programming are two well known approaches to model ambiguity and vagueness under a fuzzy decision-making environment

When the unknown data can be thought of as stochastic, it might be difficult to specify reliably data distribution, especially in many real cases where there is no enough historical data for the uncertain parameters. Indeed, the mere fact that the data are stochastic does not help unless we possess knowledge of the underlying distribution. The uncertain-but-bounded model of uncertainty also needs a priori knowledge; however, it is much easier to point out the support of the relevant distribution than the distribution itself [85]. Accordingly, robust optimization is a valid alternative to stochastic programming approaches.

Robust optimization theory provides a framework to handle the uncertainty of parameters in optimization problems that could immunize the optimal solution for any realization of the uncertainty in a given bounded uncertainty set [14].

The first step in developing the RO theory is taken by Soyster [102], who proposes a linear optimization model to construct a solution that is feasible for all data that belong to a convex set. This first non-probabilistic approach is worst-case oriented and produces solutions that are too conservative, in the sense that it gives up too much of optimality for the nominal problem in order to ensure robustness. A significant step forward in RO theory was taken by Ben-Tal and Nemirovski [11–13] and El-Ghaoui and Lebret [42]. To address the issue of overconservatism, these papers proposed models for uncertain linear problems with ellipsoidal uncertainties, which involve solving the robust counterparts of the nominal problem in the form of conic quadratic problems. This less conservative approach allows control of the degree of conservatism by adjusting a specific parameter and can be addressed as a probabilistic approach in terms of probabilistic bounds of constraint violations. Although convex, such a method has the practical disadvantage of producing nonlinear models, which are more computationally demanding than the earlier linear models by Soyster [102].

At a later time, Bertsimas and Sim present in [15] another probabilistic approach for robust linear optimization that retains the advantages of the linear framework of Soyster [102]. More importantly, this approach offers full control on the degree of conservatism for every constraint. To introduce the theoretical basis of Bertsimas and Sim [15] approach, consider the following nominal linear optimization problem:

$$\begin{aligned} \text{maximize} \quad & \mathbf{c}^\intercal \mathbf{x} \\ \text{subject to} \quad & \mathbf{A}\mathbf{x} \le \mathbf{b} \\ & \mathbf{l} \le \mathbf{x} \le \mathbf{u} \end{aligned}$$

In the above formulation, it is assumed that data uncertainty only affects the elements in the matrix $\mathbf{A}$. We assume without loss of generality that the objective function $\mathbf{c}$ is not subject to uncertainty, since the objective maximize z can be used, adding into $\mathbf{Ax} \le \mathbf{b}$ the constraint $z - \mathbf{c}^\intercal\mathbf{x} \le 0$. This approach, as well as in Soyster [102] and Ben-Tal and Nemirovski [13], is able to withstand parameter uncertainty under the following *model of data uncertainty U.*

Model of Data Uncertainty U. Consider a particular row i of the matrix $\mathbf{A}$ and let J_i represent the set of coefficients in row i that are subject to uncertainty. Each entry a_{ij}, $j \in J_i$ is modeled as a symmetric and bounded random variable $\tilde{a}_{ij}$, $j \in J_i$ (see Ben-Tal and Nemirovski [13]) that takes values in $[a_{ij} - \hat{a}_{ij}, a_{ij} + \hat{a}_{ij}]$. Associated with the uncertain data $\tilde{a}_{ij}$, we define the random variable $\eta_{ij} = (\tilde{a}_{ij} - a_{ij})/\hat{a}_{ij}$, which obeys an unknown but symmetric distribution, and takes values in $[-1, 1]$.

Consider the i_{th} constraint of the nominal problem $\mathbf{a_i^\intercal x} \le b_i$. Let J_i be the set of coefficients $a_{ij}, j \in J_i$ that are subject to parameter uncertainty; i.e., $\tilde{a}_{ij}, j \in J_i$ takes values according to a symmetric distribution with mean equal to the nominal value a_{ij} in the interval $[a_{ij} - \hat{a}_{ij}, a_{ij} + \hat{a}_{ij}]$. For every i, we introduce a parameter Γ_i, not necessarily integer, that takes values in the interval $[0, |J_i|]$. As would become clear below, the role of the parameter Γ_i is to adjust the robustness of the proposed method against the level of conservatism of the solution. Intuitively, it is unlikely that all the a_{ij}, $j \in J_i$ will change. Here, the goal is to be protected against all cases that up to $\lfloor \Gamma_i \rfloor$ of these coefficients are allowed to change, and one coefficient a_{it} changes by $(\Gamma_i - \lfloor \Gamma_i \rfloor)\hat{a}_i$. In other words, nature appears to be restricted in its behavior, in the sense that only a subset of the coefficients will change in order to adversely affect the solution. The approach described in the following has the property that if nature behaves like this, then the robust solution will be feasible *deterministically*, and moreover, even if more than $\lfloor \Gamma_i \rfloor$ change, then the robust solution will be feasible *with very high probability.* We consider the following (still nonlinear) formulation:

$$\begin{aligned} \max \quad & \mathbf{c}^\intercal \mathbf{x} \\ \text{s.t.} \quad & \sum_j a_{ij}x_j + \max_{\{S_i \cup \{t_i\} | S_i \subseteq J_i, |S_i| = \lfloor \Gamma_i \rfloor, t_i \in J_i \setminus S_i\}} \left\{ \sum_{j \in S_i} \hat{a}_{ij} y_j + (\Gamma_i - \lfloor \Gamma_i \rfloor) \hat{a}_{it_i} y_t \right\} \leq b_i \ \forall i \\ & -y_j \leq x_j \leq y_j \quad \forall j \\ & \mathbf{l} \leq \mathbf{x} \leq \mathbf{u} \\ & \mathbf{y} \geq \mathbf{0} \end{aligned} \tag{2.1}$$

If Γ_i is chosen as an integer, the i_{th} constraint is protected by $\beta_i(\mathbf{x}, \Gamma_i)$:

$$\beta_i(\mathbf{x}, \Gamma_i) = \mathop{max}_{\{S_i | S_i \subseteq J_i, |S_i| = \Gamma_i\}} \left\{ \sum_{j \in S_i} \hat{a}_{ij} |x_j| \right\} \tag{2.2}$$

Note that when $\Gamma_i = 0$, $\beta_i(\mathbf{x}, \Gamma_i) = 0$, the constraints are equivalent to that of the nominal problem (i.e. a deterministic approach). Likewise, setting $\Gamma_i = |J_i|$, corresponds to the Soyster's method (i.e. a worst-case approach). Therefore, by varying $\Gamma_i \in [0, |J_i|]$, the robustness of the method can be flexibly adjusted against the level of the conservatism of the solution.

In order to reformulate model 2.1 as a linear optimization model, the following proposition is needed.

Proposition 2.5.1. *Given a vector* $\mathbf{x}^*$*, the protection function of the* i_{th} *constraint,*

$$\beta_i(\mathbf{x}^*, \Gamma_i) = \max_{\{S_i \cup \{t_i\} | S_i \subseteq J_i, |S_i| = \lfloor \Gamma_i \rfloor, t_i \in J_i \setminus S_i\}} \left\{ \sum_{j \in S_i} \hat{a}_{ij} |x_j^*| + (\Gamma_i - \lfloor \Gamma_i \rfloor) \hat{a}_{it_i} |x_j^*| \right\} \tag{2.3}$$

equals the objective function of the following linear optimization problem:

$$\begin{aligned} \beta_i(\mathbf{x}^*, \Gamma_i) = \quad & max \quad \sum_{j \in J_i} \hat{a}_{ij} |x_j^*| z_{ij} \\ & s.t. \quad \sum_{j \in J_i} z_{ij} \leq \Gamma_i \\ & \qquad 0 \leq z_{ij} \leq 1 \qquad \forall j \in J_i \end{aligned} \tag{2.4}$$

Proof of Proposition 2.5.1. Clearly the optimal solution value of problem 2.4 consists of $\lfloor \Gamma_i \rfloor$ variables at 1 and one variable at $\Gamma_i - \lfloor \Gamma_i \rfloor$. This is equivalent to the selection of subset $\{S_i \cup \{t_i\} | S_i \subseteq J_i, |S_i| = \lfloor \Gamma_i \rfloor, t_i \in J_i \setminus S_i\}$ with corresponding cost function $\sum_{j \in S_i} \hat{a}_{ij} |x_j^*| + (\Gamma_i - \lfloor \Gamma_i \rfloor) \hat{a}_{it_i} |x_j^*|$ □

Next, model 2.1 is reformulated as a linear optimization model.

Theorem 2.5.2. *Model 2.1 has an equivalent linear formulation as follows:*

$$\begin{array}{lll} max & \mathbf{c}^\intercal \mathbf{x} & \\ s.t. & \sum_j a_{ij} x_j + z_i \Gamma_i + \sum_{j \in J_i} p_{ij} \leq b_i & \forall i \\ & z_i + p_{ij} \geq \hat{a}_{ij} y_j & \forall i, j \in J_i \\ & -y_j \leq x_j \leq y_j & \forall j \\ & l_j \leq x_j \leq u_j & \forall j \\ & p_{ij} \geq 0 & \forall i, j \in J_i \\ & y_j \geq 0 & \forall j \\ & z_i \geq 0 & \forall i \end{array} \tag{2.5}$$

Proof of Theorem 2.5.2. We first consider the dual of Problem 2.4:

$$\begin{array}{lll} \max & \sum_{j \in J_i} p_{ij} + \Gamma_i z_i & \\ \text{s.t.} & z_i + p_{ij} \geq \hat{a}_{ij} |x_j^*| & \forall i, j \in J_i \\ & p_{ij} \geq 0 & \forall j \in J_i \\ & z_i \geq 0 & \forall i \end{array} \tag{2.6}$$

By strong duality, since problem 2.4 is feasible and bounded for all $\Gamma_i \in [0, |J_i|]$, then the dual problem 2.6 is also feasible and bounded and their objective values coincide. Using proposition 2.5.1, we have that $\beta_i(\mathbf{x}^*, \Gamma_i)$ is equal to the objective functions value of problem 2.6. Substituting to problem 2.1, we obtain that problem 2.1 is equivalent to the linear optimization problem 2.5. □

It is clear by the construction of the robust formulation that if up to $\lfloor \Gamma_i \rfloor$ of the J_i coefficients a_{ij} change within their bounds, and up to one coefficient a_{it_i} changes by $(\Gamma_i - \lfloor \Gamma_i \rfloor) \hat{a}_{it}$, then the solution of problem 2.5 will remain feasible. The parameter Γ_i controls the trade-off between the probability of violation and the effect to the objective function of the nominal problem, which is what can be called *the price of robustness*.

Readers interested in more details and analysis of the Bertsimas and Sim approach, particularly on the probability bounds of constraint violation, can refer to [15] and the references therein. In conclusion, this approach has the following main features:

- It is successful in controlling *the price of robustness*
- It is computationally tractable
- It captures the trade-off between return and risk
- It applies to discrete optimization problems
- It ensures deterministic and probabilistic guarantees on constraints satisfaction

Above all, it does so in a linear framework under the *model of data uncertainty U.*

Chapter 3

Clustering and Routing in Reverse Logistics: A Two-Stage Optimization Approach

This chapter presents a two-stage model to design and operate a waste management (WM) network. The decision-maker (a regional authority) is interested in locating sorting facilities in a regional area and defining the corresponding capacities to install. The decision-maker is aware that waste will be picked up and brought to the installed facilities by independent private municipal companies. Therefore, the authority wants to foresee the behavior of these companies in order to avoid shortsighted decisions. In the first stage, the regional authority divides the clients into clusters, further assigning facilities to these clusters. In the second stage, it is defined an effective routing to serve clients' pickup demand. The main idea behind the model is that the authority aims to find the best location-allocation solution by clustering clients and assigning facilities to these clusters without generating overlaps. In doing so, the authority tries to *i)* assign clients' demand to facilities by considering a safety stock within their capacities in order to avoid shortages during the operational phase, *ii)* minimize greenhouse gases emissions, *iii)* be as compliant as possible with the solution found by the second stage problem, the latter aiming at optimizing tour lengths performed by vehicles. After properly modeling the problem, a matheuristic solution algorithm is proposed. Validation of the approach is achieved, and computational analysis is presented to highlight how the matheuristic is able to improve upon the first shortsighted solution.

3.1 Introduction

In recent years, sustainability has become the center of public attention. This global environmental concern results in new recovery and recycling targets imposed by national and international waste directives. In order to achieve these goals, specific policies must be defined and employed. The need to achieve these goals has caused an increasing interest in the recovery of materials from the waste streams [83] along with the rising prices of raw materials. Recovery of materials is a common concept of the Circular Economy, where every object that reaches an end-of-life state is put back into the stream to create additional value. In order to achieve this goal, it is vital to have technologically advanced facilities able to manage waste, although with the possible drawback of increasing costs [108]. Since the recycling industry is already characterized by low margins and high operations and logistics costs, optimizing the processes becomes critical to turn it into a feasible and profitable market.

Indeed, considerable attention has been directed toward the optimization of tasks related to Waste Management (WM). The Waste Framework Directive 2008/98/EC of the European Parliament [40] defines Waste Management as a group of several tasks, ranging from waste collection to disposal to after-care of the sites designated for disposal. Waste Management is also considered one of the main tasks of Green Supply Chain [104]. The reader can refer to the survey of Ghiani et al. (2014) [50] for a substantial knowledge of Operations Research (OR) literature related to strategic and tactical issues in solid WM. A more recent survey focused on strategic tasks in WM has been conducted by Van et al. (2020) [115]. Treating every task independently of one another could be limiting. Indeed, when dealing with a WM network, there is a concurrence of vital actions, such as collection [70], sorting, disposal, waste-to-energy practices, and recycling. Moreover, the impact of these tasks must be analyzed from an economic and environmental perspective. Therefore, the simultaneity of strategical, operational and environmental problems is highlighted.

It is also essential to focus on the potential imbalance between regions in charge of WM. Indeed, the rates at which countries manage solid waste using landfill, waste-to-energy plants, or composting facilities differ considerably at the global level [61]. Di Foggia et al. (2021) [38] try to analyze these differences, further noting that some regions struggle to achieve self-sufficiency. One of the main reasons is the level of industrialization, most strikingly characterized by a critical under-capacity. In [38], the authors underline how some regions' overcapacity counterbalances others' under-capacity. This situation generates negative environmental and economic externalities due to waste exports [38], further highlighting the importance of a proper Facility Location and Capacity Allocation. Policymakers need strategical support to address these gaps through policies that properly design networks, enabling appropriate waste handling and disposal routing.

Therefore, the purpose of the work presented in this chapter is to propose a WM network design model to sustainably achieve the recycling targets of circular economy. This model aims to provide an optimal treatment capacity distribution that limits waste movement while optimizing the overall economic and environmental impact.

3.1.1 Literature Review

Green Supply Chain Management (GSCM) is a complex field of research with several tasks involved. Some of these are Green Design, Green Manufacturing, Network Design and Waste Management [104]. Several papers tried to optimize a GSC by focusing on specific parts. Cristobal et al. (2018) [32] propose a model to prevent food waste generation, while Shoaeinaeini et al. (2021) [97] optimize a network through the study of specific pricing policies and subsidies. Bruglieri et al. (2019)[22] introduce the Green Vehicle Routing Problem with capacitated Alternative Fuel Stations (AFSs), a more realistic variant of the Green Vehicle Routing Problem where the capacity of the AFSs is addressed. Ma et al. (2020) [75] focus on green design by including the computation of carbon emitted during production. The reader can refer to the survey of Memari et al. (2016) [77] for comprehensive knowledge on modelling GSC by including CO_2 emissions. The research focus of this work is oriented to waste management only. The aforementioned survey of Ghiani et al. (2014) [50] analyses OR literature related to WM tasks, further dividing them into strategic and tactical/operational (for instance facility location and transportation, respectively). Erfani et al. (2018) [45] use operation research and geographical information systems to investigate effective factors in the storage service of municipal solid WM systems. Bautista and Pereira (2006) [7] provide a facility location model for locating collection areas for urban WM, with a real world application to Barcelona. Most of the articles in the survey deal with single-level models with single objective functions, and just a few tackle the issue with multi-objective models, such as location-routing. Although, the complexity of WM networks may be dealt with other mathematical approaches. For instance, Caramia and Pizzari [27] develop a fractional programming model to design a WM network by clustering clients by considering their demand and their general utility. They aim to maximize the clients' overall utility and minimize costs and emissions.

Concerning transportation in WM, one of the most common approaches is the Vehicle Routing Problem (VRP), which deals with a set of waste producing customers that need to be visited. These customers may have a demand to be satisfied in terms of waste to be picked up or delivered. Each customer is assigned to one route served by one vehicle. Given the limited capacity of the vehicles, several routes may be generated and each can serve different customers. There could also be several deposits instead of just one. The VRP generalizes the Travelling Salesman Problem (TSP), given the fleet of vehicles and the several routes to be optimized, instead of a single vehicle and single route. This class of problems was first introduced in 1959 by Dantzig and Ramser [34], who also presented a heuristic for the solution. Since the TSP is a particular case of the VRP, the VRP is NP-hard [48].

Over the years, several approaches have been proposed to solve the VRP, both exact algorithms and heuristics. Among the exact methods, the main ones are Branch and Bound, Dynamic Programming and Set partitioning, while for the heuristic algorithms, Sweep algorithm [51] and Cluster first-Route second can be mentioned. In recent years, metaheuristics have been thoroughly investigated for solving the VRP, given the large real-life instances, as highlighted by Elshaer and Awad (2020) [43]. For an extensive knowledge of the methods employed for dealing with VRP, the reader can refer to Laporte and Gilber (2009) [65], Braekers et al. (2016) [20], and Elshaer and Awad (2020) [43].

Among the various methods in the literature, cluster first-route second logic is a fairly standard approach for dealing with VRP. The large set of customers is firstly divided into smaller groups of customers (clusters) not to exceed the overall capacity of a vehicle. Several attributes can be taken into account when defining the clusters. Afterwards, the vehicles are assigned to specific clusters and routing is executed. Beltrami and Bodin first introduced this method (1974) [8], who used it to solve a problem concerning the municipal waste collection. Cakir et al. (2015) [25] further studied the clustering part of the problem by considering the clusters' shape. Clustering methods are studied by Comert et al. (2018) [31], too. They propose three different algorithms (K-means, K-medoids and random) to help shape the clusters. They further solve the routing via a branch-and-bound.

3.1.2 Main contributions

In terms of theoretical implications, this chapter's main contributions to the existing literature are:

- Dynamic clusters. Most articles dealing with cluster first-route second (and its counterpart route first-cluster second) define clusters that cannot be changed. Moreover, these clusters are done without taking into account information arising from the routing. In the proposed model, the clusters are updated via this information.

- The employment of cluster first-route second logic in a two-stage model. Information from the routing (second stage) will be used as a new starting point for the clustering phase (first stage).

- Fairness of capacity allocation between facilities. The issue of unbalanced capacity and the economic and environmental impact it causes has already been addressed in the introduction of this chapter.

- Penalty on capacity saturation. This feature has been included to consider the uncertainties in waste streams and to better address the issue of unbalanced capacity.

The model is tested in a real-world case scenario, namely the Lazio region, Italy. Although the real case scenario application deals with an Italian region situation, the model can provide several useful insights for other regions and countries.

The rest of this chapter is structured as follows: Section (3.2) gives the problem definition and further provides the mathematical formulation, Section (3.3) explains the mathematical approach employed for solving the model, Section (3.4) describes the computational analysis, and results for the case study. Finally, conclusions are discussed in Section (3.5).

3.2 Problem definition and mathematical formulation

This section first introduces the considered waste management problem in 3.2.1, then its mathematical formulation is presented in 3.2.2.

3.2.1 Problem definition

A regional authority, denoted for short also as RA, is involved in solving a strategical problem, hereafter denoted as SP. The SP consists of opening a set of *collection facilities* in proper geographical locations (drawn from a set F of prescribed locations). Waste must be routed after being picked up from *collection nodes*, i.e., *client nodes*, where waste and the resulting collection demand is generated. Let us denote this client set with C and demands with d_i, with $i \in C$.

Collection facilities act as hubs for the (spokes) client nodes. They may also be referred to as *sorting facilities* in case waste need to be sorted in order to be finally routed to recycling plants, incinerators or landfills for their disposal. In this chapter, however, no attention is given to the downstream part of the supply chain, which requires studying another strategic problem, as the one of Chapter 4.

Facilities to be opened by the RA have different sizes and capacities; let H be the set of sizes associated with a facility, e.g., H={small, medium, large} and let cap^f_{jh} be the capacity of a facility located in a candidate node $j \in F$ with size $h \in H$. Depending on both location and size, facilities have different opening costs c_{jh}, with $j \in F$ and $h \in H$, and a different environmental impact in terms of CO_2 emissions em^f_{jh}, with $j \in F$ and $h \in H$.

The clustering phase in the strategical problem.

In an attempt to decide which facilities have to be opened and which sizes have to be assigned to each of them, RA searches for a partition of set C into clusters, each with its own facilities. In doing so, RA aims at implementing a proximity logistic where capacities are fairly allocated to opened facilities and, consequently, to clusters, based on the following assumptions:

- h_1: demands d_i, with $i \in C$, are i.i.d. stochastic variables;
- h_2: the number of clients in each cluster is large enough to let the overall demand to be served in each cluster to follow the Central Limit Theorem.

Consider a generic cluster; let $C' \subseteq C$ be the subset of clients belonging to this cluster. Moreover, let $d(C') = \sum_{i \in C'} d_i$ be the overall cluster's demand. By hypotheses (h_1) and (h_2), $d(C')$ is a Gaussian variable with expected value $\mu(d(C'))$

equal to the sum of the expected values of the variables d_i, with $i \in C'$, and variance $\sigma^2(d(C'))$ equal to the summation of the variances of the same variables.

With this setting, `RA` can define the probability (i.e., the service level) with which an assignment of clients to a cluster will be obeying the cluster capacity, the sum of the capacities of the facilities therein assigned.

For instance, further considering the example of a cluster with a set C' of assigned clients, in order to guarantee a 0.99 service level, `RA` may impose 2.33 standard deviations of $d(C')$ from the expected cluster demand $\mu(d(C'))$ to determine the minimum capacity to be assigned to that cluster.

Hypothesis in h_1 related to the independence of the client demands appears to be realistic since clients produce waste independently one to each other; hypothesis in h_1 for which client demands are identically distributed appears to be realistic in those scenarios in which clients are represented by, e.g., comparable sets of families or commercial activities. In the case in which clients are substantially heterogeneous and, seemingly, it would be quite unrealistic to assume identical distributions, this assumption can be properly relaxed as follows (this option is denoted as option (b), as opposed to the current option (a)). Client demands d_i, with $i \in C$, are modeled as (deterministic) parameters such that $d_i = \mu d_i$, i.e., each demand is set equal to its expected value, and a safety capacity sc on the capacity of a cluster is considered, say, for instance, $\bar{cc}$, to reserve and penalize in case of being used. By means of sc, the action of the previously defined standard deviations is modeled without making use of any assumption on the client demand stochastic variables. Formally, we have

$$\sum_{i \in C'} d_i + (1 - \eta) \cdot sc \leq \bar{cc}, \tag{3.1}$$

where η is a continuous variable which should be minimized to let it be as close as possible to 0 to let, in turn, the safety capacity to be untouched. In the worst case $\eta = 1$, all the safety capacity will be used and, therefore, the cluster will be assigned a capacity only on the basis of the expected values of the demands, which would correspond to a service level of 0.5 in the case of identical distribution of the client demands.

The operational problem nested inside the strategical problem.

After opening the facilities, `RA` cannot play any role in determining how clients will be served and which facilities will be used. Moreover, it appears not to be realistic to impose clusters at an operational routing level, since carriers are free to choose routes based on their minimum cost criterion. Therefore, to minimize the risk of failing in the clustering task, `RA` tries to infer which will be the best routing to serve clients from the carrier's point of view, given the set of opened facilities; this task requires that `RA` nests a new optimization problem in their problem formulation. This new problem will be denoted as `OP`. The optimal solution of `OP` allows the calculation of miss-clustered clients to be penalized in the `SP` full objective function, i.e., a penalty arises in the case a client allocated in a cluster and to be served by the associated facilities in that cluster, is instead served by a different facility in the routing solution offered by OP.

The different nature of both SP and OP leads to define a two-stage optimization problem (denoted as TSOP) which well represents the interactions between the two problems. In order to entirely define TSOP, OP is considered in more detail. To this end, additional notation is introduced.

Let $G = (N, A)$ be a graph modeling the geographical area of the problem, where N is the node set encompassing three different subsets, i.e., $N = C \cup F \cup D$, being C the subset of node clients, F the subset of sites where facilities may be opened, and D is the subset of depot nodes. Let t_{ab} be the travelling time between nodes $a \in N$ and $b \in N$.

There is a set V of vehicles in charge of collecting wastes from clients in C. Each vehicle $l \in V$ has a capacity cv_l. The demand d_i of each client $i \in C$ has to be served by a vehicle $l \in V$. Each depot, in turn, is associated with a set of vehicles. The matrix $A \in \mathbb{Z}^{|D|\times|V|}$ stores this allocation of vehicles to depots in such a way that its generic element a_{kl} is equal to 1 if the vehicle l starts its tour from the depot k, and holds 0 otherwise.

OP have to find tours of vehicles in such a way that a vehicle $l \in V$ starts its collection tour from a depot $k \in D$, serves a subset of the clients in C obeying its capacity cv_l and then goes to an opened facility $j \in F$ of size $h \in H$. Finally, it routes back to the same depot $k \in D$. A service operated by a vehicle $l \in V$ should respect a maximum servicing time per tour, denoted as T_l.

The objective function of OP is to minimize the sum of the travelling time of all vehicles.

As mentioned earlier, the regional authority first decides which facilities to open by minimizing emissions due to installation of facilities and minimizing predicted capacity saturation. Afterwards, the authority uses this information to infer the optimal routing in the second stage, which gives feedback on the eventual miss-clustering and on the actual capacity saturation. Therefore, it makes sense to have two different objective function for the SP, namely a reduced objective function, computed in the first stage, and a full objective function, computed after the second stage.

The reduced objective function of SP is to minimize the conic combination of two functions to be minimized:

- (i) emissions due to installation of facilities
- (ii) penalty associated to the usage of the safety stock capacity of a facility

The full objective function of SP is to minimize the conic combination of three functions to be minimized:

- (i) emissions due to installation of facilities and transportation
- (ii) penalty associated to the usage of the safety stock capacity of a facility

- (iii) penalty associated to a possible miss-match between the clustering solution, represented by the solution of SP, and the assignment clients/routes, offered by the solution of OP.

Figure 3.1 briefly display the interaction between the two models. In the figure, *OF* shorten *objective function*.

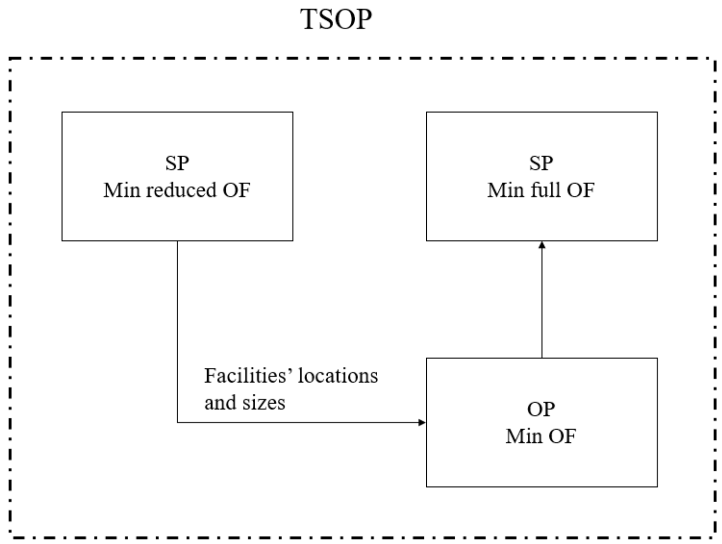


Figure 3.1. The Two-Stage Optimization Model

3.2.2 The mathematical formulation

After the definition of the problem, the mathematical formulation of TSOP is given. In order to get to the overall formulation, the constraints of SP and OP are presented separately.

The strategical problem constraints. Let S be the set of clusters the municipal firm may define, i.e., $|S|$ is an upper bound on the number of non-empty clusters defined by the problem solution. Let sc_{jh} be the safety capacity associated with a facility $j \in F$ of the size $h \in H$. The decision variables of SP are:

$$x_{is} = \begin{cases} 1 \text{ if client } i \in C \text{ is assigned to cluster } s \in S \\ 0 \text{ otherwise} \end{cases}$$

$$r_{jhs} = \begin{cases} 1 \text{ if facility } j \in F \text{ of size } h \in H \text{ is assigned to cluster } s \in S \\ 0 \text{ otherwise} \end{cases}$$

$$y_j = \begin{cases} 1 \text{ if facility } j \in F \text{ has been opened} \\ 0 \text{ otherwise} \end{cases}$$

$\eta_{jhs} \in [0,1] =$ the fraction of used safety capacity sc_{jh} associated with facility $j \in F$ of size $h \in H$ assigned to cluster $s \in S$

The constraints of SP are described in the following; note that, in defining the capacity of each cluster, they encompass option (b) (Equation 3.1).

$$
\begin{array}{llcll}
(1) & \sum_{s \in S} x_{is} & = & 1, & \forall i \in C, \\
(2) & \sum_{s \in S} \sum_{h \in H} r_{jhs} & = & y_j, & \forall j \in F, \\
(3) & \sum_{i \in C} d_i \cdot x_{is} & \leq & \sum_{j \in F} \sum_{h \in H} (r_{jhs} \cdot cap^f_{jh} - & \\
 & & & (r_{jhs} - \eta_{jhs}) \cdot sc_{jh}), & \forall s \in S, \\
(4) & x_{is} & \leq & \sum_{j \in F} \sum_{h \in H} r_{jhs}, & \forall i \in C,\ \forall s \in S, \\
(5) & \eta_{jhs} & \leq & r_{jhs}, & \forall j \in F, h \in H, s \in S, \\
(6) & \sum_{j \in F} \sum_{h \in H} \sum_{s \in S} c_{jh} \cdot r_{jhs} & \leq & B, & \\
(7) & \sum_{j \in F} \sum_{h \in H} r_{jhs} & \leq & mc, & \forall s \in S, \\
(8) & \eta_{jhs} & \in & [0,1] & \forall j \in F, h \in H, s \in S \\
(9) & x_{is}, r_{jhs}, y_j & \in & \{0,1\} & \forall i \in C,\ \forall j \in F, \\
 & & & & \forall h \in H,\ \forall s \in S.
\end{array}
$$

Constraints (1) say that every client $i \in C$ has to be assigned to one cluster in S. Constraints (2) impose that a facility $j \in F$ can have at most one size $h \in H$ and can be allocated to at most one cluster $s \in S$; moreover, in case facility $j \in F$ of size $h \in H$ is assigned to cluster $s \in S$, facility j is opened, i.e., y_j. Constraints (3) guarantee that the overall demand of clients assigned to a cluster $s \in S$ (considering demands as given parameters, see Subsection 3.2 for details) must not exceed the sum of the capacities cap^f_{jh} of all the facilities $j \in F$ (each with their own size h) assigned to cluster s minus the fractions η_{jhs} of the safety capacities sc_{jh} of the same facilities. Constraints (4) assign at least one facility to a cluster $s \in S$ if at least one client $i \in C$ is assigned to that cluster s. Constraints (5) impose that if no facility $j \in F$ is opened with size $h \in H$ and assigned to cluster $s \in S$, then no safety stock can be used. Constraint (6) imposes that the cost of locating facilities cannot exceed a given amount of budget B. Constraints (7) puts a limit on the maximum amount mc of facilities that can be assigned to a cluster. Constraints (8) and (9) define the range of feasible values for the decision variables.

The operational problem constraints. Let us now define constraints of OP. Let

$$
h^a_l = \begin{cases} 1 \text{ if vehicle } l \in V \text{ visits node } a \in N \text{ during its tour} \\ 0 \text{ otherwise} \end{cases}
$$

$$
z^{ab}_l = \begin{cases} 1 \text{ if vehicle } l \in V \text{ travels from node } a \in N \text{ to node } b \in N \\ 0 \text{ otherwise} \end{cases}
$$

$p_l^a \geq 0$; the arrival time of vehicle $l \in V$ in node $a \in N$

$v_l^j \geq 0$; the total amount of waste transported by vehicle $l \in V$ to facility $j \in F$

Constraints are as follows:

(10)	$\sum_{j\in F} h_l^j$	$=$	$\sum_{k\in D}\sum_{i\in C} z_l^{ki}$,	$\forall l \in V$,
(11)	$\sum_{k\in D} h_l^k$	$=$	1,	$\forall l \in V$,
(12)	$\sum_{j\in F} h_l^j$	$=$	1,	$\forall l \in V$,
(13)	$\sum_{l\in V} h_l^i$	$=$	1,	$\forall i \in C$,
(14)	z_l^{ij}	$=$	0,	$\forall l \in V, i \in N, j \in N : i = j$
(15)	$\sum_{i\in C} z_l^{ki}$	$\leq$	a_{kl},	$\forall k \in D,\ \forall l \in V$,
(16)	$\sum_{j\in F} z_l^{jk}$	$\leq$	a_{kl},	$\forall k \in D,\ \forall l \in V$,
(17)	$\sum_{i\in C} z_l^{ji}$	$=$	0,	$\forall j \in F, l \in V$,
(18)	$\sum_{k\in D} z_l^{jk}$	$=$	$\sum_{i\in C} z_l^{ij}$,	$\forall j \in F, l \in V$,
(19)	$\sum_{j\in C+F} z_l^{ij}$	$=$	h_l^i,	$\forall i \in C, l \in V$,
(20)	$\sum_{j\in D+C} z_l^{ji}$	$=$	h_l^i,	$\forall a \in C, l \in V$,
(21)	$\sum_{i\in C} h_l^i \cdot d_i$	$\leq$	cv_l,	$\forall l \in V$
(22)	p_l^b	$=$	$p_l^a + t_{ab}$,	$\forall l \in V, a \in D + C, b \in C + F : z_l^{ab} = 1$,
(23)	$\sum_{l\in V}\sum_{k\in D} p_l^k$	$=$	0	
(24)	p_l^a	$=$	0,	$\forall l \in V, a \in N : h_l^a = 0$,
(25)	$\sum_{j\in F} p_l^j$	$\leq$	T_l,	$\forall l \in V$
(26)	$\sum_{i\in C} h_l^i \cdot d_i$	$=$	v_l^j,	$\forall j \in F, l \in V : h_l^j = 1$,
(27)	$\sum_{l\in V} v_l^j$	$\leq$	$\sum_{h\in H}\sum_{s\in S} r_{jhs} \cdot cap_{jh}^f$,	$\forall j \in F$,
(28)	v_l^j	$=$	0,	$\forall j \in F, l \in V : h_l^j = 0$,
(30)	h_l^i	$\in$	$\{0, 1\}$,	$\forall i \in N, l \in V$,
(31)	z_l^{ij}	$\in$	$\{0, 1\}$,	$\forall i, j \in N, l \in V$,
(32)	p_l^a	$\geq$	0,	$\forall a \in N, l \in V$
(33)	v_l^j	$\geq$	0,	$\forall j \in F, l \in V$.

Constraints (10) say that if a vehicle $l \in V$ travels from depot $k \in D$, i.e., $\sum_{k\in D}\sum_{i\in C} z_l^{ki} = 1$, then it must exist exactly one facility $j \in F$ visited by vehicle l in its tour. Constraints (11) impose that each vehicle $l \in V$ must have precisely one depot $k \in D$ in its route (that is, the one for which $a_{lk} = 1$), while constraints (12) impose that each vehicle must have exactly one facility in its route. Constraints (13) impose that each client node must be visited by exactly one vehicle. Constraints (14) do not allow loops over the same node. Constraints (15) define that a vehicle $l \in V$ in a depot $k \in D$, i.e., one for which $a_{kl} = 1$, can exit from depot k to visit as immediate successors only (client) nodes $i \in C$ (i.e., facility or depot nodes are not allowed). Constraints (16) define that a vehicle exiting from a facility $j \in F$ can visit only one deposit $k \in D$ afterwards, namely the one for which $a_{kl} = 1$. Constraint (17) guarantee that a vehicle $l \in V$ cannot visit a client node $i \in C$ after having visited a facility node $j \in F$. Constraints (18) define that if a vehicle $l \in V$ has visited a facility $j \in F$, the next node visited by vehicle l must be its depot. Constraints (19) guarantee that after visiting a client, a vehicle can visit another client or a facility, while constraints (20) state that a vehicle can enter a client node only from a deposit or another client. Constraints (21) impose to respect the maximum capacity for each vehicle. Constraints (22)-(25) regulate the behavior of the variable p_l^a, i.e. the arrival time of vehicle l in node a. In detail, constraints (22) computes the arrival time at node b from node a as the arrival time at node a plus the time needed for the arc (a, b), but only if the arc (a, b) is in the route of vehicle l. Constraints (23) initializes the arrival time for each vehicle to be zero at each deposit. Constraints (24) sets the arrival time to zero for each node not visited. Finally, constraint (25) puts a limit on the time-length of a route finishing in a facility. Constraints (26) compute the overall load of a vehicle $l \in V$, linking this information to the facility $j \in F$ visited during the route. Constraints (27) are the capacity constraints for the facilities; they ensure that the vehicles' overall load does not exceed the capacity installed. Constraints (28) put the load towards the facilities not visited to zero. Constraints (30)-(33) state the feasible domain of the decision variables.

The operational problem objective function.

`OP` aims at minimizing the sum of the vehicles' travelling time. This means that the objective function associated with `OP` is:

$$of_{\mathtt{OP}} : \min \sum_{a \in D+C} \sum_{b \in C+F} \sum_{l \in V} z_l^{ab} \cdot t_{ab}.$$

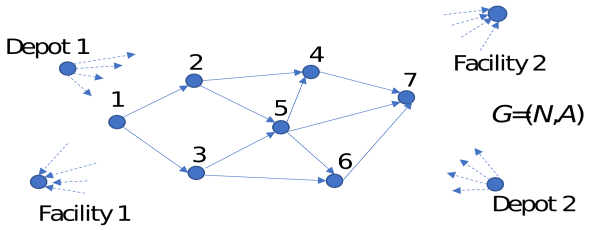
The strategical problem objective function.

This paragraph is intended to give a more in depth understanding of term (iii) mentioned at the end of Subsection 3.2; to this end, in Figures 3.2 and 3.3, a gadget example of a problem instance is illustrated.

The upper part of Figure 3.2 reports a gadget graph $G = (N, A)$ with $C = \{1, 2, 3, 4, 5, 6, 7\}$, F={Facility 1, Facility 2}, and D={Depot 1, Depot 2}. The lower part of Figure 3.2 reports a clustering solution consisting of two clusters, i.e., Cluster 1, including clients 1, 2, and 3, and Cluster 2, including clients 4, 5, 6, and 7.

Figure 3.3 shows (upper part) an example of routing operated by the company in charge of collecting the waste demands of the network, i.e., Route 1, which starts from Depot 1, visits clients 2, 5, 4, and 7, and, finally, reaches Facility 2; and Route 2, which starts from Depot 2 and visits clients 1, 3, and 6, and, finally, reaches Facility 1. Both routes, after having visited their respective facilities, end up at the initial depot.

Looking at the lower part of Figure 3.3, there is a misalignment between the cluster composition and the clients in each route. In particular, clients 1, 2, and 3, belong to the same cluster but are not served on the same route. A similar situation occurs for clients 4, 5, 6, and 7, which belong to cluster 2 but are not served on the same route. Therefore, the unmatched assignments, e.g., those related to clients 2 and 5 (same route, different clusters), or those related to clients 2 and 6 (again,



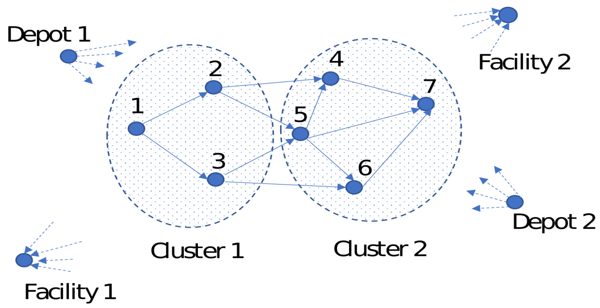


Figure 3.2. An example of a network and a clustering

same route, different clusters), will activate a penalty term in the objective function of SP.

The full objective function of SP is, therefore, the following:

$$
\begin{aligned}
of_{\texttt{SP}} : \min \quad & \gamma_1 \cdot \left(\sum_{i \in N} \sum_{j \in N} \sum_{l \in V} z_l^{ij} \cdot em_{ij}^t + \sum_{j \in J} \sum_{h \in H} \sum_{s \in S} em_{jh}^f \cdot r_{jhs} \right) + \\
& \gamma_2 \cdot \sum_{j \in F} P_j \cdot \eta_j + \gamma_3 \cdot \sum_{i \in C} \sum_{i' \in C} \sum_{l \in V} \sum_{s \in S} \max\{0, z_l^{ii'} - x_{is} \cdot x_{i's}\},
\end{aligned}
$$

where γ_1, γ_2, and γ_3 are real scalars. The first piece of the function defines the overall emissions, given by the sum of the emissions caused by transportation (the first term in the parenthesis, where em_{ab}^t is the emission for each arc (a, b)) and the sum of the emissions caused by facility locations and their assigned size (second term in the parenthesis). The second piece of the function models the amount of penalty $\eta_j \cdot P_j$ to be paid in case a fraction $0 \leq \eta_j \leq 1$ of safety capacity sc_j is used in the facility j, $\forall j \in F$, P_j being a real scalar defining the maximum penalty in a facility $j \in F$. The third term of $of_{\texttt{SP}}$ refers to the penalty defined at the beginning of this paragraph, i.e., the penalty occurring when two clients are assigned to the same route in OP but to different clusters in SP. It can be linearized by introducing:

- a real non-negative variable $g_{ii'ls}$, with $i \in C$, $i' \in C$, $l \in V$, $s \in S$,
- a binary variable $u_{ii's}$, with $i \in C$, $i' \in C$, $s \in S$,

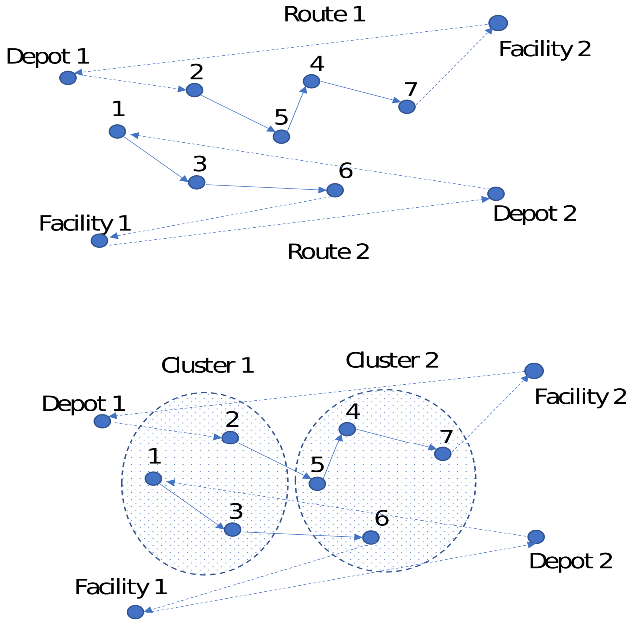


Figure 3.3. An example of routing and the associated penalty occurrence

and by adding the following constraints in SP:

$$
\begin{array}{llcll}
(34) & g_{ii'ls} & \geq & 0, & \forall i \in C,\ \forall i' \in C,\ \forall l \in V,\ \forall s \in S, \\
(35) & g_{ii'ls} & \geq & z_l^{ii'} - u_{ii's}, & \forall i \in C,\ \forall i' \in C,\ \forall l \in V,\ \forall s \in S, \\
(36) & u_{ii's} & \geq & x_{is} + x_{i's} - 1, & \forall i \in C,\ \forall i' \in C,\ \forall s \in S, \\
(37) & u_{ii's} & \leq & \frac{x_{is}+x_{js}}{2}, & \forall i \in C,\ \forall i' \in C,\ \forall s \in S, \\
(38) & u_{ii's} & \in & \{0,1\}, & \forall i \in C,\ \forall i' \in C,\ \forall s \in S
\end{array}
$$

and further rewriting the objective function as follows:

$$
\begin{aligned}
of_{\mathtt{SP}} : \min \quad & \gamma_1 \cdot \left(\sum_{i \in N} \sum_{j \in N} \sum_{l \in V} z_l^{ij} \cdot em_{ij}^t + \sum_{j \in J} \sum_{h \in H} \sum_{s \in S} em_{jh}^f \cdot r_{jhs} \right) + \\
& \gamma_2 \cdot \sum_{j \in F} P_j \cdot \eta_j + \gamma_3 \cdot \sum_{i \in C} \sum_{i' \in C} \sum_{l \in V} \sum_{s \in S} g_{ii'ls},
\end{aligned}
$$

As mentioned earlier, the first stage model also employs a reduced objective function, which is the following:

$$
of'_{\mathtt{SP}} : \min \quad \gamma_1 \cdot \sum_{j \in J} \sum_{h \in H} \sum_{s \in S} em_{jh}^f \cdot r_{jhs} + \gamma_2 \cdot \sum_{j \in F} P_j \cdot \eta_j
$$

3.3 A Matheuristic Solution Approach

Decisions taken in the first stage of the model affect decisions taken in the second stage. Furthermore, the second stage decisions affect the full objective function of the regional authority. If a simple two-stage scheme is employed, i.e. the first stage is optimally solved, then the second stage is optimally solved, and finally, the overall results are computed, several shortsighted decisions may be selected. Therefore, a matheuristic is developed in order to provide the `RA` with better solutions. The proposed matheuristic combines a Local search and a Tabu search logic. The overall framework is displayed in Figure 6.2, where the reader can easily recognize three main sectors, i.e. sector A, B, and C.

At the beginning of sector A, the `RA` solves `SP` on the reduced objective function. Information regarding opened facilities and their size is then passed upon the second stage, which is then solved. After `OP` is solved, the `RA` has the information that it needs for computing the full objective function. At the end of sector A, the `RA` checks if there are facilities whose safety stock is being used, i.e. if there are facilities that are overly used by the `OP`.

Sector B comprises all the possible actions that could be taken. The authority selects the facility that struggles the most, i.e. has the most amount of safety stock used. The authority first tries to enlarge the under-sized facility. If it is not possible, the authority checks if there are facilities whose capacity is used under a certain threshold, eventually closing them and replacing them with other facilities. The reason behind is that facilities under-used may not be attractive to the second-stage routing. Therefore, the `RA` tries to open other facilities, which may be more attractive. If there are not under-used facilities, the `RA` opens an additional facility, in order to try to assist the one in need.

In sector C, the action undertaken is then passed on to the second stage, which is again solved. Finally, the authority is able to infer if the new combination of facilities and sizes yields better results for the full objective function. If it is so, the authority continues the matheuristic. If the solution is worse than the one already obtained, the change in facilities location/size is reverted and added to a Tabu list to avoid making the same decision. When there is no more room for improvement, i.e. all facilities are acceptably used, or if there are no available moves, i.e. the Tabu list contains all the possible moves from the current solution, then the matheuristic stops.

3.4 Computational Analysis and Case Study

Both the model and the matheuristic are coded in Python3 programming language. All `SP` and `OP` problems instances are solved via branch-and-cut using the Gurobi 9.5.2 solver on a PC running an AMD Ryzen 7 4800H Processor with 16 GB of RAM. In order to test the behavior of the two-stage model and of the matheuristic before applying them to a real world case study, a set of random instances of different size is created. Table 3.1 displays the number of facilities, clients, deposits, and vehicles for each size of the instances, as well as the solver time limit (TL) for each stage of the model (expressed in seconds). For each size, 5 different instances

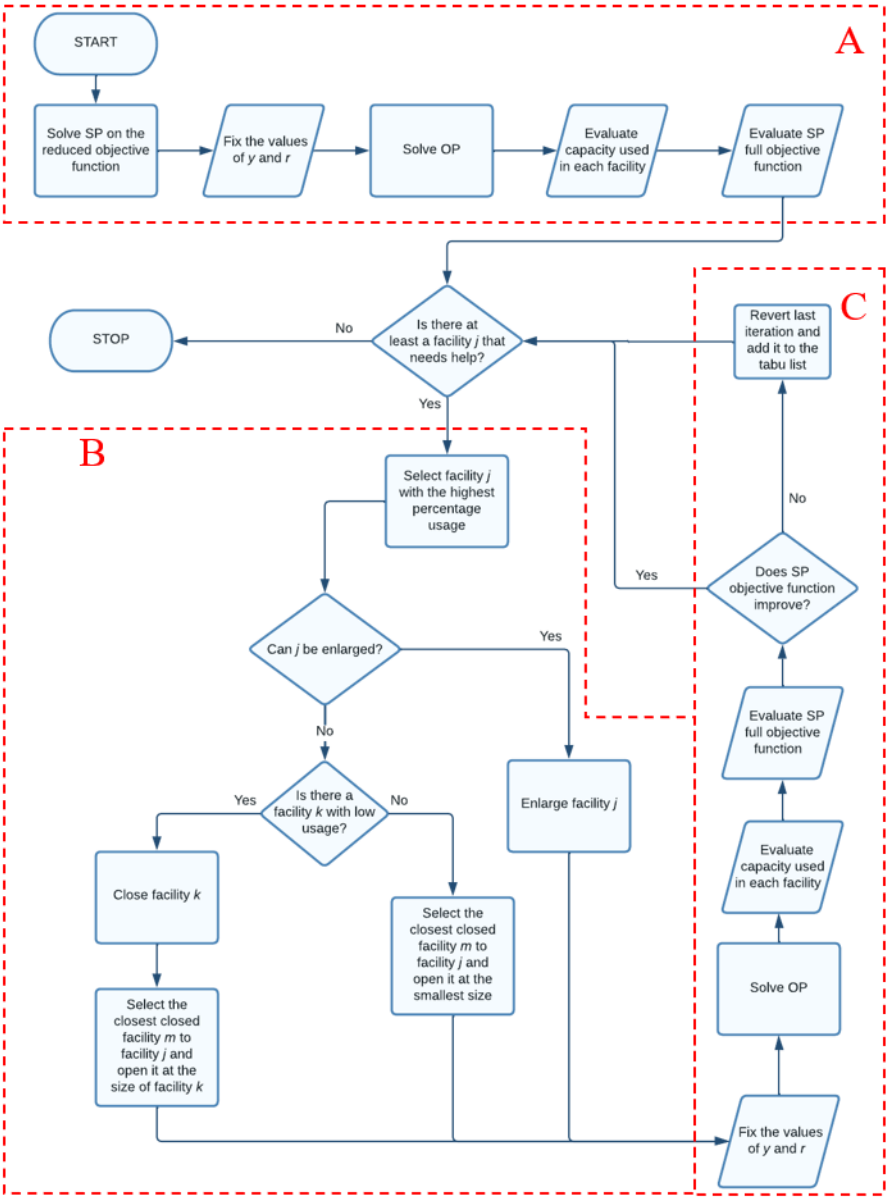


Figure 3.4. Framework of the matheuristic

are considered. For what concerns the network nodes of each instance, these are the results of different random samples of real locations of waste disposal facilities, industrial waste-clients and depots of waste companies trucks fleets. These types of nodes are all located within the Lazio region of centre-Italy. Dealing with data from a real-case scenario, the expected waste demand of served clients is computed according to 5 years (2017-2022) of waste pick-up instances obtained from a research project sponsored by the EU POR-FESR program of Lazio region, Italy [Grant No. B86H18000160002]. The attributes of the graph edges, such as travelling distance and duration, are generated by Open Source Routing Machine (OSRM), a high performance routing engine written in C++14 designed to run on OpenStreetMap data [74].

Table 3.1. Random instances - details

Instance	Facilities	Clients	Deposits	Vehicles	SP TL	OP TL
Small	5	15	2	4	25	200
Medium	10	25	5	10	35	400
Large	15	40	8	12	50	800

Table 3.2 displays the results for each random instance. Specifically, it shows the value of the full SP objective function computed in the first iteration and the best value of the objective function computed according to multiple starting points provided by the matheuristic. The improvement column shows that the proposed approach improved the results with respect to the initial solution for most instances. For the few not improved instances, the matheuristic did not start, meaning that the allocation of capacity done at the SP stage was proved acceptable by the OP. Table 3.3 shows how the SP objective function values evolve across the iterations (shorten as *It*). The underlined values highlight the instance with the best value. The results certify that the matheuristic is able to improve upon the original solution. A limit of 10 maximum iterations bounds the matheuristic test, still this limit did not come into play. Indeed, all possible starting points are explored in less than 10 iterations.

Table 3.2. SP results for the random instances

Size	Instance	First Value	Best Value	Improvement
Small	1	139.30	139.30	0.00%
	2	337.78	337.78	0.00%
	3	228.56	228.56	0.00%
	4	157.29	157.29	0.00%
	5	181.05	181.05	0.00%
Medium	6	302.96	288.69	4.71%
	7	519.48	282.58	45.60%
	8	293.13	274.13	6.48%
	9	430.69	328.50	23.73%
	10	481.95	456.53	5.27%
Large	11	457.20	443.80	2.93%
	12	545.90	543.94	0.36%
	13	465.61	441.00	5.29%
	14	557.70	557.70	0.00%
	15	544.38	506.93	6.88%

Table 3.4 displays the values of the second stage model for each matheuristic iteration. Underlined results do not represent the best OP values, they instead

Table 3.3. Evolution of the SP objective function

Instance	***It*1**	***It*2**	***It*3**	***It*4**	***It*5**	***It*6**	***It*7**	***It*8**	***It*9**
1									
2									
3									
4									
5									
6	288.69								
7	368.58	282.58							
8	274.13								
9	375.96	338.82	328.50						
10	456.53	456.53							
11	445.22	443.80							
12	581.09	548.29	567.79	587.13	600.54	589.62	549.73	543.94	558.96
13	471.42	459.84	465.69	464.62	465.21	455.44	441.00		
14									
15	506.93								

represent the iteration the RA settles on (i.e. the iteration for which the value of SP is the lowest). The SP problem was always solved at the optimum, while the OP is a more complex problem and its optimal solution is not always found in a reasonable amount of time (Table 3.5). Regarding computational times associated to the gaps in Table 3.5, the first four instances are optimally solved in less than 1 second. The solver required 30 seconds circa to close the gap for both OP problems of the instance n.6. Regarding instance n.10, the solver did not manage to find the optimum of the first OP problem, while it succeeded in the two following OPs in less than 20 and 30 seconds, respectively. All nonzero gap values of Table 3.5 refer to the solver time limits previously reported in Table 3.1.

3.4.1 Case study

The case study focuses on the Lazio region, located in the centre of Italy. Lazio region has an extension of $17,242km^2(6,657mi^2)$ and a population of 5,864,321 (Figure 3.5). Considering such a large area is indeed a challenging network design

Figure 3.5. Lazio region (highlighted in red)

problem. Therefore, only some municipalities are selected for each district. Lazio region has 5 districts, namely Rome, Viterbo, Rieti, Latina, and Frosinone. For each district, the provincial county seat and the most populated municipalities are the ones considered by the use-case application. Rome is out of this case study due

Table 3.4. `OP` results for the random instances

Instance	**First Value**	***It*1**	***It*2**	***It*3**	***It*4**	***It*5**	***It*6**	***It*7**	***It*8**	***It*9**
1	263.90									
2	580.00									
3	520.33									
4	315.79									
5	455.49									
6	477.30	477.19								
7	822.49	633.80	508.62							
8	534.36	536.54								
9	882.68	898.55	804.90	804.90						
10	848.55	812.80	812.80							
11	716.75	659.04	696.89							
12	889.32	946.32	880.58	857.95	893.93	897.05	913.71	851.05	882.91	852.76
13	653.71	687.21	650.11	663.09	651.16	656.68	644.53	631.63		
14	880.37									
15	945.42	937.89								

Table 3.5. Percentage gap of `OP` for each iteration

Instance	**First Value**	***It*1**	***It*2**	***It*3**	***It*4**	***It*5**	***It*6**	***It*7**	***It*8**	***It*9**
1	0.00%									
2	0.00%									
3	0.00%									
4	0.00%									
5	4.55%									
6	0.00%	0.00%								
7	32.87%	12.88%	2.56%							
8	9.17%	9.45%								
9	2.94%	4.25%	9.29%	9.29%						
10	6.06%	0.00%	0.00%							
11	21.07%	14.16%	12.85%							
12	11.58%	16.63%	10.13%	11.59%	11.30%	13.48%	16.15%	8.63%	11.98%	7.54%
13	7.99%	12.91%	5.80%	5.89%	4.38%	10.76%	9.08%	7.22%		
14	20.54%									
15	9.08%	8.35%								

to its size as a metropolitan city, which implies specific management approaches. Nevertheless, the author is collaborating with AMA S.p.a. (the WM operator in charge of all WM operations in Rome) to investigate optimization opportunities to better design and operate the WM network of Rome. Regarding this use-case, several facilities are selected for each province, and all data regarding waste production, population, and processing capacity has been taken from ISPRA's *Catasto dei rifiuti* (Waste cadastre)[1].

A total of 40 municipal-clients and 15 facilities are selected. They can be served by a fleet of 12 vehicles, distributed across 8 depots. Figure 3.6 displays the selected municipal-clients (green), facilities (orange), and trucks depots (blue).

Figure 3.6. Real case instance with vehicle depots, facilities, and demand points

The optimal use-case solution that results from employing the matheuristic is described in the following. In particular, Table 3.6 shows the number of opened facilities, their size, and the used capacity. Table 3.7 shows the values of the SP objective function, as well as the evolution of the matheuristic's iterations. The time limit for solving the SP is 50 seconds, while the time limit for the OP is 1800 seconds (30 minutes). Once again, the limit of 10 maximum iterations does not bound the matheuristic implementation.

Table 3.8 shows the solution results w.r.t. the OP. The number in bold corresponds to the iteration that the regional authority settles on, i.e. the third iteration, which

Facility	Size	Capacity used (%)	Safety stock used (%)
6	Small	81.94 %	39.8%
12	Small	58.66%	0
13	Large	31.17%	0
14	Large	40.43%	0

Table 3.6. Open facilities and capacity allocation in use-case application

First value	**Best value**	**Improvement**	**Iter 1**	**Iter 2**	**Iter 3**	**Iter 4**
972.17	887.78	8.60%	947.35	957.64	**887.78**	903.74

Table 3.7. Results of the `SP` in the case study

is the one with the best result for the `RA`, as shown in Table 3.7. Although the value of the `OP` in the third iteration improves upon the first solution, the second stage model could settle for an even better result in the fourth iteration.
Figure 3.7 showcases the vehicles' tour length in km for each of the twelve considered vehicles.

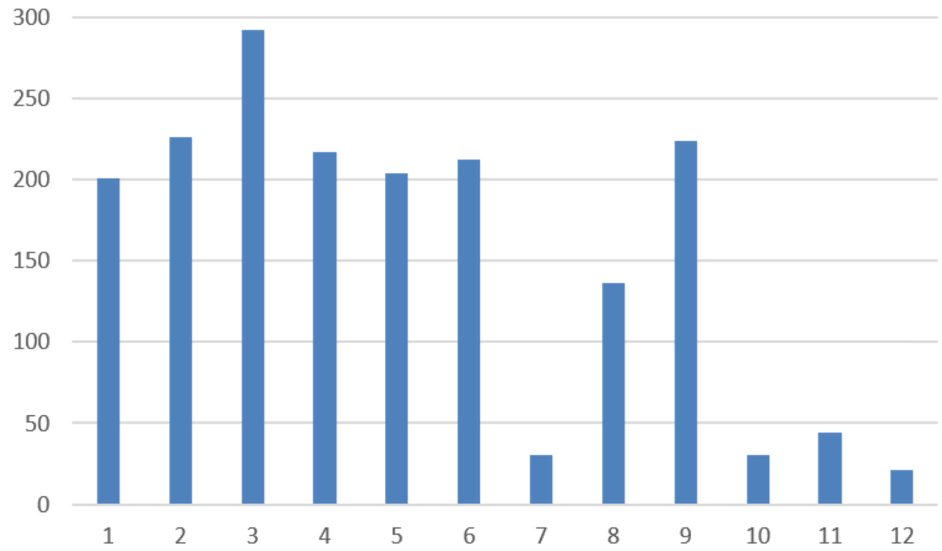


Figure 3.7. Vehicles' tour length with vehicle id in

First value of `OP`	**Iter 1**	**Iter 2**	**Iter 3**	**Iter 4**
2051.39	1901.99	1932.09	**1836.38**	1821.15

Table 3.8. Results of the `OP` in the case study

3.5 Conclusions

This chapter presented a novel two-stage model in order to assist a regional authority in designing a WM network. The authority wants to cluster clients, locate facilities for these clusters, and define the correct amount of capacity to install. The regional authority is aware that the network will then be used by independent decision-makers, i.e. the carriers in charge of picking up waste and delivering it to the opened facilities. To foresee the behavior of the operational decision-makers and to avoid possible miss-clustering or misallocation of capacity, the regional authority relies on the second stage of the model and a matheuristic.

Several random instances are used to test the two-stage optimization problem TSOP within the proposed matheuristic. Given the promising results, the TSOP and the matheuristic are then applied to a real-world case study. Once again, the model provides promising results, and the matheuristic is able to improve upon the first shortsighted solution.

Given that some tour lengths are uneven, a future research may address tour lengths balance.

Most importantly, several instances of the OP were optimally solved. For these instances, the whole TSOP model is de facto a Bilevel optimization model, which can be used with multiple decision-makers, an inherent hierarchy and a possible degree of cooperation. For these instances, the first stage can be seen as the leader, whereas the second stage could be perceived as the follower. However, the exact solution approach is not always able to close the duality gap of the second stage problem within a reasonable amount of time. For all the instances where the second stage was not optimally solved, we cannot refer to the TSOP as a bilevel optimization problem. Indeed, the optimality of the follower's problem solution is a strict requirement in order to have a feasible bilevel solution. Therefore, another future research may address these gaps in order to achieve the optimality needed for a bilevel optimization approach.

Chapter 4

Robust Optimal Planning of Waste Sorting Operations

Circular economy objectives are worthwhile and worldwide challenges concerning both the protection of the environment and the conservation of natural resources with aim of zero waste. A considerable attention has been directed over the last decade towards the optimization of planning procedures related to waste management in order to empower circular economy ambition. This chapter investigates the operations of waste recycling centers where materials are collected by a fleet of trucks and then sorted in order to be converted in secondary raw materials. The activity is characterized by low margins, difficulties to track flows and uncertainties in supplies. In [83] a formulation has been proposed to address and optimize the sorting process. However, special attention should be paid to the fact that waste streams processes are affected by several uncertainties, such as the stochastic processes regarding waste arrivals to sorting facilities. This work extends the model in [83] by introducing robustness to data uncertainties related to waste supplies. Accordingly, the main aim of this study is to develop a mixed integer linear programming model for planning and scheduling the packaging waste recycling operations, taking into consideration also the stochastic nature of waste arrivals. This is done by introducing a protection function in each constraint according to the probabilistic robust approach presented in [15] and in Section 2.5 of this dissertation. This approach ensures deterministic and probabilistic guarantees on constraints satisfaction. The model supports other strategic decisions, such as sizing of the amount of processed waste and allocating of the optimal number of operators for each shift of the sorting processes. Experiments are performed on instances taken from a real case scenario, and comparisons are made against different planning strategies.

4.1 Introduction

Performances of waste management systems have been improving thanks to a noticeable commitment of decision makers and research efforts regarding the optimization of each system component. As an example, a conventional operational task addressed by research is about waste shipment and collection trucks route optimization as in [93][19]. In the meantime, similar optimization models have been drastically reducing transportation costs, enhancing the growth of the online shopping of any sort of good. As a result, while logistic companies start serving a new magnitude of customers, also a new dimension of packaging waste started affecting the overall waste system. This leads to the need of a stronger technological and strategic decision support to packaging waste facilities in order to lower all the extra costs involved with the selective collection and sorting of this kind of waste. Not only logistic companies, but also every other kind of industry, generates a considerable amount of packaging waste. In Europe, the Directive 2004/12/EC on packaging and packaging waste laid down the European recycling and recovery targets. In particular, official reporting on packaging waste for all EU Member States was implemented in 2007 and since then Eurostat monitors also the developments of this important statistics. Therefore, the need of meeting the recovery and recycling targets imposed by EU law and the rising prices of raw materials used for packaging have resulted in an increasing interest in the recovery of materials from the waste streams. Moreover, the recycling industry is characterized by very low margins and high percentage of operation and logistics costs. For this reason, it is critical the optimization of the process in order to turn it into an economically sustainable business. Special attention should be paid to the fact that this objective is affected by several uncertainties, such as those arising in the waste streams processes. In particular, waste arrivals to sorting facilities are stochastic processes. Indeed, waste truck arrivals are subject to considerable variability that should be properly addressed when modeling scenarios including waste streams. In [83] this subject has been investigated. This work intends to expand the modeling power of the MILP presented in [83] by introducing robustness to data uncertainties related to waste supplies.

The reminder of this chapter is organized as follows: the literature review is given in Section 4.1.1; Section 4.2 is dedicated to the problem description and the MILP formulation; Section 4.3 presents the experimental results; finally, Section 4.4 gives conclusions and future research perspectives.

4.1.1 Literature review

The range of scientific literature contributions to waste management is justified by the variety of technological configurations and decision levels (mainly strategic and operational). The main type of waste flows considered are municipal solid waste, as a result the great majority of works are related to the management or the strategic definition of municipal solid waste networks, such as in [105]. The conventional operational task addressed by research is about collection trucks route optimization and waste shipment [93][19]. Besides them, a real case application is presented in [6]. A complete survey of both strategic and tactical issues in solid waste management that have been addressed by operations research methods is presented in [50]. Within the waste management paradigm, none of the previous works is close to the original operational application of mathematical programming presented in [83]. This chapter expands the value of the original work in [83] by extending the model presented therein with the introduction of robustness to data uncertainties related to waste supplies. The contents of this chapter are also published in [82], a paper co-authored by the author, Claudio Gentile and Giuseppe Stecca.

4.2 Problem definition and modeling

In this section, the main operational features covered by the nominal deterministic model are described together with the formulation of its robust counterpart. It will be clarified how the model is able to cover the main strategic decisions of the process while properly modeling the typical production dynamics of a reverse logistic setting. The production demand of the waste facility arises from the need to program and size the sorting operations of waste in order to balance the availability of the buffer of received material with the production and set-up costs of sorting operations and storage costs of all the inter-operational buffers. Therefore, the simultaneity of the scheduling problem and the lot sizing problem is highlighted.
It is important to notice that, in the considered industrial case, costs of storage are not directly measurable. Indeed, it is impossible to compute the inventory costs as proportional to the inventory value because there is no means to evaluate that value before the material is sorted. At the same time, the level of buffer storage can be such as to constitute a criticality in terms of saturation of the storage capacity. This is particularly evident when a specific level of stock is passed. Therefore, in [83] it is considered appropriate to model this dynamic through a storage cost curve which originally included a non-linearity from the exceeding of the critical stock level. The linearity of the model is indeed guaranteed using a piece-wise linear curve that approximates the real cost curve. The indications about the threshold perceived by the waste company in relation to the customer service level can also be considered.

A mixed integer linear programming (MILP) model which defines the robust counterpart to the problem introduced in [83] is described and detailed in the following. The basic notations that will be used in the MILP, such as parameters and indexes, are here listed:

$j \in \{1, \dots, J\}$: index of the J sorting stages

$p \in \{1, \dots, P\}$: index of the P time-shifts

T : time horizon partitioned in time shifts with $t \in \{1, \dots, T\} = T_1 \cup \dots \cup T_P$

C : hourly cost of each operator

σ_t : working hours for time t determined by the corresponding shift p

$C_t = C * \sigma_t$: cost of each operator at time t

f_j : set-up cost of sorting stage j

a_t : quantity of material in kg unloaded from trucks at time t

α_j : percentage of waste processed in stage $j-1$, received in input by buffer j

S_j : maximum inventory capacity of the sorting stage buffer j

LC_j : critical stock level threshold of buffer j

ρ_j : fraction of material allowed to be left at buffer j at the end of time horizon

K_j : single operator hourly production capacity [kg/h] of sorting stage j

$SK_{j,t} = K_j * \sigma_t$: operator sorting capacity in sorting stage j, at time t

M : maximum number of operators available in each time shift

E_j : minimum number of operators employed in each time shift of stage j

∂h_j^i : slope of the i-th part of linearization of the buffer j stock cost curve

The nominal deterministic model consider the following variables.

$x_{j,t} \in \mathbb{Z}^+$: operators employed in the sorting stage j at time t

$u_{j,t} \in \mathbb{R}^+$: processed quantity at stage j at time t

$y_{j,t} \in \{0,1\}$: equal to 1 if stage j is activated at time t, 0 otherwise

$I_{j,t} = I_{j,t}^{'} + I_{j,t}^{''} \geq 0$: stock level of material in buffer j at time t; for each stage j the corresponding $I'_{j,t}$ and $I''_{j,t}$ represent the inventory level before and after reaching the critical threshold respectively

$w_{j,t} \in \{0,1\}$: equal to 1 if $I_{j,t}^{''} > 0$, 0 otherwise. Indeed, these binary variables are used to model the piece-wise linear functions of the buffer stock costs.

We consider the set of parameters a_t, $t \in T$, that are subject to uncertainty, taking values according to a symmetric distribution with mean equal to the nominal value a_t in the interval $[a_t - \hat{a}_t, a_t + \hat{a}_t]$. Indeed, $\hat{a}_t$ is the maximum deviation of a_t. In order to meet the standard formulation of the nominal problem presented in [15], where parameters subject to uncertainties belong to inequality constraints only, the equality constraints of [83] regarding waste arrivals a_t are reformulated to turn them into inequality constraints. This is performed considering, for each period t, the sum of all the received and processed quantities of waste up to that period, as in constraints (4.5),(4.6),(4.7),(4.8) of the formulation presented in this section. According to the robust approach presented in [15], a parameter Γ_i is introduced for each constraint i holding one or more uncertainty coefficients. Γ_i is not necessarily integer and takes values in the interval $[0, |J_i|]$ where J_i is the set of the coefficients of constraint i being subject to uncertainty. The nominal problem presented in [83] presents only one set of T constraints considering the coefficients a_t and these are the ones reformulated as inequality constraints. Therefore, we get $\Gamma \in R_+^T$, and because of this reformulation $|J_t| = t \ \forall t \in \{1, \dots, T\}$. For each period t, Γ_t represents the number of coefficients that we consider as allowed to vary within their interval, ergo we consider nature behaving like only a subset of the coefficients will change with respect to their nominal value. Indeed, as affirmed in [15], it is unlikely that all $|J_t|$ will change; so the idea of conservative robustness is to be protected against all cases that up to $\lfloor \Gamma_t \rfloor$ of these coefficients are allowed to change, and one coefficient a_t changes by $(\Gamma_t - \lfloor \Gamma_t \rfloor)\hat{a}_t$. Note that when $\Gamma_t = 0 \ \forall t \in \{1, \dots, T\}$ we get the nominal deterministic scenario, while setting $\Gamma_t = |J_t| = t \ \forall t \in \{1, \dots, T\}$ represents solving the problem of the worst case scenario. It is clear then that by varying Γ the level of robustness can be flexibly adjusted against the level of conservatism of the solution. Considering the peculiar structure of the constraints including a_t is important: because of the telescopic expansion of each set J_t as t goes from 1 to T (i.e. $|J_{t+1}| = |J_t| + 1$), we consistently constraint Γ_t to be bigger or equal to Γ_{t-1}. The following list presents all the additional variables and parameters that are required to introduce the robustness protection functions presented in [15] and formulate the robust counterpart of the model presented in [83]:

$\epsilon_t \in \mathbb{R}^+$: extra variables multiplying $a_t \ \forall t \in T$. These variables are introduced in order to have a variable multiplying the only set of parameters that are affected by uncertainty. These are indeed constrained to be equal to 1 $\forall t \in T$.

$z_t \in \mathbb{R}^+$: variable resulted of duality within Bertsimas and Sim [15] robustness theory; when multiplied by Γ_t provides its overall contribution to the protection function of constraint t.

$p_{t,k} \in \mathbb{R}^+$: variable resulted of duality within Bertsimas and Sim robustness theory; provides its contribution to the protection function of constraint t with respect to the specific coefficient a_k.

$s_t \in \mathbb{R}^+$: variable resulted of duality and Bertsimas and Sim robustness theory; multiplied by $\hat{a}_t$ sets the lower bound of the protection function contribution in each constraint t.

Γ_t : parameter to adjust the level of robustness of each period t.

Considering a case study where $J = 2$ sorting stages, for the 1$^{\text{st}}$ sorting phase, $u_{1,t} \geq 0$ and $x_{1,t} \in \{0, 1\}$ represent the quantity of material to be selected and decision to activate the process respectively at time t. For the 2$^{\text{nd}}$ sorting phase, $u_{2,t} \geq 0$ and $x_{2,t} \in \{0, 1\}$ represent the quantity of material to be selected and decision to activate the process respectively at time t. $I_{1,t}, I'_{1,t}, I''_{1,t} \geq 0$ are the inventory levels at 1$^{\text{st}}$ phase sorting buffer while $I_{2,t}, I'_{2,t}, I''_{2,t} \geq 0$ are inventory levels at 2$^{\text{nd}}$ phase sorting buffer. As previously stated, w_1 and w_2 are used to model the piece-wise linear functions of the buffer stock costs. In detail $w_1 = 0$ if $I'_{1,t} < LC$, 1 if $I'_{1,t} = LC$ and $I''_{1,t} > 0$; similarly $w_2 = 0$ if $I'_{2,t} < LC$, 1 if $I'_{2,t} = LC$ and $I''_{2,t} > 0$. The model minimizes the sum of sorting and holding costs and is detailed as following:

$$\min Z = \sum_{j\in J}\sum_{t\in T} C_t x_{j,t} + \sum_{j\in J}\sum_{t\in T} f_j y_{j,t} + \sum_{j\in J}\sum_{t\in T}\left(\partial h_j^1 I'_{j,t} + \partial h_j^2 I''_{j,t}\right) \tag{4.1}$$

s.t.

$$E_j\ y_{j,t} \leq x_{j,t} \leq M\ y_{j,t} \qquad \forall j \in J, t \in T_p, p \in P \tag{4.2}$$

$$\sum_{j\in J} x_{j,t} \leq M \qquad \forall t \in T \tag{4.3}$$

$$u_{j,t} \leq SK_{j,t}\ x_{j,t} \qquad \forall j \in J, t \in T \tag{4.4}$$

$$I_{1,0} + \sum_{k=1}^{t} a_k \epsilon_k - \sum_{k=1}^{t} u_{1,k} + z_t \Gamma_t + \sum_{k=1}^{t} p_{t,k} \leq S_1 \qquad \forall t \in T \tag{4.5}$$

$$I_{1,0} + \sum_{k=1}^{t} a_k \epsilon_k - \sum_{k=1}^{t} u_{1,k} \geq 0 \qquad \forall t \in T \tag{4.6}$$

$$I_{1,0} + \sum_{k=1}^{T} a_k \epsilon_k - \sum_{k=1}^{T} u_{1,k} + z_T \Gamma_T + \sum_{k=1}^{T} p_{T,k} \leq \rho_1\ LC_1 \tag{4.7}$$

$$I_{1,t} = I_{1,0} + \sum_{k=1}^{t} a_k \epsilon_k - \sum_{k=1}^{t} u_{1,k} + z_t \Gamma_t + \sum_{k=1}^{t} p_{t,k} \qquad \forall t \in T \tag{4.8}$$

$$I_{j,t} = I_{j,t-1} - u_{j,t} + \alpha_j\ u_{j-1,t} \qquad \forall t \in T, j \in J \setminus 1 \tag{4.9}$$

$$I_{j,t} = I^{'}_{j,t} + I^{''}_{j,t} \qquad \forall j \in J, t \in T \tag{4.10}$$

$$LC_j\ w_{j,t} \leq I^{'}_{j,t} \leq LC_j \qquad \forall j \in J, t \in T \tag{4.11}$$

$$0 \leq I^{''}_{j,t} \leq (S_j - LC_j)\ w_{j,t} \qquad \forall j \in J, t \in T \tag{4.12}$$

$$I_{j,T} \leq \rho_j\ LC_j \qquad \forall j \in J \setminus 1 \tag{4.13}$$

$$z_t + p_{t,k} \geq \widehat{a}_t\ s_t \qquad \forall t \in T, k \in \{0, ..., t\} \tag{4.14}$$

$$-\ s_t \leq \epsilon_t \leq s_t \qquad \forall t \in T \tag{4.15}$$

$$\epsilon_t = 1 \qquad \forall t \in T \tag{4.16}$$

$$x_{j,t} \in \mathbb{Z}^+ \qquad \forall j \in J, t \in T \tag{4.17}$$

$$u_{j,t} \in \mathbb{R}^+ \qquad \forall j \in J, t \in T \tag{4.18}$$

$$y_{j,t} \in \{0, 1\} \qquad \forall j \in J, t \in T \tag{4.19}$$

The objective function (4.1) defines the minimization of the sum of the three cost terms, which are sorting, setup, and inventory costs respectively. (5.2) and (4.3) bounds the number of workers that can be assigned to each sorting station and to each time shift. Constraints (4.4) limit the quantity sorted $u_{j,t}$ to the sorting capacity dependent on the number of workers $x_{j,t}$. The following constraint sets (4.5)(4.6)(4.7)(4.8)(4.9) define and limit the inventories: constraint (4.5) defines the inventory for the first buffer, considering the cumulative inbound material a_t up to period t, the overall sorted material u_{1t} up to period t, and the uncertainties protection function made of the joint contribution of $z_t\Gamma_t$ and the sum of $p_{t,k}$ for $k \in \{1, \dots, t\}$. Constraint (4.6) sets the lower bound of the inventory for each period and (4.7) imposes the maximum unsorted material allowed to be left at the end of the planning period for the first buffer, as constraint (4.13) does for all other subsequent buffers. Equality constraint (4.8) allows the inventory of the main buffer (i.e. buffer no. 1) to be considered in the corresponding piece-wise linear part of the cost function. Constraint (4.9) defines the inventory for the other buffers corresponding to $j > 1$. Indeed, (4.9) outlines the waste flow across the sorting stages that follow one another: each subsequent inter-operational buffer j receives by the previous sorting stage $j-1$ a quantity of waste equal to a α_j percentage of the waste processed in stage $j-1$. Constraint sets (4.10), (4.11), and (4.12) define the piece-wise linear functions for inventories; in these constraints, maximum capacity level S_j and the critical stock level threshold LC_j are connected with the inventory levels through the variable $w_{j,t}$. Constraints (5.9) and (5.10) resulted from duality in [15] robustness theory; where (5.9) sets the lower bound of the protection function contribution in constraints (4.5) and (4.7).

4.3 Experimental results

This section holds the main results from the studied scenarios described in the following. All instances are created by a real-world case study from a waste sorting plant located next to Rome, Italy. All model instances are coded in Python3 and solved via branch-and-cut using the Gurobi 9.0 solver on a PC running a 1.60GHz Intel Core-i5-10210U CPU with 16 GB RAM. This has been performed in order to test the model response to different levels of robustness (i.e. different Γ selection), the corresponding price of robustness (i.e. the optimality reduction w.r.t the deterministic scenario) with respect to different weeks of scheduling time horizons. Figure 4.1 provides a first look at the model reaction to three different scenarios: the deterministic case, an intermediate level of protection and the worst-case scenario. It is evident that in the deterministic case, the protection function value remain null for each period, almost like the first buffer stock level. Indeed, the production marginal cost is less than the storage marginal cost, resulting in the processing of waste as soon as it arrives at the sorting facility. This is the reason why considering constraint (4.8) the protection function value equals for each period the first buffer stock level, and this applies for each protection scenario. Therefore, it can be reasonable to attribute a cost to the protection function value as the extra cost related to a higher level of stock in first buffer receiving the uncertain amount of waste. The robustness performance and the corresponding additional cost definitely depend on the protection strategy of choosing the vector $\Gamma \in R^T_+$ s.t. $\Gamma_t \geq \Gamma_{t-1} \forall t \in T$. In Figure 4.1 the intermediate protection relies on a moderate, still

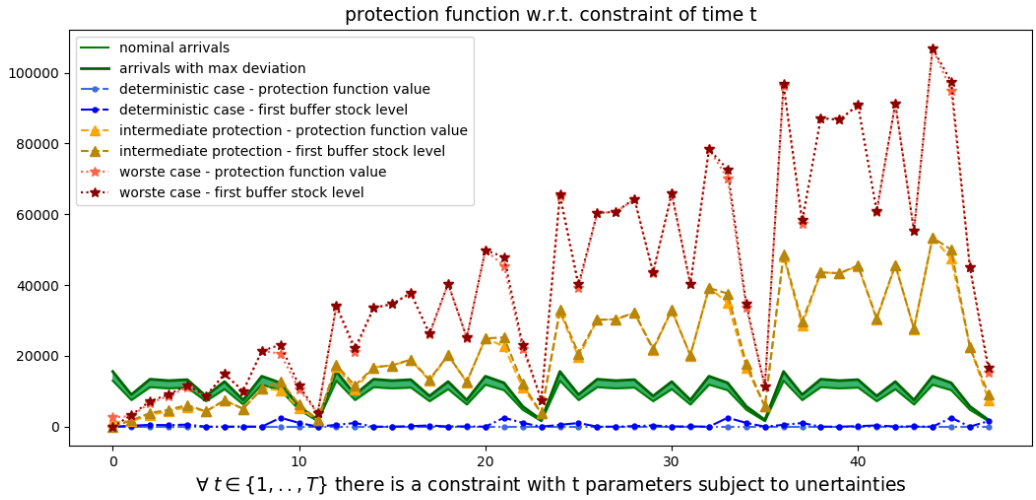


Figure 4.1. Illustration of protection function and stock level evolution over three different uncertainty's protection scenarios

continuous increase of Γ_t. This approach represents a cumulative sum of protection over the risk considered across the time horizon. Dealing with robustness to reverse demand uncertainties in a scheduling problem setting, is a suggestion to consider the seasonality of the stochastic behavior of the coefficients when setting the strategy of choosing $\Gamma \in R_+^T$. In the considered real case application, the parameters a have a one-week period (i.e. $t_{period} = 12$ when $P = 2$ working shifts a day for six working days). Therefore, a good approach is increasing Γ_t for $t \in \{1, .., t_{period}\}$ and keeping the maximum Γ_{period} for the rest of the time horizon. Figure 4.2 shows an example with a three weeks time horizon (i.e. T = 36).

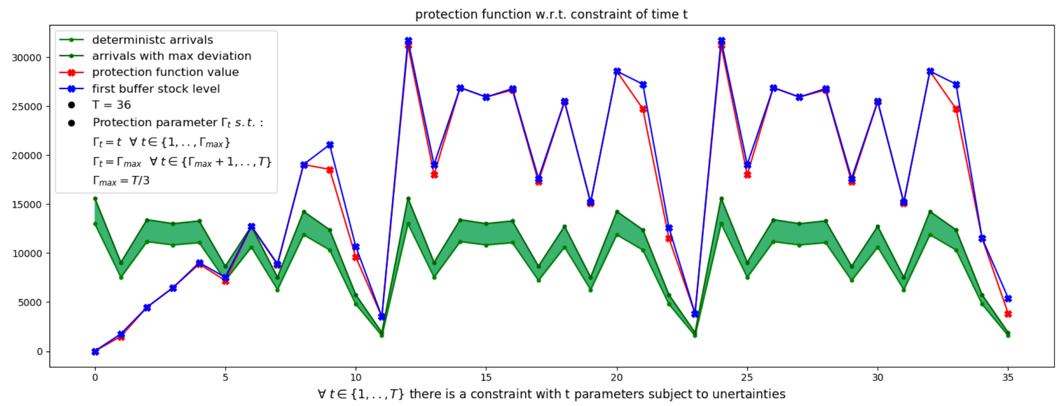


Figure 4.2. Using demand period for Γ selection strategy

The price of robustness (the optimality reduction w.r.t. the nominal deterministic problem) is tested over twenty protection magnitudes with respect to different time horizons from one to four weeks. All Γ selections linearly increase with different slopes from minimum to maximum risk protections, as shown in Figure 4.3.

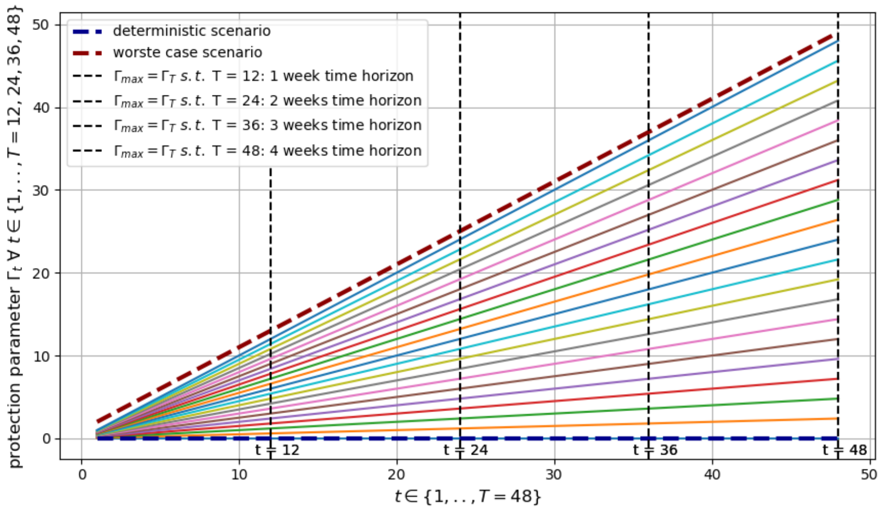


Figure 4.3. protection magnitude scenarios: from deterministic to worst-case

Results concerning the price of robustness are presented in Figure 4.4. It is clear that the evolution of the price paid for risk protection remains reasonable, and its evolution with respect to the protection scenarios strictly depend on the strategical selection of Γ. Indeed, a linear evolution of the price is obtained with a linear expansion of Γ components.

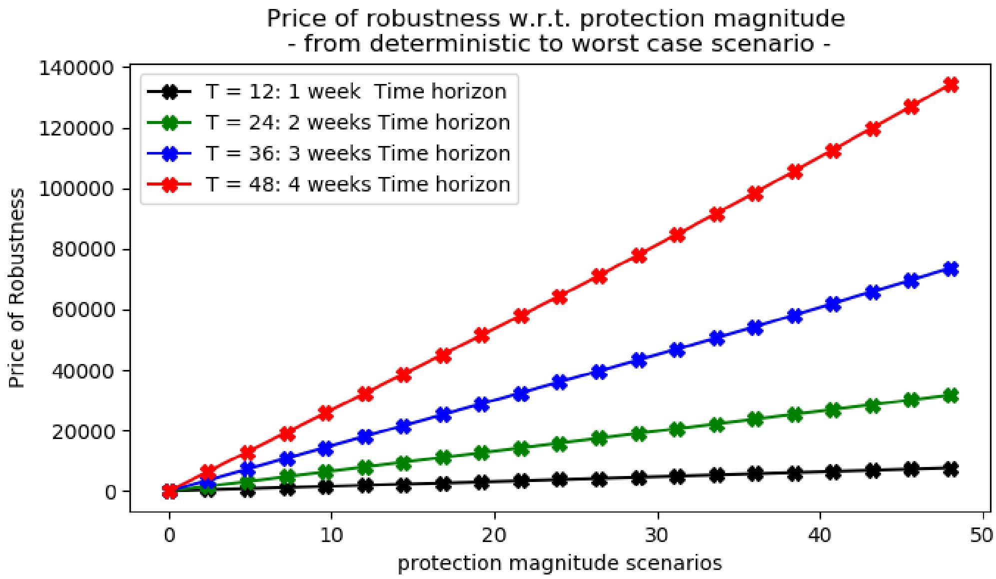


Figure 4.4. Price of robustness results

4.4 Conclusions

This chapter presented a tuned version of the model presented in [83] with additional complexity due to the introduction of robustness on the most critical parameters values. The formulation keeps supporting all the original strategic decisions that are critical in the business considered. This robust counterpart showed a good adjustable protection capacity when used in a real-world application. Findings concerning the controllable price of robustness in the considered case study are also interesting. Indeed, for the company level of service, this economical and controllable improvement is highly remarkable, taking into account the low margin of the activity. Future works may consider introducing more complexity in the formulation, such as considering production capacity dependent on the size of working teams.

Chapter 5

Price of Robustness Optimization through Demand Forecasting

Robust optimization can be effectively used to protect production plans against uncertainties. This is particularly important in sectors where variability is inherent the process to be planned. The drawback of robust optimization is the chance of producing over-conservative solutions with respect to the real occurrences of the stochastic parameters. Information can be added in order to better control the extra-cost resulting from considering the parameter variability. This work investigates how demand forecasting can be used in conjunction with robust optimization in order to achieve an optimal planning while considering demand uncertainties. In the proposed procedure, forecast is used to update uncertain parameters of the robust model. Moreover, the robustness budget is optimized at each planned stage in a rolling planning horizon. In this way, the parameters of the robust model can be dynamically updated tacking information from the data. The study is applied to a reverse logistics case, where the planning of sorting for material recycling is affected by uncertainties in the demand, consisting of waste material to be sorted and recycled. Results are compared with a standard robust optimization approach, using real case instances, showing potentialities of the proposed method. The contents of this chapter are also published in [49], a paper co-authored by the author, Claudio Gentile and Giuseppe Stecca.

5.1 Introduction

Robust optimization approaches are commonly applied in solving mathematical programming problems where a certain set of parameters are subject to uncertainty. Considering either production or procurement planning problems, these are dealing with the stochastic nature of demand, and a deterministic approach would definitely fail to provide concrete decision support when modeling those kinds of scenarios. Therefore, demand variability across the planning time horizon should be properly addressed. This can be done by introducing a protection function in each constraint according to the probabilistic robust approach presented in [15] and introduced in Chapter 2. This approach ensures deterministic and probabilistic guarantees on constraints satisfaction, and it does so in a linear framework.

In order to trade-off between optimality and level of robustness, a risk parameter has to be set to formulate the robust counterpart of the nominal model and its level of conservatism. At the same time, the level of conservatism of robust solutions can be such to constitute a significant cost in terms of optimality reduction, also known as price of robustness. This is often the case of over-conservative robust solutions, which consider demand values perturbations with low probability of occurrence. In a production planning setting, these solutions lead to extra costs resulting from additional production and storage.

Either risk-adverse or risk-taking decision makers will struggle to deal with the challenging trade-off of risk management by setting the robustness control parameter only, besides its odd interpretation. This topic is studied by the literature of robust approaches aiming at producing models better supporting the reality of decision-making in uncertain scenarios. Adjustable robust models, for example, is a branch of robust optimization introduced in [10] where some of the decision variables can be adjusted after some portion of the uncertain data reveals itself. This approach offers increased flexibility and produces less conservative solutions with respect to static robust optimization. An interesting application of this approach in scheduling problems is presented in [23]. In the aforementioned paper, the authors present an adjustable robust formulation where sequencing decisions are taken in a first stage, and scheduling decisions are made in a second stage. The reader can refer to the survey in [117] for a substantial knowledge of adjustable robust optimization (ARO) literature. Other approaches are Soft Robust Optimization [9], Light Robustness [47], Scenario-Based Robust Optimization [52] and the one proposed in [90].

Demand is the most critical information input of production planning and the main source of uncertainty as well. Addressing demand forecasting with proper time series analysis and regression models plays an important role in the overall decision processes. Features such as fitness of demand regressions models should be taken into account along with their parameters setting and forecast accuracy metrics.

Supply chain management is one of the most used scenarios to prove the potentialities of robust optimization. Some fundamental supply chain and inventory management models are revised using robust optimization theory in [16, 17]. The authors develop robust models for the optimization of the inventory in different settings and policies, such as the (s, S) case, allowing to control the level of conservatism of the solution, without assuming a specific demand distribution. The models are applied to a multi-period planning problem for single or networked warehouses, and for the uncapacitated and capacitated cases. The networked capacitated case is similar to the model studied in this work as an application case. Multi-period inventory management is addressed in detail in [94] where the concept of budget of uncertainty proposed in [16, 17] is extended for controlling the demand. This is done considering demand descriptive information such as standard deviation, seasonality and autoregressive aspects. The inventory policy introduced by the authors is solved by means of Second Order Cone Programming (SOCP).

In real case applications, robust optimization could induce over conservatism. The problem is addressed in [33] where correlation between uncertain parameters is taken into account in the definition of uncertainty sets in order to mitigate over conservatism. Another methodology used to shape the uncertainty sets based on data analysis has been proposed in [88]. The authors propose a data-driven robust approach of modeling the multi-product inventory problem with demand uncertainties. Basically, they construct an uncertainty set using historical demand data which are estimated not via demand descriptors but using a Support Vector Clustering (SVC) model.

The research work of this chapter aims to provide a mechanism for setting the level of conservatism of robust solutions according to accurate estimates of robustness costs. Thus, a framework integrating both a forecasting model and two extensions of the nominal multi-period planning model is proposed.

The central idea is to iteratively solve planning and forecasting problems, with the goal of finding the best configuration of robust parameters that minimizes the costs that result from overestimating or underestimating risk. These costs are the so-called *price of robustness* (Pr) as described in [15] and the potential extra cost resulting from overtime production (Po) whenever demand is underestimated. In the considered setting, the way of dealing with demand underestimation errors is indeed the activation of overtime production, while demand overestimation contributes to Pr costs.

In order to study the performance of the proposed method, a robust optimization problem arising from waste management and inverse production planning with demand uncertain coefficients is solved and variants of the model with different protection strategies are compared with real case instances.

The remainder of this chapter is organized as follows: Section 5.2 is dedicated to the definition of the planning problem formulations; the proposed framework aimed at the optimization of the risk considering parameters is presented in Section 5.3; Section 5.4 presents the experimental results, while Section 5.5 gives some conclusions and research perspectives.

5.2 Problems definition and modeling

This section presents the formulations of the problems used in the proposed framework, which is then detailed in the following Section 5.3.

Let τ be a planning period made of T time slots. Each time slot is indexed by

$t \in \mathcal{T} = \{1, \ldots, T\}$ and corresponds to a working shift where production can be activated. Thus, the planning consists of defining the production lot sizes and the schedules in order to meet the demand quantity d_t of each time slot t. Therefore, each planning period τ is given with a foreseen demand vector $d_T \in \mathbb{R}_+^T$.

Considering a deterministic planning problem $\mathcal{D}$, we refer to $\mathcal{R}$ as its robust counterpart, while a third model $\mathcal{E}$ replicates the same deterministic formulation of $\mathcal{D}$ and includes some additional decision variables regarding overtime production. Overtime production is the assumed strategy to counteract, with an extra cost, the uncovered demand.

The formulations of problems $\mathcal{D}$, $\mathcal{R}$, and $\mathcal{E}$ are presented in Subsection 5.2.1, Subsection 5.2.2, and Subsection 5.2.3, respectively.

5.2.1 Deterministic model $\mathcal{D}$

Dealing with a production planning setting, $\mathcal{D}$ is a mixed integer linear programming model to schedule and lot-size production operations. To better introduce a general formulation of $\mathcal{D}$, model notation for parameters and indexes is set out in the following.

T : time horizon length;

$t \in \mathcal{T} = \{1, \ldots, T\}$: index of working shifts across time

f_t : set-up cost of working shift at time t;

d_t : production demand at time t;

k_t : production capacity at time t;

c_t : unitary production cost at time t;

h_t : unitary inventory holding cost at time t;

I_0 : initial inventory level.

The model considers the following variables.

$y_t \in \{0, 1\}$: equal to 1 if production is activated at time t, 0 otherwise

$u_t \in \mathbb{R}^+$: production quantity at time t

$I_t \in \mathbb{R}^+$: inventory level at time t

The model minimizes the sum of production, setup and holding costs and is detailed as follows:

$$\min\ Z = \sum_{t \in T} c_t u_t + \sum_{t \in T} f_t y_t + \sum_{t \in T} h_t I_t \tag{5.1}$$

s.t.

$$u_t \leq k_t y_t \qquad \forall t \in \mathcal{T} \tag{5.2}$$

$$I_t = I_{t-1} - d_t + u_t \qquad \forall t \in \mathcal{T} \tag{5.3}$$

$$I_t \in \mathbb{R}^+ \qquad \forall t \in \mathcal{T} \tag{5.4}$$

$$u_t \in \mathbb{R}^+ \qquad \forall t \in \mathcal{T} \tag{5.5}$$

$$y_t \in \{0,1\} \qquad \forall t \in \mathcal{T} \tag{5.6}$$

The objective function (5.1) defines the minimization of the sum of the three cost terms, which are production, setup, and inventory costs, respectively. Constraints (5.2) bound the production quantity for each time period, and constraints (5.3) define the inventory.

5.2.2 Robust model $\mathcal{R}$

The mixed-integer linear programming model $\mathcal{R}$ defines the robust counterpart of $\mathcal{D}$ according to the robust approach presented in [15]. We first consider the parameters d_t, $t \in \mathcal{T} = \{1, \ldots, T\}$, which are subject to uncertainty, to take values according to a symmetric distribution with mean equal to the nominal value d_t in the interval $[d_t - \sigma_t, d_t + \sigma_t]$. Indeed, σ_t is the maximum deviation allowed for d_t. In order to meet the standard formulation of the nominal problem presented in [15], where parameters subject to uncertainties belong to inequality constraints only, the equality constraints (5.3) of $\mathcal{D}$ regarding demand quantities d_t are reformulated to turn them into inequality constraints. This is performed considering, for each period t, the sum of all demanded quantities up to that period, as in constraints (5.7) and (5.8) of the formulation of $\mathcal{R}$ presented in this section. According to the robust approach presented in [15], a parameter Γ_i is introduced for each constraint i holding one or more uncertainty coefficients. Γ_i is not necessarily integer and takes values in the interval $[0, |J_i|]$ where J_i is the set of the coefficients of constraint i being subject to uncertainty. The nominal problem $\mathcal{D}$ presents only one set of T constraints considering the coefficients d_t and these are the ones reformulated as inequality constraints. Therefore, we get $\Gamma \in R^T_+$, and because of this reformulation $|J_t| = t \; \forall t \in \{1, \ldots, T\}$. For each period t, Γ_t represents the number of coefficients that we consider as allowed to vary within their interval. In practice, we consider nature behaving like only a subset of the coefficients will change with respect to their nominal value. Indeed, as affirmed in [15], it is unlikely that all $|J_t|$ will change; so the idea of conservative robustness is to be protected against all cases that up to $\lfloor \Gamma_t \rfloor$ of these coefficients are allowed to change, and one coefficient d_t changes by $(\Gamma_t - \lfloor \Gamma_t \rfloor)\hat{d}_t$. Note that when $\Gamma_t = 0 \; \forall t \in \{1, \ldots, T\}$ we get the nominal deterministic scenario, while setting $\Gamma_t = |J_t| = t \; \forall t \in \{1, \ldots, T\}$ represents solving the problem of the worst case scenario. It is clear that by varying Γ the level of robustness can be flexibly adjusted against the level of conservatism of the solution.

Considering the structure of the constraints including d_t is important: because of the telescopic expansion of each set J_t as t goes from 1 to T (i.e. $|J_{t+1}| = |J_t| + 1$), we consistently constraint Γ_t to be bigger than or equal to Γ_{t-1}.
The following list reports all the additional variables and parameters that are required to introduce the robustness protection functions presented in [15] and formulate the robust counterpart of $\mathcal{D}$:

$\epsilon_t \in \mathbb{R}^+$: extra variables multiplying d_t for $t \in T$. These variables are introduced in order to have a variable multiplying the only set of parameters that are affected by uncertainty. These are indeed constrained to be equal to 1 for $t \in T$ as in constraint (5.11) of $\mathcal{R}$.

$z_t \in \mathbb{R}^+$: variables resulting from duality within Bertsimas and Sim's robustness theory; when multiplied by Γ_t, these variables provide their overall contribution to the protection function of constraint t.

$p_{t,k} \in \mathbb{R}^+$: variables resulting from duality within Bertsimas and Sim's robustness theory; they contribute to the protection function of constraint t with respect to the specific coefficient d_k.

$s_t \in \mathbb{R}^+$: variables resulting from duality and Bertsimas and Sim's robustness theory; multiplied by σ_t, they set the lower bound of the protection function contribution in each constraint t.

Γ_t : parameter to adjust the level of robustness of each period t.

The robust counterpart $\mathcal{R}$ of $\mathcal{D}$ is introduced as follows:

$$\min \; (5.1)$$

$$\text{s.t.}$$
$$(5.2), (5.4), (5.5), (5.6)$$

$$I_0 - \sum_{k=0}^{t} d_k \epsilon_k + \sum_{k=0}^{t} u_k + z_t \Gamma_t + \sum_{k=0}^{t} p_{t,k} \geq 0 \qquad \forall t \in \mathcal{T} \tag{5.7}$$

$$I_t = I_0 - \sum_{k=0}^{t} d_k \epsilon_k - \sum_{k=0}^{t} u_k + z_t \Gamma_t + \sum_{k=0}^{t} p_{t,k} \qquad \forall t \in \mathcal{T} \tag{5.8}$$

$$z_t + p_{t,k} \geq \sigma_t \; s_t \qquad \forall t \in \mathcal{T}, k \in \{0, ..., t\} \tag{5.9}$$

$$- s_t \leq \epsilon_t \leq s_t \qquad \forall t \in \mathcal{T} \tag{5.10}$$

$$\epsilon_t = 1 \qquad \forall t \in \mathcal{T} \tag{5.11}$$

Constraint (5.7) defines inventory considering the cumulative demand d_t up to period t, the overall produced quantity u_t up to period t, and the uncertainties protection function made of the joint contribution of $z_t\Gamma_t$ and the sum of $p_{t,k}$ for $k \in \{1, \ldots, t\}$. Constraint (5.7) sets the lower bound of the inventory for each period. Equality constraint (5.8) allows the inventory to be considered within the cost function. Constraints (5.9) and (5.10) resulted from duality in [15] robustness theory; where (5.9) sets the lower bound of the protection function contribution in constraints (5.7) and (5.8).

Solving model $\mathcal{R}$ allows us to evaluate the price of robustness (Pr) resulting from a specific protection Γ. This is done by computing the difference between the optimal objective function value of $\mathcal{R}$ and the optimal objective function value of $\mathcal{D}$.

5.2.3 Overtime production model $\mathcal{E}$

In the considered approach, overtime production is to be activated whenever standard scheduled production is not enough to meet the entire demand across the time horizon. For this reason, the third model $\mathcal{E}$ replicates the same deterministic formulation of $\mathcal{D}$ and includes some additional decision variables regarding overtime production. This additional production has of course a higher unitary cost with respect to standard scheduled production. Solving model $\mathcal{E}$ is intended to evaluate the need and the cost of overtime production (Po).

Considering the main decision variables of $\mathcal{D}$, such as $y_t \in \{0, 1\}$ and $u_t \in \mathbb{R}^+$, the formulation of $\mathcal{E}$ incorporates also $y'_t \in \{0, 1\}$ and $u'_t \in \mathbb{R}^+$ which correspond to the overtime production equivalent of the previous ones. These additional variables allow $\mathcal{E}$ to capture the extra costs resulting whenever the robust solution of $\mathcal{R}$ is not feasible when the true demand vector $\bar{d}$ is observed. Indeed, while both $\mathcal{D}$ and $\mathcal{R}$ are solved considering the predicted demand vector $\hat{d}$, instances of $\mathcal{E}$ are solved w.r.t. the true demand vector $\bar{d}$ and its set of standard production variables (i.e. y_t and u_t) are fixed to the values of the robust solution of $\mathcal{R}$ for the same corresponding scheduling time window. The corresponding unitary costs of these overtime production variables are $f'_t > f_t$ and $c'_t > c_t$, respectively. Therefore, the formulation of $\mathcal{E}$ is the following:

$$\min\ (5.1) + \sum_{t \in T} f'_t y'_t + \sum_{t \in T} c'_t u'_t \tag{5.12}$$

s.t.

$$u'_t \leq k_t y'_t \qquad \forall t \in \mathcal{T} \tag{5.13}$$

$$I_t = I_{t-1} - \bar{d} + u_t + u'_t \qquad \forall t \in \mathcal{T} \tag{5.14}$$

$$y'_t \in \{0, 1\} \qquad \forall t \in \mathcal{T} \tag{5.15}$$

$$u'_t \in \mathbb{R}^+ \qquad \forall t \in \mathcal{T} \tag{5.16}$$

$$I_t \in \mathbb{R}^+ \qquad \forall t \in \mathcal{T} \tag{5.17}$$

Solving $\mathcal{E}$ allows the evaluation of the cost of overtime production (Po) as the difference between the optimal objective function value of $\mathcal{E}$ and the optimal objective function value of $\mathcal{D}$. Thus, the sum P of the price of robustness (Pr) and overtime production (Po) can be computed according to a specific protection Γ (i.e. $P(\Gamma) = Pr(\Gamma) + Po(\Gamma)$). Given the above, a procedure named *Eval_P*, that generates a single evaluation of $P(\Gamma)$, is introduced. This procedure is part of the routine, detailed later in Section 5.3, aimed at the optimization of the robustness control vector Γ. The pseudocode of *Eval_P* is set out below.

$Eval\_P\left(\Gamma, \bar{d}, \hat{d}, \sigma\right)$:

1. Solve $\mathcal{R}\left(\hat{d}, \sigma, \Gamma\right)$ to get $y^*, u^*, Obj^*_{\mathcal{R}}$
2. Solve $\mathcal{D}\left(\hat{d}\right)$ to obtain $Obj^*_{\mathcal{D}}$
3. $Pr(\Gamma) = Obj^*_{\mathcal{R}} - Obj^*_{\mathcal{D}}$
4. Solve $\mathcal{E}\left(\bar{d}\right)$ where y and u are fixed to y^* and u^* respectively to obtain $Obj^*_{\mathcal{E}}$
5. $Po(\Gamma) = Obj^*_{\mathcal{E}} - Obj^*_{\mathcal{D}}$
6. Return $P(\Gamma) = Pr(\Gamma) + Po(\Gamma)$

5.3 Robustness control optimization

The main notation used in the proposed framework is defined in Table 5.1.

Table 5.1. Notation

Symbol	Description
$\tau \in \mathcal{T} = \{1 \dots N\}$	Planning time period
T	Time slots for each planning period τ
$\Gamma(\tau) \in \mathbb{R}^T_+$	Robustness control parameters vector for planning period τ
ρ	Number of planning periods used as forecasting model training data
$D(\rho, \tau)$	Demand time-series considering the planning periods from $\tau - \rho$ to τ corresponding to time slots from $(\tau - \rho)T$ to τT
$\mathcal{F}\ (D(\rho, \tau))$	Forecasting model
$\bar{d}(\tau) \in \mathbb{R}^T_+$	Observed demand vector of planning period τ
$\hat{d}(\tau) \in \mathbb{R}^T_+$	Predicted demand vector of planning period τ
$\hat{\sigma}(\tau) \in \mathbb{R}^T_+$	Predicted demand standard deviation vector
$\sigma(\tau) \in \mathbb{R}^T_+$	Maximum allowed deviation of $\hat{d}(\tau)$ from $\bar{d}(\tau)$
$\mathcal{D}\ (d(\tau))$	Deterministic version of the planning model
$\mathcal{R}\ (d(\tau), \sigma(\tau), \Gamma(\tau))$	Robust counterpart of the planning model
$\mathcal{E}\ (d(\tau))$	$\mathcal{D}\ (d(\tau))$ with additional variables modelling overtime production
$Obj^*_{\{model\}}$	Objective function value at the optimizer of a specific model
Pr	Price of robustness equal to $Obj^*_{\{\mathcal{R}\}}$ minus $Obj^*_{\{\mathcal{D}\}}$
Po	Price of overtime production equal to $Obj^*_{\{\mathcal{E}\}}$ minus $Obj^*_{\{\mathcal{D}\}}$
P	Sum of Pr and Po

The forecasting model $\mathcal{F}$ employed in the framework to evaluate the expected demand is presented in Section A of the appendix; its implementation is available as open source software, is called Prophet [110], and it uses a decomposable time series model [56] with three main model components: trend, seasonality, and holidays.

The robustness control vector Γ is learned by a routine properly built in order to achieve this parameter tuning objective. The optimization of Γ is to find the value that minimizes the sum $P(\Gamma)$ of the price of robustness $Pr(\Gamma)$ and the potential extra costs resulting from overtime production $Po(\Gamma)$. Given below is a detailed routine that seeks for the best configuration of Γ for a considered planning period τ with its corresponding demand forecast $\hat{d}(\tau)$ and its true observations $\bar{d}(\tau)$. Its pseudocode is set out below. We refer to this routine as $Optimize\_\Gamma\left(\Gamma_0, \Gamma_{step}, \bar{d}(\tau), \hat{d}(\tau), \sigma(\tau)\right)$:

1. Set $\Gamma_0 \in R_+^T$: the starting configuration of Γ
2. Set $\Gamma_{step} \in R_+^T$: a vector of the updating step sizes of each component Γ_t of Γ
3. Set $max_k = floor\,(1/\Gamma step)$: maximum number of iterations k for a complete search over the space of $\Gamma \in R_+^T$
4. Set $k = 0$; $\Gamma_k = \Gamma_0$
5. $P(\Gamma_k) = Eval\_P\left(\Gamma_k, \bar{d}(\tau), \hat{d}(\tau), \sigma(\tau)\right)$
6. Set $P^* = P(\Gamma_k)$; $\Gamma^* = \Gamma_k$
7. While $k \leq max_k$
   (a) $k = k + 1$
   (b) $\Gamma_k = \Gamma_{k-1} + \Gamma_{step}$
   (c) $P_k = Eval\_P\left(\Gamma_k, \bar{d}(\tau), \hat{d}(\tau), \sigma(\tau)\right)$
   (d) if $P_k \leq P^*$
   $P^* = P_k$
   $\Gamma^* = \Gamma_k$

Whatever setting of Γ_0 and Γ_{step} is made, this must be done according to the peculiar structure of constraints (5.7), (5.8) of the formulation of $\mathcal{R}$. Indeed, as stated in Section 5.2, before introducing model $\mathcal{R}$, the telescopic expansion of each set J_t (i.e. $|J_{t+1}| = |J_t| + 1$) constrains each component Γ_t of the protection vector Γ to be bigger than or equal to the component Γ_{t-1} and smaller than t. The setting of both Γ_0 and Γ_{step} must be consistent with these constraints. Given a scalar $\gamma_{step} \in \{0 \ldots 1\}$, a possible rule for setting each component $\Gamma_{step}(t)$ of Γ_{step}, such that the previous constraints are satisfied, is the following:

$$\Gamma_{step}(t) = \gamma_{step}\; t \qquad \forall t \in \{1 \ldots T\}$$

This *Optimize*_Γ routine can be embedded in the proposed framework for solving the multi-period planning problem under uncertainties. The purpose of this framework is to provide automated decision support to implement an appropriate robustness control vector that minimizes the aforementioned costs of over- or underestimating risk in this class of planning problems.

Referring to the most recent demand realizations, and to its corresponding time-series $D(\rho,\tau)$, we consider τ planning period as the latest T time slots part of $D(\rho,\tau)$. This demand time-series $D(\rho,\tau)$ can be used along with *Optimize*_Γ to mine what would have been the best robustness control vector Γ^* for the planning period τ. This is indeed described in the following:

1. Set ρ and τ, then consider $D(\rho,\tau)$ and get $\bar{d}\,(\tau)$
2. Solve $\mathcal{F}\ (D(\rho,\tau))$ to forecast $\hat{d}(\tau)$ and $\hat{\sigma}(\tau)$
3. Set Γ_0 and Γ_{step}
4. $\Gamma^* = \mathit{Optimize\_}\Gamma\Big(\Gamma_0, \Gamma_{step}, \bar{d}(\tau), \hat{d}(\tau), \sigma(\tau)\Big)$

The rationale of the proposed framework is the use of $D(\rho,\tau)$ and its corresponding best configuration Γ^* to solve the planning problem of the future planning period $\tau+1$. Therefore, for each observed demand time-series $D(\rho,\tau)$, the corresponding Γ^* impact in terms of $P(\Gamma^*)$ is evaluated when Γ^* is used to protect against the uncertainties of the very immediate future period $\tau+1$. Considering a sequence of framework implementations, at each of these it is reasonable to set Γ_0 starting configuration to $\Gamma^*_{\tau-1}$. The experimental results of both *Optimize*_Γ and its implementation framework are presented in Section 5.4. Performances in terms of P costs are compared with P resulting from either the deterministic and worst-case scenario approaches that we refer to as $P(\Gamma_{nominal})$ and $P(\Gamma_{worstecase})$, respectively.

5.4 Application to Waste Management

This section holds the experimental results obtained by applying the proposed methodology to a waste management (WM) setting.

With respect to the problem addressed, while it is possible to find several applications of robust optimization to supply chain and production problems, fewer research works address circular economy and reverse logistics related cases. Stochastic based approaches in waste flow optimization have been addressed in [107] and [119]. The work of [63] develops a robust model where box uncertainty and robustness budget is used to control uncertainty in a closed loop supply chain in the textile industry. The paper considers recycling operations in a networked environment, considers the over conservatism problem, but does not consider demand characteristics. In [58], p-robust constraints are used to control disruption events. In [44] a multi-objective multi-period multi-product multi-site aggregate production planning model is solved with reverse flow considerations. In this case, the robust approach is pretty standard. In [82], the same problem addressed as an application scenario of this work, is treated with classical robust theory.

In WM, the planning consists of scheduling and lot sizing each phase of a recycling material sorting process. The planning model presented in [83] is considered as the deterministic model $\mathcal{D}$ for testing the proposed framework. The formulation of $\mathcal{D}$ is reported in Section B of the appendix. This model supports several strategic decisions that are critical in the considered WM application. It can be described as a variant of a lot sizing model with non-linear costs (approximated by mean of piece-wise linear functions) with the additional features of scheduling the operations and allocating the appropriate workforce dimension. The aim of the model is finding the best allocation of operators to each working shift in order to process the recycling material quantity d_t arriving at each time slot t. In this scenario, a time slot is indeed a working shift where teams of operators may be allocated. The robust counterpart of $\mathcal{D}$ is presented in [82] and is considered as $\mathcal{R}$ for what concerns the experimental results. The formulation of $\mathcal{R}$ is reported in Section C of the appendix. Model $\mathcal{E}$ is derived from model $\mathcal{D}$ in [83] as illustrated in Section 5.2.3 and its formulation is reported in Section D of the appendix.

*Optimize*_Γ routine is supposed to densely explore the search space of Γ for an exhaustive search aimed at the optimization of P. In order to validate its performances, some preliminary experiments are performed over a set of subsequent planning periods: for each planning period τ, performances in terms of P costs resulting from applying Γ^* found by *Optimize*_Γ are compared with P resulting from the deterministic (i.e. nominal) and worst-case scenario approaches. The results are illustrated in Table 5.2 and discussed below. The accuracy of the forecast model is reported in terms of symmetric mean absolute percentage error (i.e., SMAPE), an accuracy measure based on percentage errors which is usually defined as follows:

$$\text{SMAPE} = \frac{1}{n}\sum_{t=1}^{N}\frac{|F_t - A_t|}{(|A_t|+|F_t|)/2}$$

where A_t is the actual value and F_t is the forecast value. The absolute difference between these values is divided by half the sum of absolute values of the actual value A_t and the forecast value F_t. Then the value of this calculation is summed for every fitted point t and divided by the number of fitted points n.
The table's columns present the reduction of robustness and overtime production costs P achieved by $P(\Gamma^*)$ with respect to the deterministic $P(\Gamma_{nominal})$ and worst-case $P(\Gamma_{worstecase})$ approaches. The presented values of costs reduction result from

the following expressions:

$$wrt\ nominal = \frac{P(\Gamma^*) - P(\Gamma_{nominal})}{P(\Gamma_{nominal})}$$
$$wrt\ worstecase = \frac{P(\Gamma^*) - P(\Gamma_{worstecase})}{P(\Gamma_{worstecase})}$$

The following columns of Table 5.2 present the percentage of protection guaranteed by each Γ^* considered, obtained as the ratio between the sum of the components of Γ^* and the sum of the components of the vector Γ corresponding to the worst case; the SMAPE accuracy metrics of the forecasting model; while the last column presents the sum of all the forecasting residuals of the planning period to consider forecast bias, that is overestimating (a positive value of bias) or underestimating (a negative value of bias) the future demand. Indeed, the forecast model is implicitly introducing robustness to the planning solution whenever is overestimating the demand realization. At the same time, the model $\mathcal{F}$ is incautiously fostering the importance of robust planning solutions whenever it is underestimating the demand realization. Indeed, considering systematical biased behavior of forecast models is crucial for a proper planning. Results of Table 5.2 show how Γ^* moderates its robustness contribution with respect to forecast bias over the planning period: its percentage protection remains minimal (or close to zero) for positively biased prediction in order to produce solutions close or equal to a deterministic (nominal) solution, while it is providing a stronger protection to uncertainties when dealing with underestimating demand forecasts. However, for both types of biased prediction scenarios, *Optimize*_Γ routine produces configurations of Γ minimizing risk costs with respect to either deterministic and worst-case approaches. Figure 5.1 shows an example of *Optimize*_Γ instance solving.

5.4.1 Analysis of results

As described at the end of Section 5.3, considering an observed demand time-series $D(\rho, \tau)$, the proposed framework essence is using the very close past best configuration Γ^* to protect against the uncertainties of the very immediate future. That is, solving the robust planning problem $\mathcal{R}\left(\hat{d}, \sigma, \Gamma^*\right)$ of the subsequent future planning problem $\tau + 1$. Therefore, a new set of experiments is performed to test the performance relative to the observed costs P of robustness and overtime production of the very next future. All instances are created by a real-world case study from a waste sorting plant located next to Rome, Italy. Results are shown in Table 5.3. As in Table 5.2, performances in terms of $P(\Gamma^*)$ costs are compared with P resulting from either the deterministic $P(\Gamma_{nominal})$ and worst-case $P(\Gamma_{worstecase})$ scenario approaches. Demand arising from the considered real-case study is particularly unstable, and it seems reasonable to consider this adverse feature of the time-series D particularly challenging for the proposed framework. Indeed, no autocorrelations

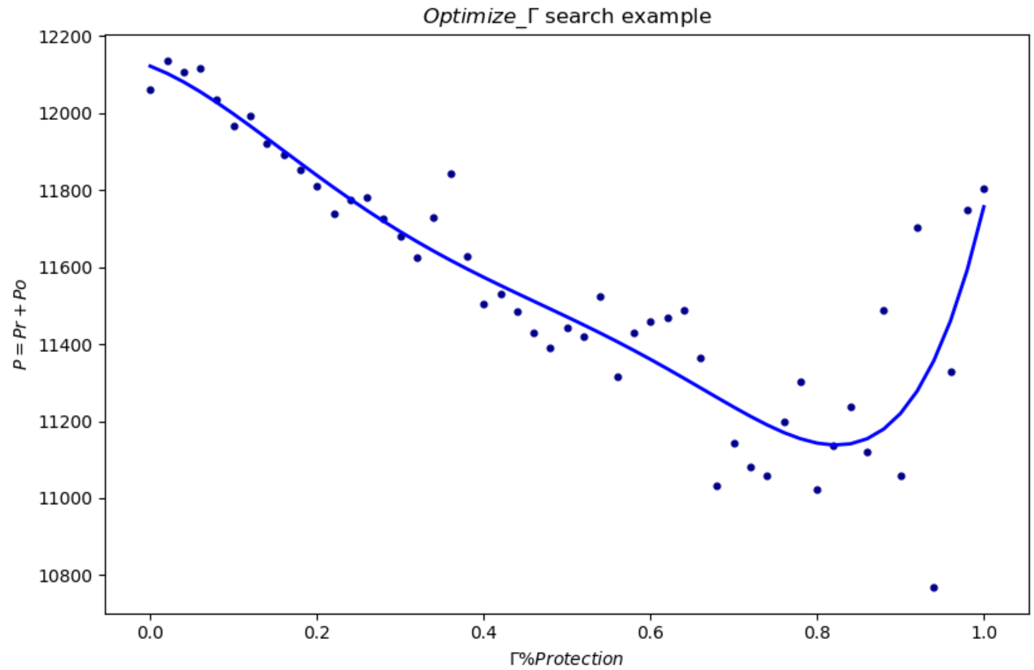


Figure 5.1. Example of an *Optimize_*Γ instance solving

are present either for small or larger seasonal lagged values of D. Therefore, the larger the planning period $\tau+1$ towards the future, the smaller the chances of a good performance of Γ^* learned over the immediate past planning period τ. Experiments presented in this section consider 50 instances of subsequent planning periods of two weeks (i.e. 12 time slots considering 6 weekly working days of 2 working shifts each). Table 5.3 highlight two main important results: the framework provides stronger protections to uncertainties (as featured in Γ^* column) for most of the occasions of underestimation of demand realization and it does so while guaranteeing a lower cost P of robustness and eventual overtime production with respect to the deterministic and worst-case approaches. Indeed, out of the 30 instances where $\mathcal{F}$ underestimates the demand, 21 of these reveal a valuable P cost reduction, that is about 70% of the occasions. At the same time, costs reduction are also observed for 7 of the remaining 20 occasions (35%) where $\mathcal{F}$ overestimate the demand. Moreover, 42 of all 50 instances (84%) prove how the framework is providing protection vectors Γ^* with smaller associated $P(\Gamma^*)$ with respect to $P(\Gamma_{worstecase})$.

5.5 Conclusions

This chapter addressed the problem of controlling the extra-costs resulting from considering demand uncertainties in planning problems. Robust optimization theory is applied to both a general production planning model in the general discussion and to a waste management use-case regarding recycling operations planning. An

wrt nominal	wrt worst-case	Γ^*	SMAPE	Tot. Pred. Bias
-0.30	-0.68	0.20	0.50	5720
0.00	-0.44	0.00	0.62	15000
0.00	-0.40	0.00	0.59	6880
0.00	-0.51	0.00	0.66	11300
-0.09	-0.38	0.08	0.55	7080
-0.20	-0.62	0.04	0.70	13380
-0.48	-0.72	0.12	0.58	8940
-0.18	-0.57	0.28	0.76	16200
-0.32	-0.41	0.30	0.60	-18400
-0.20	-0.23	0.47	0.60	-27440
-0.18	-0.31	0.30	0.49	-7040
-0.23	-0.35	0.16	0.55	-3460
-0.45	-0.56	0.12	0.80	18100
-0.14	-0.28	0.16	0.67	-4280
-0.06	0.15	0.26	0.78	-33440
-0.03	-0.28	0.32	0.61	-10260
0.00	-0.46	0.00	0.67	11240
0.00	-0.65	0.00	0.64	1820
-0.32	-0.57	0.04	0.63	25700
-0.12	-0.14	0.12	0.70	-3160
-0.31	-0.62	0.16	0.52	19140
-0.26	-0.39	0.04	0.52	-3300
0.00	-0.72	0.00	0.55	5880
-0.53	-0.58	0.02	0.79	3860
-0.19	-0.59	0.02	0.66	1220
-0.54	-0.74	0.10	0.70	3140
-0.26	-0.31	0.30	0.63	520
-0.18	-0.27	0.55	0.70	-11900
-0.12	-0.39	0.06	0.67	-11760
-0.13	-0.06	0.43	0.49	-17560
-0.14	-0.16	0.39	0.70	-30360

Table 5.2. *Optimize*_Γ validation results

$P(\Gamma^*)$	$P(\Gamma_{nominal})$	$P(\Gamma_{worstecase})$	wrt nominal	wrt worst-case	Γ^*	SMAPE	Tot.Pred.Bias
1838	3461	3062	-0.47	-0.40	0.20	0.62	-18200
2381	2586	3605	-0.08	-0.34	0.16	0.88	-3440
3225	3451	4560	-0.07	-0.29	0.14	0.48	-12160
2268	2268	3737	0.00	-0.39	0.00	0.59	6880
1579	1546	3246	0.02	-0.51	0.02	0.70	13380
1942	1708	3225	0.14	-0.40	0.16	0.76	16200
2398	3310	3402	-0.28	-0.30	0.30	0.60	-18400
3362	3890	2674	-0.14	0.26	0.30	0.60	-27440
3081	3207	3677	-0.04	-0.16	0.49	0.49	-7040
2925	2765	3305	0.06	-0.11	0.18	0.55	-3460
1301	2378	3007	-0.45	-0.57	0.16	0.80	18100
3322	3064	3946	0.08	-0.16	0.12	0.67	-4280
2634	2174	2861	0.21	-0.08	0.18	0.61	-10260
3226	1607	3042	1.01	0.06	0.32	0.67	11240
1428	1428	3945	0.00	-0.64	0.00	0.64	1820
1832	1832	2906	0.00	-0.37	0.00	0.63	25700
2646	3076	4151	-0.14	-0.36	0.10	0.70	-3160
1804	1605	3046	0.12	-0.41	0.08	0.52	19140
2509	3459	4109	-0.27	-0.39	0.02	0.52	-3300
2542	2542	2929	0.00	-0.13	0.00	0.79	3860
1797	2676	3558	-0.33	-0.49	0.37	0.65	-16540
4029	4546	4449	-0.11	-0.09	0.65	0.53	-35380
3696	3997	3759	-0.08	-0.02	0.81	0.98	-40840
1932	2289	2715	-0.16	-0.29	0.18	0.50	-3460
1431	1474	2955	-0.03	-0.52	0.02	0.66	1220
1754	2253	2190	-0.22	-0.20	0.08	0.53	-9200
2855	1758	3095	0.62	-0.08	0.06	0.70	3140
3848	3626	3906	0.06	-0.01	0.10	0.63	520
2575	2276	2525	0.13	0.02	0.35	0.70	-11900
3188	2167	3172	0.47	0.01	0.43	0.67	-11760
3747	3748	3772	0.00	-0.01	0.43	0.70	-30360
2527	3012	3548	-0.16	-0.29	0.39	0.62	-30640
2562	3041	3861	-0.16	-0.34	0.16	0.42	-12580
1039	2235	2495	-0.53	-0.58	0.12	0.55	9360
3033	3790	3925	-0.20	-0.23	0.06	0.64	-12240
1865	1620	2895	0.15	-0.36	0.22	0.49	2160
2451	2409	2863	0.02	-0.14	0.02	0.63	9860
1151	1473	2894	-0.22	-0.60	0.10	0.71	13100
3204	2746	2665	0.17	0.20	0.04	0.54	-1260
2782	3418	4385	-0.19	-0.37	0.26	0.77	-12640
2095	1600	3125	0.31	-0.33	0.20	0.67	12600
3104	3066	2850	0.01	0.09	0.02	0.74	11280
2006	1888	2675	0.06	-0.25	0.12	0.78	-6480
2946	2007	2607	0.47	0.13	0.16	0.86	9240
3060	1443	2270	1.12	0.35	0.41	0.60	-7820
2722	2722	3563	0.00	-0.24	0.00	0.64	-23260
2220	3087	2839	-0.28	-0.22	0.28	0.79	-1800
2536	1987	2802	0.28	-0.10	0.26	0.68	-3180
1754	1673	3277	0.05	-0.46	0.04	0.71	3680
2108	2216	3015	-0.05	-0.30	0.60	0.24	9580

Table 5.3. Framework results in real case application

optimization procedure determining the best possible robustness budget to use in successive planning stages is proposed. In this way it is possible to dynamically update both the estimated demand and the robustness budget, helping to balance the extra costs of robustness and extra costs due to overtime production. The framework is tested in a real case environment where demand does not follow a specific probability distribution. The results show that, most of the time, the classical robust approach is over conservative. Moreover, when the forecasts overestimate the observed demand, the robustness budget Γ can be effectively optimized. Forecasting model features and their overall effect over the protection cost are not addressed by this study and they could in a future work. Moreover, the proposed approach can be applied to different planning problems and tested against different scenario in future works.

Chapter 6

Customer Cost Forecasting through Patterns Learning of Optimal Capacity Allocation

Production, logistics, and service systems involve multiple customers being served by shared resources. Once either a process or a service concerning several customers is optimized, business sustainability and profit opportunities become a matter of contracted commercial offers and business inherent risks sharing. Commercial offers are indeed intended to cover the expected costs, be competitive without reducing net margin, and robust to risks resulting from the uncertainties affecting the business. This chapter presents a framework that integrates an operational research model providing optimal capacity allocation with a learning model performing customer cost estimation. This estimator relies on a set of input features related to each customer. The aim is to provide a cost forecasting framework for contract management that considers a fair allocation of costs to customers. Validation of the approach is done with real case instances of a pick-up and delivery routing model dealing with reverse logistic operations. The author introduces a new formulation of the considered routing problem and show the effectiveness of the proposed method. The contents of this chapter are based on a paper submitted by the author for publication and co-authored by Marco Boresta and Giuseppe Stecca.

6.1 Introduction and literature review

To meet the ambitious targets of the sustainability paradigm, new advanced information systems, digital technologies, and mathematical models are required. With the increased interest in sustainable production and services to promote economic growth and development while minimizing their adverse effects on the environment, this trend is particularly rising. At the heart of this scenario there are both smart industries, in which data flows steadily between well-connected processes, and the opportunity of using that information to better support decisions affecting each business target, including profitability and sustainability. Particularly, these latter ones should not be viewed as competing goals; rather, they should be addressed simultaneously within a comprehensive vision that adequately addresses these objectives. Organizations can achieve these goals through innovative management approaches, such as recognizing sustainable efficiency and profitability to be inextricably linked by the savings that result from an optimal capacity allocation. Savings can be of many kinds according to sustainability metrics that measure the direct impact of the social or environmental issue a company is addressing (including energy, emissions, climate, labor, water, race and gender) and business metrics such as all operational and strategic costs.

This chapter intends to extend this research area, addressing the problem of forecasting the cost of serving customers while taking into account the benefit of sharing production/service capacity for a set of independent customers. These type of benefits in cost allocation are addressed by the literature in different settings and with different approaches. In [118] a set of firms have the choice of either operating their own production/service facilities or investing in a facility that is shared; the problem is formulated as a cooperative game and there is a cost allocation that is in the core under either the first-come, first-served policy or an optimal priority policy. In [72], firms decide on the allocation of demand from different sources to different facilities to minimize delay and service-fulfillment costs. Considering logistics, the authors of [116] present a new approach to horizontal carrier collaboration: the sharing of distribution centers with partnering organizations. This approach allows transport companies to cooperate to increase their efficiency levels by, for example, the exchange of orders or vehicle capacity. The same source report that, to ensure cooperation sustainability, collaborative costs need to be allocated fairly to the different participants, and they analyze the effects of different cost allocation techniques with numerical experiments. Thus, also in the aforementioned work, capacity is shared across firms that decide to operate collectively as a coalition. Moreover, they highlight the importance of a fair cost allocation of the shared capacity. In [4], capacity sharing is exploited in the horizontal collaboration between taxis in the settings of Demand-Responsive Transport (DRP); in the paper, the authors define and solve optimization problems aimed at minimizing the total cost of the service while maintaining a balance of work among operators. In logistics applications, it is common to aggregate customers in order to optimize the service. In [106], a negotiation based scheme is used to exploit customer aggregation in a waste management application. The aggregation can be done using concepts related to clustering or creating corridors [76]. The concept of green corridors can also be used to lower the environmental impact of logistics services [26].

Capacity-sharing in logistics solutions is definitely a pathway towards sustainability. Indeed, the research effort of this work addresses (as a use-case) a logistic scenario where capacity sharing solutions ensure sustainability without collaboration between the participants. These participants are the customers sharing the transport capacity of a logistic company that provides pick-up and delivery solutions. With respect to the evaluated research, this contribution intends to provide a cost forecasting framework for contract management of logistics operators considering fair allocation of costs to customers. Customers have heterogeneous locations, visiting time windows and service variability that may represent distinctive valuable features for the customer cost forecasting model. In the considered scenario, logistic costs need to be fairly allocated to each customer in order to ensure that the forecasting model can be trained to provide fair customer cost estimates for competitive commercial offers.

Given the above, this work comes at a time when many companies are increasingly considering innovation solutions linked to sustainability challenges, and when the literature is still scarce on research incorporating non-cooperative sharing of capacity allocations.

The reminder of this chapter is organized as follows: Section 6.2 describes the learning framework and its details; a novel logistic model is presented in Section 6.3; Section 6.4 introduce a real-case scenario application of the new model in Section 6.3, Section 6.5 reports the experimental results of applying the learning framework to the application in Section 6.4, and provides insights and in-depth analysis of the customer features importance. Finally, Section 6.6 gives some conclusions and reports research perspectives.

6.2 Customer cost learning framework

This section describes a framework that integrates an operational research (OR) model providing optimal capacity allocation with a machine learning (ML) model performing customer cost estimation. This framework is presented as a general approach for any OR model allocating either capacity or resources across multiple non-cooperative customers. In Section 6.5 this framework is applied to a real-case of a reverse logistic (RL) setting regarding waste management. The RL setting is described in Section 6.4 and the considered OR model is the one detailed in Section 6.3.

The main objective of this scheme is evaluating the impact of the customer features over the customer cost that results from the optimization of the process/service concerning that customer. The same objective applies for all engineered features arising from the specific instance concerning that customer. Therefore, the idea behind this framework is considering these set of features and their inherent variability in order to evaluate their explanatory power within a customer cost regression task. Accordingly, the purpose of the regression model is providing cost forecasts for a new production/service request. This cost estimate is the essential input of any profitable and competitive commercial offer. Therefore, Explainable Artificial Intelligence (XAI) techniques are used at the very end of the framework to validate the information contribution of each considered feature. The reader can refer to the survey of Das and Rad (2020) [35] for substantial knowledge over the opportunities and challenges in XAI. The framework is illustrated in Figure 6.1 and is made of the following main components:

- Data Augmentation
- OR model
- Cost Allocation Strategy
- ML Dataset
- ML regression model
- ML model Explainability

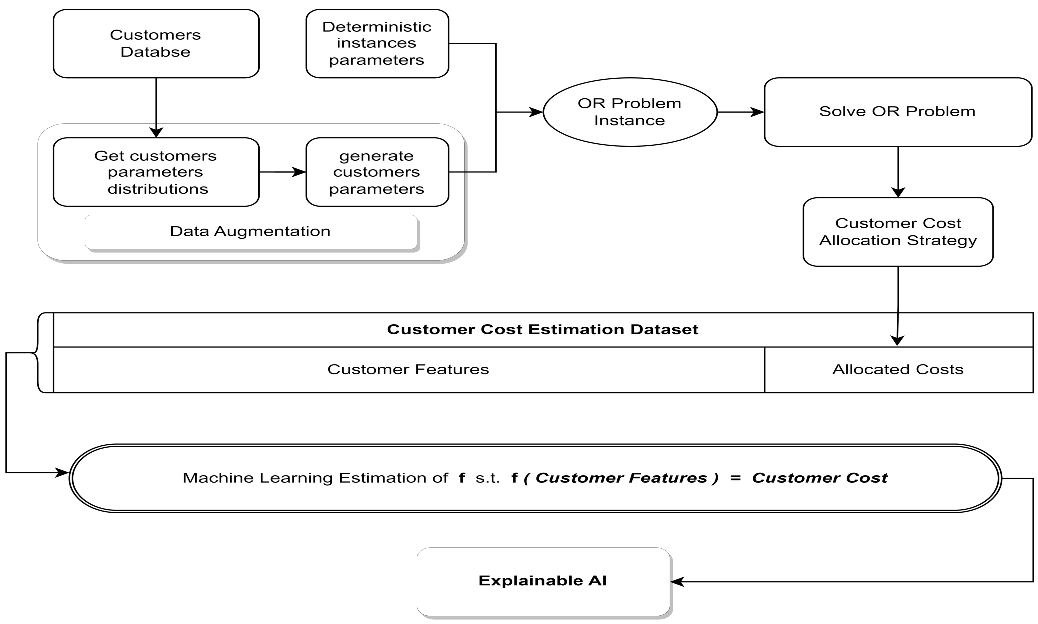


Figure 6.1. Customer Cost Patterns Learning Framework

Data augmentation (DA) in data analysis are techniques used to increase the amount of data by adding slightly modified copies of already existing data or newly created synthetic data from existing data. It acts as a regularizer and helps reduce overfitting when training a machine learning model [98]. In the proposed framework, performing DA is particularly important to ensure that the regression model is identified from a dataset containing all relevant observations of the possible customer features values. In particular, the amount and variety of data is increased by sampling values from reasonable probability distributions to be determined from a given customers database. Given the above, DA is used to produce synthetic data in order to perform a comprehensive scan of the customers variability and the associated risk.

As mentioned above, the OR model can be any model incorporating non-cooperative sharing of capacity allocations across multiple customers. Still, this work focuses on the VRP with Pickup and Delivery and with Semi Soft Time Windows that is presented in Section 6.3.

The cost allocation strategy represents one of the most important component of the presented framework, both in terms of fairness and expected regression performance. In either production or services scenarios, costs need to be fairly allocated to each customer in order to ensure that the forecasting model can be trained to provide fair customer cost estimates. This is also relevant for delivering competitive commercial offers. The following Section 6.2.1 presents an allocation strategy that combines three different approaches for the considered logistic setting.

The main types of information hold in a record of the regression dataset are the customer related features, some additional engineered features arising from the instance concerning that customer, and the allocated cost according to the selected strategy. Considering the logistic scenario, basic customer features concern pickup and delivery locations, time window bounds and width, service times, number of surrounding customers within distance thresholds in the customers database, distance and duration information between pickup node, delivery node and the depot. Moreover, some instance related features can be engineered in order to extract any relevant information to explain the allocated cost. Some examples w.r.t. the logistic setting are the vehicle tour total distance and duration, the number of costumers served within the tour, the number of surrounding customers within some distance thresholds that are served in the specific instance.

The ML regression task investigates the relationship between the set of the described features and the dependent outcome being the expected customer cost. The objective of the ML model is that of learning how to predict new, unseen data. The ability to perform well on inputs not seen during the training phase is called generalization, and it provides insights into how well the model will perform on unseen data. As a consequence of this, a data segregation stage is often used to split the dataset into training and test subsets. Although the training of the model is performed using the former and by minimizing the loss function on this set, a bigger interest is placed on the performance measures that are normally evaluated on the second set of data, the test set. Additional information can enrich the set of data within a feature engineering phase. To decrease the amount of data ingested into the training model, shorten training times, improve the generalization properties of the model and its interpretation, explanatory features with high information content can be extracted in accordance with feature selection strategies. Multiple classes of modeling architectures of various complexity can be tested with respect to their accuracy performance. Validation techniques can be employed to avoid overfitting issues and guarantee model quality aspects such as proven generalization properties, reliability and robustness to significant datasets changes. The performance of models can be assessed by comparing predictions and actual observations on the test subset using relevant accuracy metrics.

In the end, XAI techniques are used to validate the information contribution of each considered feature. Indeed, XAI methods are included in the framework in order to overcome the issues related to the lack of interpretability of ML models. XAI methods allow identifying the impact of the original interpretable features on predictions by evaluating the effect of single input features on the outcome of interest, while excluding the effect of other features. The reader can refer to a recent review of Linardatos et al. (2020) [71] on machine learning interpretability methods.

6.2.1 Fair Cost Allocation

Given the solution of a capacity allocation model, it is critical to find a way to divide the resulting overall production/service cost, in a way that is fair to all customers. Different cost allocation solutions for scenarios that can be modelled as cooperative games have been proposed [30][67]. The problem in transportation logistics is determining how much of a route's total cost should be allocated to each of the customers served. This fair division problem turns out to be very challenging and is addressed in recent literature with different strategies. From relatively simple to state-of-the-art solutions are reported in [62]. An ideal solution is well-defined and is based on the Shapley value [96] of the Travelling Salesman Game (TSG). In essence, the Shapley value of player/customer i is an average of all marginal costs due to player i, over all possible coalitions, including player i. The Shapley value is the only attribution method that satisfies the properties of Efficiency, Symmetry, Dummy and Additivity [96], which together can be considered a definition of a fair allocation and makes it a preferred choice for a fair cost allocation scheme [86]. Unfortunately, this method has exponential computational complexity, which makes it practical only for small scale examples involving few customers. In real-case applications, scenarios involving a few dozen or even a few hundred customers are more typical. This has led to substantial research effort dedicated to finding approximations with lower computational complexity. Novel methodologies to generate high-quality approximations to the Shapley values are presented in [86] and [68].

Considering the scope of this research work, the cooperative hypothesis and the computational complexity of the Shapley value, along with the amount of customers involved in the considered instances and the data augmentation requirements of the designed framework, this research work proposes a cost allocation strategy that is out of the Shapley value paradigm. The proposed allocation strategy appears to be fair and is computationally tractable in all allocation examples. Moreover, this strategy applies to the solution of a VRP with Pickup and Delivery, hence a customer i is identified by two distinct nodes: the one of pickup P_i and the one of delivery D_i.

The proposed allocation strategy provides a weighted average of the outcomes of three different allocation rules, namely:

- *Stand-Alone* (SA)
- *Neighbors Savings* (NS)
- *Extreme Neighbors Savings* (ENS)

Stand-Alone rule assigns costs in proportion to the shortest paths distances of the route that starts from the depot towards the pickup node P_i, thus to the delivery node D_i, then returns to the depot. This travelled distance can serve as a first proxy in order to allocate a proportion of the total route cost. For each customer, the SA proportion is obtained from the normalization of all travelled distances, computed in such a way, of the customers served by the same vehicle. This rule assigns a cost that is proportionate to both P_i and D_i distances and takes into account these nodes as independent of the other visited ones, embedding the non-cooperative scenario. At the same time, this represents its main downside, as SA rule does not consider the reduction in costs due to proximity to other served customers, both in terms of pickup and delivery.

Neighbors Savings rule is intended to recover the main SA downside. This is accomplished by evaluating the marginal cost of visiting P_i and D_i in the vehicle tour. With this objective, the following quantities are considered for each customer i being served by vehicle k :

C_{tot} : the total distance travelled by a vehicle k visiting customer i in its tour.

$C_{deviation}$: the sum of all travel distances to visit both P_i and D_i as deviations from the tour of k not considering customer i. This is the sum of all distances associated to the graph edges crossed by k in its tour that have P_i or D_i as either departing or arriving node.

C_{link} : the sum of all distances associated to the graph edges that k should cross to complete its tour without visiting P_i and D_i while respecting the nodes visiting order of the original solution.

$\hat{C}$: the marginal distance contribution of i being $\hat{C} = C_{tot}$ - $C_{deviation} + C_{link}$

Once these quantities are computed for all costumers served by k, NS rule assigns to customer i a portion of the cost obtained from the normalization of all marginal distance contributions $\hat{C}$ of the customers served by k. The main downside of NS rule is the risk of not being fair to customers in proximity of the depot that are involved in a tour that reaches distant locations. NS would assign a portion of cost that is related to the value of C_{tot} which is expected to be high in such a tour.

Extreme Neighbors Savings rule is intended to recover the aforementioned NS downside. This is accomplished by computing the marginal distance contribution of i without considering C_{tot}. Therefore, ENS employs the EN rule with the exception of considering $\hat{C} = max(0, C_{deviation} - C_{link})$

The final output of the proposed strategy is a cost allocation proportion that is a weighted average of the outcomes of SA, NS and ENS rules. Numerical experiments have analyzed the effects of different weights to address the fairness of this allocation technique. Intuitively, equal weights provide a fair balance between all rules objectives and downsides.

Although the proposed allocation strategy is out of the Shapley values paradigm, the Shapley value is the theoretical base of the XAI method used in the features' importance explanation of the cost forecasting framework. Indeed, a unified approach for interpreting predictions is presented in [73], is called SHAP (SHapley Additive exPlanations), and assigns each feature an importance value for a particular prediction according to Shapley values. SHAP is expolited in the XAI section of the framework and its results w.r.t. the application use-case are presented in Section 6.5.4.

6.3 Operational problem definition and modeling

This section describes in detail a novel mixed integer linear programming model for the optimization of planning routes for pick-up and delivery services. This general problem is one of the main operational tasks of supply chain management and is known as the Vehicle Routing Problem (VRP), a NP-Hard and well-known combinatorial optimization problem [111]. The presented formulation is intended to find the optimal set of routes for a single depot fleet of trucks to pick up goods from a given set of customers and deliver them to another given set of delivery nodes. A feasible solution of this model simultaneously satisfies the network system constraints, transport capacity constraints, and those associated with each customer and delivery location. Indeed, each graph node, corresponding either to a customer or a delivery node, has a time window bounding the time in which that node can be visited. Truck units are heterogeneous in terms of operating and emissions costs and can haul goods according to specific hauling capacity. Non-linear costs are considered for truck drivers, a two part tariff is made of a fixed fee plus a cost per driving hours. With and additional overnight cost, trucks can take multiple driving shifts to reach distant locations. In case the size of a node time window is particularly small, either causing infeasibility or bounding route savings, this can be extended with an additional cost per hour. Indeed, the presented formulation can be

seen as a variant of the VRP with pickups and deliveries (VRPPD) [112] that only considers penalties on late arrival while waiting on early arrival is allowed without cost, namely the Vehicle Routing and scheduling Problem with Semi Soft Time Windows (VRPSSTW) [89]. Considering a logistic service request i, this is identified by two nodes, i and $n+i$, corresponding, respectively, to the pickup and delivery stops of the request. It is possible that different nodes may represent the same geographical location. Then, denote the set of pickup nodes by $P = \{1, ..., n\}$ and the set of delivery nodes by $D = \{n+1, ..., 2n\}$. If request i consists of transporting d_i units from i to $n+i$, let $l_i = d_i$ and $l_{n+i} = -d_i$. Next, let K be the set of vehicles. The aim of the VRP is to define the routes serving all the customers, respecting vehicle and user constraints, while minimizing the total traveling costs.
To better introduce the formulation, and all its additional features w.r.t. what presented in [112] and [89], model notation for parameters indexes and variables is set out in the following.

n : number of customer to be served

$P = \{1, ..., n\}$: set of pickup nodes

$D = \{n+1, ..., 2n\}$: set of delivery nodes

$N = P \cup D$: overall set of pickup and delivery nodes to visit

o : depot as a departing node

d : depot as a returning node

$od = o \cup d$

$No = N \cup o$

$Nd = N \cup d$

$Nod = o \cup N \cup d$: overall set of graph nodes

K : set of heterogeneous vehicles

$[a_i, b_i]$: service time window for node i

$c_{i,j}$: cost of arch i, j as the sum of distance and duration costs

$t_{i,j}$: arch i, j travel time

s_i : service time at node i

l_i : pickup or delivery demand at node i

C_k : carrying capacity of vehicle k

u_k : activation cost of vehicle k related to expected operating and emissions costs

O : overnight cost

R : maximum number of driving hours in a shift

$\mathcal{Z}$: maximum number of subsequent driving shifts

Γ : time window enlargement cost per hour

The model consider the following variables.

$x_{i,j,k} \in \{0,1\}$: equal to 1 if vehicle k crosses arch (i,j), 0 otherwise

$T_{i,k} \in \mathbb{R}^+$: service starting time at node i by vehicle k

$L_{i,k} \in \mathbb{Z}^+$: load of vehicle k when leaving node i

$y_k \in \mathbb{R}^+$: bounds the time span between departure and returning to depot of vehicle k

$z_k \in \mathbb{Z}^+$: number of subsequent driving shifts of vehicle k

$o_k \in \mathbb{Z}^+$: number of subsequent overnights stay for vehicle k

$\gamma_i \in \mathbb{R}^+$: node i time window upper bound enlargement

The model minimizes the sum of several transport costs and is detailed as following:

$$\min\ Z = \sum_{k \in K} \sum_{i \in Nod} \sum_{j \in Nod} c_{i,j}\ x_{i,j,k} + \sum_{k \in K} (u_k\ z_k + O\ o_k) + \sum_{k \in K} y_k + \Gamma \sum_{i \in N} \gamma_i \quad (6.1)$$

s.t.

$$\sum_{i \in od} L_{i,k} = 0 \qquad \forall k \in K \qquad (6.2)$$

$$\sum_{k \in K} \sum_{j \in Nd} x_{i,j,k} = 1 \qquad \forall i \in P \qquad (6.3)$$

$$\sum_{j \in N} x_{i,j,k} = \sum_{j \in N} x_{j,n+i,k} \qquad \forall k \in K, i \in P \qquad (6.4)$$

$$\sum_{j \in P} x_{0,j,k} \leq 1 \qquad \forall k \in K \qquad (6.5)$$

$$\sum_{i \in D} x_{i,2n+1,k} = \sum_{j \in P} x_{0,j,k} \qquad \forall k \in K \qquad (6.6)$$

$$\sum_{i \in No} x_{i,j,k} = \sum_{i \in Nd} x_{j,i,k} \qquad \forall k \in K, j \in N \qquad (6.7)$$

$$T_{i,k} + s_i + t_{i,j} - T_{j,k} \leq M(1 - x_{i,j,k}) \qquad \forall k \in K, i \in Nod, j \in Nod, i \neq j \qquad (6.8)$$

$$a_i \leq T_{i,k} \leq b_i - s_i + \gamma_i \qquad \forall k \in K, i \in N \qquad (6.9)$$

$$T_{i,k} + s_i + t_{i,n+i} \leq T_{n+i,k} \qquad \forall k \in K, i \in P \qquad (6.10)$$

$$L_{i,k} + l_j - L_{j,k} \leq M(1 - x_{i,j,k}) \qquad \forall k \in K, i \in N, j \in N, i \neq j \qquad (6.11)$$

$$l_i \sum_{j \in N, j \neq i} x_{i,j,k} \leq L_{i,k} \leq C_k \qquad \forall k \in K, i \in P \qquad (6.12)$$

$$L_{i,k} \leq (C_k + l_i) \sum_{j \in N, j \neq i} x_{i,j,k} \qquad \forall k \in K, i \in D \qquad (6.13)$$

$$T_{|N|+1,k} - T_{0,k} \leq y_k \qquad \forall k \in K \qquad (6.14)$$

$$\sum_{i \in N, i \neq j} \sum_{j \in N, j \neq i} (s_i + t_{i,j}) x_{i,j,k} \leq R\ z_k \qquad \forall k \in K \qquad (6.15)$$

$$z_k \leq \mathcal{Z}(\sum_{j \in P} x_{0,j,k}) \qquad \forall k \in K \qquad (6.16)$$

$$z_k \geq \sum_{j \in P} x_{0,j,k} \qquad \forall k \in K \qquad (6.17)$$

$$o_k \geq 0 \qquad \forall k \in K \qquad (6.18)$$

$$o_k \geq z_k - 1 \qquad \forall k \in K \qquad (6.19)$$

$$\gamma_i \geq 0 \qquad \forall i \in N \qquad (6.20)$$

$$x_{0,j,k} = 0 \qquad \forall k \in K, j \in D \qquad (6.21)$$

$$x_{i,i,k} = 0 \qquad \forall i \in Nod, k \in K \qquad (6.22)$$

$$x_{i,0,k} = 0 \qquad \forall i \in N, k \in K \qquad (6.23)$$

The objective function (6.1) defines the minimization of the sum of the routing costs (regarding emissions and operating costs per km and hour), driving shifts activation and overnights costs, and time window enlargement costs. In addition, (6.1) includes the unit cost of the auxiliary variable y bounding the time span between departure and returning to depot for each used vehicle.

Constraints (6.2) limits each truck to be empty when exiting or entering the depot; constraints (6.3) guarantee that each customer $i \in P$ is served by one and only one truck; constraints (6.4) describe the network flow conservation and at the same time ensure that each pickup is delivered to its delivery location; constraints (6.5) guarantee that each used truck departs from the depot to reach a pickup node; constraints (6.6) force used vehicles to return to the depot; constraints (6.7) ensure network flow conservation; for all subsequently visited nodes, constraints (6.8) introduce time coherence between arrivals, service and travel times; constraints (6.9) force each node i to be visited in its time window while considering service time and the opportunity of extending the upper bound b_i; constraints (6.10) ensure that delivery occurs later than pickup; constraints (6.11) introduce truck load coherence between each subsequently visited node; constraints (6.12) and (6.13) limit truck load capacity and guarantee truck load coherence when visiting a pickup and a delivery node respectively; constraints (6.14) bounds vehicles time span between the exit and the return to depot; constraints (6.15) limit each vehicle travel time with respect to the driving shifts and their maximum driving hours; while constraints (6.16) bound the maximum number of subsequent shifts for each used truck, constraints (6.17) ensure the activation of at least one driving shifts of each used truck; constraints (6.18) and (6.19) imply that for each truck the number of overnights is zero unless is used for more than one driving shift; constraints (6.20) ensure that time windows can only be extended; constraints (6.21) avoid trucks traveling from the depot directly to a delivery node; constraints (6.22) avoid node loops and (6.23) ensure that no vehicle returns to the depot as a departing node.

With the rapid growth in the processing speed and memory capacity of computers, various algorithms can be used to solve increasingly complex instances of VRPs [109]. Indeed, while the computation time for the exact approach is adequate for smaller instances, the computation time for large-sized problems is usually very large for the exact solution technique, which favors the use of heuristics and meta-heuristic algorithms. The reader can refer to the reviews presented in [21] and [109] to find relevant literature, recent trends and solution methodologies in the field of VRPs and some well-known variants. The computational experience reported on the VRPPDTW indicates that algorithms capable of solving larger or more difficult problems are constantly being proposed. Nevertheless, computational experiments, solution methodologies and computing times are out of the scope of this work. The research work is instead aimed towards the study of a learning framework that consider some relevant customers features to forecast each customer cost.

6.4 Application to a reverse logistic service

Waste management (WM) is a worthwhile and important challenge concerning both the protection of the environment and the conservation of natural resources; it can be defined as the collection, transport, recovery and disposal of waste, including the supervision of such operations and the after-care of disposal sites, and including actions taken as a dealer or broker (Directive, 2008) [2]. The need of meeting the recovery and recycling targets imposed by EU law and the rising prices of raw materials have resulted in an increasing interest in the recovery of materials from the waste streams. This recycling industry is characterized by very low margins and high percentage of operation and logistics costs, for this reason it is critical the optimization of its processes in order to turn it in an economically sustainable business. Indeed, a considerable attention has been directed over the last decade towards the optimization of both strategic and operational tasks related to WM. In particular, performances of WM systems have been improving thanks to a noticeable commitment of decision makers and research efforts regarding the optimization of each system components. The reader can refer to the surveys of Ghiani et al. (2014) [50] and Das et al. (2019) [36] for an extensive knowledge of literature related to strategic and tactical issues in solid WM. Industrialization and consumerism are deeply affecting the amount of generated waste, leading to the need of a stronger technological and strategic decision support to waste facilities dealing with industrial waste management in order to lower all the extra costs involved with the selective collection and sorting of this kind of waste. Indeed, within WM one of the major topic of interest besides Municipal Solid Waste Management (MSWM) is Industrial Waste Management (IWM) which encompasses every task involved from collection and transportation of the waste generated in industrial sites to its process in sorting facilities where all its kinds of mixed materials are sorted to extract the so-called secondary raw materials. In the described setting, waste companies usually serve their industrial customers according to a pull logic for the waste containers' collection. Indeed, a company truck picks up the waste container of a customer whenever the company logistic services are contacted by the client for the container pick up. As planning and scheduling the operations of sorting facilities represents the main tactical task of IWM performed by OR models, the logistic cost of trucks routing to pick-up and deliver waste is the main operational cost of IWM that these models have to optimize. Accordingly, the model presented in Section 6.3 is able to optimize logistic operations of such an IWM setting. In this scenario, the model finds the optimal set of routes for a fleet of trucks in order to pick up waste containers from a given set of industrial customers and deliver them to waste sorting facilities. Taking the waste collection management as a practical background, the problem in Section 6.3 can also be considered as belonging to the class of Rollon-Rolloff Vehicle Routing Problems (RR-VRPs). The RR-VRP is studied in several papers, such as [5, 18, 69], and involves tractors pulling large containers between customer locations and disposal facilities. A feasible solution of this model simultaneously satisfies both the network system constraints and those associated with each waste producing customer and related disposal unit. Indeed, each graph node, corresponding either to a customer or a waste sorting facility, has a time window bounding the time in which that node can be visited. Truck units instead can haul either one or two waste containers, depending on each truck capacity. The following Section 6.5 presents the experimental results obtained by applying the proposed framework to the described IWM setting.

6.5 Experimental results

In this section, the integration of an operational research (OR) model providing optimal capacity allocation with a machine learning (ML) model performing customer cost estimation is described.

In order to test the proposed framework, a real case study from the IWM setting is considered. In particular, the case of an operator of a medium-sized waste company based in the province of Rome, Italy. Every day, the logistic company receives a different set of customer service requests. Accordingly, the firm determines the routes for its fleet of trucks in order to pick up waste containers from the set of industrial customers and deliver them to their designated sorting facilities. A critical aspect for both sustainable efficiency and profitability performance is related to commercial offers submitted to clients. Indeed, the business should be able to make competitive commercial offers that embed the ability of satisfying customer demand in the most efficient way.

The objective of this experiment is to provide the contract management of the WM company with a tool, in the form of a machine learning model, that produces an estimate of the costs associated to the satisfaction of the service requests, based on the information of each customer such as its demand, its position and other information that can have an impact on the operative costs of the business. Once trained, the machine learning model is able to provide profitability classification in short time, and on demand, while embedding different scenarios in which the customer can be served, considering the costs that the company must afford in different routing scenarios. Conversely, the VRP optimization tool can provide output only for a well specified instance.

As discussed in Section 6.2, the tool can be realized with the framework which includes the following steps:

1. Creation of the dataset that is the input of the OR problem, with the possible application of data augmentation techniques;

2. Resolution of the OR problem instances, with the subsequent allocation of costs across multiple customers;

3. Creation of the ML dataset.

4. Model training and performance evaluation: using Explainable Artificial Intelligence (XAI) to compute feature importance.

The above steps are discussed in detail in the following Sections.

6.5.1 Dataset creation

This section describes the dataset used for the experimental test and the data augmentation performed to increase the variability of the data and to investigate the role of variables of interest.

Original Dataset

The WM firm provided access to data ranging from January 2020 to March 2022. The data consists of daily records of customers served requests, including the list of customers served each day, their position as well as the position of each customer's waste sorting facility, and the demand, expressed as the number of containers to pick up. This dataset, in particular, covered 668 operating days, with an average of 17.3 clients served, and 27 containers picked up each day.

Data augmentation

In addition to the information at our disposal, this experiment investigates the role played by other variables that are expected to have an impact on the resolution of the VRP problem and, thus, to the operating costs of the company, but that have not been recorded and that the contract management does not currently consider when preparing a commercial offer to its clients.

In particular, it is investigated the role played by the visiting time windows of both the pickup and delivery nodes, and the service time associated to each node, as described in Section 6.3. To explore the role of such variables, different copies of each operating day of the dataset are made. For each copy, DA then uses random sampling from appropriate probability distributions to generate values for the time windows and service times for each customer. The next section describes the resolution of the OR model and the strategy used to allocate the cost to each customer.

6.5.2 OR model and cost allocation strategy

The logistic problem of the use-case application, concerning pickups, deliveries and semi soft time windows, is modeled according to the formulation described in Section 6.3.

Model instances are coded in Python3 and tested on a PC running a 1.60GHz Intel Core-i5-10210U CPU with 16 GB RAM. Considering the available data of 668 operating days, a total of 2672 instances are solved (one for each of the four DA copies that differ in the values of the time windows and service time of each client). These are solved via branch-and-cut using the Gurobi 9.5.2 solver hosted on a server running on an Intel Xeon Gold 6136 CPU @3.0 GHz with 250 GB RAM, with a solution time limit of 60 minutes.

Out of the total number of instances, 2172 (or 82% of the total) are solved with a duality gap less than 0.05. Out of them, 1433 are exactly solved finding the optimal solution.

In the following phase of the experiment, the ML model is trained only using the 2172 instances solved with a duality gap < 0.05.

To determine how much of a route's total cost should be allocated to each of the customers served, the allocation strategy described in Section 6.2.1 is used, namely the arithmetic average of three different allocation rules: *Stand-Alone rule* (SA), *Neighbors Savings* (NS) and *Extreme Neighbors Savings* (ENS).

It is important to remember that this allocation choice is just one of the possible allocation choices that can be made, and that any other allocation could be used without affecting the validity of the framework as long as it distributes costs fairly.

6.5.3 ML dataset and preliminary data analysis

This section describes the dataset resulting from the application of the proposed framework. In order to present data considerations, it also contains a preliminary data analysis. Additional details about how the dataset is used to train the machine learning model are given in the following Section 6.5.4.

The ML dataset consists of 14669 records, each corresponding to one customer served in a replica of one of the 668 operating days. For each record, while the target variable is *ServiceCost* (i.e., the routing cost allocated to the customer, expressed in Euro currency), the list of feature columns is the following:

- *demand*: number of containers that the customer asks to pick up
- *distHtoP*: shortest path distance in km from the depot (H) and the pickup node
- *distHtoD*: shortest path distance in km from the depot (H) and the delivery node
- *distPtoD*: shortest path distance in km from the pickup node and the associated delivery node
- *distSingleTour*: shortest path distance in km of the tour depot - pickup node - delivery node - depot
- *timeWindowPD*: sum of the widths of the pickup time window and delivery time window, expressed in minutes. For example, if the pickup node has a $9am - 3pm$ time window, and the delivery node has a $11am - 4pm$ time window, the variable *timeWindowPD* will have a value of $60 \cdot 6 + 60 \cdot 5 = 660$
- *serviceTimePD*: sum of the service time of the pickup node and delivery node, expressed in minutes

- *concentration20km*: number of other customers, across the whole dataset, that are within a 20 km shortest path distance from the customer
- *concentration50km*: number of other customers, across the whole dataset, that are within a 50 km shortest path distance from the customer
- *concentration100km*: number of other customers, across the whole dataset, that are within a 100 km shortest path distance from the customer

Several of these features are the result of some feature engineering. The latitude and longitude of the position of each pickup and delivery node are not used as raw values, but are used to compute the shortest path distances from and between the depot, the pickup node and the delivery node. The Open Source Routing Machine (OSRM) [74] is used to compute the shortest path distances. OSRM is an open-source router, exploiting Dijkstra's algorithm [39], and designed for use with data from the OpenStreetMap project [81].

The last columns consider all client location recorded in the database to report, for each customer, the concentration of other clients within a given distance. These features are engineered to help the model learn the allocated costs' reduction that may result from the proximity of customers. According to the proposed cost allocation, in fact, customers that are isolated are charged more than customers that, being close to each other, can be served within a more efficient route.

Considering this set of data, inductive inference is accomplished by a machine learning model that is intended for the discovery of knowledge from observations. Nevertheless, as a first analysis step, it is always advisable to examine either feature's histogram or scatter plots. This enables the examination of the data's variance and distribution in order to make some initial deductive inferences. For example, in case data distribution shows an almost null variance, most likely the corresponding feature will not add any useful information for modeling purposes. Some of the most interesting data plots that resulted from a preliminary deductive analysis are set out, and commented on, below.

Figure 6.2 displays the allocated *ServiceCost* along the vertical axis (dependent target variable) and the corresponding values of the *distSingleTour* feature along the horizontal axis (independent variable). Intuitively, this might be one of the features being mostly responsible for the service cost. Moreover, *dist single tour* stems out of one of the allocation strategy rules (SA), thus providing useful information about the allocated cost. Accordingly, Figure 6.2 shows a positive correlation between the two axis values. At the same time, for the same *distSingleTour* value, there is a highly variable result in terms of *ServiceCost*. In particular, this variance trend increase w.r.t. the magnitude of the feature values, proving that such a positive correlation is not sufficient to explain the variety of scenarios addressed by the OR model.

Figure 6.3 and Figure 6.4 are the scatter plots that relate the *concentration20km* feature and *concentration50km* feature to the target variable cost, respectively.

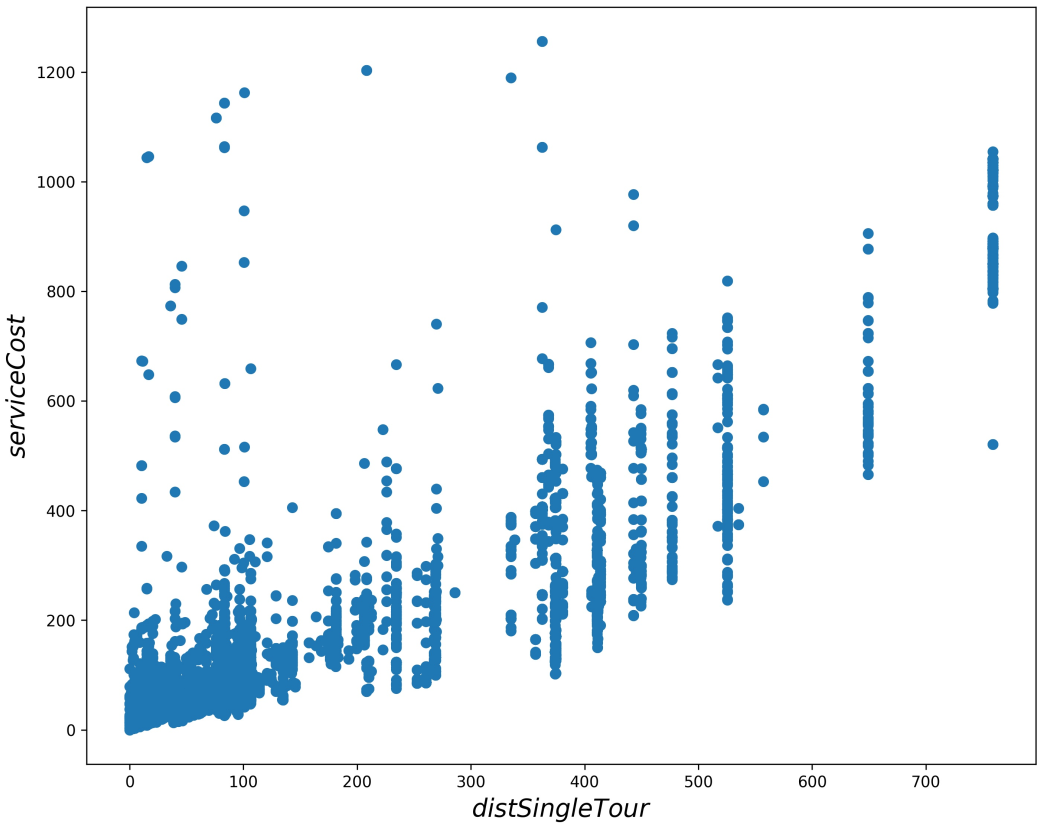


Figure 6.2. Scatter plot *service cost* - *dist single tour*

Considering a non-cooperative scenario, a customer who requests a service in an area with a high concentration of potential customers is more likely to be served by a route that is more efficient and therefore assigned with a lower allocated cost. Accordingly, Figure 6.3 shows that both the mean and variance of the customer service cost decrease as the number of close customers, across the whole dataset, increase. The same type of considerations about Figure 6.3 apply to Figure 6.4.

Figure 6.5 and Figure 6.6 are the scatter plots that relate the *time windowPD* feature and *serviceTimePD* feature to the target variable cost, respectively. It is very important to highlight that, even though both plots are scattered and no clear relation with the service cost is shown, these features do have an impact on the service cost. This is proved in Section 6.5.4 by the ML model explainability, which allows investigating the importance of all features w.r.t. the regression performance of the model. Furthermore, neither plot's observations are evenly distributed throughout the plot, making it impossible to draw any firm conclusions or even infer a non-linear relationship. This aspect supports and validates the use of a non-linear regression within the machine learning paradigm.

In the following section, the training of the ML model is described and the impact of each feature on the prediction of the service cost is analyzed.

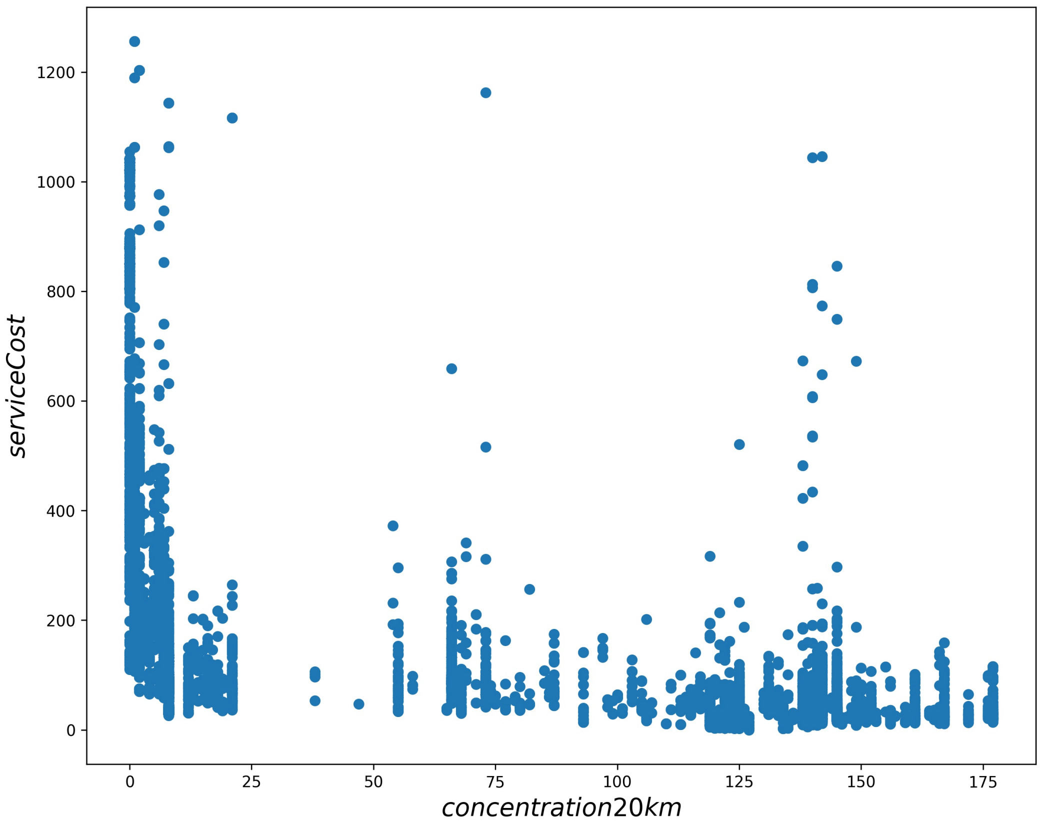


Figure 6.3. Scatter plot

6.5.4 Model training and performance evaluation

In order to learn the function that maps the aforementioned list of input features to the target variable *ServiceCost*, the XGboost model [29] is trained. This model, that belongs to the tree ensemble model class, is known to be one of the most reliable models for tabular data, often outperforming the popular artificial neural networks [99].

To train the model, data are split according to a $80-20$ proportion, with the following caution: if a record related to a customer served on a given day is in the training (or test) set, then *all* the records of *all* the replicas of that given day are also in the training (or test) set. For example, if there are 4 replicas of the operating day (instance) 1/01/2020 in which 10 customers have been served, then all of them will be part of one among the training and test set. This is done to avoid the potential information leakage that can derive from seeing two records related to the same customer-instance combination in both the training and test set. The same information leakage may apply to the case of having, in both the training and test set, two customers with similar characteristics (such as location and demand features) that are served in the same instance.

The XGboost model is implemented on Python 3.8.10. The hyperparameters

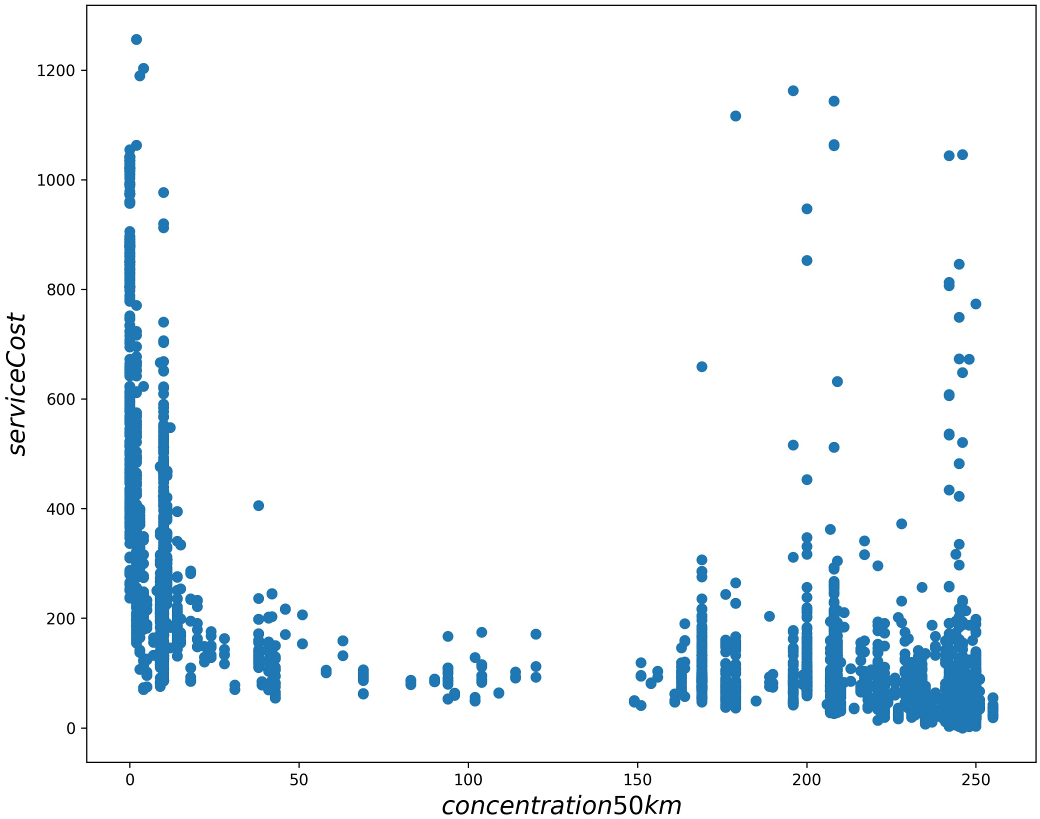


Figure 6.4. Scatter plot

	Training Set	Test Set
MAE	33.07	31.92
MAPE	0.49	0.47

Table 6.1. ML model performance

of the model are determined by means of a random search with a K-fold Cross Validation (K = 5), and the hyperparameters' combination that minimizes the average Mean Absolute Error (MAE) on the validation sets is selected. Table 6.1 reports the performance of the XGboost model trained with such combination of hyperparameters on the training set and test set. In particular, the metrics reported are MAE and Mean Absolute Percentage Error (MAPE), the latter measuring the mean absolute percentage difference between the actual and the predicted value.

Both the error metrics assume similar values in the training and test set, thus showing the ability of the model to generalize on new, unseen data, not suffering from the problem of overfitting.

To better appreciate the performance of the model w.r.t. the use-case application, it is worth to observe the distribution of the target variable displayed in Figure 6.7. It is possible to see that the *ServiceCost* values are within the range 0-1256, with

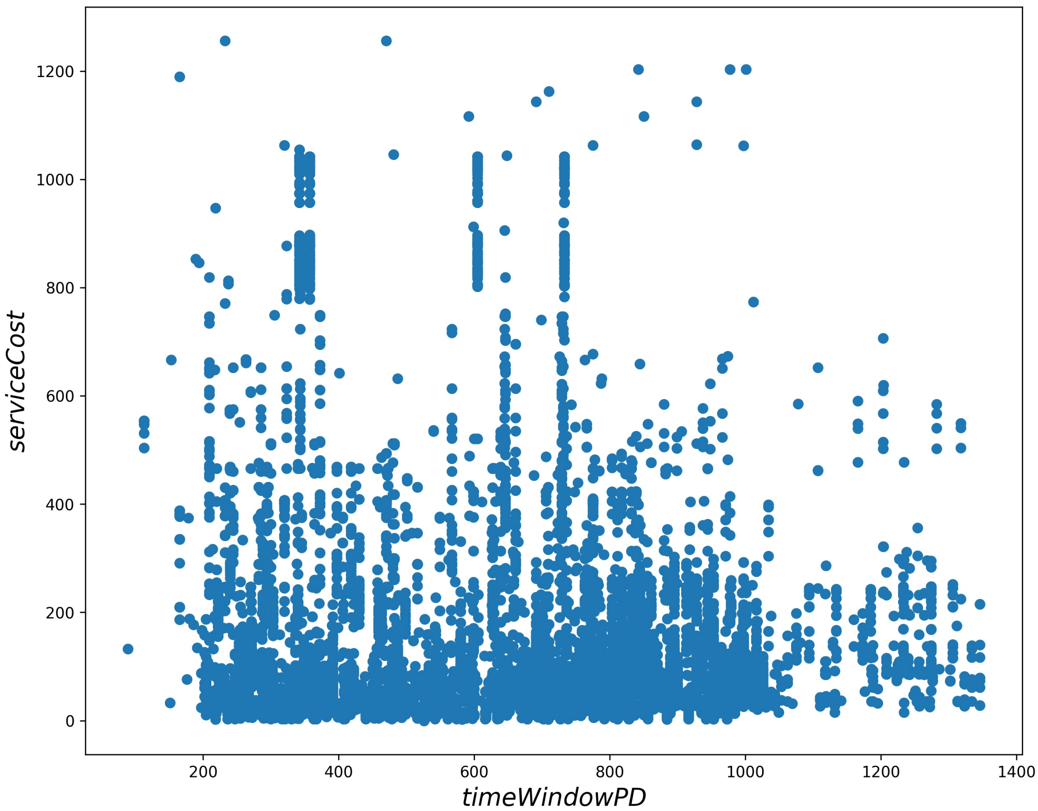


Figure 6.5. Scatter plot

the majority of records having a *ServiceCost* between 0 and 200, a discrete amount of records within a 200-600 range, and a third group of customers is served within an 800-1100 cost range. Given this distribution, a model with a MAE of 32 Euro on unseen data can be considered worthy and useful for the specific application. Nevertheless, a MAPE value of 0.49 may appear to be high without decomposing this metric w.r.t. different ranges of true observation values. Accordingly, Table 6.2 presents a breakdown of the MAE and MAPE errors on the test set for customers within various ranges of service cost values. It is interesting to observe that the highest MAPE values are associated to records with the lowest *ServiceCost* values. In other words, the lower the *real* target value, the higher the percentage error made by the model. At the same time, the mean percentage error is less than 0.3 for customers whose service cost is greater than 100 and is below 0.13 for records whose service cost is greater than 500. It is also possible to observe a sublinear increase in the MAE as the *Service Cost* rises.

When evaluating the performance of the proposed framework, an important aspect to consider is the following: throughout the course of the three years of data, the same customer is served in numerous daily instances that vary in terms of the total number of different clients requesting the service. This is the main reason why the same customer can cause a different operating cost depending on the specific

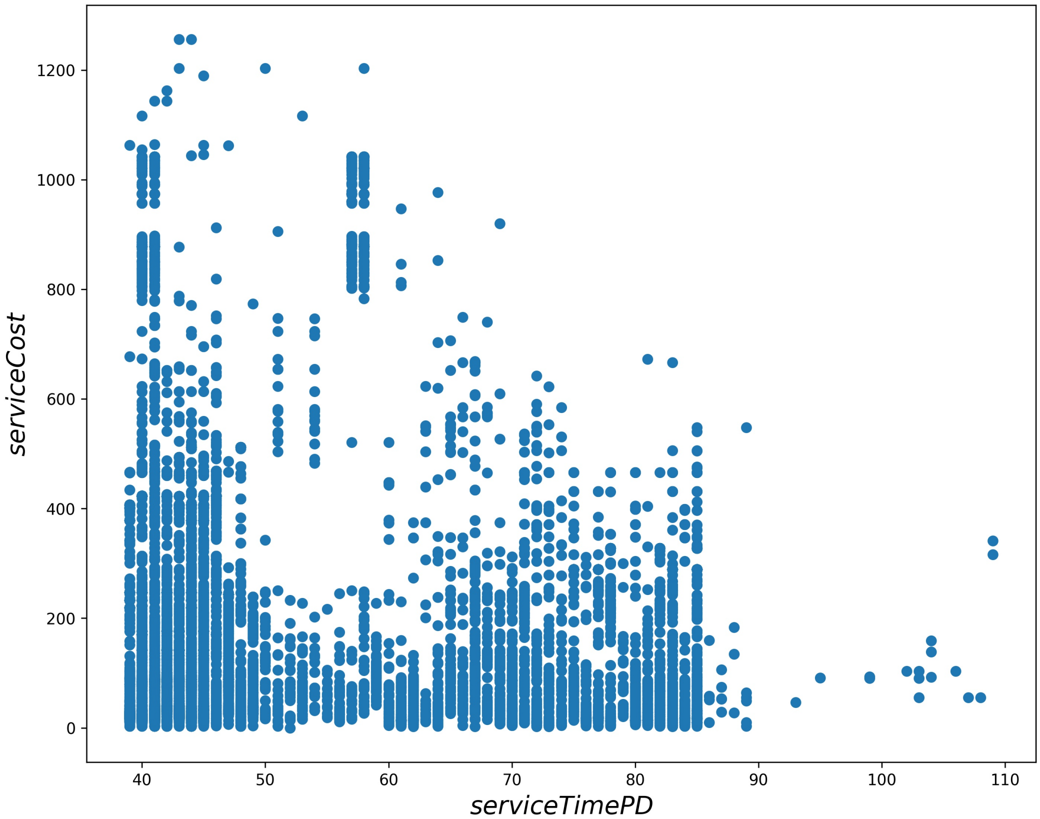


Figure 6.6. Scatter plot

daily instance. Indeed, it is the entire set of customers that determines the way in which logistics resources are efficiently assigned to each of them by the optimization model. Therefore, in the ML dataset, the variety of the costs assigned to the same customer reflects the diversity of the service instances that include that customer. Explaining this variance is the complex non-linear challenge of the regression task.

For sure, the considerations above could also apply to a different type of service provider or production environment.

To find out what importance each feature has in explaining the variation of the target variable's data, XAI techniques can be exploited. As introduced in Section 6.2.1, the XAI method used in this work to explain the model features' importance

Service Cost range	MAE	MAPE	Test records
0 - 100	17.06	0.63	1891
101 - 200	41.45	0.27	380
201 - 500	53.06	0.16	511
501 - 1256	89.59	0.12	200

Table 6.2. Breakdown of MAE and MAPE metrics

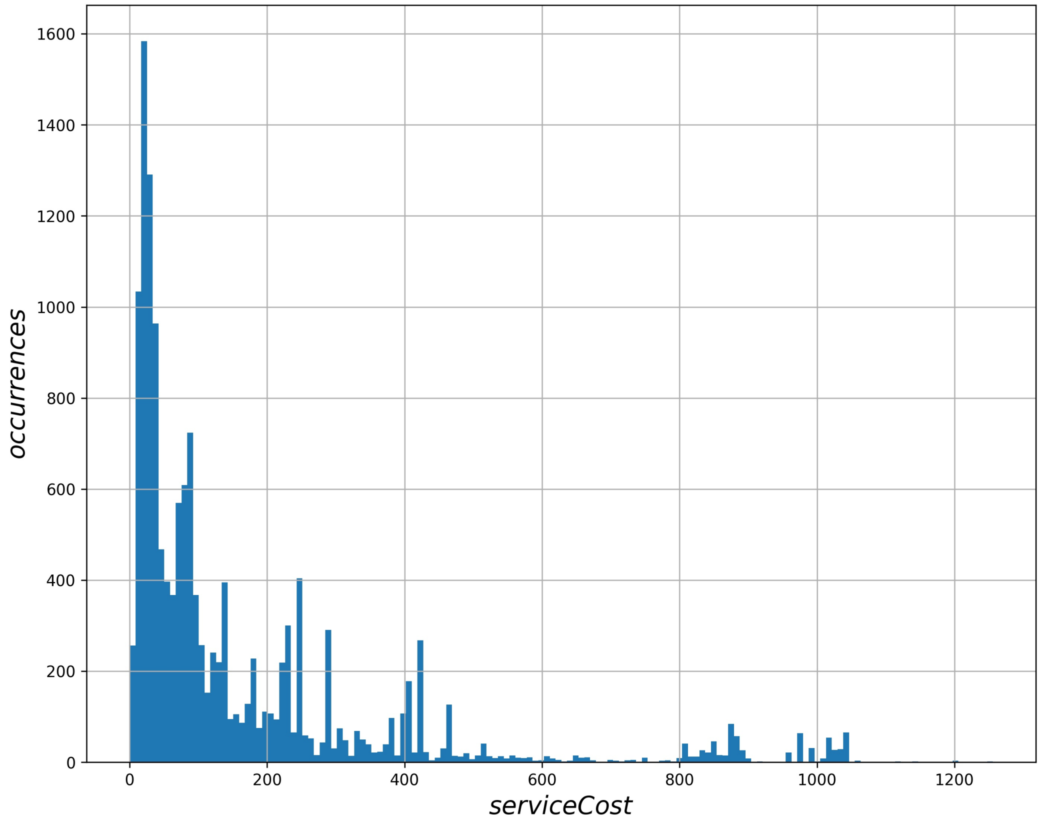


Figure 6.7. Histogram

is called SHAP (SHapley Additive exPlanations) [73], which assigns each feature an importance value for a particular prediction according to Shapley values [96]. The summary plot that combines feature importance with feature effects is shown in Figure 6.8. For each feature, every record of the dataset appears as its own point. The position on the y-axis is determined by the feature, and on the x-axis by the Shapley value. The color represents the value of the feature from low to high. Overlapping points are jittered in the y-axis direction, so we get a sense of the distribution of the Shapley values per feature. The features are ordered according to their importance [79].

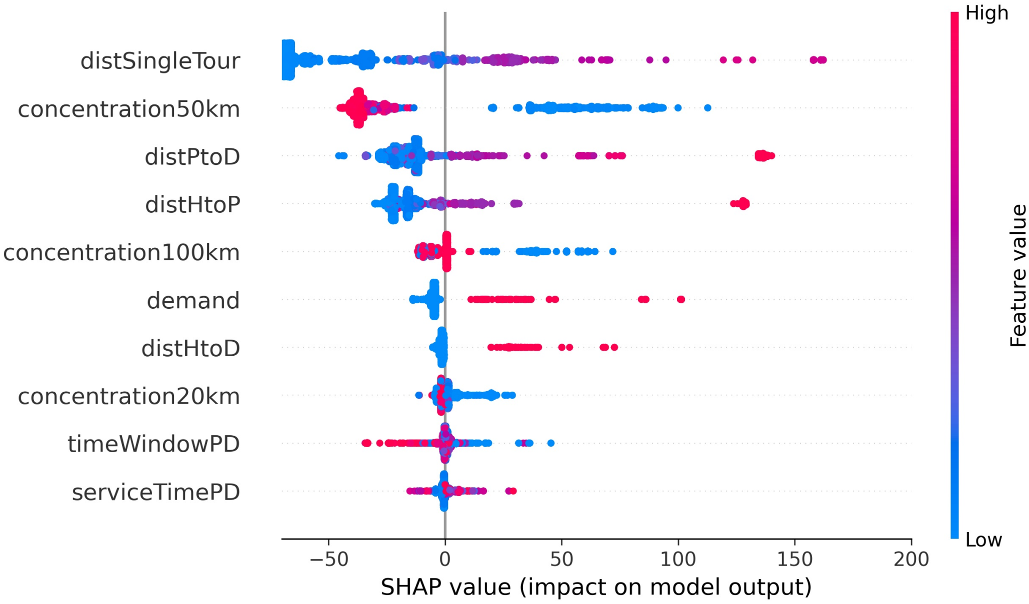


Figure 6.8. SHAP values to explain features importance

Examining the color distribution horizontally along the x-axis for each feature provides insights into the general relationship between a feature's raw values and its Shapley values.

The feature with the highest impact on model predictions is *distSingleTour*. In particular, the lower values of *distSingleTour* have negative SHAP values (the points extending towards the left are increasingly blue) and higher values of *distSingleTour* have positive SHAP values (the points extending towards the right are increasingly red). This confirms that customers having lower predicted costs are those who request a pick-up and delivery service that could be accomplished by a short distance tour. The same type of colours polarization, thus the same type of impact, applies to the features *distPtoD*, *distHtoP*, *distHtoD*. The plot reveals that the latter's impact is moderate. This is due to the fact that, in this use-case, the distance between the depot and the delivery node is frequently zero, since the depot location coincides with the delivery node of several service requests. Still, for the records in which this distance is high, the SHAP values have a positive value, indicating a higher predicted service cost.

Another set of feature that has an interesting behavior is the group of features that considers the concentration of other clients within a given distance. The most relevant of them is *concentration50km* that, for each record, counts the number of other clients within a 50 km shortest path distance from the customer of that record. It is evident how a dense cluster of records has a high feature' value (red points) with a small but negative Shapley value. Records with a low number of other customers within 50 km (blue points) extend further towards the right, suggesting that being isolated from other customers has a positive impact on the predicted service cost. This is in line with the considerations expressed in the comments of Figure 6.4, namely that a customer who requests a service in a location with a high concentration of potential customers is more likely to be served by a route that is more efficient and, as a result, assigned with a lower allocated cost.

Features *concentration100km* and *concentration20km* show a similar behavior, and the same considerations apply.

Taking the IWM application background, truck units can haul either one or two containers, and the *demand* feature is limited to a few number of containers, often one or two. Accordingly, most features values are distributed in a low value range, while the few records with a high feature value have a clear positive SHAP value. Indeed, customers requesting for a pick-up of several containers are likely being served with dedicated logistic resources.

The plot of Figure 6.8 proves that another important customer characteristic is the *timeWindowPD*. Indeed, this feature has a well-defined impact on the predicted customer cost, as reflected by the polarized distribution of its SHAP values w.r.t. the feature values. In particular, the lower feature's values have positive SHAP values and higher feature's values have negative SHAP values. Therefore, customers with a shorter time windows (both pick-up and delivery nodes time windows are considered) are expected to be served with higher costs compared to customers that allow the carrier to be visited within larger time windows. This is because the constraints on feasible, and efficient service solutions are tighter the smaller the customer's time window. This result confirms that contract management should take into account this characteristic when collecting relevant customer features.

Time is money, and even if *serviceTimePD* is the least important feature on the list, it produces a moderate but clear effect over the customer service cost: the more time spent in pickup and delivery locations, the less likely that customer can share service capacity and costs with another set of clients. Indeed, driving hours are limited for each working shift, and when roll-on-roll-off container operations are time taking, fewer customers can be served within the same truck tour, thus requiring the use of additional resources (i.e. truck units).

6.6 Conclusions

Research in mathematical programming and supply chain management incorporates studies that draw attention to the several sources of uncertainty the businesses must cope with. In addition to price, demand, and costs, other factors can be considered to be nondeterministic. Some of them are the uncertainties related to the customer characteristics, such as its location or time window. These types of uncertainties affect any business engaging multiple customers that make production or service requests unpredictably. The IWM application of this research activity is an example of such business. In this scenario, the proposed framework investigates how the operative costs are altered by the variability of the customers characteristics and their unpredictable and non-cooperative production/service requests. This is allowed by XAI methods that highlight the impacts that each considered characteristic have on the cost allocated to the single customer. In case the performance of the regression model are such to accurately forecast customers cost, then the proposed framework is also able to provide reliable and fair costs estimates that are the essential input of any profitable and competitive commercial offer. Indeed, competitive commercial offers embed the ability of satisfying customer demand in the most efficient way.

Future research may look at testing the framework when an ideal fair cost allocation is made using novel methodologies that can produce accurate approximations of the Shapley value with less computing effort. This would make it possible to apply the Shapley values cost allocation strategy in real-case application that involve several customers. Running sensitivity analyses on the features' importance results with respect to the cost allocation strategy is another interesting future work. In addition, it may be relevant to extend experimental testing to capacity allocation problems that arise from a production setting.

Appendix A

Prophet forecasting model

This appendix describe the time series forecasting model presented in [110] and designed to handle the common features of time series seen both in business and industrial scenarios. The implementation is available as open source software, is called Prophet, and it uses a decomposable time series model [56] with three main model components: trend, seasonality, and holidays. They are combined in the following equation:

$$y(t) = g(t) + s(t) + h(t) + \epsilon_t \tag{A.1}$$

where $g(t)$ is the trend function which models non-periodic changes in the value of the time series, $s(t)$ represents periodic changes such as seasonality, and $h(t)$ represents the effects of holidays which occur on potentially irregular schedules. The error term ϵ_t represents any changes which are not captured by the model and is assumed to be normally distributed. Therefore, seasonality and potential holidays are treated as additive components. The model is identified within this class of models by solving a curve-fitting problem, either using backfitting or L-BFGS [24]. This is a different approach from time series models that explicitly account for the temporal dependence structure in the data.
Regarding the trend component $g(t)$, a piece-wise constant trend provides a parsimonious and often useful model. In addition, eventual trend changes in the model are modeled with changepoints where the trend is allowed to change. The trend model $g(t)$ is indeed considering S changepoints at times s_j , $(j \in 1, ..., S)$ and a vector $\delta \in R^S$, where δ_j is the change in rate that occurs at time s_j. The rate at any time t is then the base rate k plus all of the adjustments up to that point: $k + \sum_{j:t>s_j} \delta_j$. This is better represented by considering a vector $a(t) \in \{0, 1\}^S$ such that:

$$a_j(t) = \begin{cases} 1, & if\ t \geq s_j \\ 0, & otherwise. \end{cases}$$

The trend rate at time t is then $k + a(t)^\intercal \delta$. The trend component $g(t)$ considers also an offset parameter m that must be adjusted whenever the rate k is adjusted in order to connect the endpoints of the segments. The adjustment at changepoint j

is computed as $\gamma_j = -s_j\delta_j$. Therefore, the trend component $g(t)$ can be defined as following:

$$g(t) = (k + a(t)^\intercal\delta)t + (m + a(t)^\intercal\gamma) \tag{A.2}$$

Many time series have multi-period seasonality producing evident repeated effects that should be properly addressed by a forecasting model. The model relies on a Fourier series to provide a flexible model of periodic effects [57]. Let Q be the expected regular period the the time-series (e.g. Q = 7 for weekly data), then the smooth seasonal effects component can be approximated with the a standard Fourier series:

$$s(t) = \sum_{n=1}^{N}\left(a_n cos\left(\frac{2\pi nt}{Q}\right) + b_n sin\left(\frac{2\pi nt}{Q}\right)\right) \tag{A.3}$$

Fitting $s(t)$ requires the estimation of the $2N$ parameters $\beta = [a_1, b_1, ..., a_N, b_N]^\intercal$. This is done by firstly setting N and the period Q, then constructing a matrix of seasonality vectors $X(t)$ for each value of t in both historical and future data:

$$X(t) = \left[cos\left(\frac{2\pi(1)t}{Q}\right), ..., sin\left(\frac{2\pi(N)t}{Q}\right)\right]$$

By doing so the seasonal component is then

$$s(t) = X(t)\beta \tag{A.4}$$

The authors suggest to impose a prior smoothing on the seasonality by taking $\beta \sim Normal(0, \sigma^2)$.
Incorporating holidays effects with the corresponding component $h(t)$ is made by firstly assuming that these effects are independent. Considering each holiday i, D_i is the set of past and future dates for that specific holiday and an indicator function $\mathbb{1}(t \in\ D_i)$ is defined in order to represent whether time t is during holiday i. Then, a parameter k_i is assigned to each holiday being the corresponding change in the forecast. As similarly done for seasonality $s(t)$, a matrix of regressors is defined as follows, where L is the number of yearly holidays considered:

$$Z(t) = [\mathbb{1}(t \in\ D_1), ..., \mathbb{1}(t \in\ D_L)]$$

By doing so the holidays component is

$$h(t) = Z(t)k \tag{A.5}$$

As with seasonality, the authors suggest to use a prior $k \sim Normal(0, \sigma^2)$.

Appendix B

Model $\mathcal{D}$

Dealing with a waste management setting, $\mathcal{D}$ is a mixed integer linear programming model scheduling the sorting operations of each phase of a waste sorting process. The model can be described as a variant of a lot sizing model with non linear costs (approximated by mean of piece-wise linear functions) with the additional features of scheduling the operations and allocating the appropriate workforce dimension. To better introduce the formulation of $\mathcal{D}$, model notation for parameters and indexes is set out in the following.

$j \in \{1, \ldots, J\}$: index of the J sorting stages

$p \in \{1, \ldots, P\}$: index of the P time-shifts

T : time horizon partitioned into time shifts with $t \in \mathcal{T} = \{1, \ldots, T\}$

C : hourly cost of each operator

b_t : working hours for time t determined by the corresponding shift p

$C_t = C * b_t$: cost of each operator at time t

f_j : set-up cost of sorting stage j

d_t : quantity of material in kg unloaded from trucks at time t

α_j : percentage of waste processed in stage $j-1$, received in input by buffer j

S_j : maximum inventory capacity of the sorting stage buffer j

LC_j : critical inventory level threshold of buffer j

n_j : fraction of material allowed to be left at buffer j at the end of time horizon

K_j : single operator hourly production capacity [kg/h] of sorting stage j

$SK_{j,t} = K_j * b_t$: operator sorting capacity in sorting stage j, at time t

M : maximum number of operators available in each time shift

E_j : minimum number of operators to be employed in each time shift of stage j

∂h_j^i : slope of the i-th part of linearization of the buffer j inventory cost curve

$I_{j,0}$: initial inventory level in buffer j

The model consider the following variables.

$x_{j,t} \in \mathbb{Z}^+$: operators employed in the sorting stage j at time t

$u_{j,t} \in \mathbb{R}^+$: processed quantity at stage j at time t

$y_{j,t} \in \{0,1\}$: equal to 1 if stage j is activated at time t , 0 otherwise

$I_{j,t} = I_{j,t}^{'} + I_{j,t}^{''} \geq 0$: inventory level of material in buffer j at time t; for each stage j the corresponding $I'_{j,t}$ and $I''_{j,t}$ represent the inventory level before and after reaching the critical threshold, respectively.

$w_{j,t} \in \{0,1\}$: equal to 1 if $I_{j,t}^{''} > 0$, 0 otherwise. Indeed, this binary variables are used to model the piece-wise linear functions of the buffer inventory costs.

The model minimizes the sum of sorting and holding costs and is detailed as following:

$$\min\ Z = \sum_{j \in J} \sum_{t \in T} C_t x_{j,t} + \sum_{j \in J} \sum_{t \in T} f_j y_{j,t} + \sum_{j \in J} \sum_{t \in T} \left(\partial h_j^1 I'_{j,t} + \partial h_j^2 I''_{j,t} \right) \tag{B.1}$$

s.t.

$$E_j\ y_{j,t} \leq x_{j,t} \leq M\ y_{j,t} \qquad \forall j \in J, t \in \mathcal{T} \tag{B.2}$$

$$\sum_{j \in J} x_{j,t} \leq M \qquad \forall t \in \mathcal{T} \tag{B.3}$$

$$u_{j,t} \leq SK_{j,t}\ x_{j,t} \qquad \forall j \in J, \in \mathcal{T} \tag{B.4}$$

$$I_{1,t} = I_{1,t-1} + d_t - u_{1,t} \qquad \forall t \in \mathcal{T} \tag{B.5}$$

$$I_{j,t} = I_{j,t-1} - u_{j,t} + \alpha_j\ u_{j-1,t} \qquad \forall t \in \mathcal{T}, j \in J \setminus 1 \tag{B.6}$$

$$I_{j,t} = I_{j,t}^{'} + I_{j,t}^{''} \qquad \forall j \in J, t \in \mathcal{T} \tag{B.7}$$

$$LC_j\ w_{j,t} \leq I_{j,t}^{'} \leq LC_j \qquad \forall j \in J, t \in \mathcal{T} \tag{B.8}$$

$$0 \leq I_{j,t}^{''} \leq (S_j - LC_j)\ w_{j,t} \qquad \forall j \in J, t \in \mathcal{T} \tag{B.9}$$

$$I_{j,T} \leq n_j\ LC_j \qquad \forall j \in J \tag{B.10}$$

$$x_{j,t} \in \mathbb{Z}^+ \qquad \forall j \in J, t \in \mathcal{T} \tag{B.11}$$

$$u_{j,t} \in \mathbb{R}^+ \qquad \forall j \in J, t \in \mathcal{T} \tag{B.12}$$

$$y_{j,t} \in \{0,1\} \qquad \forall j \in J, t \in \mathcal{T} \tag{B.13}$$

The objective function (B.1) defines the minimization of the sum of the three cost terms, which are sorting, setup, and inventory costs respectively. Constraints (B.2) and (B.3) bound the number of workers that can be assigned to each sorting station and to each time shift. Constraints (B.4) limit the quantity sorted $u_{j,t}$ to the sorting capacity dependent on the number of workers $x_{j,t}$. The remaining constraint sets define and limit the inventories: constraint set (B.5) defines the inventory for the first buffer, considering the inbound material d_t and the sorted material u_{1t}, while (B.6) defines the inventory for the other buffers corresponding to $j > 1$. Indeed, constraints (B.6) describe the waste flow across the sorting stages that follow one another: each subsequent inter-operational buffer j receives by the previous sorting stage $j - 1$ a quantity of waste equal to a α_j percentage of the waste processed in stage $j - 1$. Constraint sets (B.7), (B.8), and (B.9) define the piece-wise linear functions for inventories; in these constraints, level S_j and maximum capacity LC_j are connected with the inventory levels through the variable $w_{j,t}$. The last constraint set (B.10) imposes the maximum unsorted material allowed to be left at the end of the planning period for each buffer.

Appendix C

Model $\mathcal{R}$

The robust counterpart $\mathcal{R}$ of $\mathcal{D}$ is introduced as following:

$$\min \text{ (B.1)}$$

$$\text{s.t.}$$
$$\text{(B.2)} - \text{(B.4)}, \text{(B.6)} - \text{(B.13)}$$

$$I_{1,0} + \sum_{k=1}^{t} d_k \epsilon_k - \sum_{k=1}^{t} u_{1,k} + z_t \Gamma_t + \sum_{k=1}^{t} p_{t,k} \leq S_1 \qquad \forall t \in \mathcal{T} \tag{C.1}$$

$$I_{1,0} + \sum_{k=1}^{t} d_k \epsilon_k - \sum_{k=1}^{t} u_{1,k} + z_t \Gamma_t + \sum_{k=1}^{t} p_{t,k} \geq 0 \qquad \forall t \in \mathcal{T} \tag{C.2}$$

$$I_{1,0} + \sum_{k=1}^{T} d_k \epsilon_k - \sum_{k=1}^{T} u_{1,k} + z_T \Gamma_T + \sum_{k=1}^{T} p_{T,k} \leq n_1 \; LC_1 \tag{C.3}$$

$$I_{1,t} = I_{1,0} + \sum_{k=1}^{t} d_k \epsilon_k - \sum_{k=1}^{t} u_{1,k} + z_t \Gamma_t + \sum_{k=1}^{t} p_{t,k} \qquad \forall t \in \mathcal{T} \tag{C.4}$$

$$z_t + p_{t,k} \geq \sigma_t \; s_t \tag{C.5}$$
$$\forall t \in \mathcal{T}, k \in \{0, ..., t\}$$
$$-s_t \leq \epsilon_t \leq s_t \tag{C.6}$$
$$\forall t \in \mathcal{T}$$
$$\epsilon_t = 1 \tag{C.7}$$
$$\forall t \in \mathcal{T}$$

Constraint sets (C.1)(C.2)(C.3)(C.4) define and limit the inventories: constraint (C.1) defines the inventory for the first buffer, considering the cumulative inbound material a_t up to period t, the overall sorted material u_{1t} up to period t, and the uncertainties protection function made of the joint contribution of $z_t\Gamma_t$ and the sum of $p_{t,k}$ for $k \in \{1, \ldots, t\}$. Constraint (C.2) sets the lower bound of the inventory for each period and (C.3) imposes the maximum unsorted material allowed to be left at the end of the planning period for the first buffer, as constraint (B.10) does for all other subsequent buffers. Equality constraint (C.4) allows the inventory of the main buffer (i.e. buffer no. 1) to be considered in the corresponding piece-wise linear part of the cost function. Constraints (C.5) and (C.6) resulted from duality in [15] robustness theory; where (C.5) sets the lower bound of the protection function contribution in constraints (C.1) and (C.3).

Appendix D

Model $\mathcal{E}$

Model $\mathcal{E}$ replicates the same deterministic formulation of $\mathcal{D}$ and introduces some additional decision variables to model overtime production. Considering the following set of main decision variables of $\mathcal{D}$:

$$y_{j,t} \in \{0,1\} : \text{ equal to 1 if production stage } j \text{ is activated at time } t, \text{ 0 otherwise}$$

$$x_{j,t} \in \mathbb{Z}^+ : \text{ operators employed in the production stage } j \text{ at time } t$$

$$u_{j,t} \in \mathbb{R}^+ : \text{ processed quantity at production stage } j \text{ at time } t$$

The formulation of $\mathcal{E}$ incorporates also the variables $y'_{j,t}$, $x'_{j,t}$ and $u'_{j,t}$ which correspond to the overtime production equivalent of the previous ones. The corresponding unitary cost of these overtime production capacity variables (i.e. $y_{j,t} \in \{0,1\}$ and $x_{j,t} \in \mathbb{Z}^+$) are f'_j and C'_t respectively, while M' is the maximum number of operators available for overtime production. Therefore, the formulation of $\mathcal{E}$ is the following:

$$\min \text{ (B.1)} + \sum_{j \in J} \sum_{t \in T} f'_j y'_{j,t} + \sum_{j \in J} \sum_{t \in T} C'_t x'_{j,t} \tag{D.1}$$

s.t.

(B.2), (B.3), (B.4), (B.7), (B.8), (B.9), (B.10)

$$\sum_{j \in J} x'_{j,t} \leq M' \qquad \forall t \in \mathcal{T} \tag{D.2}$$

$$u'_{j,t} \leq SK_{j,t}\ x'_{j,t} \qquad \forall j \in J, t \in \mathcal{T} \tag{D.3}$$

$$I_{1,t} = I_{1,t-1} + d_t - u_{1,t} - u'_{1,t} \qquad \forall t \in \mathcal{T} \tag{D.4}$$

$$I_{j,t} = I_{j,t-1} - u_{j,t} + \alpha_j\ u_{j-1,t} + \alpha_j\ u'_{j-1,t} \qquad \forall t \in \mathcal{T}, j \in J \setminus 1 \tag{D.5}$$

$$x'_{j,t} \in \mathbb{Z}^+ \qquad \forall j \in J, t \in \mathcal{T} \tag{D.6}$$

$$u'_{j,t} \in \mathbb{R}^+ \qquad \forall j \in J, t \in \mathcal{T} \tag{D.7}$$

$$y'_{j,t} \in \{0,1\} \qquad \forall j \in J, t \in \mathcal{T} \tag{D.8}$$

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