



TALLINN UNIVERSITY OF TECHNOLOGY
SCHOOL OF ENGINEERING
Department of Mechanical and Industrial Engineering

OPTIMIZATION OF SUPPLY CHAIN USING METAMODEL-BASED SIMULATION IN PARMIDA COMPANY

Tarneahela optimeerimine metamudelil põhineva
simulatsiooni abil ettevõttes Parmida

MASTER THESIS

Student: Seyed Mohsen Tavahodi

Student code: 165623MARM

Supervisor: Kashif Mahmood

Tallinn, 2020

AUTHOR'S DECLARATION

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No academic degree has been applied for based on this material. All works, major viewpoints and data of the other authors used in this thesis have been referenced.

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Department of Mechanical and Industrial Engineering

THESIS TASK

Student: Seyed Mohsen Tavahodi, 165623MARM

Study programme: Industrial Engineering and Management(MARM

main speciality:

Supervisor: Kashif Mahmood, engineer , (+372) 620 3253)

Consultants: Marzieh Tavahodi, System Analyst , Parmida, +989111006355,

m.tavahodi@parmida.co.ir

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Student: Seyed Mohen Tavahodi "25" MAY 2020

signature/

Supervisor: Kashif Mahmood "25" MAY 2020

/signature/

Consultant: Marzieh Tavahodi "25" MAY 2020

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Head of study programme: Professor Kristo Karjust "25" MAY 2020

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PREFACE

The basis of this these topic “Optimization of supply chain using metamodel-based simulation in Parmida company “originated from my passion and initiative for solving supply chain issues, particularly in inventory control context. I was involved in researching and writing this thesis from February to May 2020. My thesis was formulated and developed together with my supervisor, Kashif Mahmood from Tal Tech.

I would like to thank, Kristo Karjust who gave me the golden opportunity to study this wonderful program at Tallinn University of Technology, also, my supervisor for his excellent guidance, and my wife for her support during this process. I also wish to thank all of employees at Parmida Company whose information helped me to complete this work.

List of abbreviations

ANN- Artificial Neural Networks

GA- Genetic Algorithm

IPA- infinitesimal perturbation analysis

LHS- Latin Hypercube Sampling

LP - Linear Programming

NP- Nested partitions

RSM- Robust Simulation Optimization

SA- Simulated Annealing

SO- Simulation optimization

SS- Scatter Search

TA- Tabu Search

TPE - Thermo-Plastic Elastomers

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INTRODUCTION

Existing research recognizes the critical role played by computer simulation in modern science, particularly in designing and analysing complex systems [1], [2], [3], [4], [5]. The advantage of this powerful tool is that it provides users with the practical feedback when designing real-world systems. The simulation system “can be used to study the dynamic behaviour of systems in situations, where real systems cannot be easily or safely applied” [6].

In light of recent development in the supply chain, the use of simulation modelling in the product supply chain is becoming extremely interesting for researchers and managers inside the firms [7]. The high complexity, uncertainty, and existence of numerous decisions making and environmental parameters in real supply chain models is contributed to a surge in employing simulation models in this context.

In broad terms simulation optimization (SO), is used as a superior term for techniques used to optimize stochastic simulations [8].

“Simulation optimization involves the search for those specific settings of the input parameters to a stochastic simulation such that a target objective, which is a function of the simulation output, is, without loss of generality, minimized” [8]. Often simulation optimization algorithmic approaches depend on input-output data from the simulation in their search for optimal input settings. The optimization approaches iterate for the simulation models until the designs with desired properties are found [9]. Given the output of the discrete simulation model has stochastic nature and sometimes is expensive to run, in terms of time and resources, the application of the classic approach of simulation for these models might not be the best option. The metamodel-based simulation approaches “simplifies the simulation optimization in two ways: the metamodel response is deterministic rather than stochastic, and the run times are generally much shorter than the original simulation” [9].

In practice, some of the inputs of simulation models are uncertain and, neglecting this uncertainty in the optimization of model might be misleading. The Taguchi robust design method can be employed in such uncertain environments [10]. This approach was initially employed in Toyota with the object of the robust automobile and achieved high success in production engineering.

This dissertation aims are firstly, to develop a multi-objective simulation model of multi-product supply chain with uncertain demand, for the supply chain process of Parmida Company and secondly to introduce a framework for designing of decisions and uncertain environments parameters which later is optimized using a robust simulation optimization approach. In this approach, the Taguchi perspective is combined with novel metamodel-based approaches in order to minimize the output of simulation (cost of the system) given to standard deviation considered

for this output. In addition, the performance of Neural network is evaluated in this approach and the result is discussed.

The overall structure of the study takes the form of 3 chapters. In the first chapter, the author focuses on the literature review of application of simulation optimization in supply chain setting. chapter two begins with reviewing of the common simulation optimization approaches then each of these approaches is discussed in detail. The second half of chapter two focuses on the common metamodel-based approaches and the introduction of robust optimization approaches based on the combination of Taguchi approach and the metamodel-based simulation optimization.

In chapter 3, the author first describes the case company under study and their supply chain problem. After briefly explaining the concepts and safety stock inventory levels in the literature of the supply chain, a mathematical model is presented as the base of the simulation model for the problem. A direct simulation optimization approach is firstly employed, and the shortages of this approach investigated. Then a metamodel-based simulation optimization method is used by creating Artificial Neural Network metamodels. These metamodels are used to predict the mean and standard deviations of the supply system cost per each combination of the input variables. Ultimately, the results provided from the Pareto-optimal plot is explained to show how this robust approach can help the decision-makers to comply with risk management.

Finally, a summary of the work performed in this thesis and the results is provided. Besides, some ideas and suggestions for further research and continuing this study is presented.

1.LITERATURE REVIEW

1.1 Simulation via optimization in supply chain

Competitiveness of companies in the current marketplace highly depends on the ability of them in reducing lead-times and costs, improving customer service levels, and enhancing product quality [11], [12]. In fact, in a dynamic business environment, instead of single companies, the entire supply chains are competing with each other [13] .

The management of supply chain networks, however, faces many challenges owing to interactions between the several entities, the length of the supply chain, differences in objectives of each department, the stochastic nature, uncertainty of demand and distribution, and the variety of decision-making parameters and limitations. Furthermore, the decision makings in supply chain management are elusive since are subject to various conflicting criteria and multiple objectives. in the business environment, a group of people, rather than a single decision-maker, is often involved in the decision-making process [14]. The decision making requires consideration of several conflicting quantitative and qualitative criteria in supply chain management [15] . Notwithstanding these complexities, managers often make decisions based on their experiences which is not always the best remedy in today's highly competitive market. Under certain conditions, the Incorrect decisions may result in decreasing competitiveness, termination of supply chain function and even the collapsing of companies [14]

With respect to these complexities, decision-makers are in need of a solid approach to help and support them in decision making and able them to evaluate the impact of these decisions before their implantation.

There is a need for the optimization of the supply chain plays a pivotal role in overcoming these challenges. The system modeling is common means for summarizing the most important details of the real systems in which the output behavior is predicted by the input parameter behavior [16]. However, very few existing analytical models are restricted to simplified versions of the problem which are based on limiting assumptions [17] In addition, traditional search methods like linear programming often fail to solve these models because of the fact that most of these models are discrete and non-linear. The optimization models, however, are flexible enough to be able to incorporate multiple disparate data sources and consider all dynamics and complexities of the supply chain systems [18].

Despite the simulation models tend to explain the relationship between input and output of a complex system, they might not be able to find a set of optimized decision-making parameters

when the objective function is predetermined. Thus, the optimization model has received considerable critical attention for decision making that determines the best alternatives.

The general form of the objective function for many businesses can be defined as bellow :

$$\begin{aligned} &\text{Optimize } f_i(x) \quad i = 1, \dots, I && (1) \\ &\text{Subject to : } g_j(x) \leq 0 \quad j = 1, \dots, J \\ &h_k(x) = 0 \quad k = 1, \dots, k \end{aligned}$$

In which $f_i(x)$ is the objective function of i , x is the environmental variables vector, $g_j(x)$ and $h_k(x)$ are the functional and set constraints. However, it is elusive to find the set of decision parameter that optimize the effectiveness since:

The relationship between system components that determine the system effectiveness is ambiguous, therefore the mathematical definition of $f_i(x)$ is elusive, if It is not impossible.

Supply chains often can encompass the multi-object functions as the result of different and often contradictory alternatives [19].

There are many decision variables and alternatives that are hard to be simulated. Thus, there is a need for more advanced optimization algorithms to find optimized solutions in a timely manner. The optimization methods should consider the uncertainty that is accompanied by the supply chain and in finding of solid and reliable solution [20] .

1.2. Supply chain

Supply chain (SC) refers to “a comprehensive network of various members that supply raw materials, convert materials into intermediate and, final products and ultimately deliver them to the end customers” [19]. As Singh and Verma stated Supply chain activities encompass the transformation of raw materials, resources, and components into a finished product that can be delivered to the end-user [21]. The value creation for ultimate customer occurs through upstream and downstream linkages, in the different processes and activities. Figure 1.1 illustrates the simplified picture of a supply chain process.

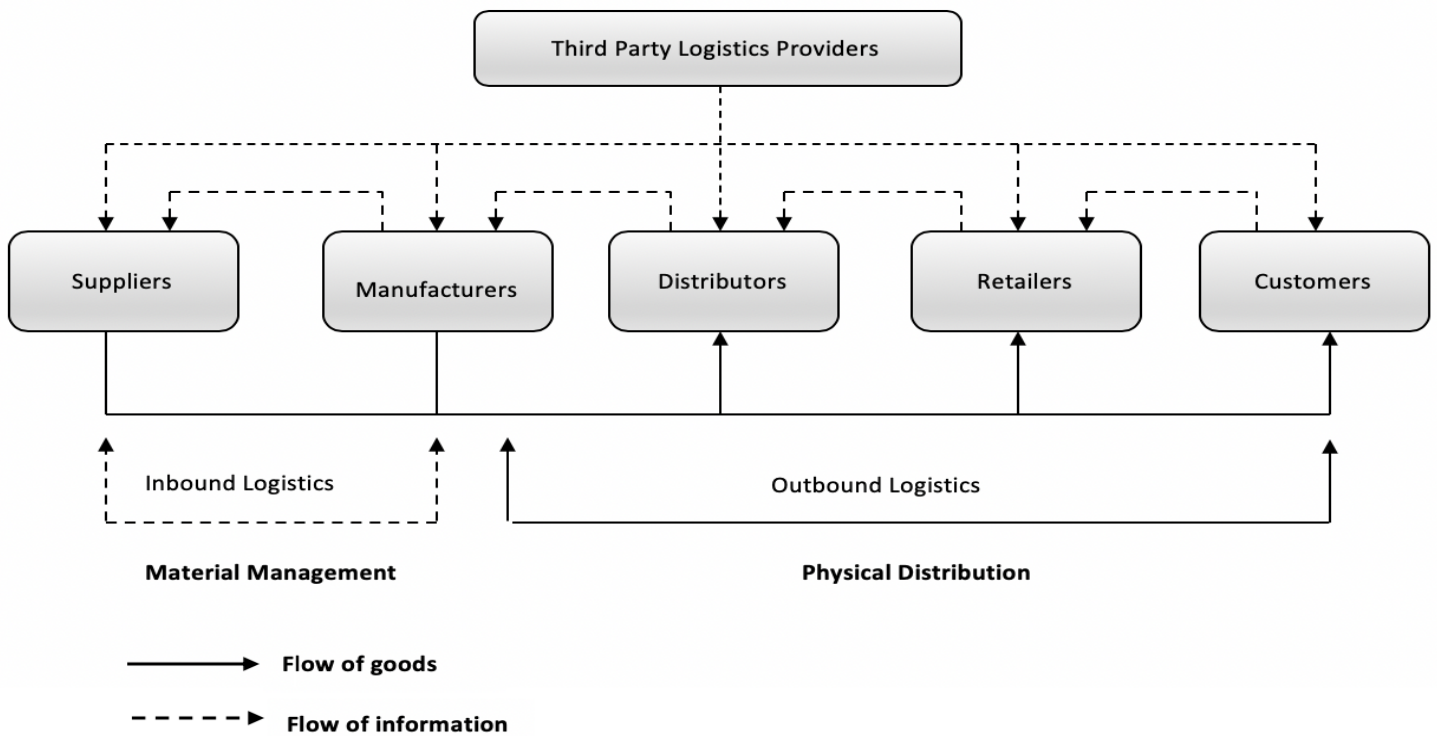


Figure1. 1 The process of supply chain [20]

A general supply chain network usually encompasses the suppliers of raw materials, producers, distributors, and retailers [22]. Multi-product supply chain networks and profitability of all supply chain components often depend on the integrated procurement, production and distribution decisions [19] [23]. Thus, for businesses seeking to survive in an increasingly competitive business world, it is crucial for each component department within the supply chain to make integrated decisions, which facilitates sustainable success and competitiveness of each supply chain member [19].

However, management of such a complex network is difficult and challenging because of various reasons such as globalization of today's market, increasing outsourcing, short product lifecycle, and advancements in information technology.

In the following section, the author gives a brief overview of optimization simulation in the supply chain. From the decision making perspective, supply chain can be divided into four main areas including Inventory management, production planning, support and logistics management, and designing and supply chain coordination. In this thesis, the research model is placed in the inventory management context, therefore, the rest of this chapter focuses on the review of the simulation optimization in the inventory management context.

1.3. Inventory Management

Inventory is one of the main parts of supply chain management that “focus on the management of inventory from supplier to customer and vice versa” [21]. Inventory is one of the most important assets of a company and inventory management as an integral part of supply chain management “plans, implements and controls the efficient, effective, forward and reverse flow and storage of goods, services, and related information between the point of origin and the point of consumption in order to meet customer's requirements” [21]. Effective management of inventory requires various decisions. The effective inventory management is a building block for achieving the competitive advantage whereas the poor decision regarding inventory can lead to the decrease of sales because of stock-outs, increase in shipment and finished product cost, and longer production time. Thus, a company survives in the long run if its managers pay special attention to the area of supply chain and Inventory. Of all the activities in a supply chain process, inventory management is the most dynamic and visible activity. Given the importance of the strategic impact of inventory on the supply chain, finding the minimum and maximum level of inventory, volume of order, and the calculation of the optimum amount of (s,S) is costly and represents a big simulation-based challenge for decision-makers inside the companies. In a (s,S) ordering policy the order is placed when the level of inventory is lower than S unit and the volume of this order is equal to the difference between maximum level of order and current inventory. Thus, the optimization helps the decision-makers to evaluate and analyze the alternatives and find the optimum amount of inventory. Jiang et al. (2015), presented an optimization model for inventory system as well as an algorithm for the optimal inventory costs based on the supply-demand balance in order to minimize the average total costs in unit time of inventory system, They succeeded to find the optimal stock and the optimal inventory costs. In addition, the result of their research showed that the uncertainty of lead time greatly influenced the optimal inventory strategy [23]. Gavirneni (2001) used infinitesimal perturbation analysis (IPA) for the calculation of the optimum level of order in a capacitated supply chain [24]. The author evaluated the advantage associated with sharing of inventory parameter data with the retailers including the ordering policies. As a result, the cost of supplier decreased from 1 to 35% [24]. Pichitlamken et al. (2006) developed a selection-of-the-best scheme known as Sequential Selection (SSM) with Memory with the goal of finding the neighborhood [25]. Köchel and Nieländer (2005) also developed an integrative simulation method and GA for determining the optimal order policy in multi-echelon inventory systems [26].

The relationship among the inventory decision variables and criteria of supply chain effectiveness can be determined using meta-models. The generated meta-models, then can be employed to determine the base-stock levels in various stages of supply chain in order to find the minimum cost

of product storage in the warehouses and maintain cost in supply chain nodes. Based on this structure, Nagaraju (2018) developed a model for optimal net revenue of the coordinated three-level supply chain incorporating ordering cost, carrying cost and transportation cost [27]. Similarly, Daniel and Rajendren (2006), integrated the GA and simulation models to determine base-stock levels, and reduced the maintenance and goods shortages cost in the entire supply chain process [28].

Determining of the optimum level of inventory is often challenging in a stochastic and environment of supply chain with several resource of uncertainty. The resource of uncertainty might be varying from the changes in customers' demands to the unreliability of external suppliers. Jung et al. (2004) employed a simulation-based optimization approach in which they used safety stock levels as a means of placing demand uncertainties in routine operation [29]. The main limitation of this approach might be related to the timely calculations where the supply chain dimensions and territories expand and termination of the relationship between inventory decision variables and effectiveness criteria gets elusive.

The research problem in this study is adopted from the supply chain model in Jung et al. (2004) research and it is associated with the multi-object inventory management using the meta-model approaches [29].

2. SIMULATION OPTIMIZATION

In the present chapter, the author clarifies the term of simulation optimization and its framework and application in decision-making. Then, introduces the several types of optimization models that have been proposed in the literature alongside optimization model's advantages and drawbacks, particularly the metal-model methods since it is the focus of this thesis. Thereafter, the author introduces the Taguchi Robust approach and its application in simulation optimization.

2.1. Simulation optimization: definition, concepts, advantages and drawbacks

Simulation is one of the most widely used and effective methods of analyzing the complex system with multiple variables. The advancement in technology and the increasing use of computers have significantly contributed to the application of simulation in solving the decision-making problems. The simulation has widely been used by the designers and analysis in various fields of science and it promises to become a useful tool for solving the complicated problems of managerial decision-making [30].

Compared with mathematical programming, simulation methods offer a number of advantages. They are a powerful tool for analyzing the complex system with a high level of uncertainty. Often managerial decision problems are highly intricate to be solved by either mathematical programming or experimentation with the actual system, even if possible, is very costly and risky. Simulation methods provide the solution by allowing experimentation with the model of the system without interfering with the real system. Simulation models are also flexible and can be modified to adjust to the changing environments of the real situation. Thus, the simulation method is widely used in various fields of science such as transportation, production, communication, supply chain, etc.

Optimization models often seek to find an answer to "how an optimal response can be found?", whereas, the simulation models looking for an answer to "what if...?" questions. In other words, simulation mostly focuses on the result of changing and substituting multiple factors in the model and analyzing the consequent changes, rather than finding the optimal response [18]. This is a very useful tool for decision-makers as they are often willing to know the impact of a change on a system. In some cases, the output of an optimization process might not be applicable for some reasons. Therefore, simulation methods can be a powerful tool for managers and analysts in an environment with high uncertainty.

One of the main features of simulation is that it ables the decision-makers to change the parameter of systems instantly and analyze the impact of these changes on the system performance. Thus, it is logical that the analyst seeks to find those changes that are influential on the improvement and optimization of system performance. This process is called simulation optimization in the literature. Amaran and his colleagues defined Simulation Optimization (SO) as “optimization of an objective function subject to constraints, both of which can be evaluated through a stochastic simulation” [8].

These authors considered term Simulation Optimization “an umbrella term for techniques used to optimize stochastic simulations”. In general, using simulation optimization, the researcher is looking for an optimum or semi-optimum response among other alternatives that their evaluation is possible through computerized simulation.

SO is widely used when:

- The objective function or constraints is stochastic in nature
- The mathematical form of object function or constraints are not available
- The measurement of object function or constrains with mathematical methods may be expensive to run, in terms of time, money, or resources

A very general simulation optimization problem adopted from Amaran et al.(2016) [8] can be formulated as below:

$$\begin{aligned}
 \min \quad & E\omega [f(x, y, \omega)] & (2) \\
 \text{s. t.} \quad & E\omega [g(x, y, \omega)] \leq 0 \\
 & h(x, y) \leq 0 \quad xi \leq x \leq xu \\
 & x \in Rn, y \in Dm
 \end{aligned}$$

In which, the f function can be evaluated via simulation for the continuous inputs x , discrete inputs y , and a realization of the random variables (the vector ω) in the simulation, ω may or may not be a function of the inputs, x and y . The problem’s constraints can be defined by the vector-valued function g that can be also evaluated with each run of the simulation. The expected values for these s functions are used in this formulation. There may be also other constraints (h) that do not include random variables, as well as bound constraints on the decision variables. The elimination of any of these conditions would make a problem that would fall under the territory of SO. The formulation above is very general, and thus a wide variety of applications fall under the scope of simulation optimization [8].

2.2. Simulation Optimization methods

As previously mentioned, the simulation optimization problems are very time consuming because finding the optimum output requires several executions of simulation models particularly when there are several decision variables. The literature on simulation optimization has introduced several approaches that mainly seek to find the optimum output with fewer executions in shorter time of solution. The simulation approaches can be categorized based on the following criteria:

- Based on the type of objective function(s): single or multiple objectives
- Based on the decision variables: discrete or continuous
- Based on the solution space: countable and uncountable
- Based on the decision variables: qualitative or quantitative

Figure 2.1 demonstrated the main simulation optimization approaches in the literature [31], [32]. In the following section, the author provides an overview of most widely-used simulation optimization approaches.

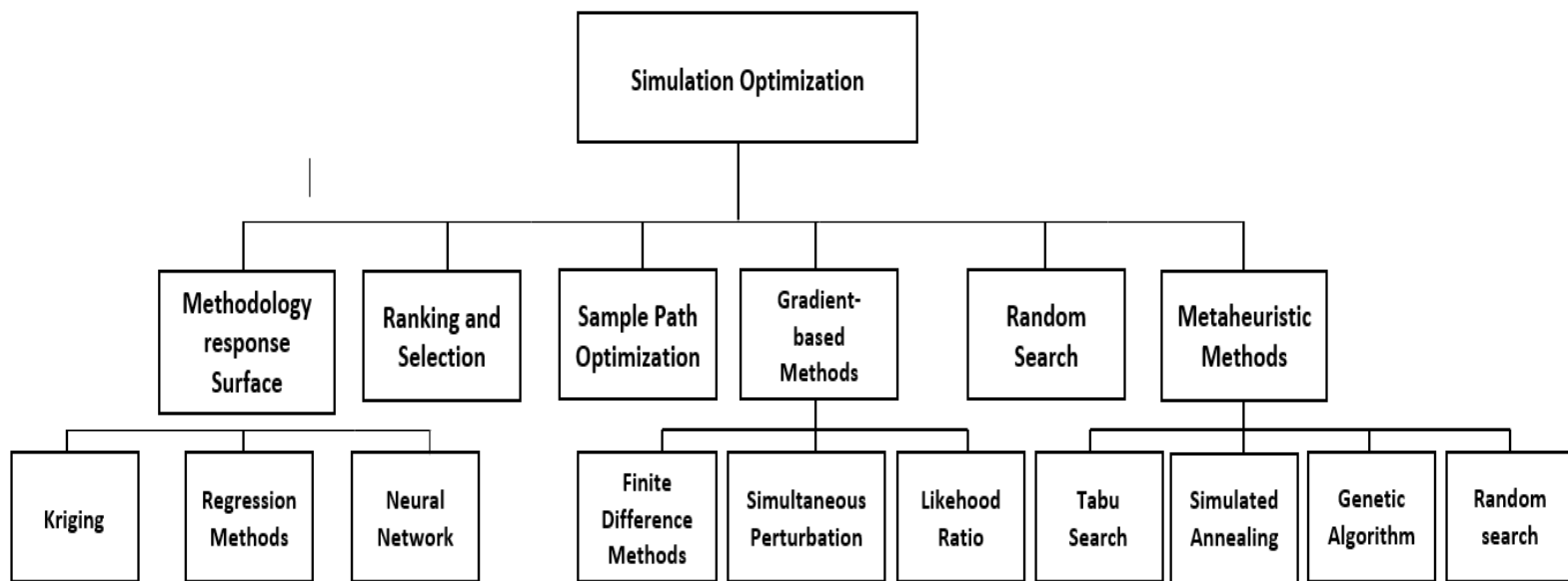


Figure 2. 1 Categories different methods of simulation optimization (Source: own illustration)

2.2.1 Gradient Methods

Deterministic optimization can be divided into Gradient search methods and direct search methods. Although the direct search methods use the value of objective function for acquiring of an optimum point regardless of object function characteristics, the Gradient-based methods are iterative methods that constantly use the gradient information of the objective function during iterations and seek to find the path to optimize the problem. The Gradient-based methods in simulation optimization perform in optimization problems similarly. However, the optimization problem in simulation is stochastic. It is widely used particularly for those problems where the decision variables are continuous [32].

2.2.2. Heuristic and metaheuristic methods

The Heuristic and metaheuristic methods are able to determine a solution with good quality approximations to exact solutions. These methods were initially based on experts' knowledge and experience that aimed to discover the search space in a convenient way" [33]. In recent years, there has been an increasing interest in using heuristic and metaheuristic methods in solving the decision-making problems. These methods can best be categorized under four headings: Simulated Annealing (SA), Genetic Algorithm (GA), Tabu Search (TA), and Scatter Search (SS). Among these GA, SA and TS are the most widely-used methods in optimization literature. Despite SS has been addressed as the most known searching method in optimization simulation software, but in terms of application it covers a limited range of problems [34].

In 2000, Shi and Olafsson introduced another heuristic method into the literature for stochastic optimization called "Nested partitions" (NP) method [35]. This method has proven an effective method for solving optimization simulation problems. The summary of steps in the Nested partitions can be listed as follow:

1. The whole solution space is considered the Most Promising Set (feasible region)
2. The most promising set is partitioned into a number of subsets unless it has only one point.
3. The independent points in each subset are selected using random sampling and evaluated later based on their performance.
4. Based on the sampled selected from each subset, the promising index is calculated for each subset (the higher promising index the better subset)
5. Based on the promising index, the most promising set out of subsets are selected. In the case that two sets have the same promising value, they are merged then the whole new sets considered the most promising set.

6. If the best value is not reached, the algorithm will not stop and start again from step 2 otherwise algorithm stops and the best response (value) will be returned.

In recent years, the metaheuristic methods have been merged into other simulation optimization methods such as R&S, RSM (metamodels), random search, etc. which shows the interesting result [36].

2.2.3 The metamodel methods

This method originates from the design of the statistical experiments and its objective is to find the relationship between the decision variable and objective function (response variable). These methods are relatively easy to implement. Since the simulation models, themselves may be complex, and therefore simpler approximations are usually constructed which are called models of the model, or metamodels [37].

In this method, first a relationship between the objective function and decision variables is determined in the form of a restricted formed function, then this approximated objective function is optimized. Since the simulation optimization problem often there might not be available, the response surface methods seek to obtain an estimation of the objective function using the input and output of the simulation. Thereafter, this approximated function is used as a substitute function during the optimization process. In recent years, the response surface is mainly used for the regression metamodels. Similarly, in this thesis, the author uses response surface as regression metamodel.

One of the advantages of this method is that after attaining the approximated function, this function can be used in solving deterministic optimization problems. In addition, this method decreases the mathematical calculations as well as time and the cost of optimization. In practice, when the process of function estimation is done on the whole response surface, the approximated function is called “metamodel” [37].

2.2.4 Neural Networks

Artificial Neural Networks (ANN) are pieces of computing models and algorithms that simulate the way that human biological neural networks process the information. They receive raw input information and produce outputs based on predefined activation function [38]. One of the main applications of these networks is the estimation of functions. These methods often consist of three or more layers as input layer, hidden (intermediate) layer, and output layer. Each layer has one or more neurons. Each neuron receives input signals and raw input data enters into the neural network through the input layer, thereafter, goes to the intermediate layer and the process procedure, the output is delivered to user through the output layer. The figure 2.2 shows a

simplified version of neural network and figure 2.3 shows a neural network with one intermediate layer.

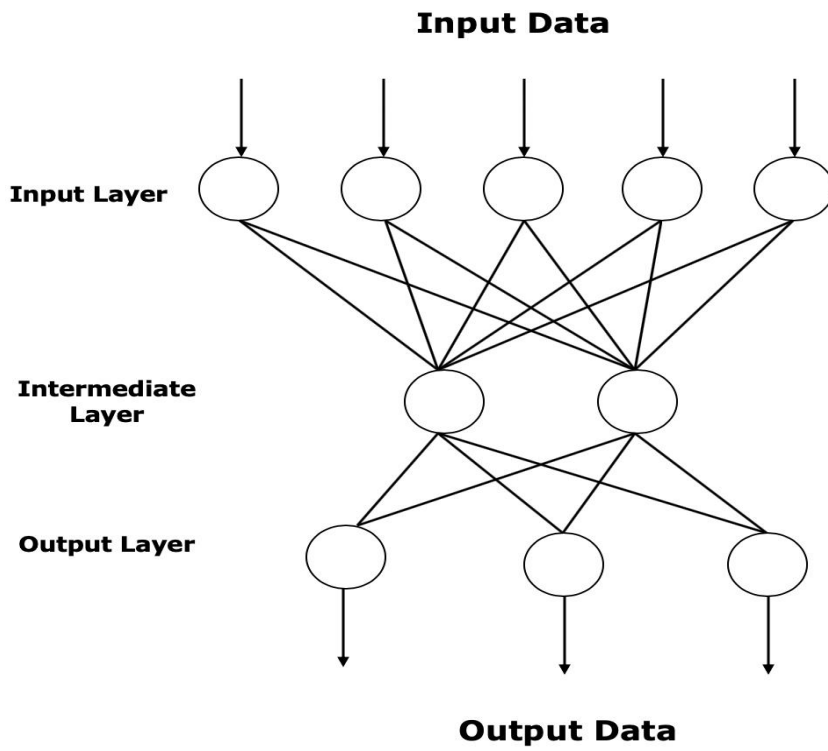


Figure 2. 2 Simplified version of a Neural Network (Source: own illustration)

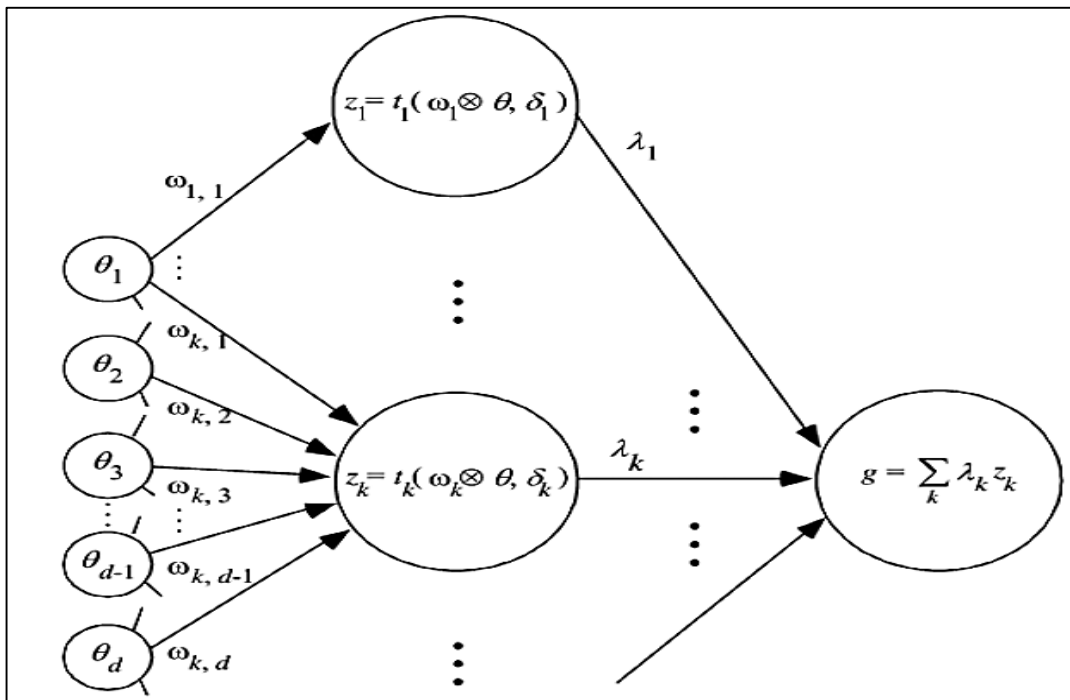


Figure 2. 3 A neural network with one Layer [38]

In figure 2.3, $\theta_1, \theta_2, \dots, \theta_d$ are the problem parameters, $\omega_{i,j}$ indicates the weight of that synapses than connects the t^{th} (neuron) of input layer to the t_j^{th} of intermediate layer, $z_m = t_m(\cdot)$ reflects the activation tm function, λ_m is the weight of intermediate t_m , and

$$\omega_m \otimes \theta = \sum_i \omega_{m,i} \theta_i$$

The number of neurons in the input and output layers depends on the problem. The number of neurons in the input layer is the same as the number of independent variables of the problem and the neuron number in the output layer is same as the number of response variables(s). However, the number of neurons in the intermediate layer mainly depends on the degree of nonlinearity and complexity of the problem. A higher number of neurons in hidden layer is associated with the network's ability in explaining the complexity of the problem.

The result of each neuron operation, after calculating the corresponding weights and aggregation of their weights, is entered into the activation function then after some changes, it enters into next layer as an input. In the cases where the neural networks are used to approximate the and predict of actual value, the linear activation function can be employed in the last layer.

Since the majority of problems that use neural networks are complex and nonlinear, in the intermediate layer the nonlinear activation functions are employed. Due to the widespread use of neural networks' ability in approximating and estimatiimg of functions, they have been the subject of many studies in the simulation optimization context. [39], [40], [41].

2.3 Metamodel Validation

The process of metamodel validation is one of the main steps in metamodel-based optimization. During the validation of metamodel, the quality of the generated model in terms of accuracy and the ability of model in estimating objective function is evaluated. The validation of a metamodel depends on the type of problem and the goal of simulation optimization. Several validation methods have been introduced in the literature over the last two decades such as:

- Coefficient of determination
- Bootstrap
- Cross-Validation

2.3.1 Coefficient of determination

The coefficient of determination is an increasingly important method for validation of metamodels that allows for the evaluation of prognosticated response variables accuracy used in the metamodel. The closer the numerical value of this statistic (R^2) is to 1, the higher the predictability of the model is possible. The value of this statistic is calculated through the following equation:

$$R^2 = \frac{\sum_{i=1}^n (\hat{y}(x_i) - \bar{w})^2}{\sum_{i=1}^n (w_i - \bar{w})^2} = 1 - \frac{\sum_{i=1}^n (\hat{y}(x_i) - w_i)^2}{\sum_{i=1}^n (w_i - \bar{w})^2} \quad (3)$$

In which n refers to the predicted points, $\hat{y}(x_i)$ denotes the value of predicted response in point x_i , w_i indicates the true (actual) value derived from the simulation, and finally \bar{w} is the Arithmetic mean of w_i (s).

The main problem with this method is that: first, the R^2 does not follow the any known statistical distribution (therefore it might not be possible to calculate a precise confidence interval for that), Second, the value of this statistic increases along with to the problem parameters, however, the prediction performance of model remains the same. There is another type of determination coefficient called the adjusted coefficient of determination, which is presented to solve the second problem and is calculated as follows:

$$R_{adj}^2 = 1 - \frac{n-1}{n-m} (1 - R^2) \quad (4)$$

In the above equation, m shows the number of metamodel parameters, and the value of R^2 is calculated using equation (3). In addition, the number of design should be bigger than the number problem parameter [42].

2.3.2 Bootstrap methods

This method introduced by Efron in 1979, is one of the most powerful methods for validation of metamodel and its ability of predict. Bootstrap observation is obtained by sampling from a series of random and independent observations. On other word, the author assumes that the set of main points is $S = \{x_1, x_2, \dots, x_n\}$, one sample of Bootstrap can be defined as $BS = \{x_1^*, x_2^*, \dots, x_n^*\}$ in which, each member is selected from S with the equal placement and probability. Thus, it might be possible that each of x_i is used more than once in BS set $i = (1, \dots, n)$. In this case, if $\xi(x_1, x_2, \dots, x_n)$ is the estimator of known standard deviation of θ , the Bootstrap estimation of this parameter is:

$$\hat{\theta}^* = \xi(x_1^*, x_2^*, \dots, x_n^*) \quad (5)$$

To approximate the standard deviation error, the process of Bootstrap sampling repeat in a determined number, and an estimation is calculated of the Bootstrap parameter in each iteration. Thereafter, the estimation of $\hat{\theta}$ error can be calculated using the following equation:

$$s. e. (\hat{\theta}) = \sqrt{\frac{\sum_{i=1}^B (\hat{\theta}_i^* - \bar{\theta}^*)^2}{B-1}} \quad (6)$$

Where, B denotes the number iteration, $\hat{\theta}_i^*$ is the approximate value for unknown parameter of ($i = 1, 2, \dots, B$) θ , and $\bar{\theta}^*$ is the Arithmetic mean of $\hat{\theta}_i^*$ in B Bootstrap iteration.

2.3.3 Cross-validatory method

The cross-validatory method is one the most powerful methods for evaluating of the accuracy of metamodel's prediction ability. The main idea of the cross-validatory method first presented by Stone in 1974. In this method, the set of raw data is be divided into two categories in the first phase. The first category called training data is used for training of metamodel and its fitting. The second category called validation data is employed to evaluate the performance of metamodel.

In order to decrease the error variance, several iterations of the above-mentioned are used with different categories, and eventually the metamodel error can be calculated considering criterion that aggregates all iteration errors.

So far there have been various algorithms developed based on the cross-validatory methods that the majority of them are different in the way they divide the design pints into training and validating categories. The simplest algorithm is known as K-fold cross-validation. In each iteration of this algorithm the following steps are performed:

The experiment points are partitioned into K similar size subsamples and experiment points in each subsample and the relevant response variables are called x_i and ($i = 1, \dots, n$), respectively.

The i subsample is excluded temporarily from the experiment points and the metamodel fit can be evaluated based on the remained points.

The value of the experiment point (the excluded pint) is predicted using the fitted metamodel in the prior step, then is called \hat{y}_{-i} .

These steps are reaped until all sets above are excluded at least once from the experiment points set. The error associated with each predicted value is calculated given (w_i, \hat{y}_{-i}) and then the error of the whole metamodel is calculated [42].

2.4 Robust simulation optimization

The main goal of robust simulation optimization is the integration of the Taguchi worldwide approach (1987) with existing simulation optimization methods (e.g. RSM). The Taguchi approach first developed in order to assist the robust automobile design (those have satisfactory performance under diverse situations) in Toyota. There have been many critiques and modifications toward the Taguchi statistical methods. For instance, Montgomery and Myers (1995), who integrated the Taguchi approach with RSM to present robust optimization. Their approach was more applicable in the real model's (not simulated) optimization where changing a factor is difficult for its different values. Dellino et al. (2010) matched the RSM of Montgomery and Myers with the simulation optimization characteristics using Latin Hypercube Sampling (LHS), which has as many values per factor as it has combinations [43]. Further they modified RSM methodology with adding Bootstrapping, Mathematical Programming, and Pareto frontier. RSM methodology uses the low-order polynomial regression metamodels that are faster than simulation models.

2.4.1 Taguchi robust approach

According to Kleijnen (2008) [42], Taguchi's approach can be described as below:

Taguchi divided the model variables into two categories:

- Decision factors (or control) that are denoted by d_j ($j = 1, \dots, k$) here
- Environmental factors (or noise) that are shown as e_g ($g = 1, \dots, c$) in this thesis.

Based on the above, the decision variables are under the control of the user. For instance, in inventory control, the amount of order (Q) can be controlled. However, the demand rate (D) cannot be controlled easily. Taguchi considers w unit output and focuses on the mean, $E(w) = \mu_w$ and variance, $var(w) = \sigma_w^2$ of the output. Dellino et al (2010), utilized Taguchi's approach for simulation optimization while modified its statistical methodologies and replaced them with RSM. The reason was that the simulation experiments enable the exploration of several factors, factor levels as well as the combinations of factor levels than real-life experiment provides. Instead of using the scalar loss function of Taguchi including signal-to-noise or mean-to-variance ratio, they let each output have a statistical distribution which is characterized through its mean and standard deviation. Then they solved the resulted problem through the Pareto-optimal efficiency frontier [43]. To do this, they considered a random output variable like w , then formulated a constrained minimization problem in which the average of this output (\bar{w}) is optimized subject to a limit on the standard deviation of this output (S_w).

2.5 Robust optimization and RSM

Montgomery and Myers (1995) [44], used a low-order polynomial function, which in fact is a second-order polynomial of multiple decision variables of d_j to estimate the optimum combination of values of these variables. For modeling of the probable impact of environmental factors of e_g , a first-order polynomial was employed. To approximate the interaction and correlation between two type of decision and environmental variables, a “noise-control” function was used, the result of that is formulated in form of regression:

$$y = \beta_o + \sum_{j=1}^k \beta_j d_j + \sum_{j=1}^k \sum_{j'>j}^k \beta_{j;j'} d_j d_{j'} + \sum_{g=1}^c \gamma_g e_g + \sum_{j=1}^k \sum_{g=1}^c \delta_{j;g} d_j e_g + \varepsilon =$$

(7)

$$\beta_o + \beta' d + d' B d + \gamma' e + d' \Delta e + \varepsilon_o$$

In which, y denotes the regression predictor of the output w , ε is residual with $E(\varepsilon) = 0$ in the case that the metamodel has no lack of fit (LOF), B shows the symmetrical matrix $k \times k$ with diameter elements of $\beta_{j;j}$ and the non-diameter of $\beta_{j;j'}/2$.

Generally, the coded variables are used in the designing of experiments which is shown as x_i . As a result, the experiments contain n main factors of z_i are that correspond to variables of d_j and e_g in the formula (7).

Unlike Montgomery and Myers (1995) [44], Dellino et al. (2010) considered more realistic assumption for error e . They considered its mean as non-equal to zero and the co-variance matrix as $cov(e) = \Omega_e$. [43]. To approximate the unknown parameters in the formula (7), the bellow linear regression model is formulated:

$$y = \zeta' x + \varepsilon \quad ; \quad \zeta = (\beta_o, \beta, b, \gamma, \delta)' \quad (8)$$

In this model, b denotes the vector with the $k \times (k + 1)/2$ iterations between the decision factors plus their k purely quadratic effects, and $k \times c$ shows the control-by-noise interactions. It should be mentioned that the equation (8) is linear with the ζ parameters, while is not linear with the decision variables of d . Then equation (8) gives the Least Squares (LS) estimator:

$$cov(\hat{\zeta}) = (X'X)^{-1} \sigma_w^2 \quad (9)$$

The presented metamodel RSM metamodel (7) implies on that equality of σ_w^2 and σ_ε^2 . This variance is approximated using the Mean Squared Residuals (MSR)

$$MSR = \frac{(\hat{Y}-W)(\hat{Y}-W)}{n-q} \quad (10)$$

In which, $\hat{Y} = \hat{\zeta}'X$

In addition, Dellino et al. (2010), assumed that y has normal distribution which means that ε and e are distributed normally in (7) [43]. Thus, the approximated regression parameters of ζ Can be tested through t statistics below with degrees of freedom

$$t_{n-q} = \frac{\hat{\zeta}_j - \zeta_j}{s(\hat{\zeta}_j)} ; j = 1, \dots, q \quad (11)$$

In which, the denominator is the square root of the j th element on the main diagonal of $cov(\hat{\zeta})$ with σ_w^2 approximated using (10). To construct confidence intervals for the robust optimum, Parametric Bootstrapping is used in the simulation model. It requires the distribution of the relevant random variable to be known. bootstrapping is a simple numerical method for acquiring the approximated density function of a statistic for a parent distribution (non-Gaussian). To determine if the RSM model (7) adequately approximates the true Input/output function defined by the simulation model, Dellino et al. (2010) employed the Leave-one-out cross-validation [43]. In this approach, in each stage one of combination i from the complete set of n combinations are omitted, and using the rest of combination, the RSM is recomputed. Then, these steps are repeated until all n combinations are processed. Thereafter, using a scatterplot with the n pairs, it can be judged whether the metamodel is adequate. In addition, the relative prediction errors can be calculated through $\widehat{y}_{(-i)}/w_i$ where $\widehat{y}_{(-i)}$ is regression predicational for simulation outputs when the i^{th} combination among existing combination of output/input, is deleted.

3. ANALYSIS

3.1 Problem definition and solution algorithm

In this chapter, the author presents a stochastic multi-product supply chain with multiple suppliers and suppliers using Taguchi and metamodel-based stimulation optimization with the goal of optimization as well as the introduction of a framework for designing experiments and rebuts optimizing of a similar problem in the supply chain and inventory control contexts. In this thesis, using case study strategy author evaluate a supply chain problem found in an industrial company performing in the automobile industry. Using the collected data from this company, the author tests the possible simulation model of the problem. In addition, the impact of random demand is evaluated on the average cost of the system. The weakness of the classic simulation approach is evaluated, and the metamodel-based approach is used for rebuts optimization of the problem. In the following section, the author presents a brief history of the company, the research case.

PARMIDA Rubber Industries Co. (from 1984 till now) is the biggest manufacture of various types of multi-components EPDM rubber strips in Iran that produces two-component and three-component rubber strips for various industries, particularly for the automotive industry.

Along with the fast growth of the automotive industry, and in order to respond to high market demand for the latest standards, using the most sophisticated machinery, PARMIDA produces the new generation of weather strips based on Thermo-Plastic Elastomers (TPE).

For the time being, the company proves sealing systems for all internal-made automobiles including various brands such as Peugeot, KIA, Renault, IK, Mazda, and different heavy trucks. During recent years, this company has also focused on supplying the demand of different industries such as home appliances, railway, oil and gas, construction, and petrochemical industry. PARMIDA rubber industry was one of the few companies that have been nominated as Grade "A" by Iranian auto-manufacturers. Developing high quality products employing, this company employs trained personnel, modern top rate machineries and up-to-date laboratory equipment. PARMIDA rubber industry vision is to develop into international market and export products to auto manufacturers across the World.

However, the industry that this company performs in, accompanies with a great deal of uncertainty in product demand, the raw material price, raw material order time, production and distribution of the final product, and the issues in the production line and quality control. Among them, the uncertainty o of demand plays most influential role in company's profit and customer satisfaction.

the uncertainty in demand might lead to over- or under-production of products that result in the extra inventory and maintenance cost and non-responded customer demand respectively.

In the supply chain previous research, the level of customer satisfaction is defined as the customer expected level of supplier ability in supplying of products. In the competitive market, the customer satisfaction level is an important index for companies that need be evaluated and kept in a highest level. The increase in customer satisfaction can be fulfilled with a big amount of inventory to respond the demand uncertainty, which lead to high inventory cost. The balance between these factors can be achieved through a probable multistage optimization in which both production and inventory levels are key variables of optimization. Since even the most definitive models of such problems are challenging with conventional solution methods, practical alternative methods are required.

Applying such alternative approaches requires using of the safety stock concept: safety stock refers to the extra stock that is a time-independent that is maintained to alleviate the risk of stockout and covers some of the uncertainty in demand.

In fact, in the literature of the supply chain, there is a significant amount of research focused on the determination of safety stock based on classical inventory theory. Although, the analytical methods were remarkably simplified in these researches, the majority of the unable to explain the key issues in the real supply chain, for instance when the production of multiple products happen in multiple factories, while demand comes from multiple sales regions.

Moreover, in the contemporary world of supply chains, the level of inventory depends on various factors such as the probabilistic distribution of demand, ratio demand to capacity ratio, the general level of customer satisfaction associated with the demand for multiple different goods manufactured in the same factory, and also the periodicity that the planning and production of factory's production is updated. The combination of these factors leads to complexities that do not correspond to classical models of inventory.

The automobile industry and the companies related to this industry often use the Linear Programming (LP) and complex integer linear programming (MILP) for planning and scheduling. Practically, the demand uncertainty and many other different factors are evaluated implementing models called "Horizon Rolling". In this method, the operational horizon is categorized into a certain number of periods, the planning model can be solved by predicting the appropriate definite demand to obtain the target rate of production in every single period. The objects of first periods are used as the input to definite models that ultimately provide us with time-based production and sequence responses. Once the first period ends, the system mode such as inventory level is updated, and the planning and scheduling cycle is repeated along the horizon of another period.

The safety stock concept can embed in such planning models considering the low level of product inventory or various factories.

Since generating customer satisfaction is uncertain quantity inherently, integrating this criterion to the model can be difficult.

3.2. The impact of safety stock on the supply chain problems

In figure 3.1, the conceptual relationship between customer level of satisfaction and safety stock of a product under uncertain demand is illustrated [45].

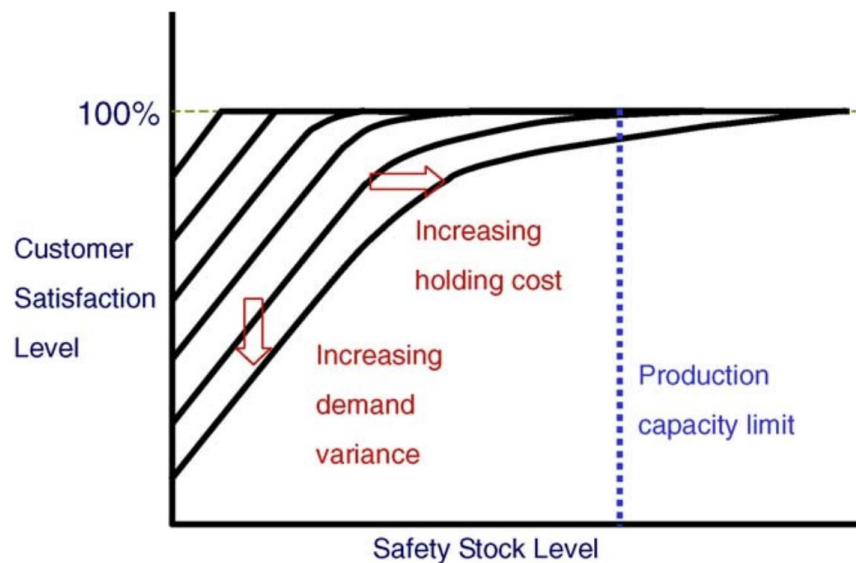


Figure 3. 1 The conceptual relationship between customer satisfaction level and safety stock [45]

In one hand, the safety stock protector allows the production system to adapt to a sudden change in demand. if there is a limited capacity of production rate, when demand changes are higher than certain level, it cannot be expected that any level of safety stock meets the customers’ demand. Therefore, making a balance between the optimizing of customer level of satisfaction and minimize of safety stock should be based on the limitation of production capacity that results in the constrained stochastic optimization problem.

The difference amount of expected demand ratio to production capacity leads to the creation of three different operational systems. In the first system, in which the ratio of demand to production capacity is small enough, the manufacturer factory has sufficient extra capacity to cover the sudden change in the demand. Therefore, in this system, a relatively small or even zero safety stock is needed to achieve the desired level of customer satisfaction. In the second system, with the medium amount of ratio of expected demand to the production capacity, the capacity of production might be completely limited when there are sudden increases in the various product in

different times. In this system, even with the safety stock, for some goods that are produced in a joint factory (between multiple factories), the customer satisfaction level might not reach the desired level. Finally, in the third system, the ratio of demand to production capacity is so high that the combined demand from different customers cannot be easily met, and as a result, there might be a competition between these demands for productive resources. In this system, the safety stock and production resources must be strategically allocated to meet the demands of priority customers. In this thesis, the levels of safety stock appropriate to the conditions of the first and second systems will be discussed. Determining the safety stock levels in the third system includes quota allocation strategies and prioritizing customer demand, which is beyond the scope of this research.

The problem under study with the above assumptions is essentially a multi-stage probabilistic problem involving a set of operational and structural constraints.

In this formulation, the level of safety stock is not directly demonstrated but are implicitly demonstrated in individual product inventory variables.

The direct solution of multi-stage probabilistic scheduling problems with the mathematical planning methods, given to the dimension and complexity of horizon rolling, is not feasible. For instance, even the deterministic structure of this problem utilizing the approximate scenario-based solutions leads to a problem that is beyond the ability of MILP and LP solution techniques.

3.3. The introduction of model and the definition of parameters

The problem under study addresses the management of the automobile industry supply chain. The main problem is presented as a company that performs in the automobile industry that has multiple factories and each of these factories consists of multiple units of production.

Customers of the company's products are located in multiple and separate sales regions, and product demand forecasts are determined based on these sales regions. The uncertainty of demand associated with each product can be modeled by the normal distribution, as a prediction of deterministic demand is considered as the mean of this normal distribution and historical data is used to measure the standard deviation of this normal distribution. This standard deviation can be defined in terms of the requested (demanded) products (these assumptions will be explained in detail in the experimental design section). All sales regions can be supplied by each of the factories or production sites, and the transportation of products is always possible. However, there are some limitations for instance due to the limitation in the transportation system, the aggregated amount of order for all products by all sales centers for each factory is high and each factory has the ability to produce a certain amount for each product based on the current process units.

In this formulation, the aggregated cost of the supply chain is minimized given to certain constraints, and the level of customer satisfaction index will be maximized which is associated with the outsourcing of customer demand if company is unable to meet this demand. In the other word, it is assumed that customers will be more satisfied if the main manufacturer meets their demand rather than outsourcing (from another supplier). Production volume in each process unit and amount of supply from each warehouse to sales regions are presented as decision variables.

P_{ijt} : amount (volume) of production of product i in the factory j in period t

c_{ij} : cost per unit of product i in factory j

S_{ijst} : amount of supply of product i in factory j to sales regions s in period t

t_{js} : cost of transportation of each unit of product from factory j to sales regions s

d_{js} : distance from factory j to sales area s

Ψ_{ist} : amount of product i for customer in sales region s in period t that should be outsourced because of inadequate supply of product

Ω_{is} : price of product i outsourcing for sales region s

I_{ijt} : inventory level of product i in factory j at the end of period t

h_{ijt} : storage cost per product i in factory j in period t

R_{ijt} : efficiency rate of production of product i in factory j in period t

H_{ijt} : available time for production in factory j in period t

T : total number of time periods considered in the model

ω_{ist} : uncertain demand for product i from sales regions s in period t

Z_{ist} : Binary variables for determination of those sales regions that their domain is meet through outsourcing.

D_{max} : maximum amount of demand for a specific sales region in one period.

D_{min} : minimum amount of demand for a specific sales region in one period.

Then the optimization model will be defined as follow:

$$\text{Min } \sum_{i,j,t} c_{ij} P_{ijt} + \sum_{i,j,s,t} t_{js} d_{js} S_{ijst} + \sum_{i,j,t} \Omega_{is} \Psi_{ist} + \sum_{i,j,t} h_{ijt} I_{ijt}$$

S.t:

$$P_{ijt}, S_{ijst}, \Psi_{ist}, I_{ijt} \geq 0$$

$$P_{ijt} \leq R_{ijt} H_{ijt}$$

$$I_{ijt} = I_{ij(t-1)} + P_{ijt} - \sum_c S_{ijst} \quad \text{for all } i, j, t$$

$$M_{min}(1 - Z_{ist}) \leq \Psi_{ist} \leq M_{max}(1 - Z_{ist})$$

The Satisfaction level criterion addressed in the problem description can be imposed on the model in two ways.

First, adding extra weight to the outsourcing part in the model. Then, impose a heavier fine on these products to consider customer dissatisfaction. Second, through adding following constraints into the model:

J_i : level of satisfaction of customer for product i

N_s : number of sales regions

N_t : number of time periods

$$J_i = E \left[\frac{\sum_{s,t} Z_{ist}}{N_s N_t} \right] \geq r \quad 0 \leq r \leq 1$$

Where the J_i denotes the mathematical expectation of the number of periods in which the shortage of product i occurred.

3.4. The simulation implementation and determination of initial responses

For problem simulation model implementation, author considered each period of simulation as a month, and set the number of periods in each run to 12, so that the simulation will run for one year. The limitation associate with the level of customer satisfaction is applied in such a way that for each product, in accordance to its significance, to maintain customer satisfaction, a penalty for the mathematical expectation of the number of periods that facing the product shortage is determined, then it is embedded to the problem's objective function.

Whenever an order is placed, the closest factory to the sales unit where the order registered will be selected. In the case that the inventory is the factory is responsive to the demand, the next demand is met. Otherwise, the next nearest factory is selected, and the demand is fulfilled. In the case that none of factories can respond to the demand, the extra demand for that period is added outsourced for those sales areas. At the beginning of each simulation implementation, for each factory, the total demand expectation for products related to the 3 nearest sales centers is determined, and this amount is considered as the target inventory for that factory ($SS_{i,j}^0$). This parameter embeds the concept of safety stock that is needed for facing the sudden change in the demand of products. When a period begins, if the volume of available inventory is more that target inventory, the production of that product will not be paused. Otherwise, the production will continue until the inventory amount reaches the target inventory. Other constant simulation parameters are presented below.

Simulation Model Parameters for our case study derived from the information provided by the company and study of the same industry data which are available online and some others are arbitrarily determined. It must be noted that some this data (especially cost-related ones) are multiplied in a constant factor due to obligation for confidentiality. These parameters are as follows:

- Number of periods per simulation run (T): 12 (months)
- Number of factories: 2
- Number of sales centers: 5
- Number of products produced at the company: 6
- Production cost of product unit in thousand dollars (C_i): [0.2, 0.6, 0.5, 0.3, 0.2, 0.7]
- Shipping cost per unit of product per unit distance (t): 0.04
- Inventory cost of each product unit in a period (h_i): [0.1, 0.3, 0.2, 0.1, 0.1, 0.4]
- Outsourcing cost of each product unit (Ω_i): [0.4, 1.2, 1.0, 0.6, 0.4, 1.4]
- Penalty by product for not satisfying customer demand (ω_i): [1, 3, 2, 1.5, 1, 4]
- Distance matrix for factories and sales centers (d_{js}):

	Sale Center 1	Sale Center 2	Sale Center 3	Sale Center 4	Sale Center 5
Factory 1	286	264	475	603	367
Factory 2	214	487	756	444	973

- Expected values matrix for product demand in each sales center per 1000 pcs (μ_{is}):

	Sale Center 1	Sale Center 2	Sale Center 3	Sale Center 4	Sale Center 5
Product A	18	18	30	7	16
Product B	20	14	28	5	16
Product C	12	22	7	28	10
Product D	24	9	7	29	28
Product E	16	10	25	20	25
Product F	24	8	19	12	22

Based on the above data, and the method, the author explains for calculating the initial values of safety inventory stock levels in the simulation ($SS_{i,j}^0$) is computed as the following matrix:

	Product 1	Product 2	Product 3	Product 4	Product 5	Product 6
Factory 1	26	25	22	30	26	27
Factory 2	21	19	31	31	23	22

3.5 The impact of indeterministic input variables on the simulation model

As is mentioned in chapter 3, based on the Taguchi's perspective, the input variables of simulation can be categorized into two sets; first, the decision or control variables (d) and second, the environmental variables (e) that are indeterministic here because of stochastic nature of the simulation model. In the simulation of the studied supply chain, it is assumed that the uncertainty of demand in terms of product exists in each period, which means that the demand of sales center s for the product i in each period has normal distribution $N(\mu_{is}, \sigma_i)$. It is also hypothesized that these fluctuations are similar for each product in all sales centers. Therefore, the environmental variable can be defined based on products, as the amount of deviation from the average of demand, which would be 6 variables (number of products) as $\Sigma = \{\sigma_1, \dots, \sigma_6\}$.

Given the production and supply policies are usually decided before the simulation based on the target inventory, the decision variable can be expressed as the target inventory level for every single product in each factory when a period starts. So that, each decision variable can be defined as a certain coefficient of the initial level of target inventory ($SS_{i,j}^0$). This decision variable is defined as above in the form of $\Theta = \{\theta_1, \dots, \theta_6\}$ since the type of objective function in terms of customer satisfaction that is expressed by the product allows for the smaller solution space (with the values in the proposed model, from 0.2 to 3 variables) and simplifies the design of the experiment in the next steps to adequacy (fit) of the meta-model.

To illustrate the effect of demands variations on the objective function, and to visualize the effect of this fluctuation on creating the metamodel for response surface of this objective function, author plot a regression response surface metamodel for the original simulation model after fixing model parameters, by defining just two environmental variables as the demand variations for only two products. In this simulation, the values of input for the model are set equal to $\Sigma = \{\sigma_1, \dots, \sigma_6\}$ and $\Theta = \{\theta_1, \dots, \theta_6\}$.

In figure 3.2 (a), because of the probabilistic nature of the model and existence of fluctuation in the response surface, the numbers of design points are not adequate for the model's fit. In figure 3.2 (b), the metamodel depicts the reasonable response surface in terms of various amount of demand variance for products 1 and 2 (The limits of these $\sigma(s)$ are set in the range [0.5, 3]).

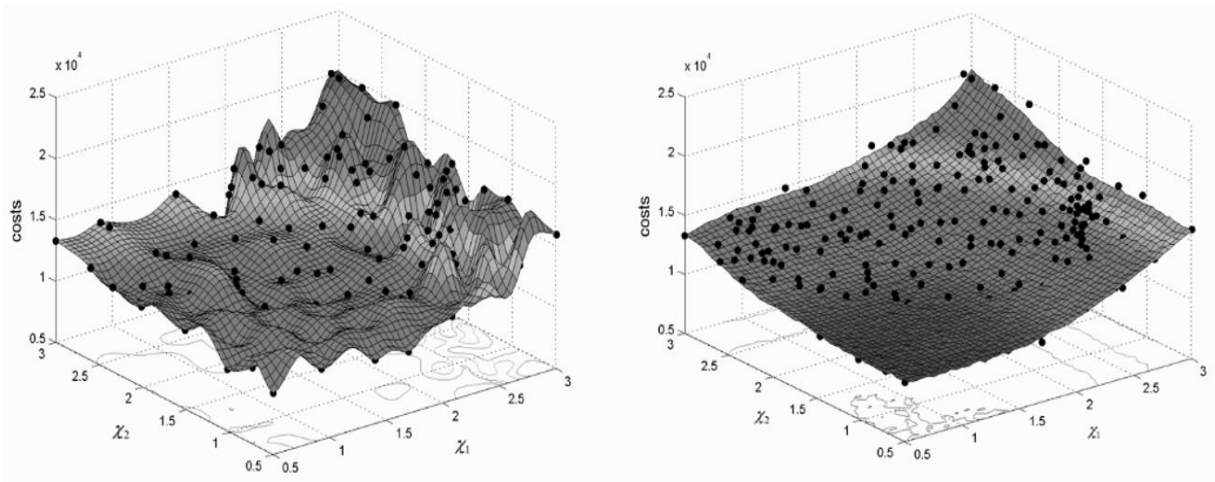


Figure 3. 2 Metamodel built on design points for different values of demand variations: (a) Metamodel for 131 design points, (b) Metamodel for 257 design points

The author can conclude that by increasing the number of design points to an adequate quantity, the resulting metamodel is smoother and fits better to predict the response surface. It is clear that if the changes in demand decrease, the simulation model is more deterministic, and the cost of the supply chain system is lower. On the other hand, as demand fluctuates, if the changes in demand increase, the cost of storing surplus inventory to meet these fluctuations as well as the cost of outsourcing and customer dissatisfaction increase.

3.6. Solution of model with a deterministic approach

The presented probabilistic simulation model can be optimized with a deterministic approach. In approach using the high number of iterations of running the simulation (Run length) per design point, the average value of the output response is considered as a deterministic answer with appropriate approximation. Then, using the common Gradient-based, Heuristic, and metaheuristic methods the optimum or close to the optimum point are identified. A sample of simulation optimization model of the supply chain is presented below along with the similar standard deviation for the demand change of all product ($\Sigma = [2,2,2,2,2,2]$) using Simulated Annealing (SA) algorithm. The amount of the target inventory levels that are given to the algorithm is the initial answer and the starting point of optimization are the same values as the starting point of the simulation ($(SS_{i,j}^0)$).

The optimized values of target inventory level through SA algorithm is as follows:

22.97932	22.6625	14.96924	22.5618	29.38156	29.7243
18.56022	17.2235	21.09302	23.31386	25.99138	24.2198

And the value of the target object is 2401.3615.

There are two main weaknesses associated with this approach. First, the robustness of response is not taken into account in this method. This means that the sensitivity of the response to changes in the values of the input variables and therefore the risk of adopting such a policy is quite unclear. Another weakness is that due to the fluctuation of the response level, a high number of reconstructions may be required to find the mathematical expectation of the output value for each combination of input variables; therefore, searching for optimum or close to the optimum point in using method that is based on searching for solution space is quite time-consuming.

Figure 3.3 illustrates the convergence of the mean of our two objective functions, namely average cost and customer dissatisfying cost, according to the number of replications of the simulation model. The runtime showed for fixed values of inputs variables both environmental and decision. environmental [2,2,2,2,2,2], decision [1,1,1,1,1,1] on the plot is for running model on a machine with Core i7- 8650 CPU processor and 16 Gb RAM memory. Based on the exponentially growth of the relevant runtime needed to implement the simulation, the author can conclude that this direct simulation optimization method is not efficient, especially when considering the fact that this supply chain model is relatively small compared with many other similar cases with hundreds number of products, manufactories, and distribution centers.

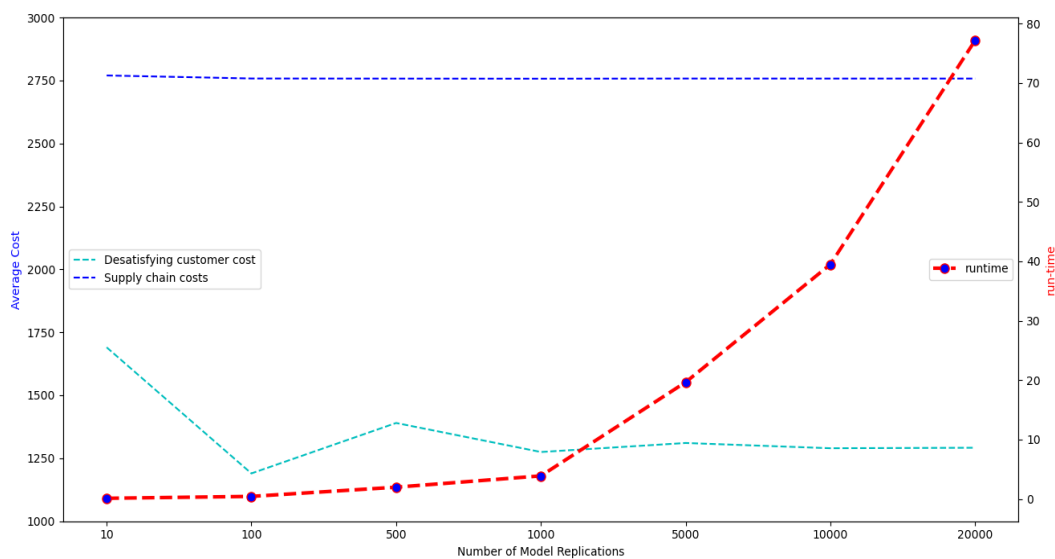


Figure 3. 3 the convergence of the mean of the average cost and customer dissatisfying cost, and the runtime for different number of replications

3.7. The metamodel-based optimization; integration of Taguchi approach and Artificial Neural Network

To robust solution of the supply chain simulation model, the author uses a neural network metamodel-based approach. Then evaluate the effectiveness of this approach given to the type of employed meta-model.

In this approach that is adopted from Dellino et al. (2010) research, two meta-models are fitted to the simulation model, one for estimating the mean of response and the other for the standard deviation [43]. Both metamodels are fitted based on simulation input/output data. As it is common in Taguchi design, the designed cross of the compound experiment for the decision and input variables allows for the determination of the combination of the input points of the simulation model.

Which means that combines the n_d number of design point from the decision variable of d with the n_e number of points from the environmental variables.

The designing points of n_e are sampled from input distribution of these variables. For sampling "Latin Hypercube Sampling" method is used. The running of simulation with using the compound of $n_d \times n_e$ results in the output of $f_{i,j}$ so that $i = 1, \dots, n_d$ and $j = 1, \dots, n_e$

These input and output data are calculated as follows for the calculation of average and conditional variances:

$$\bar{f}_i = \frac{\sum_{j=1}^{n_e} f_{i,j}}{n_e} \quad (i = 1, \dots, n_d) \quad (20)$$

$$s_i^2 = \frac{\sum_{j=1}^{n_e} (f_{i,j} - \bar{f}_i)^2}{n_e - 1} \quad (i = 1, \dots, n_d) \quad (21)$$

It should be mentioned that these two estimators are not biased since they utilize the direct input/output data of the simulation model (and not the metamodel prediction).

3.7.1 Creation of metamodel for the mean and standard deviation based on simulation estimation data

To design the experiment and determine the design points in the simulation model of the supply chain, first the limits of decision variables and environmental variables are determined. The decision variables here are the coefficients of target inventory levels of product inside the factories and environmental variables refer to the demand standard deviation for each product in sales centers.

To select the samples from environmental variables, a simple space-filling scheme called a rectangular grid has been used. In this design, it is assumed that the under-experiment area of $D \in R^n$ has a rectangular shape that is defined with dimensions $l_j \leq x_j \leq u_j, j = 1, \dots, n$.

The simplest distribution of experiment points obtained by the different form of combinations of these dimensions is expressed as follows:

$$s_j^{(i)} = l_j + k_j^{(i)} \frac{u_j - l_j}{v_j}, \quad k_j^{(i)} = 0, 1, \dots, v_j \quad (22)$$

Where v_j (s) are integer. If for all dimensions we have $v_j = v$, the number of design points are equal to $(v + 1)^n$.

Given that for random variables of demand for each product in each area, the statistic of $N(\mu_{is}, \sigma_i)$ is considered. Then, in order to sample the design point, the author sets the dimension of desired space as $[\mu_{ic} - \sigma_i, \mu_{ic} + \sigma_i], i = 1, \dots, 6$, and set the parameter $v=2$. As a result, the total number of design point is $(2 + 1)^6 = 729$.

For Environmental variables, the upper and lower limit for each of the 6 variables considered $[0.2, 2]$, then the Latin Hypercube Sampling (LHS) methods used for sampling. In this space-filling method, a kind of strategy is adopted to produce random points to ensure that all components of the vector space are included in the sampling.

Within the lower and upper limits, 500 numbers of points from the decision variable space are selected. Finally, the acquired designs for σ and θ are cross-combined that results in the number of $729 * 500 = 364,500$ combinations of the total number of input variables of the simulation model. Running the simulation model per each of these sample points, provides the input/output data required to train and fit the metamodel for the mean and standard deviation of the simulation model, based on equations 20 and 21.

As mentioned earlier, the neural network is one of the most widely used and effective methods for estimating a variety of functions. A properly designed neural network is capable to estimate most complicated models with high accuracy. Two important factors in designing the structure of the

neural network are the appropriate choice of the number of middle layers as well as the number of neurons in each layer.

Since there is no exact method available for the optimal design of this structure, the trial and error methods are used usually by the researcher to design the most desirable structure. The problem with this approach is that, firstly, there is no guarantee that an ideal design will be achieved, and on the other hand, without having enough information about the level of response and its complexity, it may take a long time to find an acceptable structure.

Furthermore, to calculate network error, the criterion of Mean Square Error (MSE) is usually used in literature:

$$MSE(y, \tilde{y}) = \frac{1}{n} \sum_{i=1}^n (y_i - \tilde{y}_i)^2 \quad (23)$$

Where y_i and \tilde{y}_i denote the actual value and the predicted value of response by neural network for i^{th} product, respectively.

In this study, besides the researches taken to find benchmarks in the literature for settings instances applied on similar case problems, almost all neural network structures, or NN hyper-parameters, the aforementioned trial and error approach has been used to find a good-enough metamodel. However, to explain the methods used for comparing the resulting NN metamodels, here, first describe the process of creating two different NN metamodels (regarding their hidden layer activation function). Then, the performance of these NN metamodels is compared.

The composition of decision and environmental variables for network creation is determined as before. Thus, the 500 points that were ultimately identified as estimates for mean and standard deviations of simulation output, per different values of environmental variables, are used to construct two neural network metamodels, one for the mean and the other for the standard deviation. After constructing the neural network metamodel for the mean cost of the system, the accuracy of this metamodel is evaluated. Using Latin Hypercube sampling experimental design, 100 combinations of the model's decision variables are identified, and the output of the simulation for these points, with considering the standard deviation of 2 for the demand for all products in sales centers ($\Sigma = [2,2,2,2,2,2]$), and the metamodel output are compared. In order to accurately estimate the average system costs, the number of running of simulation for combination of input decision variables is set to 10,000.

For the first NN metamodel, the author considers the Rectified Linear Unit activation function, known as ReLU function for the hidden layer of network. ReLU is one of the most popular functions for neural networks, which is a piecewise linear function that will output the input directly if it is positive, and zero if otherwise [39].

For the first NN metamodel, the author considers another activation function, known as Softplus function for the hidden layer of network. Softplus is generally similar to ReLU function, except it uses an exponential function in order to obtain a smooth and curvy behavioral for outputting direct input or zero, instead of a piecewise linear one [39].

Figure 3.4 illustrates the comparison of the responses of simulation and metamodel for the 100 sample points designed by LHS experimental design.

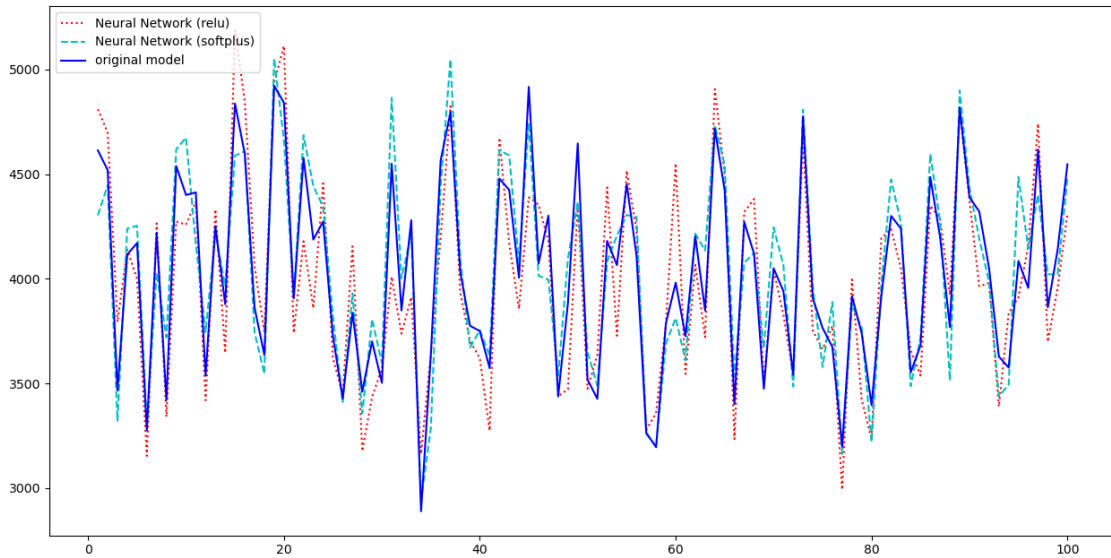


Figure 3. 4 comparison of the responses of simulation and metamodel for 100 sample points

Besides, to have an adequate metric to compare the performance of the prediction model, the Coefficient of Determination statistic is used. This statistical measure, also known as R-squared, is the percentage of the predicted value variation that is explained by a linear model and is always between 0 and 1. A zero value for the Coefficient of Determination means the model cannot predict any of the variability of the output data around its mean, and a value of 1 indicates it can explain all of these variabilities.

Using Coefficient of Determination statistical measure to compare the resulting NN metamodels, the author obtains the corresponding values for R^2 of the NN metamodel predictions and the response values points (derived from the simulation output) per the input 100 sample, as shown in table 3.1. These values indicate that the NN metamodel created by using the Softplus activation function works slightly better to predict the response values. Comparison of two NN metamodels using R^2 measure:

Neural Network Activation function	Coefficient Determination (R ²)
ReLU	0.77968
Softplus	0.88333

Table 3 1 Comparison of two NN metamodels using R2 measure

Once the metamodel is created based on the sampled data, it should be validated. The purpose of metamodel validation is to assess its ability to imitate the function of the objective function at all points in the response level. In other words, if the fitted metamodel does not pass the validation stage, it is not possible to ensure its optimal performance in new locations (the points that metamodel has not observed before). This is associated with the generalizability of the metamodel, and the purpose of the validation stage is to examine the desirability of this property.

Given the fact that the Coefficient of Determination might not be an adequate and good criterion for validating non-regression metamodels [42], in this thesis, the author uses 10-fold Cross-Validation and Root Relative Square Error (RRSE) validation methods for the validating the model. In this method, each time the algorithm is executed to calculate the degree of cross-validation error, the existing samples are divided into 10 equal-sized subcategories and each time, one subcategory is selected and metamodel is created using the data in the 9 other subcategories. Thereafter, the predictability of metamodel is tested using the calculation of RRSE error in the 10th category. The RRSE is calculated as follow:

$$RRSE(y, \tilde{y}) = \sqrt{\frac{\sum_{i=1}^n (y_i - \tilde{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}} \quad (23)$$

Where y_i and \tilde{y}_i denote the actual and predicted value of response variable, respectively.

Here, the validation of the fitted models for standard deviation of simulation costs is disregarded and it is assumed that the result of validation for the mean can also be generalized to standard deviation. Then in this case the neural network metamodel is used for prediction.

Taguchi (1987) [46] proposed his robust approach, considering a single output like w and focused on the ratio of the average of this output to the variance of this output.

This criterion is known in the literature as the Signal/Noise Ratio:

	<i>RRSE</i>	
Cluster Number	ReLU	Softplus
1	0.437679326	0.345416413
2	0.393478387	0.33227307
3	0.480890449	0.323954066
4	0.432811699	0.349301508
5	0.438187175	0.366030453
6	0.524790642	0.325737471
7	0.50973201	0.340714925
8	0.446367713	0.333333585
9	0.483282975	0.323498453
10	0.465071973	0.30921385
Average	0.461229235	0.334947379

Table 3.2 Cross validation comparison of two NN metamodels

3.8 Pareto-optimal Efficiency Frontier for average and standard cost deviation

In this thesis, another index used by Delino et al. (2009) replaces this scalar loss function. They used a nonlinear programming (NLP) model, in which the simulation output average (system cost) is expressed as a target function for minimization. In addition, the target output' standard deviation is imposed in the form a constraint to this optimization model:

$$\begin{aligned}
 & \text{Min}_d E(w | \mathbf{d}) \\
 & \text{st} : \\
 & s_w \leq T
 \end{aligned} \tag{24}$$

In this formula, $E(w|\mathbf{d})$ denotes the mean of output w under different values of the environmental variables e , and this mean is controlled by the decision variables d . The reason for using standard deviation as a constraint on the formula (24) is its identical unit with the mean. In the metamodel-based approach, the values of $E(w|\mathbf{d})$ and s_w are replaced by their corresponding metamodel predictions. changing the values of the right side of constrain (T), the Pareto-optimal Efficiency

Frontier is determined, which shows the equilibrium values between the standard deviation and the mean criteria.

In this thesis, a genetic heuristic optimization algorithm has been used to determine the Pareto-optimal diagram of the mean and standard deviation of the cost of the supply chain model. This algorithm has the advantage that instead of starting from a single point of origin, it considers a population of search space points as the initial population to start with and tries to improve the next generation with genetic operators. In the simplest version of this algorithm, a limited population of fixed-length strings, called genes, is processed. The two main operators of the algorithm are crossover-gene displacement and genetic mutation. The crossover-displacement operator, combining the genes of the two strands, tries to visit different parts of the justified area, and the mutant operator tries to escape from the optimal local points by making a small change in a selected field. The efficiency of the genetic algorithm is related to the combined use of these two operators [47].

Open-source packages available for Python programming language provide user-friendly platforms for using the operators and setting different parameters of the Genetic algorithm. The options used for these settings are shown in Table 3.3.

Hyper-Parameter	Options	Selected
Select Function	Stoch. Uniform	Roulette
	Remainder	
	Roulette	
	Uniform	
Crossover Function	Scattered	Intermediate
	Single Point	
	Two Point	
	Intermediate	
Mutation Function	Gaussian	Gaussian
	Uniform	
Population Size	-	50

Table 3.3 Hyper-parameters of Genetic algorithm

Figure 3.5 demonstrates the optimal Pareto diagram for the values of the mean and standard deviation of supply chain costs at 27 points which are opted by the optimization algorithm. In this figure, the horizontal axis indicates the system's average cost (\bar{C}), and the vertical axis indicated the cost standard deviation (S_C). As shown in the figure, the less considered the standard deviation of system costs (i.e., determine the lower values for the upper limit of cost changes (T) in the model (24), the higher is the optimal values of the corresponding cost.

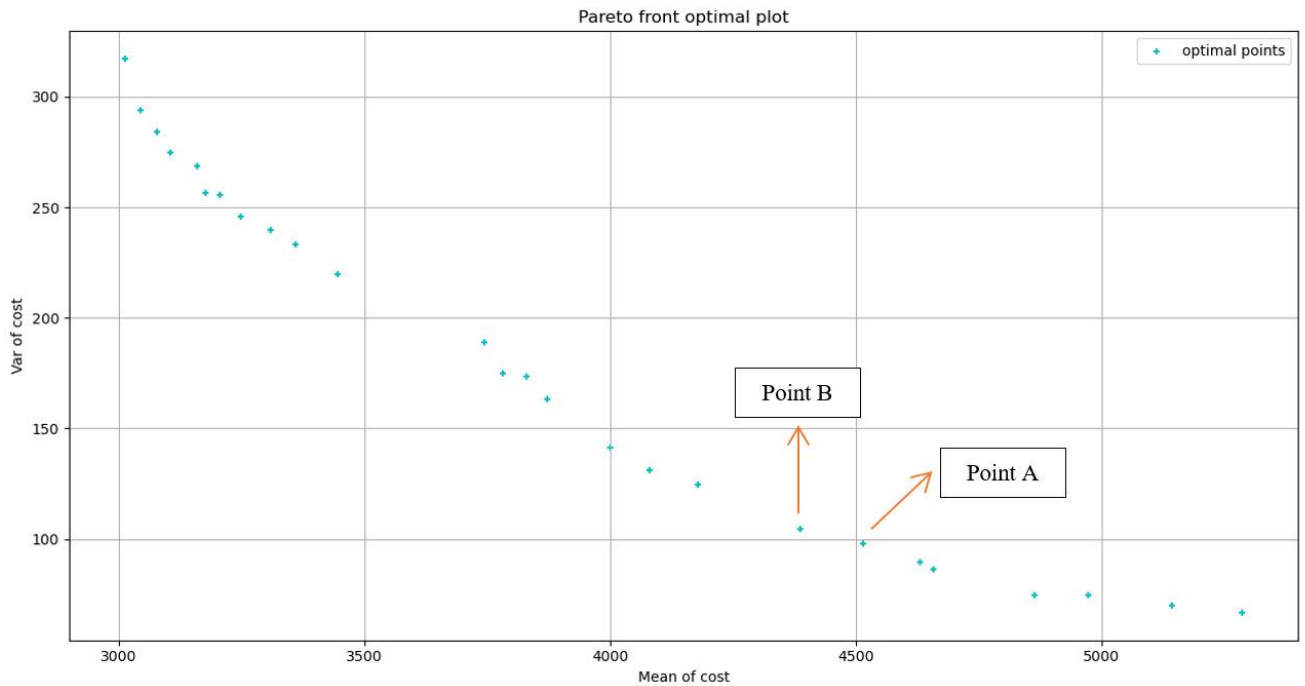


Figure 3. 5 Pareto Optimal frontier plot for the two objectives: (1) Average and (2) Variation of the supply chain system's cost

This system output's behavior is perfectly consistent with the true nature of the supply chain's behavior. So that if the system management tries avoiding taking risks, the less changeable system cost is preferred. The riskier the management of the system, the less changeable the cost of the system. This needs higher levels of safety stock to cover the risk of changes in customer demand, which in turn increases the costs associated with producing and maintaining inventory.

To sum up, it can be argued that one of the main advantages of employing an optimized simulation approach for the supply chain is providing a suitable platform for decision-makers and managers based on the level of risk-taking. This context makes it possible to apply all the analytical approaches in the field of risk analysis and management analysis, which are not mentioned here.

Another advantage of using a robust approach over classical simulation optimization methods is the provision of a kind of sensitivity analysis in determining the optimal values of system decision parameters. To explain this, an example is given below. Suppose management intends that the

standard deviation of the total cost of the supply chain system in the coming year be less than 400 units, and at the same time the decision parameters are determined in such a way that this cost is minimized.

According to Pareto's optimal chart, the best offer that can be made to management to meet its demand is shown in Table 3.4. This table shows the safety stock for each product in each factory, corresponding to the optimal decision point.

		Product					
		1	2	3	4	5	5
Factory	1	33.4664	23.8433	29.0908	58.3031	33.6974	40.5836
	2	27.0305	18.1209	40.9916	60.2466	29.8093	33.0681
\bar{C}		4513.848549					
S_C		97.99141874					

Table 3.4 Solution values corresponding to point A

According to the Pareto plot, it can be immediately concluded that there is another point close to the point A, which can be another option for the management because its relevant standard deviation is not much higher than the desired of 100 units. However, in this point B, which corresponding information is described Table 3.5. the standard deviation of system cost is slightly higher than the optimal point A, but its average cost is considerably less than point A.

		Product					
		1	2	3	4	5	5
Factory	1	33.0959	23.9197	27.1447	59.4216	34.0969	42.1301
	2	26.7313	18.179	38.2494	61.4023	30.1626	34.3282
\bar{C}		4387.188617					
S_C		104.3034535					

Table 3.5 Solution values corresponding to point B

Furthermore, it should be noted that each of the adjacent points provided in the Pareto plot has close performance measures of average and deviation of the system cost while offering different products inventory levels at each factory. This would provide the management of ability for decision-making by bringing up other assumptions and considerations existed in the real system but not included in the simulation model.

CONCLUSION AND IMPLICATIONS

In this thesis, the author employed a robust metamodel-based simulation optimization approach to solve an inventory problem in a multiple-products supply chain case study.

After reviewing the application of simulation optimization models in supply chain literature, the author explained the position of the problem under study in the literature. Thereafter, various simulation optimization methods are described followed by the integration of the Taguchi approach with metamodel-based methods. In order to implement this method in the supply chain problem, the decision variables and environmental variables of the simulation model are defined based on Taguchi approach in such a way that limits the solution space, and in the same time, capable to represent the model behavior for different values of these input variables.

Then, by running the simulation model on the compounds obtained from a cross-experimental design and by combining different points of decision and environmental variables, the required input/output data are provided and the metamodels are adjusted to the average and standard deviation of the system cost. After gathering enough input/output data from a space-filling experimental design, training, and test datasets applied to create two different Neural Network metamodels, with different activation functions of their hidden layers, to predict the average and standard deviation of the supply chain costs.

Afterward, the effectivity and efficiency of these artificial neural network metamodels are determined and compared, in terms of their accuracy and ability of prediction of outcome value in complex supply chain models. To do so, besides statistical measures like the Coefficient of Determination (R^2) and Root Relative Square Error (RRSE), a 10-fold cross-validation implemented to compare the accuracy and validation of the two ANN metamodels. The one with a better performance (built with Softplus activation function) has been selected.

To have a robust optimization approach, the metamodel is placed in a nonlinear programming model in which the average cost is limited by a high limit for the minimum standard deviation. Using the Genetic algorithm as a meta-heuristic, the Pareto-optimal frontier is derived by changing the cost deviation constraint on the average cost objective function.

Finally, the author conducted analyzes on the obtained results to explain the advantages of this approach over the classical methods of simulation optimization, specifically for the company case under study.

This study was limited by the shortage of the time, many of the methods and improvements that have come to the mind of the author along the way and might have very good results in the early stages have not found a place in the report.

Thus, future researches can expand this thesis by focusing on below:

1. Embedding more practical assumptions and constraints to the supply chain simulation model; For instance, considering a higher number of products and customers, or restrictions on the various production processes in each factory.
2. Using more efficient experimental design algorithms to increase the accuracy of the metamodel construction process
3. Employ proposed methods in the literature such as Particle Swarm optimization algorithm (PSO), to optimize the hyper-parameters of the Artificial Neural Network, in order to create more accurate metamodels.

KOKKUVÕTE

Antud töös autor uuris laoseisu probleeme mitmetootelises tarneahela kaasuses kasutades metamudelil baseeruvat simulatsiooni.

Esmalt tutvus autor kirjandusega simulatsioonipõhise optimeerimise mudelitest tarneahelas ning tutvustas probleemipüstitust kirjanduse põhjal. Töös tutvustati mitmeid eri simulatsioonipõhise optimeerimise meetodeid kaasa-arvatud Taguchi lähenemise integreerimist metamudelitel põhinevates meetodides. Erinevad otsustus ja keskkonna muutujad koguti Taguchi meetodil ning seeläbi limiteeriti lahendusruum ja kindlustati, et mudeli käitumine erinevate väärtuste korral on jälgitav.

Seejärel, eksperimendiülese kujunduse abil saadud ühendite simulatsioonimudeli käitamisel ja erinevate otsustuspunktide ning keskkonnamuutujate kombineerimisel saadakse vajalikud sisend- ja väljundandmed ja metamudelid kohandatakse süsteemi maksumuse keskmise ja standardhälbega. Pärast piisavalt sisend- ja väljundandmete kogumist ruumi täidetavast eksperimentaalsest kavandamisest, rakendati koolitus- ja testiandmekogumeid kahe erineva neurovõrgu metamudeli loomiseks, mille peidetud kihtide erinev aktiveerimisfunktsioon on ette nähtud, et ennustada tarneahela kulude keskmist ja standardhälvet.

Seejärel tehakse kindlaks ja võrreldakse nende kunstliku närvivõrgu metamodellide efektiivsust ja tõhusust, pidades silmas nende täpsust ja tulemuste väärtuse prognoosimise võimet keerukates tarneahelamudelites. Lisaks statistilistele meetmetele, nagu näiteks määramiskoeffitsient (R^2) ja juur-suhtelise ruutviga (RRSE), rakendati 10-kordset ristvalideerimist, et võrrelda kahe ANN-i metamudeli täpsuse ja valideerimise täpsust. Valitud osutus see, millel on parem jõudlus (ehitatud koos Softplusi aktiveerimisfunktsiooniga).

Robustse optimeerimismeetodi saamiseks paigutatakse metamudel mittelineaarsesse programmeerimismudelisse, milles keskmisi kulusid piirab minimaalse standardhälbe kõrge piir. Kasutades geneetilist algoritmi meta-heuristikuna, tuletatakse Pareto-optimaalne piir, muutes keskmise kulu eesmärgi funktsiooni kulude kõrvalekalde piirangut.

Lõpuks viis autor läbi saadud tulemuste analüüsi, et selgitada selle lähenemisviisi eeliseid simulatsiooni optimeerimise klassikaliste meetodite ees, eriti uuritava ettevõtte juhtumi puhul.

Seda uuringut piiras aja nappus, paljud meetodid ja parandused, mis on autori meelest meelde tulnud ja millel võib olla väga häid tulemusi varases staadiumis, pole raportis kohta leidnud.

Seega saavad tulevased uurimistööd seda lõputööd laiendada, keskendudes alljärgnevale:

1. Praktiliste eelduste ja piirangute kinnistamine tarneahela simulatsioonimudelid; Näiteks arvestades suuremat arvu tooteid ja kliente või piiranguid igas tehases erinevatele tootmisprotsessidele.
2. Tõhusamate eksperimentaalsete kujundusalgoritmide kasutamine metamudeli koostamise protsessi täpsuse suurendamiseks.
3. Kunstliku närvivõrgu hüperparameetrite optimeerimiseks, et luua täpsemaid metamudeleid, kasutage kirjanduses välja pakutud meetodeid, nagu näiteks osakeste sparmi optimeerimise algoritm (PSO).

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