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Optimal Supply Chain Configuration for the Additive Manufacturing of Biomedical Implants

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By

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In this dissertation, we study two important problems related to additive manufacturing (AM). In the first part, we investigate the economic feasibility of using AM to fabricate biomedical implants at the sites of hospitals AM versus traditional manufacturing (TM). We propose a cost model to quantify the supply-chain level costs associated with the production of biomedical implants using AM technology, and formulate the problem as a two-stage stochastic programming model, which determines the number of AM facilities to be established and volume of product flow between manufacturing facilities and hospitals at a minimum cost. We use the sample average approximation (SAA) approach to obtain solutions to the problem for a real-world case study of hospitals in the state of Mississippi. We find that the ratio between the unit production costs of AM and TM (ATR), demand and product lead time are key cost parameters that determine the economic feasibility of AM.

In the second part, we investigate the AM facility deployment approaches which affect both the supply chain network cost and the extent of benefits derived from AM. We formulate the supply chain network cost as a continuous approximation model and use optimization algorithms to determine how centralized or distributed the AM facilities should be and how much raw materials these facilities should order so that the total network cost is minimized. We apply the cost model to a real-world case study of hospitals in 12 states of southeastern USA. We find that the demand for biomedical implants in the region, fixed investment cost of AM machines, personnel cost of operating the machines and transportation cost are the major factors that determine the optimal AM facility deployment configuration.

In the last part, we propose an enhanced sample average approximation (eSAA) technique that improves the basic SAA method. The eSAA technique uses clustering and statistical techniques to overcome the sample size issue inherent in basic SAA. Our results from extensive numerical experiments indicate that the eSAA can perform up to 699% faster than the basic SAA, thereby making it a competitive solution approach of choice in large scale stochastic optimization problems.

Keywords: Additive manufacturing, biomedical implants, stochastic programming model, continuous approximation, large scale supply chain, deployment configuration, sample average approximation, enhanced sample average approximation, clustering

DEDICATION

Dedicated to my wonderful and beloved family: nuclear and extended.

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CHAPTER I

INTRODUCTION

The provision of on-demand personal care specifically tailored to the need of a patient is an important aspect of high-quality and efficient healthcare delivery. Due to the fact that the anatomy of every single patient is unique, there is a significant need to customize such biomedical implants as hip implants, knee implants dental crowns and braces, cardiovascular stents and other implants for surgical procedures. These patient-specific customized implants usually possess complex features which are laborious to produce using the conventional traditional manufacturing (TM) methods which are subtractive in nature. However, advanced manufacturing techniques such as additive manufacturing (AM) provide the opportunity to fabricate the implants from the ground-up, layer-by-layer using a variety of metallic, plastic or ceramic materials, on a patient-by-patient basis. With additive manufacturing, one can employ computer tomography to obtain a patient's anatomy data, from which a CAD model of the implant is generated and used to build a patient-specific customized implant. Among the customized implants produced using AM technology include skull ([142], [158], [37], [141]), knee joint ([59]), elbow ([151]), and hip joint ([116]). These devices possess a combination of relatively high value and small physical volume which is suitable for the applications of AM. Specifically, Kablooe Design has used AM to manufacture a device for the treatment of benign prostatic hyperplasia (BHP) [146] while Siemens has switched to

AM technology for the production of customized hearing aids. Moreover, Dental labs have used AM to produce customized dental crowns for patients. The AM technology has enabled these companies to localize the manufacture and distribution of end products, shorten the production time of the customized devices by up to 80%, and significantly reduce labor cost [34]. The US military has identified the use of AM within the combat field whereby thousands of different surgical instrument designs, customized instruments and sterile surgical kits stored on digital media or remotely accessed via the Internet, could be printed and used in field surgical settings [74].

Instead of ordering traditionally-manufactured implants from suppliers who are usually located far away from the hospitals, adopting AM technologies for fabricating biomedical implants at the site of operational hospitals may lead to faster response, lower inventory level, and reduced delivery costs [59]. In the case of TM-supplied implants, there is a long waiting time between when an implant is ordered and when it is received for use in surgery due to the need of customization [148]. The customization requirement makes keeping safety stock of products at the warehouse of TM vendors either impossible or extremely expensive. In other words, a large portion of the products may stay in the warehouse for a long period thereby ting up capital in inventory, increasing obsolescence risk and reducing stored product quality due to oxidation.

Despite the obvious benefits of AM, the decision to switch from TM to AM is not straightforward and requires a careful analysis. For one, the AM machines are expensive and require a significant initial investment outlay as well as maintenance and operating cost. Besides, implants manufactured via AM usually require expensive raw materials and may even undergo post-processing steps such as surface cleaning, smoothing or even heat treatment after fabrication which could involve additional traditional manufacturing technologies and supply chain network. All these factors significantly drive up the production cost of AM in comparison to TM. Consequently, a decision support system is needed to help decision makers in making objective make-or-buy decisions.

Costs associated with AM can be grouped into two categories: process-level or well-structured costs such as labor, material, and machine costs; and system-level or ill-structured costs related to inventory, transportation, delivery, etc [162]. Most of the existing studies focus on the analysis of process-level costs, which are usually evaluated based on individual AM processes. For example, some researchers examined the costs associated with AM machines and materials ([122], [17], [8], [4], [83], [84]); while others considered the costs of energy consumption ([94], [98], [145]). Some studies provided qualitative and general discussion regarding the designs and management policies of AM supply chains ([95], [17], [60]). However, no studies, to the best of our knowledge, have performed a quantitative investigation of the supply chain's integrated cost with AM facilities. Cost reduction arising from these system-level cost parameters could result in significant benefits in the production of biomedical implants in ways that have not yet been fully envisaged ([59], [65]). Therefore, quantifying the supply chain level costs of AM, benchmarked against its TM counterpart, is essential to better assess the feasibility of adopting AM supply chains for the biomedical implant application, identifying the system level barriers that hinder the adoption of AM technologies, and recommending the specific applications in which the adoption of AM technologies may be economically beneficial. In Chapter II, we propose a stochastic cost model to quantify the supply-chain level costs associated with the production of biomedical implants using AM techniques, and investigate the economic feasibility of using such technologies to fabricate biomedical implants at the sites of hospitals. The problem is formulated in the form of a two-stage stochastic programming model, which minimizes the total cost of using TM and AM and determines the number of AM facilities to be established and volume of product flow between manufacturing facilities and hospitals. A customized Sample Average Approximation (SAA) approach is developed to obtain the solutions. We apply the cost model to a real-world case study that focuses on the use of biomedical implants for hospitals in the state of Mississippi (MS), and identify the conditions and cost parameters that have significant impact on the economic feasibility of AM. We find that the ratio between the unit production costs of AM and TM (ATR), as well as product lead time and demands, are key cost parameters that determine the economic feasibility of AM. A manuscript based on the content of this chapter has been published in Additive Manufacturing in July, 2016.

In a large network coverage area, an important factor that influences the extent of benefits reaped by the patient, hospital and the AM provider is the AM deployment configuration. AM deployment determines how close the manufacturing point is to a hospital and this can have a huge impact on the supply chain cost. This is particularly true when we extend the network beyond the state of Mississippi to cover the states in the southeastern region of the country or the entire country. The choice of deployment approach (central, distributed, or hybrid) remains an open question that requires a careful investigation due to the relatively high AM machine, raw material and personnel costs, as well as uncertainties in the demand of implants in the future ([60], [86]). A centralized deployment whereby the AM facility is centrally located will save on machine investment cost and personnel cost but incur extra transportation cost since the manufacturing point will generally be located farther away from the hospitals. A distributed deployment on the other hand will result in lower transportation cost but higher initial investment in AM machines and personnel costs. Khajavi et al. [70] are among the few researchers that have conducted a quantitative study on AM deployment. However, the authors compare only two extreme ends of the AM deployment configuration spectrum: one centralized AM location; and an AM facility at all the customer locations, and apply their study to the AM of military aircraft spare parts. It is reasonable to observe that for expensive raw materials such as the ones used in the manufacture of biomedical implants and which are usually not available locally, their procurement and inventory decisions need to be incorporated in the AM deployment problem to enhance the realization of the full benefits of AM. In Chapter III, we propose a continuous approximation (CA) model that quantifies the supply chain network cost associated with AM-produced biomedical implants and incorporates raw material procurement quantities in the model. We present an optimization algorithm that calculates the locations of the AM machines and the hospitals that they serve (otherwise known as the AM facility's influence area), and the quantity of raw materials to be kept in inventory at a central raw material warehouse (CRW) and distributed AM facilities to minimize the total network cost and achieve a satisfactory level of patient satisfaction. We apply the cost model to a real-world case study that focuses on the use of biomedical implants in hospitals in 12 states of southeastern USA, and identify the conditions and cost parameters that have significant impact on both the AM technology deployment methods and total network cost. We find that the demand for biomedical implants in the region, fixed investment cost of AM machines, labor cost for operating the machines and transportation cost raw materials and implants are among the major factors that determine how distributed the AM facilities should be, and impact the AM supply chain network cost. A manuscript based on this chapter has been submitted to Additive Manufacturing in September, 2016.

The continuous approximation approach in Chapter III provides a means of modeling a large scale problem where a large number of hospitals and demand points are distributed in a wide area and obey the slow-varying property. However, in Chapter IV, we present an enhanced sample average approximation (eSAA) technique which significantly improves the SAA approach utilized in Chapter II and yields solutions faster without assuming the slow-varying property of demand and hospital locations. In the basic SAA method, choosing an inappropriate sample size can lead to the generation of low quality solutions with high computational burden, and determining the right sample size can be quite challenging ([73], [61]). In order to overcome this challenge, our eSAA method utilizes clustering techniques to dynamically update the sample sizes and offers high quality solutions in a reasonable amount of time. We apply the proposed approach to three test problem types (facility location problem, single-sink transportation problem and supply transportation problem). A number of numerical experiments (e.g., impact of different clustering techniques, fixed vs. dynamic clusters) are performed for various problem instances to illustrate the effectiveness of the proposed method. Results indicate that on average, eSAA with fixed clustering size and dynamic clustering size solves our test facility location problem almost 631% and 699% faster than the basic SAA technique, respectively. The promising result shows that formulating our AM deployment problem of Chapter III as a mixed integer programming problem and applying the eSAA could be a strong alternative to the continuous approximation approach utilized therein. A manuscript based on the content of this chapter has been accepted for publication in the International Journal of Production Economics in September, 2016.

Thus, the proposed contributions of this dissertation are as follows:

1. In this research, we formulate a more realistic model that captures both process-level and system-level costs. This model is used to quantitatively study and analyze the economic feasibility of using AM technology in the fabrication of biomedical implants at various demand levels, and provide managerial insights on key cost parameters that affect AM initiatives. The hospitals in the state of Mississippi are used as a case study. Such a model can be modified to suit similar analysis in other application areas such as automotive, aviation and energy production.

2. This research is the first to formulate a continuous approximation model that recommends the optimal configuration that minimizes the total network cost in the deployment of AM facilities for the manufacture of biomedical implants. This model takes into account that the expensive raw materials used in these implants are usually not locally available and must be ordered from remote sources, thereby necessitating the inclusion of reliable inventory decisions in the AM deployment problem. We apply our model to a large network involving the entire southeastern region of USA, and conduct sensitivity analysis on the factors that affect how centralized or distributed the AM facilities should be.

3. This research proposes a novel algorithmic approach that enhances the sample average approximation technique with the aim of yielding fast solutions for large scale stochastic programming problems. We apply our proposed approach to three optimization problems and the performance of the technique shows a promising results that could make it applicable to solving large scale AM facility deployment problems that involves all the hospitals in the entire USA.

CHAPTER II

ADDITIVE MANUFACTURING OF BIOMEDICAL IMPLANTS: A FEASIBILITY ASSESSMENT VIA SUPPLY-CHAIN COST ANALYSIS

2.1 Introduction

Providing personal care tailored to the specific needs of patients is a promising approach for delivering high-quality and economically efficient healthcare in terms of on-demand production and customization. Because the anatomy of every single patient is unique, there is a significant need for customizing products in the biomedical sector for replacing hip/joint implants, dental work, vessel stents, and other biomedical implants. Additive manufacturing (AM) provides the opportunity to fabricate customized biomedical implants from the ground-up using a variety of metallic, plastic or ceramic materials, and on a patient-by-patient basis (i.e. 'on-demand'). With additive manufacturing, one can employ computer tomography to obtain patient anatomy data, from which a CAD model of the implant to-be-manufactured is generated and used to build a patient-specific customized implant. Custom implants can possess truly complex features which are difficult to machine using conventional, subtractive methods. Singare et al. [142] has demonstrated the superior functionality of AM biomedical implants, as well as the aesthetical appeal. Custom implants produced using AM technology have been used for a variety of applications including skull ([142], [158], [37], [141]), knee joint [59], elbow [151], and hip joint [116].

The adoption of AM technologies for fabricating biomedical implants at the site alongside of operational hospitals, instead of ordering from off-site suppliers of traditionally-manufactured (TM) implants, may lead to faster response, lower inventory level, and reduced delivery costs [59]. This is partially because of the fact that many TM suppliers tend to locate outside of the state, or even the country, of hospitals. For instance, major hospitals in the state of Mississippi (United States) procure biomedical implants from suppliers and manufacturers located outside of Mississippi that use TM technologies for production, as shown in Figures 2.1 and 2.2. For TM, products can be ordered when they are needed in surgeries, and usually require a long waiting time (up to months) due to the need of customization [148]. A safety stock of products is kept at the warehouse of TM vendors/suppliers to accelerate the service. Thus, a large portion of the batched products may stay in the warehouse for a long period, which tends to tie up a large amount of capital in the form of inventory, increase the obsolescence risk and reduce the surface quality of the stored products or parts due to susceptibility to oxidation. Hence, fabricating biomedical implants at the sites of hospitals using AM technologies, instead of ordering products from supplier of traditionally-manufactured parts out of the state, may have the potential to significantly improve the operational efficiency of healthcare delivery systems, ultimately lowering the costs of medical service and improving patient well-being and satisfaction.

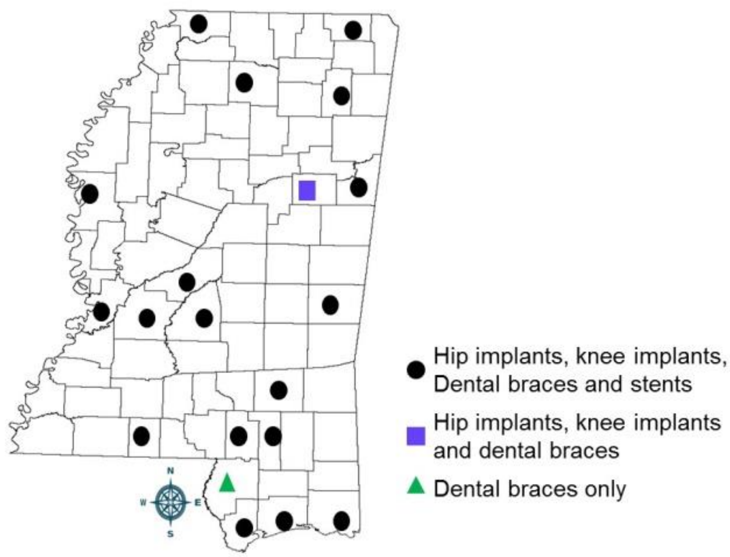

Figure 2.1 Location of major hospitals (by county) in the state of Mississippi

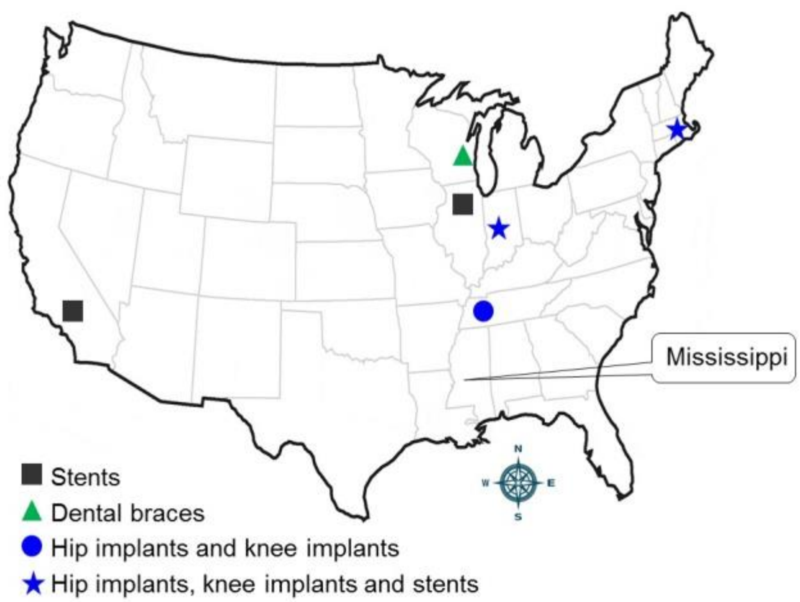

Figure 2.2 Current suppliers of biomedical implants in contiguous United States (mainland) via traditional manufacturing

Despite the potential benefits of using local AM technologies over outsourcing for TM parts, the "make-or-buy" decisions are not straightforward and require careful investigation because of the existence of conflicting cost parameters. On one hand, the transportation costs of product delivery using AM may be reduced because of the shortened distance between suppliers (i.e., third parties close to the hospitals) and users (i.e., hospitals). In addition, the inventory cost will be reduced since the raw materials for AM production are the only stock required when fabricating parts on demand. Moreover, the lead time of products fabricated via AM is significantly shortened [59]. However, the initial investment of AM machines is relatively high. According to a report by Thomas and Gilbert [148], the average costs of machines for metal printing can account for about 60% of the total production cost related to AM over the machine lifetime. Besides, AM performed on site may require surface cleaning, smoothing or even heat treatment after fabrication. These possible post-processing steps usually require the use of certain traditional manufacturing technologies, which will add to the production cost as well as the total lead time of AM parts. Therefore, the realization of a fully functional supply chain integrated with AM facilities requires comprehensive understanding and quantification of cost parameters associated with AM.

Costs associated with AM can be categorized into two types: process-level costs associated with labor, materials, and machines; as well as system-level costs related to inventory, transportation, delivery, etc. Process- and system-level costs are also referred to as well- and ill-structured costs, respectively, by Young [162]. Most of the existing studies focus on the analysis of process-level costs, which are usually evaluated/calculated based on individual AM processes. For instance, some researchers examined the costs associated with AM machines and materials ([122], [17], [8], [4], [83], [84]); while others considered the costs of energy consumption ([94], [98], [145]). However, very few researchers have investigated system-level costs, which depend on the supply chain configuration. Some studies provided qualitative, general discussion regarding the designs and management policies of AM supply chains ([95], [17], [60]). However, no studies, to the best of authors' knowledge, have performed a quantitative investigation or analysis of the supply chain's integrated cost with AM facilities, e.g., inventory cost, transportation cost, product lead time, etc. Cost reduction associated to these system-level cost parameters could be significant and result in tremendous benefits in the production of biomedical implants in ways that have not yet been fully realized ([59], [65]). Therefore, quantifying the supply chain level costs of AM, benchmarked against its TM counterpart, is essential for truly assessing the feasibility of adopting AM supply chains for the biomedical implant application, identifying the system level barriers that hinder the adoption of AM technologies, and recommending the specific applications in which the adoption of AM technologies may be economically beneficial.

Different from the existing studies that focus on process-level costs only, the objective of our study is to model how various cost parameters (e.g., inventory, transportation, demand, lead time, etc.) contribute to the system-level cost, and investigating the economic feasibility of using AM technologies to produce biomedical implants at the sites of hospitals. Due to the conflicting nature of cost parameters, existing conceptual cost analysis, as presented in the literature, may not be sufficient to characterize the overall manufacturing costs and recommend a more viable means of manufacturing. We propose a two-stage stochastic programming model to characterize the impacts of various cost parameters on the overall manufacturing cost, which can be further used to provide a guideline of the buy-or-make decisions for decision makers. Specifically, the output of the stochastic cost model recommends the number of AM facilities to be built, which could be zero if AM is not economically feasible, as well as the amount of products to be ordered from either traditional suppliers or local AM centers, by minimizing the overall costs. It is worth noting that solving such a stochastic programming problem is usually NP-hard (non-deterministic polynomial-time hard), meaning that there are no known algorithms to solve the problem in polynomial time [90]. A sample averaging approximation (SAA) is implemented in an algorithm to obtain the corresponding solutions. Based on the developed cost model, we further identify the cost parameters that may significantly impact the economic feasibility of AM part production for biomedical applications, which is captured by the number of AM centers to be established in our example case study.

The rest of this paper is organized as follows: Section 2.2 reviews the existing literature related to the cost analysis of AM technologies; Section 2.3 presents a manufacturing cost model based on stochastic programming that quantifies and compares the overall manufacturing costs of AM and TM technologies; Section 2.4 implements a SAA to obtain the number of AM facilities to be located and track the flow of products between manufacturing facilities and hospitals by solving the optimization model presented in Section 2.3; Section 2.5 applies this optimization model to the real-world case study of biomedical implants in the hospitals in the state of Mississippi; and Section 2.6 provides concluding remarks and possible future work.

2.2 Literature review

A large number of AM studies focus on the characterization of material properties and machine development ([135], [80], [161]), among which several papers have investigated the economic feasibility of applying AM for rapid tooling ([41], [72], [100]). Nevertheless, limited research efforts have been dedicated toward understanding the cost parameters of direct fabrication of metallic end-usable parts. In this section, we review papers related to the cost analysis of AM end products and categorize the related literature into two groups: process-level costs associated with labor, materials, and machines; and system-level costs related to inventory, transportation, delivery, etc.

2.2.1 Literature related to process-level cost studies

Several cost models have been developed to estimate the machine, material, and energy consumption costs of AM. For example, Hopkinson and Dickens [63] developed an initial cost model based on Selective Laser Sintering (SLS), which estimates the production of identical parts. However, this model may not be used to estimate the cost of products that consist of a mixture of parts with different geometries. Ruffo et al. [130] added to this model the direct and indirect costs such as overhead costs and presented a saw-tooth like curve for the costs of the parts in dependency of their quantity, resulting from a significant increase of the processing time for new parts. Ruffo further advanced his model in Ruffo et al. [131], which allows for the calculation of production cost for the case of simultaneous production of different shapes in the same build job. A more comprehensive model was presented by Rickenbacher et al. [122], in which authors incorporate the costs of pre- and post-processing steps linked to a mixed build job.

Besides the machine, materials, and overhead costs, some researchers studied the energy consumption and environmental impacts of AM. Mognol et al. [94] investigated the optimal sets of AM process parameters (e.g., building orientation and patterns during fabrication) that minimize the electrical energy consumption of a build. Authors reported the absence of general guidelines for the minimization of electrical energy consumption, and suggested that each AM system needs to be tested individually to identify parameters that minimize energy consumption. Morrow et al. [98] studied the environmental emissions and energy consumption for the manufacture of molds and dies using Direct Metal Deposition, compared to TM technologies. It is shown that AM has great potential to reduce cost and environmental impact simultaneously. Kreiger and Pearce [75] performed a life cycle analysis on three plastic products to quantify the environmental impact of distributed manufacturing using 3D printers. The authors compared the resulting energy and emissions with that from conventional large-scale production in low-labor cost countries, and found that distributed manufacturing using open-source 3D printers has a lower environmental impact than conventional manufacturing for the products considered. Baumers et al. [17] estimated the process energy consumption and costs occurring during AM for Selective Laser Melting and reported that the average production costs, as well as energy consumption, increase as the production volume decreases. Le Bourhis et al. [82] proposed a predictive model for environmental assessment of AM which considers electric, fluid and raw material consumptions in a direct metal deposition process. The model evaluates many manufacturing strategies to produce a part, and selects the one that has the lowest environmental impact based on the amount of electricity, fluid and raw material consumed. Kellens et al. [68] proposed a parametric model to estimate the environmental impact of selective laser sintering in the production phase considering energy and resource consumption as well as process emissions. Using the part's build height and volume as parameters, the model is able to compare AM processes and conventional manufacturing and make manufacturing method decision from environmental point of view based on the amount of energy saved and amount of waste reduced.

Wittbrodt et al. [159] studied the life-cycle economic analysis (LCEA) of self-replicating rapid prototypers (RepRaps) technology for an average US household. The authors found that using this distributed additive based manufacturing technology is already an economically attractive investment for the average US household that would save cost against commercial printing service. Pearce et al. [113] examined the capabilities and economic viability of open source 3-D printers and their use by local communities to create objects. The authors found that with improvements in local feed stock availability, size of printed parts, material properties, and the use of renewable energy systems, the technology has the potential to assist in driving sustainable development. Gebler et al. [54] provided a qualitative and quantitative assessment of 3-D printing from a global sustainability standpoint. The authors found that AM has the potential of inducing changes in labor structures and generating shifts towards more digital and localized supply chains. They showed that by 2025, the technology can reduce cost, total primary energy supply and CO_2 emissions by up to USD 593 billion, 9.30 EJ and 525.5 Mt, respectively. An overview of the challenges and research opportunities related to the sustainability, especially energy consumption, of AM can be found in Sreenivasan et al. [145].

2.2.2 Literature related to system-level cost studies

Among the very few studies that have investigated system-level costs (e.g., inventory, transportation, lead time, etc.), some research groups have studied the potential impact of AM on the supply of spare parts in the commercial aircraft industry. Holmstrom et al. [60] provided qualitative analysis for the potential benefits of using AM in aircraft industry, by comparing the on-demand production of spare parts using both centralized AM, which requires few AM facilities, and distributed AM, which requires a larger number of AM facilities. Authors also took into account cost parameters such as materials and production, distribution and inventory obsolescence, and life-cycle. The benefits and advantages of both approaches were discussed. It is found that when the demand for spare parts is relatively low, centralized AM productions may be more beneficial to allocate the demand from multiple locations; however, requiring longer delivery time and high inventory cost. In situations, where the demand is relatively high and short lead time is essential, distributed AM production may be more advantageous. Similar findings were echoed by Khajavi et al. [70], in which the authors investigated the production of spare parts for the air-cooling ducts of the environment control system for the F-18 Super Hornet fighter jet. The authors reported in their case study that the expected total cost per year for centralized production using AM was $1 million, compared to $1.8 million for distributed production via AM. As a direct extension of Khajavi et al. [70], Mohajeri et al. [95] performed a conceptual cost-benefit analysis on various AM supply chain strategies in a spare parts industries, and proposed several supply chain management strategies that could potentially mitigate the obstacles of distributed AM implementation and reduce the relative operation cost, including building hubs of AM production, postponing production, internet-based customization, and distribution.

Thanks to the existing research efforts, the potential economic benefits of AM technologies, especially cost saving related to supply chains, have begun to be realized. To further understand how AM technologies may reshape the modern supply chain networks as well as the corresponding cost benefits, mathematical models are needed to quantify the benefits and shortcomings of AM technologies, compared with TM approaches. However, to the best of our knowledge, all of the existing studies for AM-integrated supply chain are only presented at the ideation and conceptual level due to the lack of relevant data. We collect real-world data for the use of biomedical implants from major hospitals in the state of Mississippi and public databases, and propose a stochastic cost model to investigate the economic feasibility of manufacturing biomedical implants at the sites of hospitals. The detailed stochastic programming model is presented in Section 2.3.

Table 2.1 Acronyms and mathematical notations used in the optimization model

Notations & Acronyms	Explanation
TM_i	i^{th} traditional manufacturing facility
AM_j	j^{th} additive manufacturing facility
HL_k	k^{th} hospital in Mississippi
PT_p	p^{th} product type
Sets	
P	set of products (e.g., hip implants, dental braces, stents)
I	set of TM facilities
J	set of potential AM facilities
K	set of hospitals
L	set of AM center capacities
Ω	probability space of demand scenarios
Parameters	
$\Psi_{\ell j}$	fixed cost to locate an AM facility with capacity $\ell \in L$ at location $j \in J$
β_{pj}	unit production cost of producing product PT_p at AM_j
β_{pi}	unit production cost of producing product PT_p at TM_i
c_{pjk}	unit transportation cost of transporting product PT_p from AM_j to hospital HL_k
c_{pik}	unit transportation cost of transporting product PT_p from TM_i to hospital HL_k
γ_{pk}	monetary value per unit of lead-time of product PT_p at hospital HL_k
t_{pjk}	lead time of product PT_p between AM_j and hospital HL_k
t_{pjk}	lead time of product PT_p between TM_i and hospital HL_k
h_{pj}	unit inventory holding cost for product PT_p at AM_j
h_{pi}	unit inventory holding cost for product PT_p at TM_i
f_{pjk}	service frequency for product PT_p between AM_j and hospital HL_k
f_{pik}	service frequency for product PT_p between TM_i and hospital HL_k
d_{pk}	deterministic demand of product PT_p at hospital HL_k
ω	realization of demand scenarios
ρ_ω	probability of scenario $\omega \in \Omega$
$d_{pk\omega}$	demand of product PT_p at hospital HL_k under scenario $\omega \in \Omega$
$s_{p\ell j}$	supply capacity of product PT_p at AM_j of capacity level $\ell \in L$
s_{pi}	supply capacity of TM_i of product PT_p
Variables	
$Y_{\ell j}$	binary variable that takes the value 1 if an AM facility of size ℓ is established at location AM_j, 0 otherwise
X_{pjk}	production volume of PT_p from AM_j to HL_k with deterministic demand
X_{pik}	production volume of PT_p from TM_i to HL_k with deterministic demand
$X_{pjk\omega}$	production volume of PT_p from AM_j to HL_k under demand scenario $\omega \in \Omega$
$X_{pik\omega}$	production volume of PT_p from TM_i to HL_k under demand scenario $\omega \in \Omega$

2.3 Cost models with deterministic and stochastic demands

We propose a stochastic programming model to characterize the costs of biomedical implants from AM facilities and TM suppliers. Hospitals may choose to order products from TM suppliers or establish an AM facility, which may be shared by nearby hospitals and fabricates biomedical implants at the sites of hospitals. In what follows, we begin with a deterministic programming model to characterize the total costs of production using either TM or AM with deterministic demand in Section 2.3.1, which is further generalized in Section 2.3.2 to account for uncertain and dynamic demands.

2.3.1 Cost model with deterministic demand

The proposed supply chain network consists of hospitals, TM facilities (current suppliers), and possible AM facilities. We denote by AM_j the j^{th} location of possible AM facilities; TM_i the location of the i^{th} TM facility; and HL_k the location of the k^{th} hospital. Here, $J, I,$ and K represent the set of the indices of AM facilities, TM facilities, and hospitals, respectively, i.e., $j \in J$, $i \in I$, $k \in K$. Each manufacturing facility may produce multiple types of products, the p^{th} type of which is denoted by PT_p. The mathematical optimization model for the total costs can be expressed as below. The notation is summarized in Table 2.1.

$$\min_{\boldsymbol{Y},\boldsymbol{X}} \sum_{\ell \in L} \sum_{j \in J} \Psi_{\ell j} Y_{\ell j} + \sum_{k \in K, j \in J, p \in P} \left(\beta_{pj} + c_{pjk} + \gamma_{pk} t_{pjk} + \frac{h_{pj}}{2 f_{pjk}} \right) X_{pjk} +$$

$$\sum_{k \in K, i \in I, p \in P} \left(\beta_{pi} + c_{pik} + \gamma_{pk} t_{pik} + \frac{h_{pi}}{2 f_{pik}} \right) X_{pik} \quad (2.1)$$

in which, we focus on the following two groups of decision variables:

i. $Y_{\ell j}$, binary variable that takes value 1 if an AM facility of capacity level ℓ is to be built at location AM_j; 0 otherwise. If $Y_{\ell j} = 0$ for all possible locations AM_j, no AM facility will be built, and all products are to be purchased from TM service providers. On the other hand, if $Y_{\ell j} \neq 0$, for a certain combination of ℓ and j values, it suggests to build an AM facility of capacity level ℓ at AM_j.

ii. X_{pjk} and X_{pik}, are the volume of product flow for product PT_p from suppliers AM_j and TM_i to hospital HL_k, respectively, with deterministic demand. Given product PT_p and hospital HL_k, if $X_{pik} = 0$ for all TM locations, this means that hospital HL_k does not order from TM facilities. In other words, all products are manufactured using AM facilities. Similarly, $X_{pjk} = 0$ for all AM locations, hospital HL_k only order from TM facilities.

These two groups of decision variables suggest (a) whether AM facilities should be built at a certain location, (b) what types of products to be produced at AM facilities, and (c) which hospitals will use AM for biomedical part production. Values of these decision variables are chosen by minimizing the overall costs, including inventory, transportation, production, and initial investment of AM machines. We also take into account of potential costs/penalty resulting from product lead time because short response time is very essential to patients waiting for implants. The detailed cost parameters are summarized below:

i. We denote denote by $\Psi_{\ell j}$ the initial investment of AM facilities with capacity level ℓ at location M_j . The total initial investment across all possible AM locations is $\sum_{\ell \in L} \sum_{j \in J} \Psi_{\ell j} Y_{\ell j}$. $\Psi_{\ell j}$ mainly consists of the cost of AM machines. For example, in 2015 the market price of a Selective Laser Melting (SLM) system used for the production of biomedical implants ranges from USD400,000 to USD1,000,000, depending on the original equipment manufacturer, machine dimensions, effective build volume of the machine and its operational build speed. This data is from quotations received by the Department of Mechanical Engineering of the Mississippi State University on the price of SLM machines. Such a range in price due to similar factors is in line with the data from [63], [83], [7], [14] and [17]. We assume an average price of $500,000 which is reasonable for the price of the machine that can produce the identified bio-medical implants. A similar example can be found in [14], in which the authors recorded an annual maintenance and investment cost of $110,320/year over 10 years for a similar machine with a purchase price of $700,000. We use the equivalent annual cost (EAC) model to calculate the average annualized investment and maintenance cost. There is a wide range of depreciation methods in literature. The simplest method is the straight line method which calculates the annual depreciation cost by dividing the machine purchase price by its expected life. The more complex methods such as the accelerated depreciation, equivalent annual cost (EAC) and remaining value percentage (RVP) methods, use models that take into account factors like machine age, salvage value, size, usage, manufacturer, condition, interest rate and region of deployment to calculate annual depreciation cost. Jones and Smith [67] provided an overview and historical perspective of the EAC. The detailed discussion of multiple variations of RVP models can be found in Cross and Perry [36], Hansen and Lee [57], Unterschultz and Mumey [153], and Dumler et al. [43]. We calculated the average annualized investment and maintenance cost based on a life-span of ten years, resulting in an average annualized investment and maintenance cost of $75,000 for a small capacity AM center. It is worth noting that for such a fast evolving technology, a faster replacement policy may be implemented (e.g., 5 year replacement), which will result in a higher annualized investment. The annualized investment and maintenance cost for medium and large capacity AM facilities could be $135,000 and $182,000, respectively.

ii. β_{pj} and β_{pi} represent the unit production cost of product PT_p from AM_j and TM_i, respectively. This term includes material, labor, energy consumption, pre- and post-processing costs, etc. The total production cost of product PT_p for hospital HL_k from all manufacturing facilities is represented by $\sum_{j \in J} \beta_{pj} X_{pjk} + \sum_{i \in I} \beta_{pi} X_{pik}$. The exact values for the AM and TM unit production cost of biomedical implants are usually unavailable due to proprietary nature of the data. We estimate β_{pi} using the unit cost of implants obtained from hospital database, as shown in Table 2.2; for AM, we let β_{pj} represent the combination for costs of materials, energy consumption, and labor. To identify the conditions in which AM production of implants may be economically beneficial, we investigate various ratios of $\frac{\beta_{pj}}{\beta_{pi}}$, referred to as ATR hereafter, and examine its impacts on the decision variables $Y_{\ell j}$, X_{pik}, and X_{pjk}.

iii. c_{pjk} and c_{pik} represent the unit transportation cost of delivering product PT_p from AM_j and TM_i to hospital HL_k, respectively. The transportation cost depends on the characteristics of product, such as shape, weight, fragility, etc., as well as the distance between the manufacturing facility and hospital. TM facilities are usually distant from hospitals. Actually, as shown in Figure 2.1, all TM facilities are outside of state of Mississippi. Also, a safety stock of biomedical implants is kept at the warehouse for TM. These parts can be ordered when they are needed in implant surgeries and usually require a short delivery time (e.g., overnight) to ensure fast service. Thus, the unit transportation cost from TM facilities c_{pik} tends to be much higher than c_{pjk}, the counterpart from AM facilities.

iv. h_{pj} and h_{pi} represent the daily average unit inventory holding cost for product PT_p at AM_j and TM_i, respectively. TM requires a long time to produce parts on demand, which results in a high level of inventory of infrequently ordered parts. These unused products tie up capital and resources in the forms of space, warehouse, security, land, and rent, utility costs, insurance, taxes , respectively [148]. On the other hand, on demand production of these products using AM may reduce or even eliminate the need for maintaining the high inventory level and associated costs. The TM production of several types of medical implants requires batch production. As pointed out in the case study by Trotman [150], machining partners in TM of orthopedic implants using CNC machines require a minimum of two month's supply of stock at all times. In this case, the warehouse is necessary for TM production. On the other hand, since AM's operations generally stay closer to end-product point of use, AM is able to achieve a leaner and more cost-effective supply chain that relies less on safety stock and requires less inventory holding costs [143]. This is mainly because AM does not require multi-steps production operations or any additional tooling and minimizes the need for inventory. This leads to reduced costs and lead times, especially for small volumes and complex parts as in orthopedics. Similar evidence can be found in a report published by a medical manufacturing company, Conformis [32], which indicates that TM production of medical implants requires manufacturers to commit more money on the overhead for inventory and warehousing of adequate levels of a range of fixed sizes of implants. As a summary, avoiding cost in excess inventory is one way that AM achieves a superior demand-based manufacturing advantage over TM in the production of metallic medical implants. As pointed out in a NIST report [105], when only 50 to 100 of a particular implant are needed in a given year and the minimum order from a financial feasibility standpoint is 500, this creates a huge inefficiency. AM offers the ability to make only the number that is needed, and thus helps to achieve a huge reduction in inventory holding cost. AM may significantly bring down the inventory level, which frees up capital and reduces expenses. Therefore, we assume that holding costs at AM facilities is much lower than TM facilities, i.e., $h_{pj} \ll h_{pi}$.

v. f_{pjk} and f_{pik} represent the ordering frequency of product PT_p by HL_k from AM_j and TM_i, respectively. Thus, the average inventory hold cost during the time horizon of interest is $\frac{h_{pj}}{2f_{pjk}}$, for product PT_p between AM_j and hospital HL_k. Similarly, the average inventory hold cost between TM_i and hospital HL_k is $\frac{h_{pi}}{2f_{pik}}$.

vi. t_{pjk} and t_{pik} represent the product lead/waiting time required for product PT_p from AM_j and TM_i to hospital HL_k, respectively. Even though AM products require some post-processing time, in general, AM may significantly shorten lead time when compared to TM [59]. Since post-treatment varies significantly depending on the products, we do not model it explicitly. Instead, we incorporate it into the production lead time. In the biomedical/dental applications, a specific type of biomedical implant is infrequently ordered; however, when one is ordered, it is needed quite rapidly to ensure patient health and satisfaction. The TM orthopedic implant may need two to three months of lead time, including interpreting the CT scans, making rough prototypes of the component in clay or wax, shipping it to the surgeon, and awaiting approval or input [148] . In contrast, AM has the potential to rapidly manufacture parts on demand and may considerably reduce the waiting time to several weeks. Hence, we assume that $t_{pjk} \ll t_{pik}$. For healthcare applications, the waiting time may be very crucial to the health of patients; and thus excessive waiting time incurs additional procedures and extra need of medical service. We model such penalty using a variable γ_{pk} that represents the monetary value per unit of waiting time of product PT_p at hospital HL_k. We assume that the monetary value per unit of lead-time of a biomedical implant is 10% of its market price. Hence, the total penalty for product type PT_p at hospital HL_k

is $\gamma_{pk}t_{pjk}$ and $\gamma_{pk}t_{pik}$ for products from a manufacturing facility AM_j and TM_i.

Table 2.2 Data used in parameter values

	TM	AM	Unit	Comments
Production cost, β_{pj}	Hip implants: 2308 [a] Knee implants: 1863[a] Dental braces: 100[a] Stents: 249 [a]		$/unit $/unit $/unit $/unit	Based on 30% of the price hospitals pay for the implant
Build time		Hip implants: 12 [b] Knee implants: 11 [b] Dental braces: 0.25 [b] Stents: 0.4 [b]	hours/unit hours/unit hours/unit hours/unit	
Fixed investment cost, Ψ_{lj}		Small: 75,000 [c] Medium: 135,000 [c] Large: 182,000 [c]	$/year $/year $/year	
Transportation cost, c_{pjk}	Dental braces and stents [d] $28.5 + 0.02a_{jk}$ Hip and Knee implants [d] $35.4 + 0.02a_{jk}$		$/unit $/unit	Estimated from carrier data
Inventory holding cost, h_{pj}	25%	2.5%	Of inventory value or revenue	
National mean demand data, d_{pk}	Hip implants: 332,000 [e] Knee implants: 719,000 [e] Dental braces: 1,000,000 [f] Stents: 1,000,000 [g]		units/year units/year units/year units/year	Assume demand based on County population and national demand

Table 2.2 (continued)

Lead-time, t_{pjk}	60 [g]	14 [h]	days	Includes AM post-processing time
Lead-time cost, γ_{pk}	10% - 270%		Of implant price	Assumed
Supply capacity	No capacity constraint	Hip implants: 416 Knee implants: 453 Dental braces: 19,968 Stents: 12,480	units/year units/year units/year units/year	Estimated from build time

[a] Invoice of Oktibbeha County Hospital, Starkville, Mississippi.
[b] Calculated based on the relative volume of parts using SLM state-of-the-art machines for year 2015.
[c] Quotation of Selective Laser Melting systems, 2015.
[d] FedEx Get rates and transit times tool. Available at https://www.fedex.com/ratefinder/home?link=4&cc=US&language=en . Accessed on July 03, 2015
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[h] Huang, S. H., Liu, P., Mokasdar, A. & Hou, L. (2013). Additive manufacturing and its societal impact: A literature review. International Journal of Advanced Manufacturing Technology, 67, 1191-1203.

The solution to the optimization model, described by Equation (2.1), is subject to multiple constraints below:

1. The demand for each product type should be met for any hospital, HL_k, i.e.,

$$\sum_{j \in J} X_{pjk} + \sum_{i \in I} X_{pik} \geq d_{pk} \;\; \forall p \in P, k \in K \tag{2.2}$$

where d_{pk} represents the deterministic demand for product PT_p from hospital HL_k. We estimate the average annual demand of the biomedical implants in each MS county based on the average annual national demand of the implant. We also assume that patients from counties that do not have the capability to perform a certain procedure use hospitals from nearby counties. In other words, the demand of implants from counties that cannot perform a certain procedure is distributed to nearby counties.

2. The product volume of product PT_p, manufactured from any AM facility, should not exceed its total capacity of production, i.e.,

$$\sum_{k \in K} X_{pjk} \leq \sum_{\ell \in L} s_{p\ell j} Y_{\ell j}, \forall p \in P, j \in J \tag{2.3}$$

where $s_{p\ell j}$ represents the supply capacity of product PT_p at AM_j of capacity level ℓ.

3. Similar to Constraint (2.2), the production volume from TM facilities is also limited by their capacity, i.e.,

$$\sum_{k \in K} X_{pik} \leq s_{pi} \;\; \forall p \in P, i \in I \tag{2.4}$$

where s_{pi} represents the supply capacity of product type p at TM facility i.

4. For each location, a maximum of one AM facility can be built.

$$\sum_{\ell} Y_{\ell j} \leq 1. \forall j \in J \tag{2.5}$$

5. Decision variables of AM facility location are binary

$$Y_{\ell j} \in \{0, 1\} \; \forall l \in L, j \in J \tag{2.6}$$

6. Production volumes are non-negative

$$X_{pjk} \geq 0, X_{pik} \geq 0. \forall p \in P, j \in J, i \in I, k \in K \tag{2.7}$$

The cost model described by Equations (2.1) – (2.7) characterize the overall costs of a product, including machine/system investment, production, transportation, inventory, and waiting penalty when the product demand in deterministic and known. However, in many situations, the product demand may be unknown or varying over time. For example, an increase in the aging population may potentially increase the number of cardiovascular and orthopedic cases that require the use of more stents and knee and hip implants for treatment. Conversely, it is also possible for the demand of some biomedical implants to decrease when people start to live healthier lifestyles that to some extent may reduce the need of surgeries. In the next subsection, we extend the deterministic cost model to account for the scenarios, in which demand may be unknown or vary over time. This situation can be found in many real-world medical applications.

2.3.2 Stochastic model for uncertain demand

We further extend the cost model with deterministic demand as described in Section 2.3.1 to account for the uncertainty in the demand variable d_{pk}. The optimization model in Equation (2.1) can be formulated as a two-stage stochastic program, where the first-stage decisions correspond to the location and capacity selection of the AM centers and the second stage decisions correspond to the optimal routing of the products considering a particular realization. We let Ω represent the probability space that consists of all possible scenarios of demand, and ω be a sample/realization of scenarios, the probability of which is ρ_ω. In this context, for each product type PT_p, $d_{pk\omega}$ is a random variable representing the future demand at hospital HL_k, and $X_{pjk\omega}$ the corresponding product flow under scenario $\omega \in \Omega$. On the other hand, $Y_{\ell j}$, are long-term decisions that do not involve uncertainty since once AM centers are established the infrastructure does not change over time. As a result, we use the same set of decision variables $Y_{\ell j}$ as the deterministic demand model for the locations and size of AM facilities. Therefore, the corresponding two-stage stochastic programming model can be formulated as follows:

$$\min_{Y,X} \sum_{\ell \in L} \sum_{j \in J} \Psi_{\ell j} Y_{\ell j} + \sum_{\omega \in \Omega} \rho_\omega E(Y,\omega) \quad (2.8)$$

with $E(Y,\omega)$ as the solution of the following second-stage problem:

$$E(Y,\omega) = \min_{\boldsymbol{Y},\boldsymbol{X}} \sum_{k \in K, j \in J, p \in P} \left(\beta_{pj} + c_{pjk} + \gamma_{pk} t_{pjk} + \frac{h_{pj}}{2pjk}\right) X_{pjk\omega} + \sum_{k \in K, i \in I, p \in P} \left(\beta_{pi} + c_{pik} + \gamma_{pk} t_{pik} + \frac{h_{pi}}{2pik}\right) X_{pik\omega} \quad (2.9)$$

subject to the constraints below, which are similar to constraints in the model of deterministic demand, except that $X_{pjk\omega}$ and $d_{pk\omega}$ are defined for each possible realization of scenario ω.

$$\sum_{l\in L} Y_{\ell j} \leq 1, \forall j \in J \quad (2.10)$$

$$\sum_{j\in J} X_{pjk\omega} + \sum_{i\in I} X_{pik\omega} \geq d_{pk\omega}\ \forall p \in P, k \in K, \omega \in \Omega \quad (2.11)$$

$$\sum_{k\in K} X_{pjk\omega} \leq \sum_{l\in L} s_{p\ell j} Y_{\ell j}\ \ \forall p \in P, j \in J, \omega \in \Omega \quad (2.12)$$

$$\sum_{k\in K} X_{pik\omega} \leq s_{pi}\ \forall p \in P, i \in I, \omega \in \Omega \quad (2.13)$$

$$Y_{\ell j} \in \{0.1\}\ \ \forall l \in L, j \in J \quad (2.14)$$

$$X_{pjk\omega} \geq 0, X_{pik\omega} \geq 0\ \forall p \in P, j \in J, i \in I, k \in K, \omega \in \Omega \quad (2.15)$$

This stochastic programming model is a non-deterministic polynomial-time hard (NP-hard) problem [90]. Hence, it is extremely challenging and expensive to solve this model directly. To address this issue, we propose in the next section a customized solution approach to efficiently solve this model.

2.4 Sample average approximation

We use the sample average approximation (SAA) to find solutions to the two-stage stochastic programming problem as described by Equations (2.8) – (2.15). We also demonstrate the computational advantage of implementing SAA over using a general-purpose commercial solver in Section 2.4.1. SAA is a sampling strategy that seeks to quickly compute high quality solutions to large-scale stochastic programming problems with a large number of scenarios. The idea of the SAA algorithm is to generate random sample ω and approximate the expected value function $\sum_{\omega\in\Omega} \rho_\omega E(Y,\omega)$ by the corresponding sample average function. The SAA algorithm is renowned not only for providing high quality feasible solutions but also for providing a statistical estimation of their optimality gap. SAA algorithm was applied previously to solve large scale supply chain related problems ([29], [136]). Kleywegt et al. [73] conducted extensive analysis to prove the convergence properties of the SAA algorithm. Other studies such as Mak et al. [91], Norkin et al. [106], Norkin et al. [107] evaluated the statistical performance of the SAA algorithm.

2.4.1 Steps of SAA

The main difficulty in solving the stochastic problem (2.8) – (2.15) lies in computing the expectation of the linear programming value function $E(Y, \omega)$. This is extremely difficult, if not impossible, for continuous distributions as they involve multiple integrals. For discrete distributions, it involves solving a large number of linear programs, one for each scenario of the uncertain parameter realization. The SAA method provides a means for dealing with this problem by approximating the expectation $E(Y, \omega)$ using the sample average function $\frac{1}{|N|}\sum_{n=1}^{N} E(Y, n)$ with a random sample of $|N|$ realizations of the random scenario parameter ω. The problem. (2.8) – (2.15) is then approximated by the following SAA problem:

$$\min_{\boldsymbol{Y},\boldsymbol{X}} \sum_{\ell\in L}\sum_{j\in J}\Psi_{\ell j}Y_{\ell j} + \frac{1}{|N|}\sum_{n\in N}\sum_{k\in K, j\in J, p\in P}\left(\beta_{pj} + c_{pjk} + \gamma_{pk}t_{pjk} + \frac{h_{pj}}{2p_{jk}}\right)X_{pjkn} + \frac{1}{|N|}\sum_{n\in N}\sum_{k\in K, i\in I, p\in P}\left(\beta_{pi} + c_{pik} + \gamma_{pk}t_{pik} + \frac{h_{pi}}{2p_{ik}}\right)X_{pikn} \tag{2.16}$$

Kleywegt et al. [73] showed that the optimal solution of problem. (2.16) eventually converges with probability of one to the solution obtained from the original problem. (2.8) – (2.15) as the size of $|N|$ increases. Below, we discuss the detailed steps of the SAA algorithm:

Step 1 (<u>Sampling</u>): Generate M independent demand sample scenarios each of size N. Denote the m^{th} demand sample scenario by $\{\boldsymbol{d}_1^m, \boldsymbol{d}_2^m, \dots, \boldsymbol{d}_{|N|}^m\}$ for $m = 1, \dots, M$. Here, $\boldsymbol{d}_n^m$ represents the set of demand realizations in each scenario, i.e., $\boldsymbol{d}_n^m = \{d_{pkn}^m, \forall p \epsilon P, k \epsilon K\}$, for $m = 1, \dots, M$ and $n = 1, \dots, |N|$. We solve the SAA problem as expressed in Equation (2.16) subject to constraints (2.17)-(2.22) below:

$$\sum_{l \in L} Y_{\ell j} \leq 1, \forall j \in J \tag{2.17}$$

$$\sum_{j \in J} X_{pjkn} + \sum_{i \in I} X_{pikn} \geq d_{pkn} \; \forall p \in P, k \in K, n \in N \tag{2.18}$$

$$\sum_{k \in K} X_{pjkn} \leq \sum_{\ell \in L} s_{p\ell j} Y_{\ell j} \;\; \forall p \in P, j \in J, n \in N \tag{2.19}$$

$$\sum_{k \in K} X_{pikn} \leq s_{pi} \; \forall p \in P, i \in I, n \in N \tag{2.20}$$

$$Y_{\ell j} \in \{0, 1\} \; \forall l \in L, j \in J \tag{2.21}$$

$$X_{pjkn} \geq 0, X_{pikn} \geq 0 \; \forall p \in P, j \in J, i \in I, k \in K, n \in N \tag{2.22}$$

Denote by v^{N_m} and $\widehat{\boldsymbol{Y}}^{N_m}$ the objective value and optimal solution of the m^{th} problem, respectively.

Step 2 (<u>Estimating the lower bound</u>): Compute the average of all optimal objective function values from the SAA problems, μ_M^N and its variance $\sigma_{\mu_M^N}^2$:

$$\mu_M^N = \frac{1}{|M|} \sum_{m \in M} v^{N_m}$$

$$\sigma_{\mu_M^N}^2 = \frac{1}{(|M| - 1)|M|} \sum_{m \in M} v^{N_m} - \mu_M^N$$

The average objective function value μ_M^N provides a valid statistical lower bound on the optimal objective function value of the original problem (2.8) – (2.15).

Step 3 (<u>Estimating the upper bound</u>): Choose a feasible solution $\widetilde{\boldsymbol{Y}}$ from the above computed solutions $\widehat{\boldsymbol{Y}}^{N_m}$**.** We fix $\widetilde{\boldsymbol{Y}}$ and estimate the optimal solution of the original problem (2.8) – (2.15) as follows:

$$\mathrm{Min}_{\boldsymbol{X}} v_{N'}(\widetilde{\boldsymbol{Y}}) := \sum_{\ell \in L} \sum_{j \in J} \Psi_{\ell j} \tilde{Y}_{\ell j} +$$

$$\frac{1}{|N'|} \sum_{n \in N} \sum_{k \in K, j \in J, p \in P} \left(\beta_{pj} + c_{pjk} + \gamma_{pk} t_{pjk} + \frac{h_{pj}}{2 f_{pjk}} \right) X_{pjkn} +$$

$$\frac{1}{|N'|} \sum_{n \in N} \sum_{k \in K, i \in I, p \in P} \left(\beta_{pi} + c_{pik} + \gamma_{pk} t_{pik} + \frac{h_{pi}}{2 f_{pik}} \right) X_{pikn}$$

where N' is another set of samples generated independently for the demand scenarios. Typically, the sample size $|N'|$ is chosen to be much larger than the sample size $|N|$ used in the SAA problems. Note that $v_{N'}(\widetilde{\boldsymbol{Y}})$ gives an estimate on the upper bound of the original problem defined in (2.8) – (2.15). We now estimate the variance of $v_{N'}(\widetilde{\boldsymbol{Y}})$ as follows:

$$\sigma^2_{\mu N'}(\widetilde{\boldsymbol{Y}}) = \frac{1}{(|N'|-1)|N'|}\sum_{n\in N'}\left\{\sum_{\ell\in L}\sum_{j\in J}\Psi_{\ell j}\tilde{Y}_{\ell j} + \frac{1}{|N'|}\sum_{p\in P}\sum_{j\in J}\sum_{k\in K}\left(\beta_{pj}+c_{pjk}+\gamma_{pk}t_{pjk}+\frac{h_{pj}}{2f_{pjk}}\right)X_{pjkn} + \frac{1}{|N'|}\sum_{p\in P}\sum_{i\in I}\sum_{k\in K}\left(\beta_{pi}+c_{pik}+\gamma_{pk}t_{pik}+\frac{h_{pi}}{2f_{pik}}\right)X_{pikn} - v_{N'}(\widetilde{\boldsymbol{Y}})\right\}^2$$

Step 4 (<u>Estimating the optimality gap</u>): Compute the optimality gap using the lower bound and upper bound estimates from **Steps 2** and **3**:

$$gap_{N,M,N'}(\widetilde{\boldsymbol{Y}}) = v_{N'}(\widetilde{\boldsymbol{Y}}) - \mu_M^N$$

If $gap_{N,M,N'}(\widetilde{\boldsymbol{Y}}) < \epsilon$, stop. The decision variables for the optimal solution are $\widetilde{\boldsymbol{Y}}$**.** A common choice for the error threshold is $0.005v_{N'}(\widetilde{\boldsymbol{Y}})$. Otherwise go to **Step 1**.

The most computationally expensive part of the SAA algorithm (described in **Step 1**) is to solve the two-stage stochastic integer programming problem (2.18) – (2.22) involving $|N|$ scenarios. Cutting plane algorithms such as Benders decomposition by Benders [20] and dual decomposition by Rockafellar and Wets [124] can also be used to solve this class of problems. However, in our study since the size of $|L|$ and $|J|$ is relatively small, we use CPLEX, a mathematical optimization software provided by IBM to solve linear and integer programs, to solve this part of the SAA algorithm.

2.4.2 Computational efficiency of the proposed algorithms

We study the computational efficiency of the proposed model and algorithm in this subsection. The dimensions of the deterministic equivalent problem are presented in Table 2.3

Table 2.3 Problem size of the deterministic equivalent of the model

$\|P\|$	$\|I\|$	$\|J\|$	$\|K\|$	$\|L\|$	No. of Binary Variables	No. of Continuous Variables	No. of Total Variables	No. of Constraints
4	4	20	20	3	80	1920	2000	196

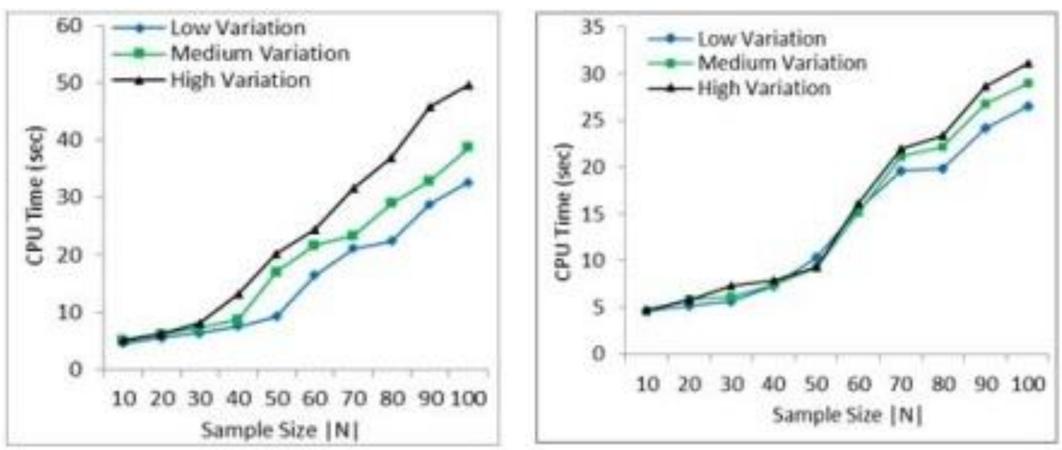
We use the following criteria to terminate the SAA algorithm: *(a)* the gap between the upper and lower bounds falls below a threshold limit ε, i.e., $\varepsilon = |UB - LB|/UB = 0.005$ *(b)* the maximum time limit is reached i.e., $t_{max} = 36{,}000$ seconds, and *(c)* the maximum iteration limit is reached i.e., $n_{max} = 100$. We conduct two sets of experiments to evaluate the convergence behavior of the SAA algorithm. In the first set of experiments (shown in Table 2.4), we test the performance of the SAA algorithm by varying the size of the scenario set $|N'| = 50, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1000$ while fixing the sample size $|N|$ to 30. The second set of experiments tests the performance of the SAA algorithm by varying the sample size $|N| = 10, 20, 30, 40, 50, 60, 70, 80, 90, 100$ while fixing the scenario set size $|N'|$ to 1000. Furthermore, we present results to evaluate the efficiency of the SAA algorithm when the demand is generated randomly using a normal and a uniform distribution. In all experiments, the best running time between CPLEX and SAA algorithm is identified by boldface letters; each can be solved with less than a 0.5% optimality gap; otherwise, the smallest optimality gap is highlighted.

Table 2.4 compares the computational performance between CPLEX and SAA algorithm under different sample sizes and demand variation levels. We change the standard deviation of demand to obtain three different demand variation levels: (-5.0 to 5.0)% for low demand, (-10.0 to 10.0)% for medium demand, and (-15.0 to 15.0)% for high demand variations. Our computational performance indicates that both CPLEX and SAA algorithm are capable of solving all the problem instances within the pre-specified optimality gap (0.5%). However, the running time of the SAA algorithm is significantly faster compared to CPLEX. On average, SAA algorithm is 245 times faster than CPLEX under low demand variations, 296 times faster under medium demand variations, and 256 times faster under high demand variations.

Table 2.4 Computational performance of the solution algorithm: Normal and Uniform distributions

$\|N'\|$	Normal Distribution				Uniform Distribution			
	CPLEX		SAA		CPLEX		SAA	
	Avg. Gap (%)	Avg. CPU (sec)	Avg. Gap (%)	Avg. CPU (sec)	Avg. Gap (%)	Avg. CPU (sec)	Avg. Gap (%)	Avg. CPU (sec)
50	0.47	13.5	0.49	**11.0**	0.47	**5.3**	0.22	5.5
100	0.25	25.9	0.15	**11.5**	0.01	28.1	0.08	**7.0**
200	0.24	126.0	0.23	**13.0**	0.02	76.4	0.15	**10.5**
300	0.23	256.5	0.15	**14.5**	0.48	109.3	0.13	**12.5**
400	0.39	362.6	0.45	**17.5**	0.10	292.7	0.16	**14.5**
500	0.29	668.9	0.22	**19.0**	0.15	432.5	0.15	**16.5**
600	0.24	853.4	0.02	**20.5**	0.11	510.7	0.10	**17.0**
700	0.18	2083.3	0.40	**23.5**	0.47	1076.5	0.23	**21.0**
800	0.23	2392.9	0.31	**25.5**	0.18	1199.7	0.13	**23.5**
900	0.14	3738.2	0.15	**27.5**	0.49	1852.1	0.14	**25.5**
1000	0.46	4307.1	0.35	**31.0**	0.46	2220.2	0.04	**29.5**

Figure 2.3 (a) and (b) present the total CPU time required for the SAA algorithm under different sample sizes $|N|$ for both the normal and uniform distributions, respectively. Additionally, Figure 2.3 evaluates the performance of the SAA algorithm under different sample sizes with three demand variation levels: low, medium and high. Computational results indicate that the running time of the algorithm increases as the variation in demand increases for both normal and uniform distributions. All computations are coded in GAMS 24.2.2 on a desktop with Intel Core i7 3.60 GHz processor and 16.0 GB RAM. The optimization solver used is ILOG CPLEX 12.6.



3(a) Normal distribution 3(b) Uniform distribution

Figure 2.3 Effect of sample size on CPU time

2.5 Numerical study

We apply the proposed stochastic cost model, as described by Equations (2.8) – (2.15), and the SAA algorithm to a real-world case study, in which we investigate the use of AM technologies to fabricate biomedical implants for hospitals in the state of

Mississippi (MS). In particular, we conduct a series of numerical studies to investigate the economic feasibility of using AM technologies for manufacturing biomedical implants, and identify the cost parameters that may pose significant impacts on the economic feasibility. (1) One key cost parameter to be considered is the ratio between unit production costs of AM and TM, $\frac{\beta_{pj}}{\beta_{pi}}$, referred to as ATR, which describes how expensive it is to produce a unit using AM relative to TM (i.e. conventional methods). For example, if ATR = 2.0, it means that the unit production cost of an implant using AM is twice the unit production cost of the implant using TM. For a high ATR value, it is more expensive to produce a unit product using AM than TM, discouraging the initiation of AM facilities. One goal of this study is to identify the critical minimal ATR value that makes AM economically beneficial, by testing various levels of ATR values. (2) The initial investment of AM, mainly consisting of the cost of AM machines, is known to be another cost parameter that constitutes a large portion of the total AM costs. We investigate whether it is economically beneficial to use AM technologies for manufacturing of biomedical implants with the current level of the initial investment. If not, we identify to what extent the future improvement of manufacturing technologies, which may make AM systems more affordable, will affect the economic feasibility of AM production. (3) Another cost parameter is the demand of each biomedical implant. Considering the high costs of AM systems, it may not justify the initial investment when the overall demand level is very low. We study the effect of various demand levels (i.e., low, medium, and high) on the number of AM facilities to be located. Last but not least, (4) product lead time and product penalty cost for the biomedical implants could be essential for the adoption of AM. Shorter product lead time may result in faster response and help with the recovery of patients. For different procedures, the urgency of a specific product, characterized by the lead time penalty coefficient, may vary. We will identify how much improvement of product lead time is needed, and how urgent the implants are desired to justify the costs of AM production. At last, the computational efficiency of the proposed algorithm is also reported.

2.5.1 Case study for additive manufacture of biomedical implants

We focus on four biomedical implants in which additive manufacturing has already been implemented for their manufacture: hip and knee joint implants, dental braces, and vessel stents. We collected data from major hospitals, as well as the nearby clinics, about the use of these four biomedical implants in the 20 most populous counties of MS, as shown in Figure 2.1. Most hospitals can perform procedures for all four implants of interest. However, select hospitals do not have the capacity to perform specific procedures. For example, the Oktibbeha County Hospital can only perform the implantation procedure of hip/knee joint implants and dental braces, but not stents. In this case, the demand in this county will be distributed to its neighborhood counties. The average demands of these four types of biomedical implants in Mississippi are estimated as the corresponding proportion of Mississippi–USA population in 2010, multiplied by the nationwide demands of these four biomedical implants, published by Centers for Disease Control and Prevention. The mean demands of all four types of biomedical implants for each county of Mississippi are demonstrated in Figure 2.4.

We have also collected information about the suppliers of these four biomedical implants via TM, as demonstrated in Figure 2.*2*. The data related to the use of biomedical implants, as well as the data source, are summarized in Table 2.2. At present, MS hospitals procure biomedical implants from suppliers and manufacturers located outside of MS who use TM methods to manufacture the parts, the prices of which are estimated based on the invoice of hospitals in Mississippi. We investigate whether it is beneficial to fabricate these biomedical implants at the sites of hospitals using AM technologies. The prices of AM systems are estimated based on the quotation of Selective Laser Melting (SLM) system in 2015. We choose the SLM system because of its widely documented use for the fabrication of biomedical implants. The build time for each part is estimated using the relative volume of parts using SLM state-of-the-art machines for year 2015. We assume that the biomedical implants are delivered using FedEx, and the costs of transportation are calculated using the online tool provided by FedEx Get Rates.

2.5.1.1 ATR analysis

We vary the ATR value and use it as input in the developed stochastic programming model, described by Equation (2.8)-(2.15), to examine the number of AM facilities to be established in each scenario and how much product to supply via AM and/or TM. Results are reported in Figure 2.5. We observe that these economic decisions largely depend on the ATR value. Lower ATR value tends to encourage the initiation of more AM centers, favoring the use of AM technology to produce more parts and decreases the average cost of production.

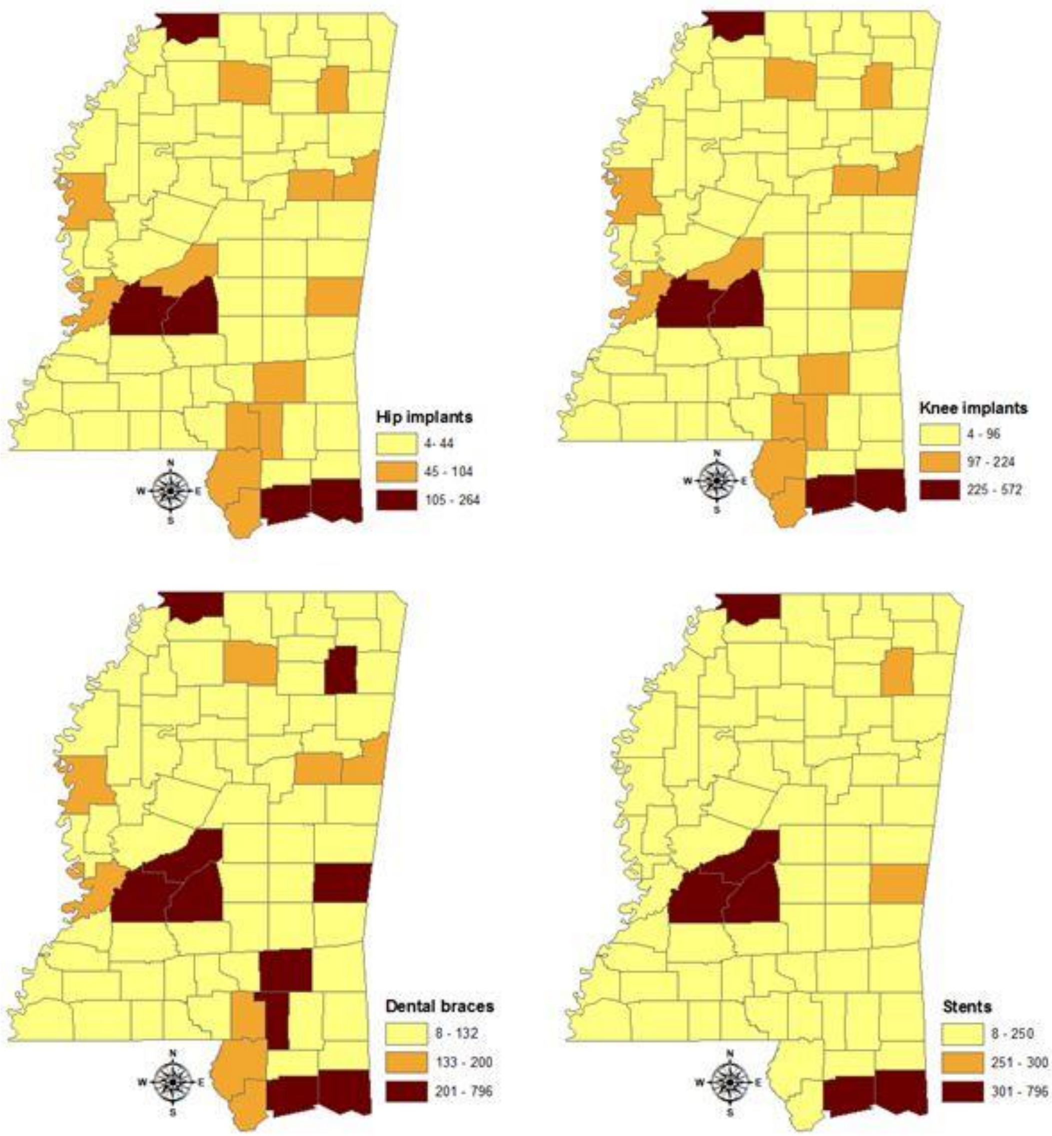
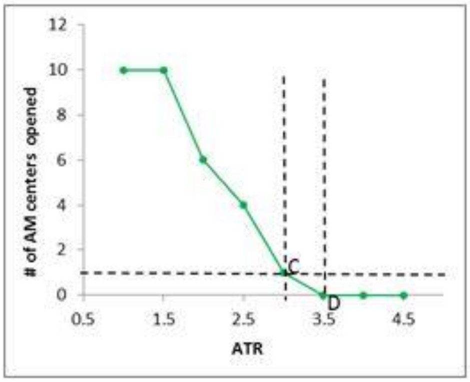
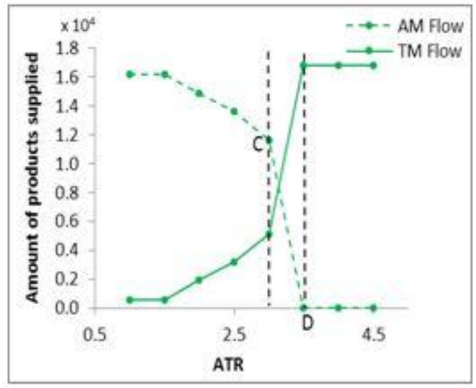


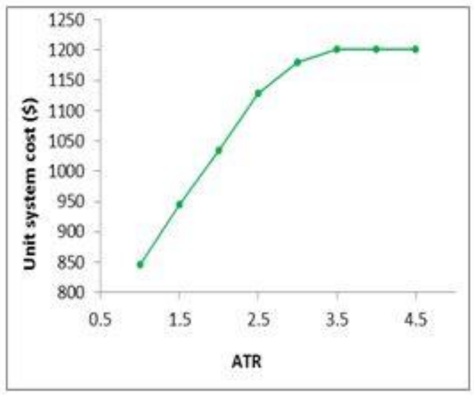
Figure 2.4 Estimated annual demands of biomedical implants for Mississippi



5(a) Number of AM centers located



5(b) Amount of products from AM and TM



5(c) Average unit production cost using either AM or TM

Figure 2.5 Effects of ATR on the economic decisions of production

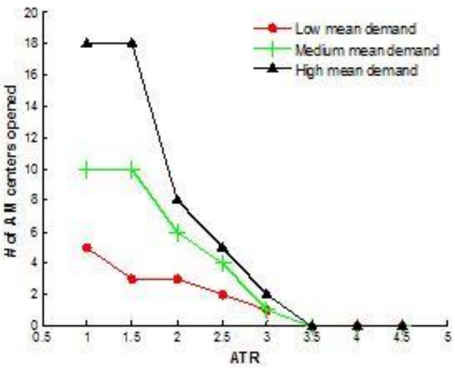
Figure 2.5(a) suggests that the ATR value should be no higher than 3.0 for any AM center to be established (point C in Figure 2.5(a)). At this point, the number of AM centers located is one. At points to the left of the critical point with lower ATR values, more AM centers would be recommended, whereas to the right of the critical point, where $ATR \geq 3.5$, no AM centers are recommended as shown by point D in Figure 2.5(a). This can be explained by considerably high unit production cost of AM for $ATR \geq 3.5$ which overshadows the benefits of AM, e.g., low inventory and short lead time. Accordingly, all of the products are economically beneficial to be supplied from

TM. Similar observations are made for the production volumes as shown in Figure 2.5(b). The amount of products supplied from AM essentially decreases as ATR increases, while the amount of products supplied from TM increases as the ratio increases. At point D and beyond (i.e., $ATR \geq 3.5$), all products are supplied via TM because no AM center is suggested to be located based on these ATR values. When the ATR decreases, the amount of products supplied from AM increases, because more AM facilities are to be established to supply medical implants together with TM. The average unit cost, using either AM or TM production technologies, increases as ATR increases as shown in Figure 2.5(c). For $ATR < 3.5$, AM is used to produce biomedical implants. On the other hand, for $ATR \geq 3.5$, no AM facilities are suggested to be established and the average unit production cost becomes stable since all products are manufactured from TM suppliers.

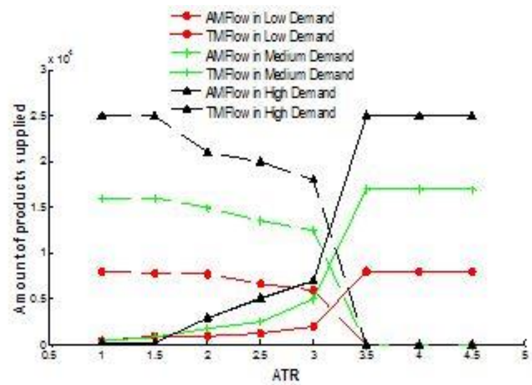
2.5.1.2 Demand Analysis

We conduct a set of experiments to further investigate the economic decisions with various scenarios of product demand, which could be varying and dynamic over time. We take the current demand data for medical implants at Mississippi hospitals as the medium/baseline demand level, and consider a low demand level (50% of baseline) and a high demand level (150% of baseline). Similar to the previous ATR studies, we determine the number of AM facilities to be established and the number of products to be produced from each manufacturing facility, with various demand levels. The results of the experiments are demonstrated in Figure 2.6.

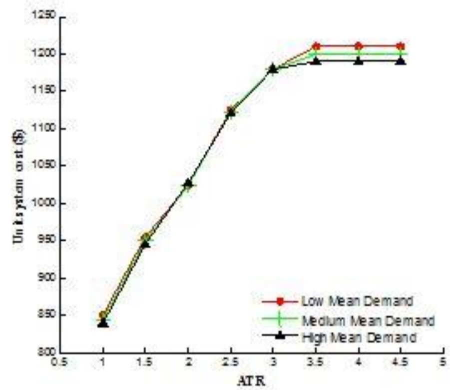
Figure 2.6(a) shows the number of AM centers to be established for the three levels of demand. It may be observed that when AM is chosen to manufacture biomedical implants, higher demand levels result in more AM centers. For example, when ATR = 2.5, two, four and five AM centers are needed to satisfy the low, medium and high levels of demand, respectively. This is echoed in Figure 2.6(b), which plots the quantity of products shipped from AM and TM suppliers to hospitals. The average unit cost for each demand level tends to increase as ATR increases and remain at a constant level for $ATR \geq 3.5$ is presented in Figure 2.6(c). When ATR < 3.5, the average unit production costs are very similar for various demand levels which may be explained by the fact that AM is mainly used for production at this regime and the production cost of AM is not sensitive to production volumes and demand levels. For $ATR \geq 3.5$, in which case only TM is chosen, the average unit production cost branches out for various demand levels and decreases as the demand level increases. This is because TM typically benefits from the scale of economics and batch production.



6(a) Number of AM centers located

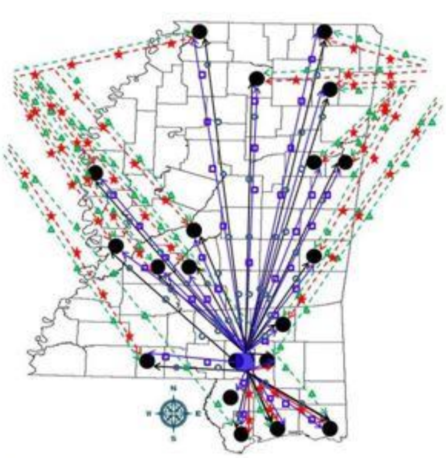


6(b) Amount of products from AM and TM

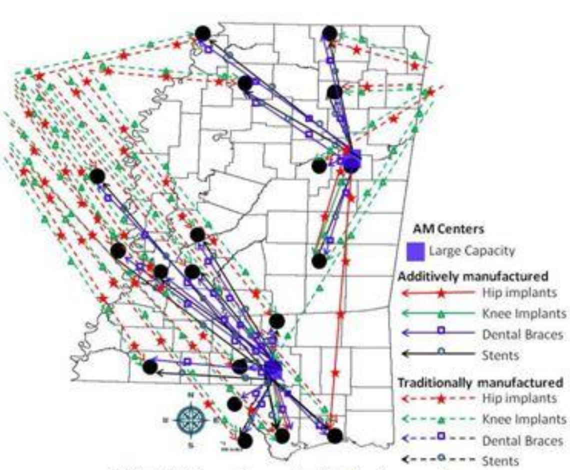


6(c) Average unit production cost (in USD) using either AM or TM for various ATRs

Figure 2.6 Number of AM centers, production volume, and average unit product cost for various demand levels



7(a) AM locations for low and medium demand



7(b) AM locations for high demand

Figure 2.7 Location of AM centers and routing of products when ATR < 3.5

When ATR < 3.5, i.e., AM production is feasible and our model recommends the potential optimal locations for AM facilities and the corresponding product flow lines, as depicted in Figure 2.7. When the demand level is low, one AM facility is sufficient to satisfy the need for production, as shown in Figure 2.7(a). This AM facility is recommended to be located in Forrest County, the southern part of Mississippi, to supply AM implants to all hospitals of the state. This location is chosen because of its physical proximity to about 80% of the major hospitals in MS, and thus may help to reduce transportation cost and product lead time. When the demand level increases to medium, this AM facility is sufficient to satisfy the need of production, and thus results in the same configuration of supply chain and location of AM centers. In other words, the increase in demand from low to medium is not enough to justify the cost to be incurred from locating an additional AM center. However, when the demand level becomes high, another large capacity AM center is situated in the northeastern part of the state in Lowndes County, which is capable of supplying to nearby hospitals. Even though the additional AM facility incurs an extra investment cost, it increases responsiveness and provides the necessary capacity to meet high product demand while reducing both transportation cost and lead time cost.

2.5.1.3 Result discussion

Based on the ATR and demand analysis, AM would be economically feasible for the production of biomedical implants for the state of Mississippi under the critical condition that ATR < 3.5. However, when AM is more expensive ($ATR \geq 3.5$), AM would not be an economically feasible option regardless of the demand, in which case, all hospitals of Mississippi are recommended to order biomedical implants from TM out of the state as demonstrated in Figure 8. At the current stage of AM technologies, the AM unit production cost tends to be much higher than that of TM, i.e., ATR > 3.5 [148]. This may explain why AM is currently mainly used for the purpose of prototyping and product design for biomedical implants, instead of manufacturing of end products. In what follows, we will investigate and identify the cost parameters that may potentially affect the economic feasibility of AM via extensive sensitivity analysis of the proposed model.

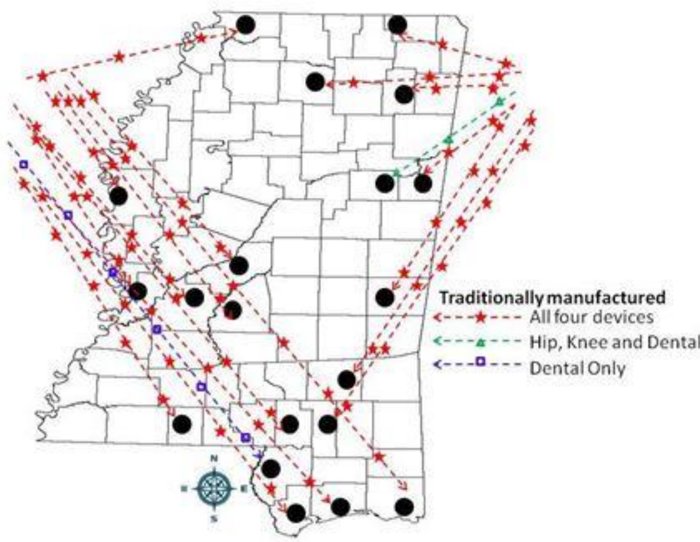


Figure 2.8 Routing of products when ATR > 3.5

2.5.2 Cost parameters impacting economic decisions

In this subsection, we will determine the cost parameters that can potentially make AM economically beneficial and recommend how much change/improvement is needed, via a series of numerical studies. We focus on the cases, in which ATR > 3.5 and AM is not readily feasible. We study the impacts of fixed initial machine cost, inventory holding cost, required lead time, and lead time penalty coefficient. To do so, we vary each cost parameter when ATR > 3.5 and apply our proposed model to decide the number of AM centers to be located. The impacts of such changes of these cost parameters (in percentage) are reported in Table 2.5

We first vary the cost of initial machine investment by reducing the machine cost by 0%, 10%, 20% … 100%. At each level of the initial machine cost, we examine one by one if the changes of each other cost parameter could affect the economic feasibility of AM production. We use the symbol of × to represent the case in which AM is infeasible at the specific level of machine cost, regardless how other parameters are varied. The symbol of ○ is used to represent the case in which AM may be economically feasible, given the reduction of the machine cost and the necessary changes in other parameters. For example, when the cost of AM machine is reduced by 60%, as shown in the highlighted row of Table 2.5, the changes in the inventory holding cost solely does not impact the feasibility of AM production. However, when the product lead time of AM is reduced by 60%, or the penalty of product waiting time is increased by 20%, it would be economically beneficial to use AM production.

It can be observed that (1) the AM machine cost is essential for the feasibility of AM production. The metal-based machine cost of the considered implants needs to be reduced by at least 60% to make AM production profitable. This may be possible considering the trend exhibited in the cost of AM machines in the past two decades: the price of some plastic-based AM machines has decreased 51% between 2001 and 2011 after adjusting for inflation [148]. It is not unlikely that metal-based AM machines will follow a similar trend in the future as research and technology advance.

Table 2.5 Combined effect of fixed cost and other costs on AM center location for ATR > 3.5

Initial Machine Cost	Inventory holding cost		Lead time		Lead time cost	
Change (%)	Impact	Change (%)	Impact	Change (%)	Impact	Change (%)
0	×	NA	×	NA	✓	+270
-10	×	NA	×	NA	✓	+240
-20	×	NA	×	NA	✓	+210
-30	×	NA	×	NA	✓	+180
-40	×	NA	×	NA	✓	+130
-50	×	NA	×	NA	✓	+70
-60	×	NA	✓	-60	✓	+20
-70	✓	0	✓	0	✓	0
-80	✓	0	✓	0	✓	0
-90	✓	0	✓	0	✓	0
-100	✓	0	✓	0	✓	0

×: Infeasible. No AM is located no matter the change given the decrease in fixed cost.
✓: Feasible and the given decrease in fixed cost is enough to locate.
NA: Not Applicable.

(2) The lead time cost penalty coefficient, related to the urgency of the product, is another important factor. Since the monetary value of a delayed procedure is uncertain and complicated to quantify, we have assumed the lead time cost as a percentage of the market price of the implants. For the health sectors, some medical procedures can be delayed without drastic consequences, in which case, we assume a low penalty of 10%. However, in other medical procedures, the delay of biomedical products may cause escalated injury; delaying the process of recovery. When it comes to life-or-death situations (e.g. 270% lead time penalty), AM may be a suitable tool for fast response regardless of the high production and machine cost. (3) It can be also observed that the impacts of AM inventory holding cost and product lead time tend to be secondary to the

feasibility of AM production. This may be because of the facts that the current inventory holding cost of AM is already at a reasonably low level, constituting only a relatively small portion of the overall production cost; and that the AM lead time is already much shorter as compared to its TM counterpart. Further improvements of these two parameters may not be of highest priority.

2.6 Conclusions

In this paper, we have developed a stochastic cost model to quantify the supply-chain level costs associated with the production of biomedical implants using Additive Manufacturing (AM) technologies, and investigate the economic feasibility of using these technologies to fabricate biomedical implants at the sites of hospitals within the state of Mississippi. Different from the existing studies that mainly focus on the process-level costs, such as machine, materials, labor, energy consumption, etc., our model mainly focused on modeling system-level costs such as inventory, transportation, etc. We also factor in the effects of product lead/waiting time on the overall transportation costs and account for the stochastic nature of product demands, resulting in a two-stage stochastic programming model. The developed cost model was then used to determine the number of AM facilities to be initiated and volume of product flow between manufacturing facilities and hospitals. Note that such a model is NP-hard and very expensive to solve. We develop a tailored SAA algorithm to efficiently obtain solutions. The resulting model and algorithm are applied to a real-world case study that focuses on investigating using AM for the on-demand production of biomedical implants for hospitals in the state of Mississippi.

1. This study mainly focused on the use of biomedical implants in the implants and hospitals that can perform similar procedures in the neighboring states. However, the proposed mathematical decision model can be applied to a larger supply chain network, such as the southeast region or the entire country of US, and account for other types of products, as long as the corresponding demand and supply data are collected. The solutions of the larger scale cost model (i.e., the locations of AM facilities) may still be obtained using the Sample Average Approximation algorithm by virtue of its scaling property. The model and algorithm proposed in this paper may be used as an initial analysis tool for decision makers to understand the supply chain cost parameters involved in the adoption of AM technologies for the purpose of infrastructure designing and planning. Once AM is identified to be feasible for production, a business case study may be followed up for a more thorough investigation.

2. Our analysis indeed recommended an AM facility with high capacity within the state of Mississippi when the demand is high. In other words, this facility can house multiple AM machines to satisfy the demands. Note that, in this study, we focus on identifying possible opportunities of establishing AM facilities in the state of Mississippi only. The transportation costs within the state may not be high. As a result, our analysis indicates that such a centralized AM supply chain layout may be more beneficial than having multiple AM facilities over the state of Mississippi, which will require much higher overhead costs. However, for a larger supply chain network (e.g., national supply chain network), it may be more profitable to establish multiple AM facilities to reduce the costs of transportation overall the country.

3. Our study suggested a harmonious implementation of AM and TM production, given the current state of AM and TM technologies. Demands of biomedical implants may be filled using both AM and TM facilities depending on the required product lead time, locations of patients, capacity of the AM facilities, and other factors. This scenario may be subject to changes when the cost parameters vary.

4. We have identified the conditions and cost parameters that have significant impact on the economic feasibility of AM. A key cost parameter is the ratio between unit production costs of AM and TM (ATR), including material, labor, energy consumption, pre- and post-processing costs, etc. When ATR < 3.5, hospitals would benefit from the use of AM technologies to fabricate biomedical implants, instead of ordering products from TM suppliers out of the region. Even though it may be more beneficial to use TM suppliers when ATR > 3.5, several cost parameters may still change the economic feasibility. For instance, our studies indicate that when the machine cost is reduced by 60%, the AM may be feasible even when ATR > 3.5. Cheaper AM machines may be possible considering the decreasing trend in the price of AM machines during the past decade.

5. Another key parameter is the urgency of the product. When a biomedical implant is needed in a short time window (e.g., in a life-or-death situation), TM suppliers may not have the parts with specific features (e.g., dimensions, shapes, etc.) in stock, and may require an additional lengthy customization process. In this case, AM may be a viable option because of the short response time and the capability of mass customization, irrespective of the high cost.

6. An advantageous feature of AM production is the capability of producing parts of complex geometries, which either may not be possible to fabricate using TM or requires multiple TM processing steps. Our model does not explicitly characterize the complexity of parts to be fabricated. However, the effect of part complexity is inexplicitly captured by the product lead time. Note that the production time needed by AM is generally insensitive to the complexity and shapes of parts by virtue of its layer-by-layer nature of fabrication. On the other hand, it may require a sequence of processes to fabricate a complex part using TM, if not impossible, and thus leads to much longer production time. Our study shows that the difference between the product lead times of AM and TM production could be a crucial parameter that affects the economic feasibility of AM production because AM has shorter lead time for complex parts even when post-treatment times are included.

7. Future work is needed to study the AM deployment approaches that can ensure that the full economic benefits of AM are realized. Especially, when the network of biomedical implants supply involves an area larger than the state of Mississippi such as the southeastern region of the country or the entire country of USA, such a study will guide decision makers on how centralized or distributed such a deployment should be. Moreover, future work may be needed to account for the cost analysis of assemblies. AM allows for the production of multiple parts simultaneously in the same build, making it possible to produce an entire product. TM often includes production of parts at multiple locations, where an inventory of each part might be stored. The parts are shipped to a facility where they are assembled into a product. AM has the potential to replace some of these steps for some products, as this process might allow for the production of the entire assembly. This would reduce the need to maintain large inventories for each part of one product. It also reduces the transportation of parts produced at varying locations and reduces the need for just-in-time delivery.

CHAPTER III

DISTRIBUTED OR CENTRALIZED? HYBRID SUPPLY CHAIN CONFIGURATION OF ADDITIVELY MANUFACTURED BIOMEDICAL IMPLANTS FOR SOUTHEASTERN US STATES

3.1 Introduction

The affordability of medical care service is essential to the coverage and performance of healthcare systems. According a recent Commonwealth Fund ranking, Southern states in US (e.g., Mississippi, Louisiana, Oklahoma, and Arkansas) have lowest coverage and service quality in the nation [71]. A major issue is the high costs associated with medical care. **There is an urgent need to provide affordable healthcare service while maintaining or even improving the service quality.** The technology of Additive Manufacturing provides a potential solution in terms of bringing down the costs of biomedical implants while ensuring implant quality based on customized needs. The use of additive manufacturing (AM) in the fabrication of medical devices has been gaining popularity in the medical technology industry. In 2012, about 16.4% of the total system-related revenue for the AM market was realized from medical applications [160]. (1) First, AM, unlike conventional manufacturing, provides a high level of customization which makes the technology very suitable for custom-fitting products to individual patients and enhances an economically efficient delivery of high-quality personalized healthcare products. Customized biomedical implants can possess complex features which are difficult to machine using conventional, subtractive methods. Singare et al. [142] has shown the superior functionality as well as the aesthetical appeal of AM biomedical implants compared to conventional manufactured biomedical products. (2) Second, the medical technology industry is well-funded and as such may provide for resources to invest in new AM technology initiatives. In 2012, the industry's estimated revenue, expected annual growth and 15-year total shareholder return (1998–2012) was about USD121.6 billion, 5.4 %, and 7.8%, respectively [49]. The 15-year total shareholder return statistic surpasses Standard & Poor 500's average of 5.2%. (3) Last but not least, there is a tremendous market of healthcare providers and consumers distributed across a broad geographic and population base, who need such medical devices as surgical implants, hearing aids, dental crowns, and more. Custom implants produced using AM technology have been used for a variety of applications including skull ([142], [158], [37], [141]), knee joint ([59]), elbow ([151]), and hip joint ([116]). These devices possess a combination of relatively high value and small physical volume which is suitable for the applications of AM.

A major driving factor contributing to the possible cost reduction of additively manufactured biomedical implants is the promise **of reduced logistic costs associated with compressed supply chains**. There is a consensus that the greatest disruption that could emerge from widespread adoption AM technology would be restructured supply chains ([120], [33]). The supply chain would be more local as the product will be manufactured closer to the end customer. In particular, deploying AM facilities at locations close to operational hospitals generally leads to faster response, and reduced delivery costs [59]. However, the investment cost of establishing each facility has to be taken into consideration. The impact of AM technology on the supply chain management is still unknown. Businesses need to understand such impacts to make supply chain decisions pertaining to the enhancement of their expansion and maintenance of their marketplace competitiveness.

One key decision that an AM provider will make is the capacity of AM to be deployed and the configuration of deployment. In other words**, how close should the AM be located to the customers**? One approach that has been suggested in literature is centralized deployment ([60], [96]). Using a centralized approach, the AM facility is centrally located to serve all the hospitals. The products are manufactured on-demand at a central location and then delivered to the hospital that made the demand. A second approach suggested is the distributed AM. In this case, an AM facility is located locally to serve a hospital or group of hospitals in the same area. In the distributed AM approach, the digital models of the medical devices can be distributed from a central database via information network to the local AM facilities where the biomedical implants are manufactured. This approach is recommended when the response time is critical and the risk of inventory stock out is high [60]. It is also suitable for isolated systems such as the space station in orbit or military equipment in battlefields where AM can be used to produce spare parts on site and on demand. **These approaches represent two extremes of AM deployment spectrum. In reality, a more hybrid approach may be more suitable. However, there is no study, to the best of our knowledge, providing a quantitative method for analyzing the logistic costs associated with AM supply chain with the goal of determining its optimum deployment configuration.** In this paper, we develop a continuous approximation cost model and implement an optimization algorithm that helps to determine the best AM deployment configuration to minimize the total supply chain network cost for biomedical implants. A case study using hospital and biomedical implant demand data from Southern US states has been investigated to prove the concept of the proposed method and algorithm.

The rest of this paper is organized as follows: Section 3.2 reviews the existing literature pertaining to the biomedical applications AM and cost analysis. The integrated facility location and inventory policy model for additively manufactured bio-medical implants Section 3.3 presents a mathematical optimization model based on continuous approximation that quantifies the supply chain network cost of additively manufactured bio-medical implants; Section 3.4 implements a two-phase approximation approach and a two-stage solution approach that solves the model presented in Section 3.3 to locate AM facilities and obtain their area of influence and raw material ordering amount. Section 3.5 applies the optimization model to the real-world case study of biomedical implants in the hospitals in the southeastern region of USA; and Section 6 provides concluding remarks and possible future work.

3.2 Literature review

We provide a literature review on the application of AM in the medical industry, as well as approaches to supply chain cost analysis.

3.2.1 Biomedical applications of AM

There are many examples of AM use in medical applications. 'Kablooe Design', an engineering firm that specializes in the creation of sophisticated medical devices has used AM to create a less invasive device for the treatment of benign prostatic hyperplasia

(BHP) [146]. Siemens has switched to AM technology for the production of customized hearing aids at several of its factories. The technology has enabled the company to localize the manufacture and distribution of end products, shorten the production time of the customized devices by up to 80%, and significantly reduce labor cost [34]. Dental labs have used AM to produce customized dental crowns for patients. Using scanned data and dental software to design a CAD model of a patient's crown, technicians can produce up to 450 crowns and bridges per day compared with only 20 when using traditional methods. In the US military, the standard procedures for making surgical equipment available on the battlefield raise challenges in terms of time of delivery, quantity, cost and matching supply with demand. Consequently, it has identified the use of AM within its combat site surgical setting, and found that thousands of different surgical instrument designs, customized instruments and sterile surgical kits stored on digital media or remotely accessed via the Internet, could be printed and used in field surgical settings [74]. AM technology only requires electrical power, raw material and digital design file for military surgeons to be able to produce these devices in such a way that reduces the required inventory and bottlenecks surrounding supply levels on the battlefield. AM has also been used in customized visualization aids in preparation for surgical procedures on kidney, liver, bones and various body cavities [108]. Sols uses AM to produce custom insoles that help to reduce a patient's foot pain and improve posture. The patient's foot is scanned using a smartphone app and uploaded to the company's database from where it is transferred to an AM machine for production. The technology has helped to streamline the production process, replace the need for error prone human touch-points and create a unique opportunity for mass-customization [123].

3.2.2 Supply chain cost analysis - qualitative approaches

The literature on AM supply chain can be divided into two broad categories: qualitative approaches to identify the factoring impacting of the supply chain of AM products and quantitative approaches to model these impacts

Most works in the literature have focused on the qualitative approaches. For example, Fisher [51] developed a framework for supply chain strategy by categorizing products into two: functional products and innovative products. According to the author, while the supply chain design for functional products with relatively predictable demand should be mostly based on efficiency, that for innovative products like AM products which require shorter lead times, high level of variety, flexibility and customization should rely on responsiveness. According to Berman [21], AM favors on-demand and small production batches and achieves customization by layer manufacturing instead of modularization or postponement. By avoiding modularization as a means of attaining mass customization, AM is able to reduce the need for supply chain integration and the number of suppliers needed in the manufacturing process. Moreover, since there is no more need to produce separate parts for assembly, costs related to assembly and inspections are virtually eliminated. Cooke [33] suggested that contrary to traditional off-shoring practices inherent in conventional manufacturing, AM requires a more regional supply chain network which can fundamentally impact total cost through reduced emissions, pipeline inventory and safety stock. However, for expensive raw materials which are not locally available such as in the manufacture of bio-medical devices, procurement and inventory decisions need to be made to ensure that the full benefits of AM are realized. According to Reeves, AM will result in a shift from the production-distribution-retail model to a model where the retailer is substituted by the end customer [121]. This is increasingly possible with the modern information and communication technologies and web-based retail transactions. In such a model, rather than the major transportation cost emanating from shipping the finished goods to the retailer, it will arise from transporting raw materials to the AM sites since these sites could be strategically scattered near customers in order to significantly decrease lead time. Holmstrom et al. [60] proposed two different deployment methods to integrate AM technology in the aircraft spare parts supply chain. The first approach called centralized AM uses capacity to replace inventory holding. In this approach, AM machines are deployed in centralized distribution centres to produce slow moving spare parts on demand. The authors found that the advantage of using centralized AM comes from the aggregation of demand from various regional service locations which ensures that the investment in AM capacity is well utilized as the parts are produced in a centralized location. However, the disadvantage is that the produced parts have to be shipped to distant service stations thereby increasing both transportation cost and response time. The second approach is the distributed or decentralized approach, in which AM technology is deployed at each service location. While this approach leads to a substantial fixed investment cost in the AM machines as well as personnel cost, it results in the drastic reduction in inventory holding and transportation cost. Mellor, Hao, and Zhang [92] suggested decentralized AM as a direct digital manufacturing (DDM) implementation approach that could reduce transportation impact and support local community involvement in the supply chain. The authors based their analysis on a qualitative normative structural model that includes supply chain, operations, strategy and organization change. While the qualitative approaches have subjective views to analyzing the AM deployment configurations, they do not provide numerical basis, on which this important long term decision should be made.

3.2.3 Supply chain cost analysis - quantitative models

Among the very few studies that have taken a quantitative route in investigating the impact of AM on supply chain, Khajavi et al. [70] extended the work of Holmstrom et al. [60] where the authors evaluated the potential impact of AM improvements on the configuration of spare parts supply chains of military aircraft parts. They used scenario modeling method to analyze the impact of AM deployment configuration on supply chain cost. A total of four scenarios arising from two AM deployment alternatives and two time dimension are investigated. However, the scenario modeling proposed by the authors does not include inventory decisions such as the reorder quantity of AM raw materials or amount to keep in inventory. Similarly, Liu et al. [86] explored the potential of introducing AM technology into the aircraft spare parts supply chain, and quantitatively analyzed the impact on supply chain safety inventory, using a supply chain operation reference (SCOR) model. They found that centralized AM is suitable for spare parts with low average demand, longer manufacturing lead time and relatively high demand fluctuations while distributed AM is recommended for parts with high average demand and stable demand. Due to the on-demand capability of AM, the authors also found that distributed AM is more beneficial than centralized AM for parts with very short manufacturing lead time even if their demand is low and unpredictable. Chiu and Lin [31] used simulation based approach to study the benefits of integrating design for AM (DfAM) and design for supply chain (DfSC) in the production of personalized lampshades of a lamp manufacturing company. The authors found that AM improves supply chain performance in terms of both lead time and total cost. In particular, their simulation results in the case study show that lead time can be shortened by up to 35%, while the total cost can be reduced by 10%, 6% and 3% for low, middle and high demand fluctuation levels, respectively. However, the authors have neither integrated facility location in their study nor considered the investment cost of AM machines in their cost model. Moreover, they did not consider raw material inventory cost which could affect supply chain decisions in situations where the raw materials used in AM were expensive. More recently, Augustsson and Becevic [9] has studied the impact of AM on the spare parts supply chain cost and customers service level of the automotive industry. Using a case study of a heavy truck manufacturing company, this study finds that adopting AM can reduce the lead time by up to 50% and increase profitability from reduced transportation cost to 23.3%. The author used a simple linear cost model that includes machine cost, labor cost and material cost to analyze the impact of AM on customer service level and supply chain cost. Achillas et al. [1] utilized a multi-criteria decision aid (MCDA) and data envelopment analysis (DEA) to study the inclusion of AM into the production portfolio of an electronics manufacturer. The authors consider production cost, lead time and quality from various manufacturing alternatives, and find that AM provides an efficient manufacturing solution for small production volumes of plastic housing units, with high demand fluctuations. Emelogu et al [45] developed a mathematical model that helps to quantitatively analyze the economic feasibility of integrating AM and TM in the supply chain network of biomedical implants. In this paper, we assume that only AM is utilized in the fabrication of the biomedical implants and extend their work in two directions. We improved the optimization model to include inventory decisions which we realize are necessary in the case of biomedical implants with expensive raw materials. The authors applied their model to a case study of hospitals in Mississippi State. However, in this paper, we propose a solution approach that solves the problem for hospitals in the southeastern region of United States relatively faster.

3.2.4 Scalability issue of supply chain models

All the AM supply chain literature dedicated to quantitative methods uses linear models to formulate the problem. However, these models do not provide realistic solutions as the amount of data that can be added to the model is often limited. **Increased amount of data in discrete models often leads to model inaccuracy and increased computational complexity**. Continuous approximation (CA) approach can be used to overcome this problem. CA requires less data to generate near approximate solution. This approach defines decision variables in terms of continuous functions and in turn reduces the complexity of the model. Newell [104] demonstrated the idea of applying continuum techniques to finite-dimensional operational research problems. Blumenfeld and Beckmann [24] developed an analytical framework for estimating the cost of distributing freight from one origin to many destinations. This analysis used a continuous space modeling approach, which requires only the spatial density of destinations and the average and variance of demand. This approach allowed distribution costs to be determined analytically in terms of a few easily measured parameters. Langevin et al [81] presented an overview of continuous approximation models used for freight distribution problems. The authors provided taxonomy of six classes to differentiate the problem and a brief review of each paper is provided. Geoffrion [55] studied a continuous model for warehouse location in which warehouse serves demand that is distributed uniformly over a plane. Erlenkotter [47] extended the work of Geoffrion [55] and Newell [104] where a general optimal market area (GOMA) was used to determine the optimal area served by a single production unit while demand was assumed to be distributed uniformly. A number of refinements of the GOMA model were discussed by Rutten et al. [132] to determine the optimal number of depots serving a set of uniformly distributed customers in a particular area. An analytic method was developed by Burns et al. [27] that used the spatial density of customers to minimize the transportation and inventory cost of freight. This study analyzed and compared two distribution strategies: direct shipping and peddling. Dasci and Verter [39] presented a framework that was based on the use of continuous functions to represent spatial distributions of cost and customer demand. However, their approach did not consider inventory works. This work was a generalization of the work done by Geoffrion [55] and Erlenkotter [47] as well as an extension of the CA model for the facility design problem proposed by Verter and Dincer [155]. A CA framework developed by Murat et al. [101] presented a methodology where the market demand was modeled as a continuous density function and the resulting formulation was solved by means of calculus. This methodology prioritized the allocation decisions rather than location decisions.

No **study, to the best of the authors' knowledge, has carried out a quantitative investigation on AM deployment alternatives in the medical industry or considered an integrated approach where AM facility location and inventory allocation decisions are included in the problem**. Moreover, this work is the first to apply a continuous approximation model to an AM supply chain problem. The centralized and distributed approaches identified in literature belong to two opposite extremes of the deployment spectrum, either of which may not be optimal. Our continuous approximation deployment model presents a hybrid solution that is able to determine the optimal number of AM facilities to establish, the hospitals each facility serves and the amount of raw materials to order for on-demand manufacture of medical implants so that the total network cost including investment, production, inventory and transportation costs is minimized while maintaining a high customer service level.

3.3 Model formulation

In this section, we develop a mathematical model that solves the integrated facility location and inventory policy model for additively manufactured bio-medical implants. The logistics network that is represented by the mathematical model is a three level distribution network where at level 2, **central raw material warehouses (CRW)** that store the AM raw materials are established. At level 1 are the AM facilities where the fabrication of AM products takes place, and at level zero end customers which in our case are hospitals serving patients are situated. Note that an AM facility at level 1 could be situated in a hospital or very close to a hospital, but from this facility the AM bio-medical implants are supplied to other hospitals.

Let us consider a continuous two dimensional space S$\subseteq R^2$ where an AM facility can be built at any location $x \in S$ with a fixed operating cost, F_s. There are predefined location of CRW's and hospitals in $x \in S$. The decision variables are the number of AM facilities and ordering quantity for each CRW and AM facilities. But before developing cost functions for this integrated facility location and inventory policy model, it is important to make a number of assumptions about the overall network structure, level of customer demand, and inventory policies on the overall network. This integrated model is a complex model and these assumptions simplify the model and help solve this model comparatively easily. The assumptions made in this model are influenced by Ganeshan [53], Teo and Shu [147], Dasci and Verter [39], and Tsao et al. [152]. The assumptions are stated as follows:

Assumption 1: Each AM facility can serve multiple hospitals but the opposite is not allowed. This type of network is termed as 'arborescence network'.

Assumption 2: Demand at each AM facility is a Poisson process as it is generated by the demand originating from hospitals in its influential area.

Assumption 3: Demand per unit time for hospitals in cluster C_i is independent and identically distributed Poisson process with rate θ_i.

Assumption 4: Each unit of product is analyzed separately and independently. Demand for single unit of product is considered in this study.

Assumption 5: Lateral shipment of products among distribution centers and customer demand points is not allowed in the model. All the shipments between distribution centers to the customer demand points are via direct shipment.

Assumption 6: The location of CRW's and hospitals is known beforehand.

Assumption 7: Euclidean distance measure is used to calculate the distance between an AM facility and hospitals.

Assumption 8: The influence area of each AM facility is assumed to be circular. Moreover, each AM facility is located at the center of the influence area.

Assumption 9: Capacity limitation of facilities is not considered at any of the network levels.

Assumption 10: CRW's and AM facilities operate under Type-1 service policy.

Assumption 11: Continuous inventory review policy is maintained for both CRW and AM facilities.

Assumption 12: Pipeline inventory cost is not considered.

Assumption 13: There is no reorder cost at the hospitals. The demand at the hospitals gets passed over to the AM facilities on a per item basis.

We modeled all the cost functions of the logistics network based on the above assumptions. Table 3.1 shows the notations and symbols used in the model. In continuous space S, let $\gamma_i(x)$ denote the discrete hospital location in cluster C_i which is expressed as a spatial density slow varying function and $A_{v_i}(x)$ denote the influential area associated with each AM facility in cluster C_i. The customer demand at each point $x \in S$ can now be expressed as a product of hospital density and demand at hospitals which can be expressed as $\gamma_i(x)\theta_i(x), x \in S$. So, the expected demand per unit time experienced by each AM facility v in cluster C_i can be expressed as $\gamma_i(x)\theta_i(x)A_{v_i}(x), x \in S$. Simultaneously, the total number of AM facilities can be estimated by $N_{v_i}(x) = \frac{S}{A_{v_i}(x)}$.

A total of six cost components have been considered while modeling the logistics network i.e. total AM facility opening cost, inbound transportation cost for AM facility/outbound transportation cost for CRW's, outbound transportation cost for AM facility, average inventory cost for AM facilities, production cost at AM facilities, and average inventory cost for CRW's. All the cost functions in this section are modeled using continuous approximation technique. This essentially means that the entire logistics network can be expressed in terms of smooth continuous functions. We summarize the notations used in the cost function in Table 3.1. Section 3.3.1 details the steps for calculating the cost components of the network and Section 3.3.2 presents the final model.

Table 3.1 Acronyms and mathematical notations in the optimization model

Parameters	**Explanation**
θ_i	Demand of product per unit time for hospitals in cluster C_i
C_i	Cluster i
F_r	Fixed opening cost for each AM facility
γ_i	Discrete hospital locations in cluster i
C_f	Fixed transportation cost per inbound shipment
C_p	Variable transportation cost per item for each inbound shipment
τ	Planning horizon
C_d	Delivery cost per mile per item
K_v	Distance metric and shape constant for the service region
R_v	Reorder cost incurred by each AM facility
R_n	Reorder cost incurred by the CRW
h_v	AM facility inventory holding cost per item over τ
h_n	CRW inventory holding cost per item over τ
α_{v_i}	Service level at each AM facility
μ_v	Mean of lead time at each AM facility
σ_v^2	Variance of lead time at each AM facility
p	Production cost per unit product excluding labor cost
l	Annual personnel salary
α_n	Service level at CRW
μ_n	Mean of lead time at CRW
σ_n^2	Variance of lead time at a CRW
Variables	
A_{v_i}	Size of influence area associated with an AM facility in cluster i
Q_{v_i}	Ordering quantity for AM facility, v, in cluster i
Q_n	Ordering quantity for CRW

3.3.1 Total network cost function

We present, in more details, the six cost components that make up the total cost function used to model the biomedical implant AM supply chain.

3.3.1.1 Total AM facility cost

A fixed opening cost F_v is incurred for opening and operating each AM facility, *v*. To calculate the total AM facility cost, opening and operating cost of each AM facility, $v \in V$, has to be multiplied by total number of AM facilities, $N_{v_i}(x)$, and is given by

$TAC(x) = F_v N_{v_i}(x)$

3.3.1.2 Inbound transportation cost for AM facility

The inbound transportation cost for AM facility and outbound transportation cost for CRW is the same. Inbound transportation cost component can be divided up into two parts i.e. fixed cost and variable cost. The fixed cost can be broken down into costs like managing the trucks, drivers etc. The variable cost is the cost per item. Let C_f be the fixed cost per inbound shipment, C_p be the variable cost per item for each inbound shipment, and $Q_{v_i}(x)$ be the ordering quantity for each AM facility, *v*, in cluster C_i. The transportation cost of a single inbound shipment to a single AM facility can be expressed as

$$SC(x) = C_f + C_p Q_{v_i}(x)$$

Taking τ as the length of the planning horizon, the total inbound transportation cost can now be calculated as

$TIAC(x) = SC(x) \frac{\tau \gamma_i(x) \theta_i(x) A_{v_i}(x)}{Q_{v_i}(x)} N_{v_i}(x)$, where $\frac{\tau \gamma_i(x) \theta_i(x) A_{v_i}(x)}{Q_{v_i}(x)}$ is viewed as the expected number of inbound shipment to a single AM facility, *v*, in cluster C_i during τ.

3.3.1.3 Outbound transportation cost for AM facility

Let C_d be the delivery cost per mile per item and K_v be a constant that depends on the distance metric and the shape of the service region in S. Hence, the total outbound transportation cost for AM facility can be expressed as

$$TOAC(x) = K_v C_d K_v \sqrt{A_{v_i(x)}} \tau \gamma_i(x) \theta_i(x) A_{v_i}(x) N_{v_i}(x)$$

$$= C_d K_v \sqrt{A_{v_i(x)}} \tau \gamma_i(\text{x})\ \theta_i(x) S$$

Note that, $K_v\sqrt{A_{v_i(x)}}$ is the average distance from the AM facility v to a hospital in the influence area, provided that the AM facility v is at the center of the influence area (see [39]).

3.3.1.4 Average inventory cost for AM facility

Each inventory cost component consists of two costs, i.e. reorder cost and holding cost. Let, R_v denote the reorder cost incurred by each AM facility while ordering each batch of raw materials that can be used to manufacture $Q_{v_i}(x)$ units. Then, the total reorder cost, for all the AM facilities over τ can be defined as

$$TRAC_v(x) = N_{v_i}(x) R_v(x) \left(\frac{\tau \gamma_i(x)\ \theta_i(x) A_{v_i}(x)}{Q_{v_i}(x)}\right)$$

To calculate the inventory holding cost, let μ_v and σ_v^2 be the mean and variance of lead time respectively and α_v be the service level at each AM facility. Note that, inventory holding cost itself consists of two unique costs, i.e. cycle inventory cost and safety stock cost. Taking h_v as the single AM facility inventory holding cost per item over τ, cycle inventory cost can be calculated as

$$CI(x) = h_v \frac{Q_{v_i}(x)}{2}$$

Similarly, safety stock cost can be calculated by

$SS(x) = h_v z_{\alpha_v}\sqrt{Var[D_{r_v,LT}]}$

where $Var[D_{r_v,LT}]$ is the variance of demand over the lead time. Now, $Var[D_{r_v,LT}]$ can also be reformulated as

$Var\left[D_{r_v,LT}\right] = \mu_v\gamma_i(\mathrm{x})\theta_i(x)A_{v_i}(x) + \sigma_v^2(\gamma_i(\mathrm{x})\theta_i(x)A_{v_i}(x))^2$

Then, total average inventory cost for AM facilities' can be illustrated by

$\mathrm{TI}_v(x)$= $\mathrm{TRAC}_v(x)$+ $\mathrm{CI}_v(x)N_{v_i}(\mathrm{x})$ + $\mathrm{SS}_v(x)\ N_{v_i}(\mathrm{x})$

3.3.1.5 Production cost at AM facilities

One advantage of AM is that it facilitates on-demand production of personalized medical implants at faster rate than traditional manufacturing. However, due to post processing operations required in AM, especially in the case of delicate bio-medical implants, significant lead time is required between when a hospital makes an order an when it receives it. The raw materials for bio-medical applications are usually chosen with care and are generally expensive. Moreover, AM machines are more sophisticated than their TM counterparts and as such require a more advanced skill set for operating them. Thus, the personnel/labor cost in AM is also significant in the operating cost of an AM facility. We include these factors in calculating the total production cost at the facilities. Let *p* be the production cost of each unit of product, *cap* be the capacity of each machine, and l be the labor cost per machine per year. Then the production cost for each AM facility can be given by

$$\mathrm{TPC}_v(x) = \tau\gamma_i(x)\theta_i(x)A_{v_i}(x) * p * N_{v_i}(x) + \frac{\tau\gamma_i(\mathrm{x})\theta_i(x)A_{v_i}(x)}{cap} * l * N_{v_i}(x).$$

3.3.1.6 Average inventory cost for CRW

The inbound cost for the CRW's is not considered in the model; instead this cost in incorporated into the reorder cost. Let, R_n be the reorder cost incurred by each CRW while ordering each batch of product with $Q_n(x)$ unit equivalent of raw materials on it. Then the reorder cost for each CRW over τ can be expressed as

$TR_n(x) = R_n(x)(\frac{\tau\gamma(x)\theta(x)S}{Q_n(x)})$, where $\tau\gamma(x)\theta(x)S$ is the total expected demand at the CRW during τ. Now, to calculate the inventory holding cost at each CRW, let h_n be the inventory holding cost per item during τ, μ_n and σ_n^2 be the mean and variance of lead time respectively, and α_n be the service level at each CRW. Hence, total inventory holding cost for CRW can be expressed as

$TH_n = h_n(\frac{Q_{n(x)}}{2} + Z_{\sigma_n}\sqrt{var[D_{n,LT}]}\,) + TR_n$ where $var[D_{n,LT}] = \frac{\sum_S \mu_n \gamma_i(x)\,\theta_i(x) A_{v_i}(x)}{Q_{v_i}(x)^2}$).

3.3.2 Final CA network cost model

The cost expression derived in Section 3.2.1 are in terms of each point *x* in the service region S$\subseteq R^2$. Each expression of the cost functions captures fine details of the logistics network model. Based on the above cost functions we can now define our logistics network as

Minimize

$$\int_0^S \big(TNC(x)\big)dx = \int_0^S (TAC(x) + TIAC(x) + TOAC(x) + TI_v(x) + TPC_v(x) + TH_n(x)) \qquad (3.1)$$

subject to

$$N_{V_i}(x).A_{V_i}(x) = S \qquad (3.2)$$

$$Q_n(x) \geq 0 \tag{3.3}$$

$$Q_{v_i}(x) \geq 0 \tag{3.4}$$

$$A_{v_i}(x) \geq 0 \tag{3.5}$$

$$Q_n(x), Q_{v_i}(x) \in Z^+ \tag{3.6}$$

where $Q_n(x), Q_{v_i}(x)$ and $A_{v_i}(x)$ are the decision variables. Constraints (3.2) are the area coverage constraints which ensure that the entire service region is covered by the sum of the distribution centers influence area. Constraints (3.3), Constraints (3.4), and Constraints (3.5) are non-negativity constraints for decision variables $Q_n(x)$, $Q_{v_i}(x)$ and $A_{v_i}(x)$. Constraints (3.6) are integer constraints.

To get any feasible solution of the optimization problem, all the decision variables $Q_n(x), Q_{v_i}(x)$ and $A_{v_i}(x)$ should be strictly greater than zero. So, adding Constraints (3.3), Constraints (3.4), and Constraints (3.5) do not change the nature of the problem and solution. If the value of the decision variables is zero, the objective function value explodes and feasible solution cannot be obtained. So, adding these constraints in the model is justifiable.

3.4 Solution methodology

We have investigated the southeastern states of USA, shown in Figure 3.1, as potential test bed for the study. The logistics network that covers the hospitals and clinics in the region with distribution shown in Figure 3.2 contains discrete data which cannot be approximated and hence becomes extremely challenging to solve. To overcome this challenge, a two phase approximation approach developed in Tsao et al. [152] is used. This approximation approach is basically an extension of the work done by Daganzo [38] where he demonstrated different ways to model complex logistics network using continuous approximation approach.

With a close observation of the logistics network shown in Figure 3.2, it becomes clear that the hospitals location is not uniformly distributed, which necessarily means that hospital density does not follow a homogenous Poisson process. As a result, customer demand at each point cannot be declared as $\gamma_i(\mathrm{x})\ \theta_i(x)$, $\mathrm{x} \in S$ that is slow varying. However, it can be stated that within a small sub-region, this function can be considered as slow varying. In Phase 1 of the two phase approximation approach, the whole distribution network is divided into smaller sub region such that the hospital density within that sub-region satisfies the slow varying property of input parameters of the model. Next, in Phase 2, the mathematical model is implemented over these sub-regions to get the optimal value of Q_n, Q_{v_i} and A_{v_i}.

3.4.1 CRW service region and grid cover-couple approach

We have investigated the southeastern states of USA, shown in Figure 3.1, as potential test bed for the study. Let us suppose that there is only one CRW in the service region that we have investigated. The raw materials for manufacturing medical implants are generally not available locally. In some cases, they have to be sourced from overseas which makes storing them in one location or few regional central locations from where they could be delivered to the AM facilities a viable option. The next job is to divide this region in such a way that the slow varying property of the input functions hold. The grid cover approach can be an effective way to achieve that. To do that, a mesh of equal sized squares is created to cover the service region. The next step is to choose the feasible size of the grid. A trial and error method is used to choose the size of the grid where the smallest level of detail is captured at the county level. Note that the county with the highest variability in demand is chosen as the size of the grid. A density can be assigned to each and every square grid as the hospital density in each county is known beforehand.

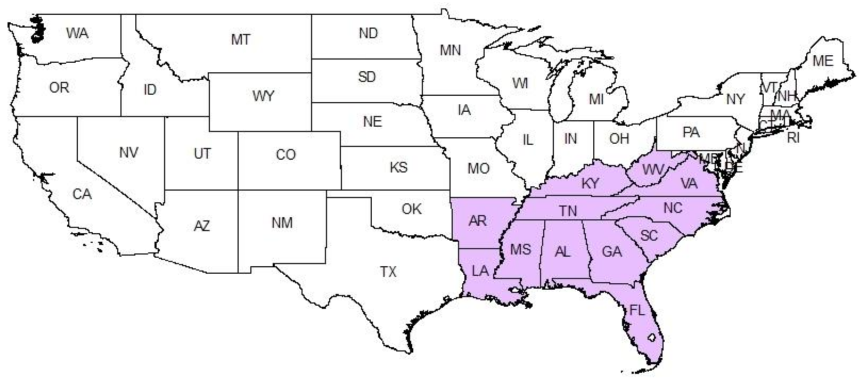


Figure 3.1 The AM supply chain covers the southeastern region of USA

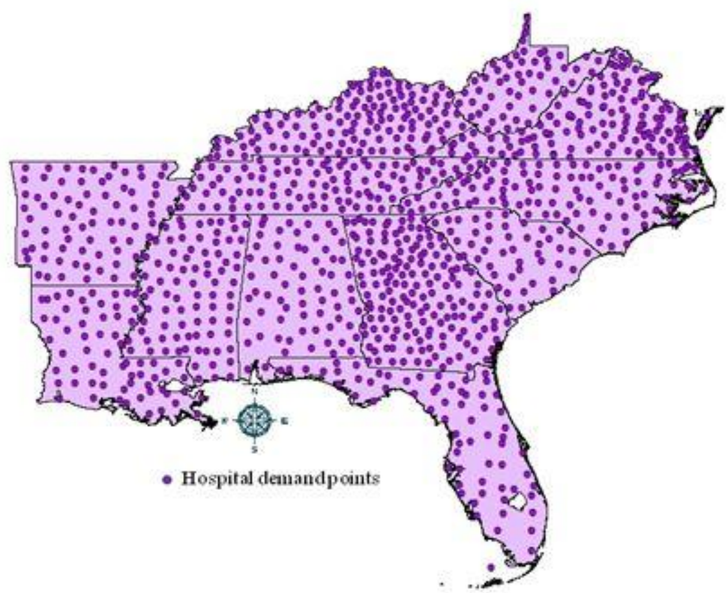


Figure 3.2 Distribution of hospitals and clinics by counties in the southeastern states

The next step in the grid cover-couple approach is to create clusters within the created square grids. Grids with similar densities can be clustered together to define areas where the hospital density function is slow varying. To do so, a tolerance limit (ϵ) is specified which measures the level of similarity among grids. More specifically, if two grids density is at most ϵ apart, these two grids can be labelled as similar and clustered together. However, the choice of ϵ solely depends on the hospital density pattern at the logistics network under study. Hospital density considered in this study is fairly similar to one another in most of the counties; hence ϵ is taken to be very small. Using this ϵ value, the entire region is divided into smaller clusters. Within each of these clusters, the hospital density is slow varying. Figure 3.3 illustrates this procedure.

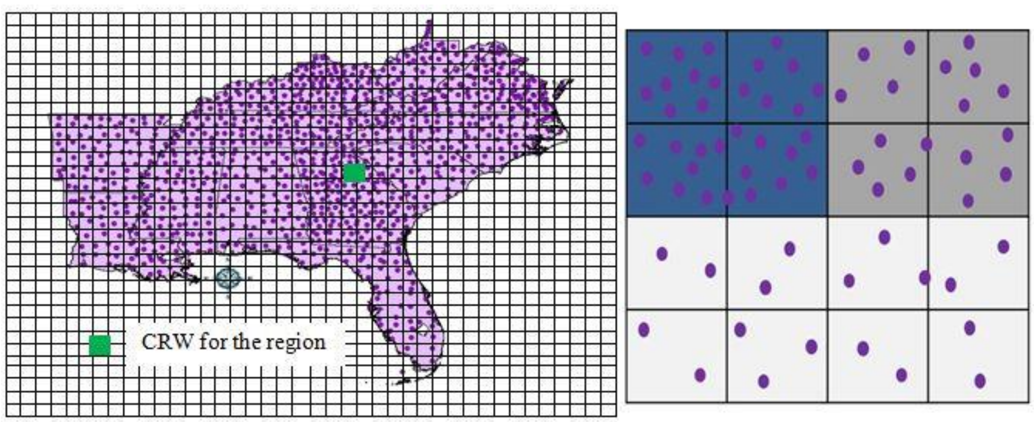


Figure 3.3(a): Grid cover for the southeastern region with one CRW

Figure 3.3(b): Coupling grids into clusters

Figure 3.3 Grid cover and coupling

3.4.2 AM facility influence area using continuous approximation approach

In this phase, the optimization model developed in Section 3.2 is used for modeling the total logistics cost in each cluster. Continuous approximation approach is used to solve this optimization model and obtain the optimal size of the circular influence area (A_{v_i}) for AM facility, and ordering quantity for AM facility (Q_{v_i}) and CRW (Q_n) respectively. By determining the size of the influence area for a particular cluster, one can easily determine the total number of AM facilities needed to serve the entire cluster. A sample influence area for an AM facility is shown in Figure 3.4.

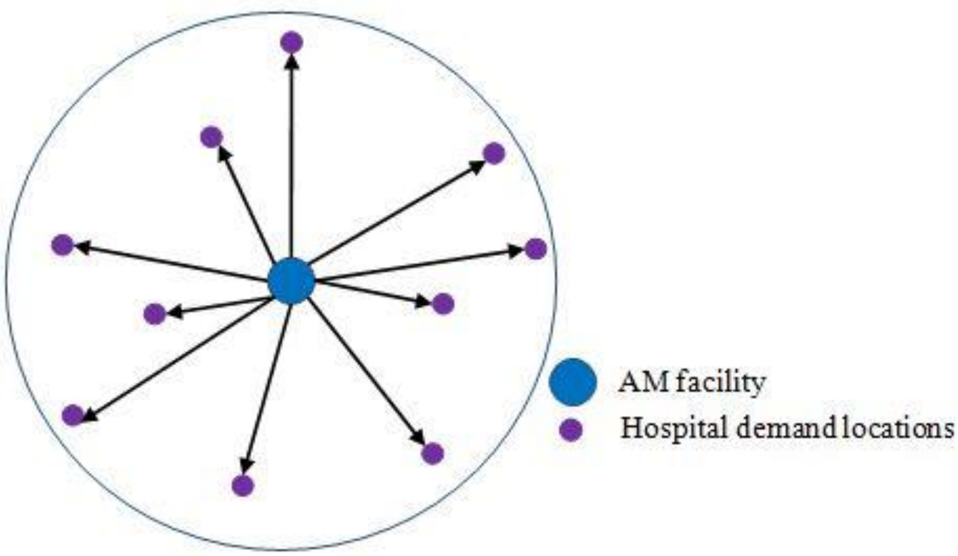


Figure 3.4 Influence area for an AM facility

Note that, to develop the continuous approximation model, the dependence of all continuous functions on parameter x can be ignored as each cluster within a given CRW has slow varying property. For the remaining portion of this study, we use Q_{v_i}, A_{v_i}, Q_n, γ_i, and θ_i instead of $Q_{v_i}(x)$, $A_{v_i}(x)$, $Q_n(x)$, $\gamma_i(x)$, and $\theta_i(x)$. Taking $C_1, C_2, \dots, C_N$ as the number of clusters within the service region under the CRW, the logistics network model formulation shown in Equation (3.1) now becomes

$$TNC(A_{v_i}, Q_{v_i}, Q_n) = \sum_{i=1}^{N} F_v \frac{C_i}{A_{v_i}} + (C_f + C_p Q_{v_i}) \left(\frac{\tau\gamma_i\,\theta_i}{Q_{v_i}}\right) C_i + \sum_{i=1}^{N} C_d (K_v \sqrt{A_{v_i}} \tau\gamma_i\,\theta_i C_i)$$

$$+ \sum_{i=1}^{N} C_i\, R_v\, \left(\frac{\tau\gamma_i\theta_i}{Q_{v_i}}\right) + \sum_{i=1}^{N} h_v \frac{Q_{v_i} C_i}{2A_{v_i}} + \sum_{i=1}^{N} h_v \frac{C_i Z_{\alpha_{v_i}}}{A_{v_i}} \sqrt{\mu_v\gamma_i\,\theta_i A_{v_i} + \sigma_v^2 (\gamma_i\theta_i A_{v_i})^2} \; +$$

$$\tau\gamma_i\theta_i \mathrm{p} C_i + \frac{\tau\gamma_i\,\theta_i}{cap} l C_i + R_n \left(\frac{\tau\gamma_i\,\theta_i C_i}{Q_n}\right) + h_n \left(\frac{Q_{n(x)}}{2} + Z_{\alpha_n} \sqrt{\sum_{i=1}^{N} \frac{\mu_n\tau\gamma_i\,\theta_i C_i}{{Q_{v_i}}^2}}\right) \quad (3.7)$$

subject to

$$Q_n(x) \geq 0 \quad (3.8)$$

$$Q_{v_i}(x) \geq 0 \quad (3.9)$$

$$A_{v_i}(x) \geq 0 \quad (3.10)$$

$$Q_n(x), Q_{v_i}(x) \in Z^+ \quad (3.11)$$

3.4.3 Solution approach

There are three decision variables in the model; Q_n, Q_{v_i} and A_{v_i}. To solve the problem, first we solve the problem for Q_n. Let us assume that, Q_{v_i} and A_{v_i} is known. Hence, we have

$$\frac{d^2 TNC(Q_n \backslash A_{v_i}, Q_{v_i})}{dQ_n^2} = \frac{2R_n \sum_{i=1}^{N} \tau\gamma_i\,\theta_i C_i}{Q_n^3} > 0$$

As the hessian of the function of *TNC* is greater than zero, we can say that the function is strictly convex with respect to Q_n and is positive definite. This means than we can calculate the optimal value of Q_n by equating the gradient of *TNC* function to zero. This means that

$$Q_n^* = \sqrt{\frac{2R_n \sum_{i=1}^{N} \tau\gamma_i\,\theta_i C_i}{h_n}} \quad (3.12)$$

Substituting the value of Q_n^* in Equation (3.7) we get

$$TNC(A_{v_i}, Q_{v_i}, Q_n) = \sum_{i=1}^{N} F_v \frac{C_i}{A_{v_i}} + (C_f + C_p Q_{v_i}) \left(\frac{\tau\gamma_i\,\theta_i}{Q_{v_i}}\right) C_i + \sum_{i=1}^{N} C_d (K_v \sqrt{A_{v_i}} \tau\gamma_i\,\theta_i C_i)$$

$$+ \sum_{i=1}^{N} C_i R_v \left(\frac{\tau\gamma_i\theta_i}{Q_{v_i}}\right) + \sum_{i=1}^{N} h_v \frac{Q_{v_i} C_i}{2A_{v_i}} + \sum_{i=1}^{N} h_v \frac{C_i Z_{\alpha v_i}}{A_{v_i}} \sqrt{\mu_v \gamma_i\,\theta_i A_{v_i} + \sigma_v^2 (\gamma_i \theta_i A_{v_i})^2}$$

$$+ \tau\gamma_i\theta_i \mathrm{p} C_i + \frac{\tau\gamma_i\,\theta_i}{cap} l C_i + \sqrt{2h_n R_n \sum_{i=1}^{N} \tau\gamma_i\,\theta_i C_i} + h_n \left(Z_{\alpha_n} \sqrt{\sum_{i=1}^{N} \frac{\mu_n \gamma_i\,\theta_i C_i}{{Q_{v_i}}^2}}\right) \tag{3.13}$$

Now, this model becomes a non-linear function with two unknown variables Q_{v_i} and A_{v_i}. Note that in the last term of Equation (3.13), there is ${Q_{v_i}}^2$ in the denominator which makes the evaluation of convexity very challenging. To overcome this exacting nature of the problem, a two stage solution approach developed in Tsao et al. [152] is proposed. The detail of the two stage solution approach is provided below:

Stage 1: In stage 1 of the solution approach, we first eliminate the ${Q_{v_i}}^2$ term from the last term of Equation (3.13). This makes the problem linear and makes it easy to evaluate the convexity property. So, Equation (3.13) can be rewritten as

$$TNC^E(A_{v_i}, Q_{v_i}) = \sum_{i=1}^{N} F_v \frac{C_i}{A_{v_i}} + (C_f + C_p Q_{v_i}) \left(\frac{\tau\gamma_i\,\theta_i}{Q_{v_i}}\right) C_i + \sum_{i=1}^{N} C_d (K_v \sqrt{A_{v_i}} \tau\gamma_i\,\theta_i C_i)$$

$$+ \sum_{i=1}^{N} C_i R_v \left(\frac{\tau\gamma_i\theta_i}{Q_{v_i}}\right) + \sum_{i=1}^{N} h_v \frac{Q_{v_i} C_i}{2A_{v_i}} + \sum_{i=1}^{N} h_v \frac{C_i Z_{\alpha v_i}}{A_{v_i}} \sqrt{\mu_v \gamma_i\,\theta_i A_{v_i} + \sigma_v^2 (\gamma_i \theta_i A_{v_i})^2} +$$

$$\tau\gamma_i\theta_i \mathrm{p} C_i + \frac{\tau\gamma_i\,\theta_i}{cap} l C_i + \sqrt{2h_n R_n \sum_{i=1}^{N} \tau\gamma_i\,\theta_i C_i} + h_n \left(Z_{\alpha_n} \sqrt{\sum_{i=1}^{N} \mu_n \gamma_i\,\theta_i C_i}\right) \tag{3.14}$$

Note that, the optimal solution to $TNC^E(A_{v_i}, Q_{v_i})$ is the initial solution used in stage 2. To solve Equation (3.14), let us assume that A_{v_i} is given and so the hessian of $TNC^E(A_{v_i}, Q_{v_i})$ with respect to A_{v_i} is given by

$$\frac{\boldsymbol{d}^2 \mathrm{TNC}^E(Q_{v_i} \backslash A_{v_i})}{\boldsymbol{d}Q_n^2} = \frac{\mathbf{2}(C_f + R_v)\,\tau\gamma_i\,\theta_i C_i}{Q_{v_i}^3} > 0, i = 1, 2, \ldots, N$$

Since $\mathrm{TNC}^E(A_{v_i}, Q_{v_i})$ is also a convex function of Q_{v_i}, the estimated value of $Q_{v_i}^E$ can be obtained by

$$\frac{dTNC^E(Q_{v_i} \backslash A_{v_i})}{dQ_{v_i}} = 0$$

Hence, estimated value of Q_{v_i} is

$$Q_{v_i}{}^E(A_{v_i}) = \sqrt{\frac{2A_{v_i}(C_f+R_v)\,\tau\gamma_i\,\theta_i}{h_v}} \tag{3.15}$$

Substituting the value of $Q_{v_i}{}^E$ into Equation (3.14), we get

$$TNC^E(A_{v_i}) = \sum_{i=1}^{N} F_v \frac{C_i}{A_{v_i}} + \sum_{i=1}^{N} C_p \tau\gamma_i\,\theta_i C_i + \sum_{i=1}^{N} C_d (K_v \sqrt{A_{v_i}} \tau\gamma_i\,\theta_i C_i) +$$

$$\sum_{i=1}^{N} h_v \frac{C_i Z_{\alpha_{v_i}}}{A_{v_i}} \sqrt{\mu_v \gamma_i\,\theta_i A_{v_i} + \sigma_v^2 (\gamma_i \theta_i A_{v_i})^2} + \tau\gamma_i\theta_i \mathrm{p} C_i + \frac{\tau\gamma_i\,\theta_i}{cap} l C_i +$$

$$\sqrt{2h_n R_n \sum_{i=1}^{N} \tau\gamma_i\,\theta_i C_i} + h_n (Z_{\alpha_n} \sqrt{\sum_{i=1}^{N} \mu_n \gamma_i\,\theta_i C_i}) + \sum_{i=1}^{N} \sqrt{\frac{2h_v(C_f+R_v)\tau\gamma_i\,\theta_i}{A_{v_i}}}\, C_i.$$

Now, Algorithm 1 determines the optimal estimated values for $Q_{v_i}{}^E$ and $A_{v_i}{}^E$. Algorithm 3.1 is illustrated in detail below:

Algorithm 3.1

Step 1: verifying $\frac{d^2TNC^E(\mathrm{A}_{\mathrm{r_i}})}{dA_{r_i}^2} > 0$, local minimum points are determined by solving for

$$\frac{dTNC^E(\mathrm{A}_{\mathrm{v_i}})}{d\mathrm{A}_{\mathrm{v_i}}} = 0$$

Step 2: Choose the local minimum point that gives the smallest value of $TNC^E(\mathrm{A}_{\mathrm{v_i}})$.

Step 3: Determine the estimated value of Q_{v_i} by Equation (3.15)

Step 4: Adjust $Q_{v_i}^E, i = 1{\sim}N$ and get the nearest integer values.

Stage 2: In Stage 2, a search-based algorithm is used to solve the original problem, starting with the initial estimated solution, $Q_{v_i}^E$ which we found in Algorithm 3.1. It is assumed that the optimal solution of $TNC^E(\mathrm{A_{v_i}}, \mathrm{Q_{v_i}})$ is very close to the optimal solution of $TNC(\mathrm{A_{v_i}}, \mathrm{Q_{v_i}})$ since Equation (3.13) is similar to Equation (3.13) except for the safety stock term. This ensures that by applying Algorithm 3.2 we can efficiently find the optimal solution.

Algorithm 3.2

Step 1: Let $Q_{v_i}^{j=1} = Q_{v_i}^E$, find the value of $A_{v_i}^{j=1}$ to minimize $TNC(\mathrm{A_{v_i}}|Q_{v_i}^1)$ and compute $TNC(A_v^1, Q_{v_i}^1)$ by Equation (3.13).

Step 2: Let $Q_v^{j+1} = Q_{v_i}^j + 1$, find the value of $A_{v_i}^{j+1}$to minimize $TNC(A_{v_i}^1|Q_{v_i}^{j+1})$ and compute $TNC(A_{v_i}^{j+1}, Q_{v_i}^{j+1})$ by Equation (3.12).

Step 3: If $TNC\left(A_{v_i}^{j+1}, Q_{v_i}^{j+1}\right) < TNC(A_{v_i}^j, Q_{v_i}^j)$, then let $Q_{v_i}^j = Q_{v_i}^{j+1}$ and go to Step 2; otherwise, go to Step 4.

Step 4: Let $Q_{v_i}^{j+1} = Q_{v_i}^j - 1$, find the value of $A_{v_i}^{j+1}$to minimize $TNC(A_{v_i}^1|Q_{v_i}^{j+1})$ and compute $TNC(A_{v_i}^{j+1}, Q_{v_i}^{j+1})$ by Equation (3.13).

Step 5: If $TNC\left(A_{v_i}^{j+1}, Q_{v_i}^{j+1}\right) < TNC(A_{v_i}^j, Q_{v_i}^j)$, then let $Q_{v_i}^j = Q_{v_i}^{j+1}$ and go to Step 4; otherwise, go to Step 6.

Step 6: Compute $\mathrm{Q_n^*}$ by Equation (3.12) and adjust $\mathrm{Q_n^*}$ to get the nearest integer value.

Step 7: Let $TNC\left(A_{v_i}^*, Q_{v_i}^*, \mathrm{Q_n^*}\right) = TNC(A_{v_i}^j, Q_{v_i}^j, \mathrm{Q_n^*})$. The optimal solution is $(A_{v_i}^*, Q_{v_i}^*, \mathrm{Q_n^*})$.

3.5 Numerical study

We apply the proposed network cost model, as described by Section 3.3, and the CA-based solution approach discussed in Section 3.3 to a real-world case study, in which we investigate the optimal deployment configuration of AM facilities and the raw material inventory policy of the CRW's and AM facilities. Twelve states in the southeastern region of USA which include Alabama (AL), Arkansas (AR), Florida (FL), Georgia (GA), Kentucky (KY), Louisiana (LA), Mississippi (MS), North Carolina (NC), South Carolina (SC), Tennessee (TN), Virginia (VA), and West Virginia (WV) are adopted as test bed in this study..

In particular, we conduct a series of numerical studies to determine where AM facilities for the fabrication of medical implants should be located to serve the hospitals and clinics in this region at the minimum cost, and identify the cost parameters that may pose significant impacts on this decision.

(1) One of the cost parameters to be considered is the unit transportation cost or delivery cost per mile per item, C_d. It is expected that if this cost is high, AM facilities should be sited closer to the hospitals to reduce the total transportation cost.

(2) The initial investment cost of AM, mainly consisting of the cost of AM machines, constitutes a significant part of the total network cost. A high fixed cost means that less number of AM facilities should be opened to curtail the total fixed cost. This means that the manufacturing sites will be located further from the hospitals and results in higher transportation cost. We investigate how these types of conflicts impact the location decisions and total supply chain network cost. (3) Reorder cost and inventory holding cost are other cost parameters that can affect the reorder frequency and total

inventory cost. We investigate how various values of these parameters affect the AM facility distribution and total network cost in the region.

(4) Personnel cost which contributes to the total production cost is another cost parameter that affects how many AM facilities are located. This cost can be tied to the automation level of AM machines where a high personnel cost is construed as a low level automation level where one staff is able to operate only fewer machines. In another light, it can be related to the level of availability of the skill sets required to operate AM machines which are usually sophisticated. We expect that a high personnel cost will discourage the location of many AM facilities.

(5) The demand level of bio-medical implants is a parameter that affects the distribution of AM facilities. Due to the high cost of AM systems, it may not make economic sense in commercial applications to locate AM facilities if there is not enough demand to justify their utilization. It makes sense to visualize the demand of bio-medical implants in the region increasing or decreasing in the future. An increasing aging population will likely increase the demand for hip and knee implants as well as cardiovascular stents. However, improvements in personal lifestyles and other treatment alternatives may diminish the demand for procedures that require AM bio-medical products. We investigate how various demand levels impact AM deployment decisions.

(6) Customer service level impacts any supply chain network cost. A high service level means increased responsiveness by the business which may be achieved by keeping lots of inventory to ensure there is no stock out or locating AM facilities very close to the customer. Any of these approaches results in a high supply chain cost. We conduct

experiments to study how different service levels affect the total network cost and the location of AM facilities.

(7) The last but not the least of this study compares the benefits of our novel AM deployment model with other approaches in literature. The closest quantitative approaches of AM supply chain to our method consider centralized and distributed deployment which we understand to be at two ends of the deployment spectrum. Our opinion is that the best deployment approach lies between these two extremes which our model is able to determine. We investigate the status quo savings in total network cost when our model is used to select the best AM facility distributions in the southeastern region vis-a-vis the approaches in literature. Furthermore, we study what happens to the savings in various future scenarios of cost parameters.

3.5.1 Data description

We focus on four biomedical implants, which are known to have been manufactures using AM: hip and knee joint implants, dental braces, and vessel stents. We collected data from major hospitals in the southeastern region, as well as the nearby clinics, about the use of the four biomedical implants. We confirm that for each state, the average demand matches with the estimate derived by multiplying the nationwide demand of the implants by the proportion of the state's-USA population, published by the Centers for Disease Control and Prevention. We find that both the demand density for the products and hospital density are unique for each state and are slow varying, necessary conditions that justify the use of the CA model. Since the inventory at the CRW's and AM facilities are mainly at the raw material level, we derive an equivalent amount for the raw materials used in producing these four products by consolidating them into an aggregate unit. We use the ratio $0.4: 0.4: 0.12: 0.08$ for weight of AM raw materials used to produce a unit hip implant, knee implant, dental implant and stent, respectively. This data is shown in Table 3.2.

In order to estimate the fixed investment cost of an AM facility, we assume that the location cost mainly consists of the cost of AM machines. Consequently, we use the prices of AM systems based on the quotation of Selective Laser Melting (SLM) systems in 2015. We choose the SLM system because of its widely documented use for the fabrication of bio-medical implants. The build time for each part is estimated using the relative volume of parts using SLM state-of-the-art machines for year 2015. We take the build time and post processing time into consideration and set the lead time to two weeks. For example, depending on the original equipment manufacturer, machine dimensions, effective build volume of the machine and its operational build speed, the market price of an SLM system used for the production of biomedical implants ranged from USD 400,000 to USD 1,000,000 in 2015. We obtained this data from quotations received by the Department of Mechanical Engineering of the Mississippi State University on the price of SLM machines. Such a range in prices from similar factors agree with the data from Hopkinson and Dickens [64], Atzeni et al. [7], Bartolo [14], Lindemann et al. [83], and Baumers et al. [17]. We assume an average price of $500,000 for one AM machine which is reasonable for the price of the machine that can produce the identified bio-medical implants. A similar example can be found in Bartolo [14], in which the authors recorded an annual maintenance and investment cost of $110,320/year over 10 years for a similar machine with a purchase price of $700,000. Using the equivalent annual cost (EAC) model, we calculate the average annualized investment and maintenance cost.

There is a wide range of depreciation methods in literature. The simplest method is the straight line method which calculates the annual depreciation cost by dividing the machine purchase price by its expected life. The more complex methods such as the accelerated depreciation, equivalent annual cost (EAC) and remaining value percentage (RVP) methods, use models that take into account factors like machine age, salvage value, size, usage, manufacturer, condition, interest rate and region of deployment to calculate annual depreciation cost. Jones and Smith [67] provided an overview and historical perspective of the EAC. Cross and Perry [36], Hansen and Lee [57], Unterschultz and Mumey [153], and Dumler et al. [43] presented a detailed discussion of multiple variations of RVP models. We calculated the average annualized investment and maintenance cost based on a life-span of ten years, resulting in an average annualized investment and maintenance cost of $75,000 for a small capacity AM facility. It is worth noting that for such a fast evolving technology like AM, a faster replacement policy may be implemented (e.g., 5 year replacement), which will result in a higher annualized investment. The annualized investment and maintenance cost for medium and large capacity AM facilities could be $135,000 and $182,000, respectively. We take the cost of the large capacity AM as the annual fixed cost since it is enough to meet the production capacity requirement of each AM facility influence region demand.

We assume that the biomedical implants are delivered using FedEx, and the costs of transportation are calculated using the online tool provided by FedEx Get Rates. The fixed transportation cost for inbound shipment (C_f), variable transportation cost per item (C_p) and delivery cost per item per mile (C_d) are $80.00, $34.02 and $1.00, respectively. We assume a planning horizon of one year and an annual raw material inventory holding cost per item at both AM facility and CRW of $40. The production cost per unit product (p) excluding labor cost is taken as $1000. This cost is mainly the cost of raw material and energy consumption which is usually high for biomedical implants. At $1000, the production cost results in an ATR ratio much less than 3.0 which is required to encourage investment in AM technology for biomedical implants [45]. The annual salary is $60,000 per staff which is commensurate with the skill of an engineering graduate. One employee is able to operate three AM machines located at each facility which means an automation level of 1:3. The fixed reorder cost for raw material at each AM facility and CRW are $100 and $200, respectively. The mean lead time at each AM facility and CRW are one week and two weeks, respectively while the variance is 0.5 at both AM facility and CRW. We require a service level of at least 95% at both locations. We use a distance metric and shape constant factor of 0.4, a value that Dasci and Verter [39] recommend for use in circular areas of influence. Table 3.2 gives a summary of the data used in the base case study of the hospitals and clinics in the southeastern part of USA.

Table 3.2 Data used in parameter values

	AM Facility	CRW	Unit	Comments
National mean demand data, d_{pk}	Hip implants: 332,000[a] Knee implants: 719,000[a] Dental braces: 1,000,000[a] Stents: 1,000,000[a]		units/year units/year units/year units/year	Annual national demand figures for medical implants
Build time	Hip implants: 12[a] Knee implants: 11[a] Dental braces: 0.25[a] Stents: 0.4[a] Aggregate product: 4.11		hours/unit hours/unit hours/unit hours/unit hours/unit	Aggregate product build time based on individual implant build time and national demand
cap	1265		units/year	Based on 20hrs/day, 5 workdays/week and 52 weeks/year
Production cost (excluding labor cost), p	Hip implants: 2308[a]; Knee implants: 1863[a]; Dental braces: 100[a]; Stents: 249[a]; Aggregate product: 1,000		hours/unit	Production cost of aggregate product based on build time ratio of 12:11:0.25:0.4 from raw material
Fixed investment cost, F_r	182,000[a]	hours/unit	\$/year	Annual depreciation and maintenance cost for large capacity AM facility
Transportation cost	Fixed (C_f): \$80.00; Variable (C_p): \$34.02 Variable (C_d): \$1		\$/unit \$/unit/mile	Estimated from carrier data
Inventory holding cost	h_v: 40	h_v: 40	\$/unit	2.5% interest rate on cost of raw material
Reorder cost	R_v: 100	R_n: 200	\$/unit	More raw material required at CRW than at AM facility

Table 3.2 (continued)

Lead-time, μ_v	7[a] ; Variance (σ_v^2):0.5	14[a] ; Variance (σ_n^2):0.5	days	Lead time when ordering raw materials
***Service level factor,* (α)**	5%	5%		$Z_{\alpha_{v_i}} = 1.65$, $Z_{\alpha_n} = 1.65$
Personnel salary, l	$60,000		$/employee/year	One employee can operate 3 AM machines
***Hospital density,* γ_i**	AL: 0.0013; AR: 0.0014; FL: 0.0010; GA: 0.0027; KY: 0.0030; LA: 0.0012; MS: 0.0017; NC: 0.0019; SC: 0.0014; TN: 0.0023; VA: 0.0031; WV: 0.0023		/square mile	Data of hospital locations in each state
***Demand per unit time,* θ_i**	AL: 2.692; AR: 1.474; FL: 11.231; GA: 2.385; KY: 1.3689; LA: 2.709; MS: 1.355; NC: 3.728;SC: 3.951; TN: 2.579; VA: 2.340; WV: 1.245		units/hospital /week	Based on national mean demand data and hospital data

[a] Retrieved from Emelogu et al. (2016)

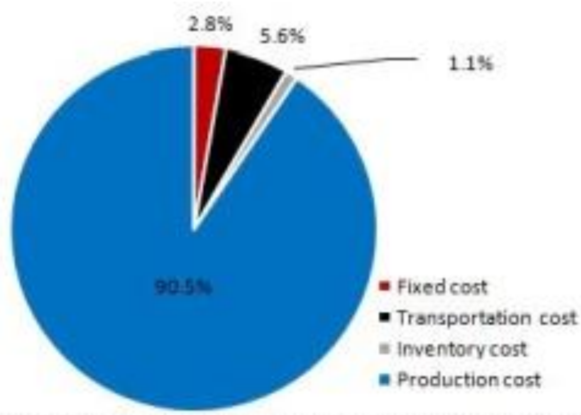
3.5.2 Solution approach illustration

We present the results obtained with base cost parameters after applying Algorithm 3.1 and Algorithm 3.2 of Section 3.3 to the network cost model developed in Section 3.2. A total of 27 AM facilities is needed in the region for the fabrication of medical implants, with Florida having the highest number of AM facilities established in it and Arkansas, Mississippi and West Virginia having the least. The model tends to establish more AM facilities if there are more hospitals and customers that need to be served. Figure 3.5(a) shows the distribution of these AM facilities in the region while Table 3.3 shows the size of their influence areas of the AM facilities and their order quantities. The total network cost is USD 177,138,273 which is essentially an aggregation of total inbound transportation cost for AM facility, total outbound transportation cost for CRW, total average inventory holding cost of AM facilities and CRW, and total production cost of AM facility. The contribution of these costs as a percentage of the total AM supply chain cost for biomedical implants is shown in Figure 3.5(b). The production cost, making up 90.5% of the total network cost, is higher than any other cost component due to the high cost of raw materials for implants, labor cost and post-processing costs which may involve its own supply chain. Inventory cost, constituting 1.1% of the total cost, represents the least cost component in AM supply chain network for biomedical implants in the region. In the following subsections, we investigate the impact of changes in model parameters on these cost components and other supply chain decisions.

Table 3.3 AM supply chain decisions for the 12 states in the region

State	A_{v_i}	Q_{v_i}	No. of AM facilities
AL	27062	2250	2
AR	38496	2201	1
FL	12431	2419	5
GA	18018	2326	3
KY	24324	2268	2
LA	28429	2243	2
MS	35780	2210	1
NC	16907	2341	3
SC	19939	2305	2
TN	19032	2315	2
VA	16642	2344	3
WV	24230	2217	1
	Q_n		12590
	TNC ($)		177,138,273

5(a): Distribution of AM facilities



5(b): Contribution of cost components to total network cost

Figure 3.5 Recommended distribution of AM facilities and resulting supply chain cost in the region

3.5.3 Parameters affecting the optimal decision

In this subsection, we will investigate how changing demand and cost parameters affect the optimal influence area for each AM facility A_{v_i}, the ordering quantity for each AM facility Q_{v_i}, the ordering quantity for the CRW Q_n, and the total network cost, *TNC*. Tables 3.4 - 3.7 and Figures 3.6 - 3.8 illustrate the result of varying parameters in the model and these results are summarized as follows:

3.5.3.1 Demand analysis

We conduct a set of experiments to investigate how the economic decisions will be affected by various demand levels of medical implant. We take the current demand data for medical implants at hospitals in southeastern USA as the medium/baseline demand level, and consider demand level from -75% to 100% while keeping every other parameter constant. A -75% change in demand signifies a 75% decrease in demand which can be achieved by multiplying θ_i by 0.25 in our model whereas a 100% change is an increase in demand obtained by multiplying the parameter by 2.0. The solution from our model gives the number of AM facilities to be established in each state of the region, as well as the contribution of each cost component to the total network cost for each demand level. We find that

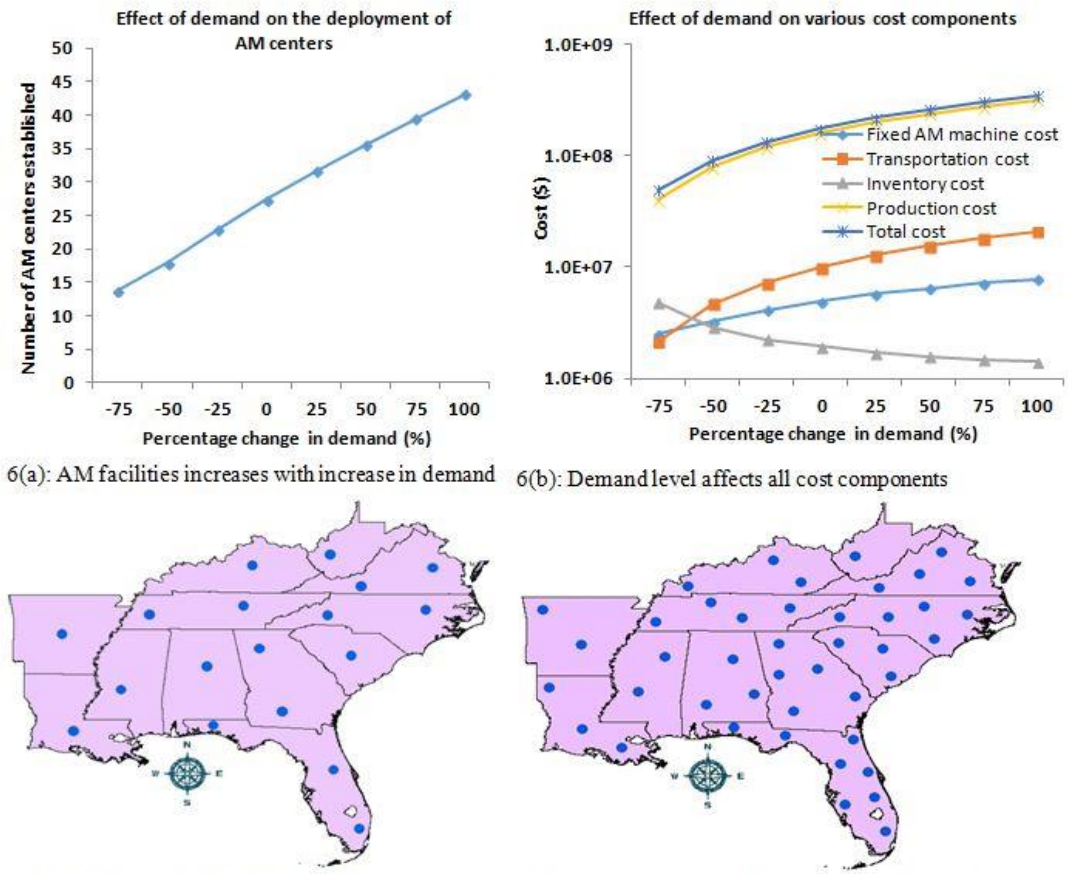
(1) The demand level has a significant effect on the number of AM facilities located in the region and the network cost components. At the current level of demand, a total of 27 AM facilities need to be deployed in the region. Florida has five AM facilities located in it which is higher than any other

state's whereas Arkansas, Mississippi and West Virginia have one each, the least among all the states.

(2) When the demand level doubles the number of AM facilities deployed in the region increases to 43, an increase of more than 59%. This results in a total network cost increase of 98%. When the demand level reduces by 50%, only 18 AM facilities are required in the entire region, which represents a decrease of 33%.

(3) The decrease in demand causes a 49% decrease in the total network cost.

When the demand for the biomedical implants increases, the number of AM facilities established also increases due to more capacity being needed to satisfy the demand. The result is an increase in the investment cost in AM machines which adds to the total network cost. Moreover, both the production and transportation cost also increase with increase in demand because more raw materials are bought and shipped from one point to the other to manufacture implants needed to satisfy the additional demand. Obviously, the production cost dominates every other cost component due to the high cost of raw materials for medical implants, labor cost and energy consumption of AM technology. However, the total inventory cost decreases when the demand increases. As more implants are needed, the raw materials kept at both the AM facilities and CRW's are depleted fast thereby reducing inventory holding cost. These results are portrayed in Figure 3.6.



6(a): AM facilities increases with increase in demand

6(b): Demand level affects all cost components

6(c): Deployment of AM facilities when demand level decreases by 50%

6(d): Deployment of AM facilities when demand level increases by 100%

Figure 3.6 Impact of demand levels on supply chain network cost and AM deployment configuration

3.5.3.2 Effect of delivery cost, C_d

In order to measure the effect of changes in the delivery cost per mile per item, (C_d), on the supply chain decision, we vary the delivery cost per mile per item (C_d) from \$1 (base case) to \$2, and finally to \$3, while keeping all other parameters constant in our model. At each level of the delivery cost per mile per item, we examine for each of the 12 states what impact a change in C_d has on A_{v_i}, Q_{v_i}, Q_n *and* TNC. We observe that

(4) Both A_{v_i} (the influence area size of each AM facility in a given state) Q_{v_i} (the recommended order quantity at the AM facility) decrease, Q_n (the order quantity at the CRW) remains the same and the total network cost increases as C_d increases. Specifically, when the delivery cost per mile per item increases from \$1 to \$2, the average influence area of each AM facility decreases by 36% which translates to an increase of 57% in the number of AM facilities established.

(5) The average order quantity at the AM facilities decreases by 35% whereas the total network cost increases by about 4%.

As C_d increases, the model responds by locating AM facilities closer to customers in an attempt to minimize the delivery distance covered. The resulting decrease in an AM facility's influence area implies that it attends to fewer customers which necessitates it to reduce its ordering quantity. However, as the influence area reduces with increase in C_d, more AM facilities need to be established to satisfy the customer demands of hospitals within the service region. The additional cost from increased number of AM facilities established outweighs any decrease in transportation cost accrued by locating the AM's closer to the customers, thus the increase in total network cost as C_d increases. Since there is no change in demand level and the CRW still serves the same entire southeastern region, its order quantity does not need to change, hence, Q_n remains the same for all values of C_d. This result is shown in Table 3.4.

Table 3.4 Effect of C_d

$C_d = 1$			$C_d = 2$			$C_d = 3$		
A_{v_i}	Q_{v_i}	No. of AM facilities	A_{v_i}	Q_{v_i}	No. of AM facilities	A_{v_i}	Q_{v_i}	No. of AM facilities
27062	2250	2	17046	1444	4	13007	1126	5
38496	2201	1	24245	1392	3	18500	1084	3
12431	2419	5	7831	1622	9	5976	1267	12
18018	2326	3	11350	1524	6	8661	1189	7
24324	2268	2	15321	1463	3	11692	1141	4
28429	2243	2	17906	1436	3	13664	1119	4
35780	2210	1	22536	1402	3	17196	1092	3
16907	2341	3	10650	1539	6	8127	1201	7
19939	2305	2	12560	1502	3	9585	1172	4
19032	2315	2	11989	1512	4	9149	1180	5
16642	2344	3	10484	1543	5	8000	1204	6
24230	2217	1	19488	1399	2	14871	1109	2
Q_n		12590	Q_n		12590	Q_n		12590
TNC ($)	177,138,273		*TNC*	184,191,380		*TNC*	190,099,534	

3.5.3.3 Effect of ordering costs, $\mathbf{R_v}$ and $\mathbf{R_n}$

We measure the effect of changes in the ordering costs, (R_v and R_n) on the decision variables by varying their values in our models while keeping all other parameters unchanged. We increase R_v and R_n from their base values of $100 and $200 to $150 and $250 respectively in the first experimental instance. In the second experimental instance, the value of R_v and R_n are further increased to $200 and $300, respectively. We observe that

(6) Q_{v_i} (the recommended order quantity at the AM facility), Q_n (the order quantity at the CRW) and *TNC* increase with increase in the reorder costs of each AM facility and CRW whereas there is no significant effect on the influence area, A_{v_i}. Specifically, in the second experimental instance, where

R_v and R_n were increased by 100% and 50%, respectively, Q_{v_i}, Q_n and TNC increase by 26%, 22% and 0.1%, respectively.

The result makes intuitive sense because if R_v and R_n increase, the CRW and AM facilities will increase their respective ordering quantities to reduce ordering frequency, and minimize their total ordering cost. This decision generally should not affect the size of the influence area the AM facility controls, hence the number of AM facilities remain the same for all ordering cost values. The 0.1% increase in TNC by a 100% and 50% increase in R_v and R_n implies that the ordering cost is not a major cost factor in the AM supply chain decision. In other words, given an ordering cost, the model will choose an ordering quantity for the Am facilities and CRW so that the net effect on the total supply chain cost will be minimal. This result is shown in Table 3.5.

Table 3.5 Effect of R_v and R_n

$R_v = \$100, R_n = \$200$			$R_v = 150, R_n = \$250$			$R_v = \$200, R_n = \$300$		
A_{v_i}	Q_{v_i}	No. of AM facilities	A_{v_i}	Q_{v_i}	No. of AM facilities	A_{v_i}	Q_{v_i}	No. of AM facilities
27062	2250	2	27072	2581	2	27079	2834	2
38496	2201	1	38511	2540	1	38521	2769	1
12431	2419	5	12434	2721	5	12438	3056	5
18018	2326	3	18023	2644	3	18028	2934	3
24324	2268	2	24332	2596	2	24338	2857	2
28429	2243	2	28439	2575	2	28446	2824	2
35780	2210	1	35794	2548	1	35803	2781	1
16907	2341	3	16912	2656	3	16916	2953	3
19939	2305	2	19945	2627	2	19950	2906	2
19032	2315	2	19037	2635	2	19042	2919	2
16642	2344	3	16647	2659	3	16651	2957	3
24230	2217	1	24230	2565	1	24230	2778	1
Q_n		12590	Q_n		14080	Q_n		15420
TNC ($)		177,138,273	*TNC*		177,242,781	*TNC*		177,379,843

3.5.3.4 Effect of unit inventory holding costs, h_v *and* h_n

In the next experiment, we investigate whether increasing inventory holding cost of AM facility, h_v and CRW, h_n has any effect on A_{v_i}, Q_{v_i}, Q_n and TNC. Initially, the value of both h_v and h_n are taken as $40. In second and third experimental instances, we increase them to $60 and $80, respectively. We find that

(7) Q_{v_i} and Q_n decrease with increase in inventory holding costs at the AM facilities and CRW whereas TNC increases. However, there is no significant effect on the size of the influence areas, A_{v_i}, and the deployment configuration of the AM facilities. When the unit inventory holding cost increase by 50% to $60, the order quantities at the AM facilities and CRW reduce by 19% and 18%, respectively. The total network cost increases by only 0.6%.

The rationale behind this is that, if inventory holding cost is high, both the CRW and AM facilities tend to order less to ensure that they have less items to keep in inventory. Holding less inventory will eventually result in less inventory holding cost. While the models tries to maintain a balance between the unit inventory holding cost and the order quantities, most of the time a slight mismatch is unavoidable. In a situation where the unit holding cost is high, it results in a slight increase in total network cost, hence the 0.6% increase in *TNC*. The result is shown in Table 3.6.

Table 3.6 Effect of h_v and h_n

h_v= \$40, h_n = \$40			h_v= \$60, h_n = \$60			h_v = \$80, h_n = \$80		
A_{v_i}	Q_{v_i}	No. of AM facilities	A_{v_i}	Q_{v_i}	No. of AM facilities	A_{v_i}	Q_{v_i}	No. of AM facilities
27062	2250	2	27082	1821	2	27095	1502	2
38496	2201	1	38527	1778	3	38548	1465	2
12431	2419	5	12438	1966	6	12443	1628	6
18018	2326	3	18029	1886	4	18037	1559	4
24324	2268	2	24341	1836	2	24352	1515	2
28429	2243	2	28450	1814	2	28464	1496	2
35780	2210	1	35809	1786	2	35828	1472	2
16907	2341	3	16918	1899	4	16925	1570	4
19939	2305	2	19952	1868	2	19961	1543	2
19032	2315	2	19044	1876	3	19052	1550	3
16642	2344	3	16652	1902	3	16659	1572	3
24230	2217	1	24230	1784	1	24230	1470	1
Q_n		12590	Q_n		10280	Q_n		8900
TNC (\$)	177,138,273		*TNC*	178,215,731		*TNC*	179,871,313	

3.5.3.5 Effect of required customer service levels

We investigate what impact various service levels will have on the decision variables and AM supply chain network cost. Initially, we assumed that demand at hospitals will be satisfied 95% of the time, (i. **e.**, $\alpha_v = \alpha_n = 5\%$). We reduced the service level to 90% in the first experimental instance and increased it to 99% in the second experimental instance. We find that for the service levels considered,

(8) There is no significant change in the number of AM facilities located in the region. However, there is a significant impact on the inventory cost, with higher service levels attracting higher inventory cost. Specifically, when the service level is increased from 95% to 99%, the total inventory cost increased by 63%. This means a 0.47% increase in total network cost.

(9) **When the service level was reduced from 95% to 90%, total inventory cost reduced by 29.2%. This translates to 0.15% reduction in the total network cost.**

We note that the increase in inventory cost and total network cost as service level increases occurred despite that Q_{v_i} significantly reduced. We attribute the resulting high cost to the fact that the AM facilities need to order more frequently to maintain high level of service. Q_n remains unchanged for all three experimental instances. Table 3.7 shows the effect of changes in service levels on A_{v_i}, Q_{v_i}, Q_n *and TNC*.

Table 3.7 Effect of α_v and α_n

α_v=10%, $\alpha_n = 10\%$			α_v=5%, $\alpha_n = 5\%$			α_v=1%, $\alpha_n = 1\%$		
A_{v_i}	Q_{v_i}	No. of AM facilities	A_{v_i}	Q_{v_i}	No. of AM facilities	A_{v_i}	Q_{v_i}	No. of AM facilities
27053	2618	2	27062	2250	2	27081	1872	2
38482	2601	2	38496	2201	3	38524	1820	2
12427	2664	6	12431	2419	6	12439	2051	6
18011	2641	4	18018	2326	4	18029	1953	4
24315	2624	2	24324	2268	2	24340	1891	2
28419	2616	2	28429	2243	2	28448	1864	2
35768	2604	2	35780	2210	2	35806	1830	2
16901	2645	4	16907	2341	4	16918	1967	4
19932	2635	2	19939	2305	2	19952	1930	2
19025	2638	3	19032	2315	3	19044	1940	3
16636	2646	3	16642	2344	3	16652	1971	3
24230	2587	1	24230	2217	1	24230	1827	1
Q_n		12590	Q_n		12590	Q_n		12590
TNC	176,873,230		*TNC*		177,138,273	*TNC*		177,969,031

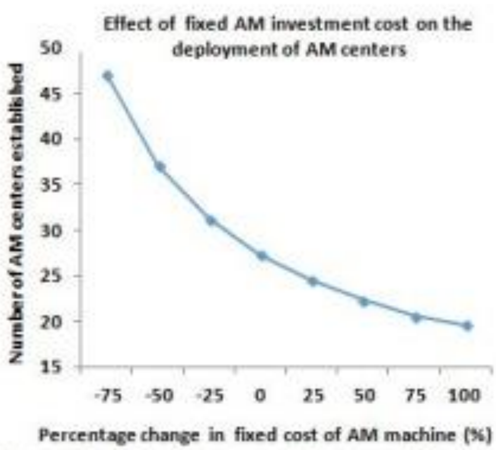
3.5.3.6 Effect of fixed AM machine cost

The high cost of AM machines is usually one of the inhibiting factors that discourage businesses from investing in AM technology. We conduct experiments to investigate the impact of various initial AM investment cost levels on AM deployment in the region. We vary $\boldsymbol{F_r}$ in our model while keeping other parameters constant. The result shows that

(10) As the cost of AM machines reduces, the number of AM facilities increases whereas at high fixed AM machine cost, few AM facilities are located. Specifically, when the annualized fixed investment cost of AM machines of USD 182,000 reduces by 50%, the number of AM facilities deployed in the region increases by 37%. If the investment cost increases by 100%, the number of AM facilities will decrease by 26%.

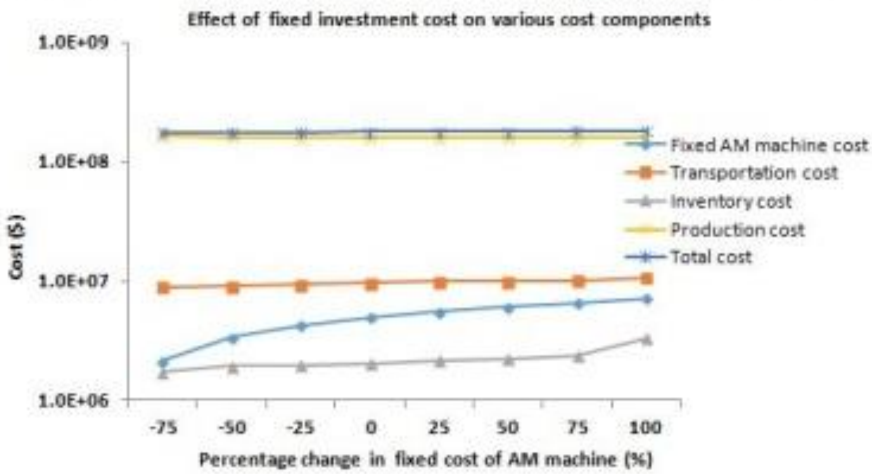
(11) Moreover, fixed investment cost of AM machines impacts the total network cost. The total network cost decreases by 0.8% when the fixed investment cost reduces 50% from USD 177.1 million , and increases by 1.2% when the fixed investment cost doubles.

Having few AM facilities means that the manufacturing locations are further away from the hospitals and CRW which results in a higher transportation cost whereas more AM facilities brings manufacturing much closer to the customers and leads to a lower transportation cost as shown in Figure 3.7(c). It is more likely that the price of AM machines will decrease in future as research in the AM technology leads to further improvements. Therefore, we show in Figure 3.7(b), the distribution of 37 AM facilities which the model recommends when the fixed cost of AM machine reduces by 50%. The total inventory cost reduces as the fixed AM cost decreases. This means that establishing more AM facilities significantly reduces the amount of inventory in the network by ordering just the right amount of raw materials and producing only the number of implants needed on-demand. This result goes to support the claim that AM facilitates lean manufacturing concepts. We observe that the total production cost slightly increases as the fixed investment cost in AM decreases. Since the same amount of raw material is utilized due to the fact that demand of the implants does not change, the slight increase in the production cost comes from the increased number of personnel required to operate the additional AM facilities located. Overall, the total network cost decreases as the fixed investment cost in AM decreases. This result means that as AM technology improves and the cost of AM machines decreases, the economic advantage from reduced transportation and inventory cost when bio-medical implant AM facilities are established much closer to the hospitals outweigh the personnel cost of operating the machines.



7(a): AM facilities increases with decrease in fixed investment cost

7(b): Deployment of AM facilities when the fixed investment cost decreases by 50%



7(c): Effect of AM fixed investment cost

Figure 3.7 Effect of fixed AM machine cost on supply chain network cost and AM deployment configuration

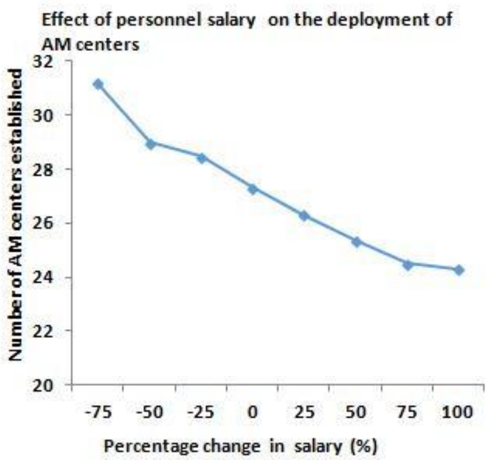
3.5.3.7 Effect of annual personnel salary

We investigate the impact of changes in the cost of labor on the deployment of AM facilities and total network cost. Annual labor cost can take a positive or negative direction in future. It can increase as a result of change in national policies that increase the minimum wage or due to scarcity of the required manpower to operate the sophisticated AM machines. Apart from the possibility that more well-trained personnel can be available in the future to give businesses a negotiating power for reduced personnel salary, we can also view a decrease in labor cost from high machine automation level that can arise due to future improvements in AM technology. In high automation, one employee can operate more machines thereby requiring few personnel in the AM workforce. We simulate changes in the annual salary by varying the value of *l=$60,000* which contributes to the total production cost in the model. We find that

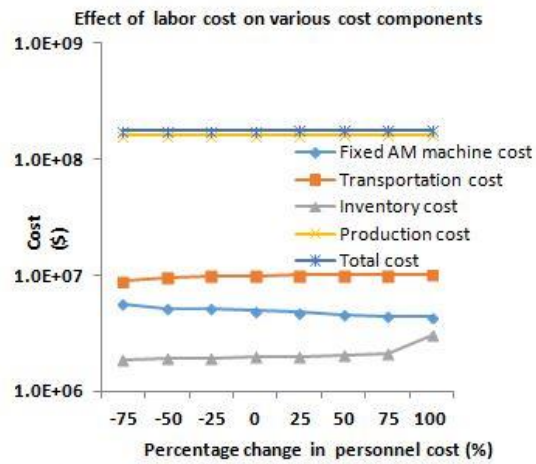
(12) An increase in the annual personnel cost results in increase in total inventory cost, increase in total transportation cost, slight increase in production cost and a decrease in total fixed AM investment cost. Overall, an increase in personnel salary leads to a higher total supply chain cost while a decrease results in higher total network cost. When the annual personnel salary decreases by 50% from USD 60,000 to USD 30,000, *TNC* decreases by 0.3% from USD 177.1 million. If personnel salary increases by 100%, *TNC* increases by 0.46%.

(13) Moreover, decreasing the personnel salary by 50% leads to a 7.4% increase in the number of AM facilities established while a 100% increase results in 11.1% decrease in the number of AM facilities.

This can be seen in Figure 3.8(a). The decrease in total fixed AM cost from high personnel cost is due to locating few AM facilities. The raw materials and medical implants have to travel a longer distance in the network. Besides, since one AM facility has to attend to more hospitals, it needs to keep more raw materials in safety stock to hedge against demand uncertainties. This explains the concomitant high transportation cost and inventory cost. According to Emelogu et al. [45], a low production cost in AM of biomedical implants results in a low ATR, which encourages investment in AM technology. Therefore, it is not surprising that the model suggests locating more AM facilities as the personnel cost decreases. Figure 3.8(c) and Figure 3.8(d) show how the AM facilities are distributed in low ($30,000) and high ($120,000) annual personnel salaries, respectively.

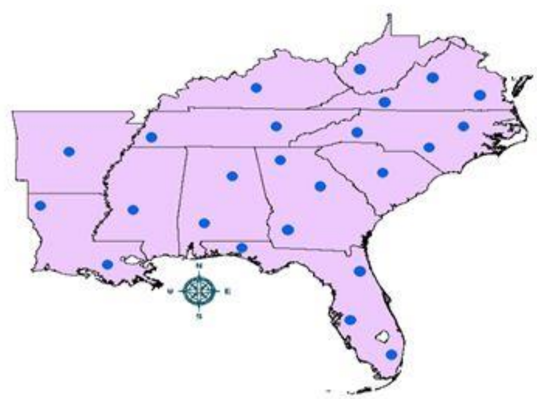


8(a): AM facilities increases with decrease in fixed investment cost



8(b): Personnel salary affects all cost components

8(c): Deployment of AM facilities when labor cost decreases by 50%



8(d): Deployment of AM facilities when labor cost increases by 100%

Figure 3.8 Effect of personnel cost on supply chain network cost and AM deployment configuration

3.5.4 Cost advantage of the CA model

We now conduct experiments to investigate the cost savings achieved from using our CA model to determine the optimal AM deployment configuration versus other approaches. We call the optimum configuration chosen by our CA model CONFIGOPT. We describe six scenarios and three possible configurations that have been suggested in literature. The six scenarios include the present baseline values of the model parameters and five other conditions that can arise in future due to changes in the model parameters. The three possible configurations indicate how distributed or centralized the AM facilities are deployed. We describe the configurations as follows:

CONFIG 1 Core centralized: One AM facility is located to serve the entire 12 states. This can be viewed as extreme centralization in which minimal investment is made on AM machine procurement. Despite its huge saving in total fixed investment cost and personnel cost, this configuration, which Khajavi et al. [70] recommends for AM deployment in present supply chain of military jet spare parts, may not be optimal. This is due to the resulting high total transportation and inventory costs.

CONFIG 2 Core distributed: This configuration, which can be conceived as extreme distributed deployment has an AM facility established in every county in every state in the southeastern region. While this configuration brings the manufacturing locations very close to the hospitals thereby having a high propensity of reducing the trio of lead time cost, inventory cost and transportation cost, the enormous capital required to invest in each AM machine may make it too expensive to be worthwhile. We investigate how this configuration measures with that identified by the CA model in the six scenarios.

CONFIG 3: One AM facility is located at each state in the region to serve all the hospitals in that state. This results in 12 AM facilities for the southeastern region of USA. Although this configuration is somewhere between the two extremes described above, it may still be a matter of luck for it to be optimal.

We describe the scenarios that we use to investigate the performance of our CA model. Scenario SP represents the status quo base values of the bio-medical implant supply chain cost parameters. Scenarios S1-S5, described below, are five other situations which can arise in future due to changes in the supply chain cost parameters.

SP: This is the present scenario where the annual personnel salary, $l = \$60{,}000$; annual fixed cost of AM investment, $F_r = \$182{,}000$; and the demand of the biomedical implants in the southeastern region is as presented in Table 3.2.

S1: In this scenario, we model a future when the personnel salary decreases by 50%, the fixed cost of AM machine reduces by 50% and the demand for bio-medical implants in the region remains constant.

S2: This scenario models a future when the personnel salary, AM machine fixed cost, and demand level all decrease by 50%.

S3: In this scenario, both the personnel cost and fixed cost of AM machine decrease by 50% while the demand for the implants increases by 100%.

S4: Here, both the personnel salary and demand increase by 100% while the cost of AM machine investment decreases by 50%.

S5: In this scenario, we model a future when both the fixed cost of AM machine and demand decrease by 50% whereas the annual personnel salary increases by 100%.

The results from our experiments show that CONFIGOPT, the AM deployment configuration decision provided by the CA model outperforms any other option for all the scenarios considered. As shown in Figure 3.9, the closest option to it is CONFIG3 which involves locating one AM facility in each to make total of 12 AM facilities in the region while the worst option is CONFIG2, locating an AM facility in every county. Given the current cost parameters in the study, 59%, 7% and 6% of the total network cost is saved if CONFIGOPT is used instead of CONFIG2, CONFIG1, and CONFIG3, respectively. This is shown in Figure 3.10. Moreover, CONFIGOPT saves up to 14% of the total cost incurred from using CONFIG1. This occurs in scenario S3 where there is high demand level, low AM investment cost and low personnel cost. These are conditions that favor distributed AM deployment more than centralized option, and thus, justify why CONFIG3 performs poorly here and makes CONFIGOPT to have a significant saving of up to 14% over it. The least saving is achieved in S5 where 4% of the total is saved. This scenario contains two of the factors that encourage centralized AM deployment of AM: low demand level and high personnel cost. Thus, CONFIG1 performs better in S5 than in any other s scenario thereby making CONFIGOPT to have the least saving against it in this scenario.

When CONFIGOPT is used as the deployment configuration instead of CONFIG2, the highest saving of 71% occurs in scenario S5 while the lowest saving of 25% is achieved in S3. In S3 there is high demand level, low AM investment cost and low personnel cost all of which are factors that encourage the distributed deployment of AM factors. Hence, CONFIG2 performs its best in that scenario thereby making the cost saving from CONFIGOPT lower than in any other scenario. Comparing CONFIGOPT with CONFIG3, the most significant saving occurs in scenarios S1, S3, AND S4 where 7% of the total network cost from using CONFIG3 is saved. The least saving is in scenario S5 where only 1% of the cost is saved.

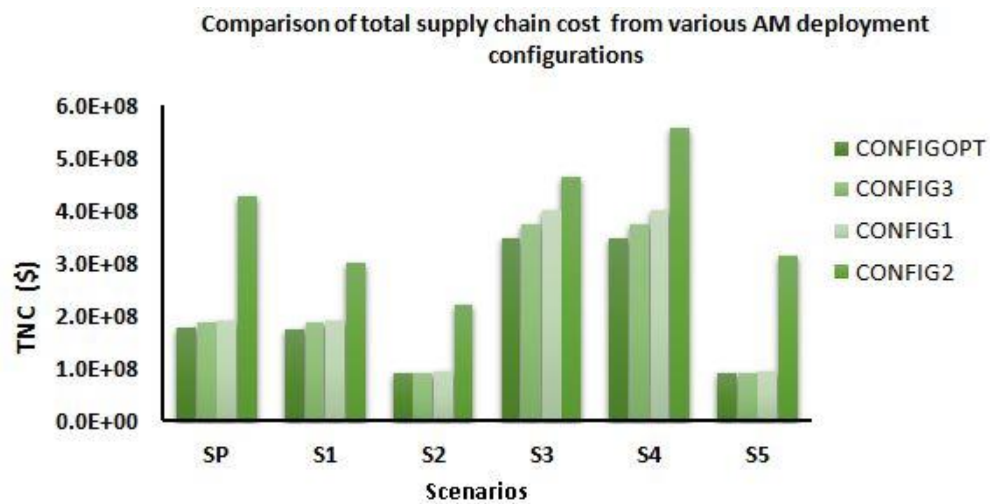


Figure 3.9 Comparing CONFIGOPT with other deployment configurations

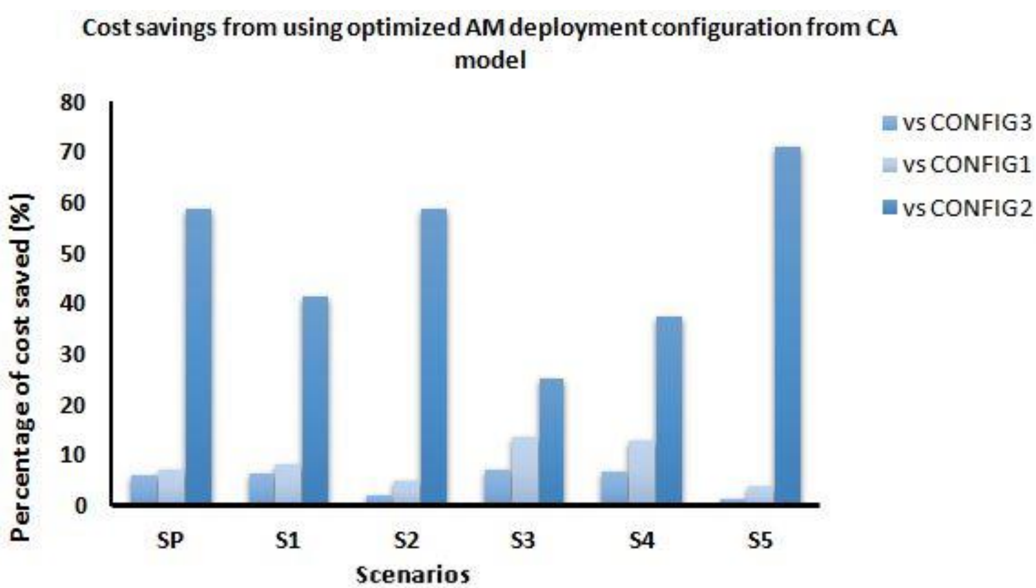


Figure 3.10 Cost savings from CONFIGOPT as a percentage of total network cost

Figure 3.11 shows CONFIGOPT, the optimal distribution of the AM facilities in the region as determined by our CA model to achieve the cost savings described above while Table 3.8 ranks the scenarios according to the number of AM facilities deployed in them.

Table 3.8 Ranking the Scenarios in a non-decreasing order of number of AM facility

Scenario	Personnel salary	Fixed AM cost	Demand	Number of AM facilities	Rank
S5	Increased	Decreased	Decreased	19	1
S2	Decreased	Decreased	Decreased	27	2
SP	Constant	Constant	Constant	27	3
S1	Decreased	Decreased	Constant	43	4
S4	Increased	Decreased	Increased	47	5
S3	Decreased	Decreased	Increased	68	6

We observe that the demand level of the bio-medical implants is the major factor that drives the number of AM facilities in the region, and thus how distributed the deployment should be for the simulated scenarios. The higher the demand, the more AM facilities to be established and the more distributed the network should be. Conversely, the lower the demand the less number of AM facilities and the less distributed. This corroborates the finding by Holmstrom et al. [60], Khajavi et al. [70] and Emelogu et al. [45]. Holmstrom et al. [60] and Khajavi et al. [70] find that enough demand for military jet spare parts at the service locations is required for distributed AM to be considered. Emelogu et al. [45] find that at higher demand levels of bio-medical implants, more AM facilities are established in a hybrid AM/TM supply chain. Given the present values of the supply chain cost parameters (Scenario SP), 27 AM facilities are located in the southeastern region with the states of Arkansas, Mississippi and West Virginia having the minimum number of one AM facility each, and the state of Florida having the maximum number of five AM facilities. The number of AM facilities deployed more than doubles to 68 in Scenario S3 where the demand is increased and both annual personnel salary and fixed AM machine investment cost decrease. In this case, the number of AM facilities located in West Virginia, Mississippi, Arkansas, and Florida increases to 2, 3, 4 and 13, respectively. We notice that the same number of AM facilities and configuration in SP is also used in Scenario S2 despite that the demand decreased. This is because both the annual personnel salary and the fixed AM investment cost decreased in S2 thereby compensating for the decrease in demand and making 27 AM facilities to be established as well.

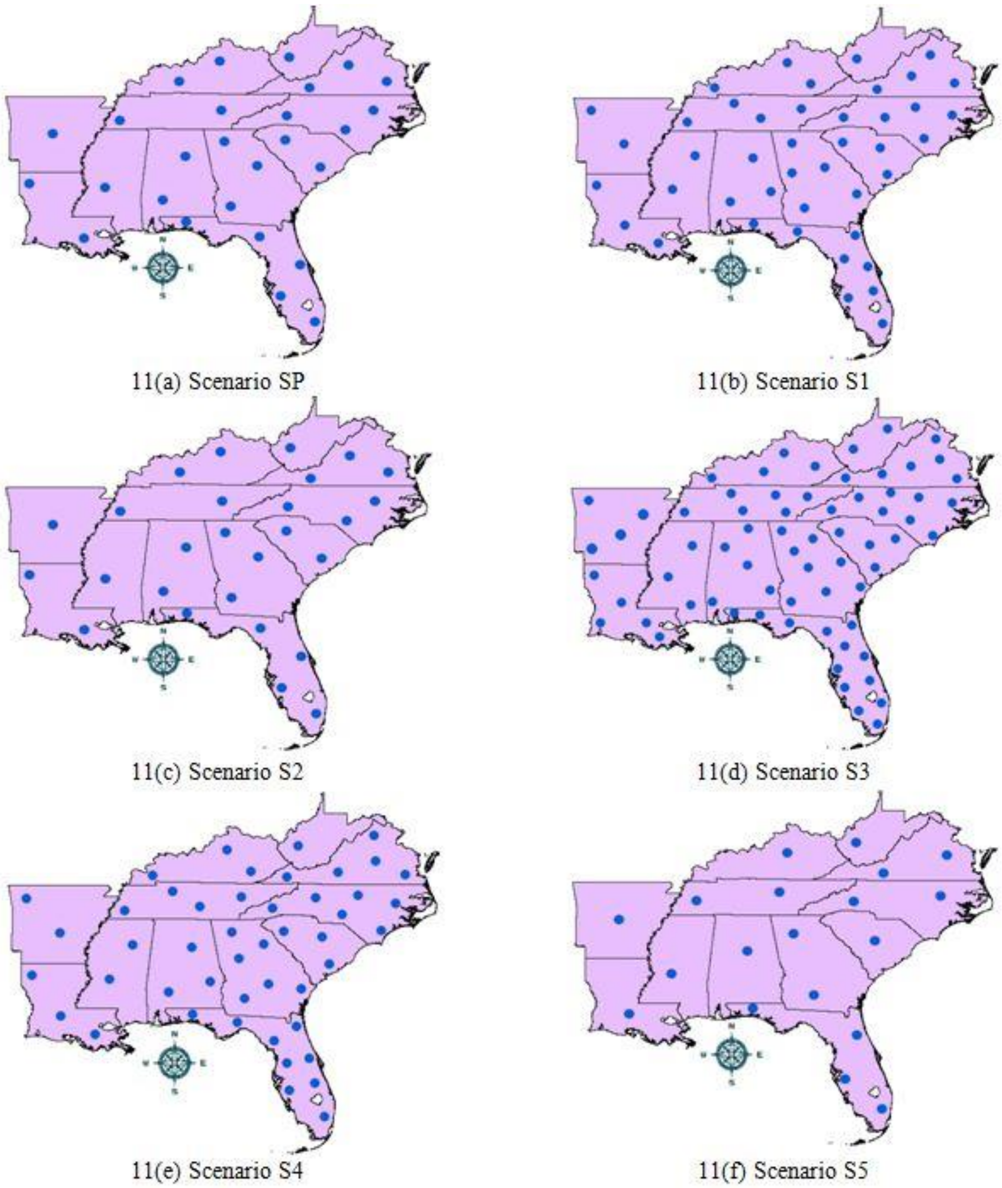


Figure 3.11 Optimal AM facility deployment in the southeastern USA for various scenarios

3.6 Conclusions

In this paper, we have developed a continuous approximation cost model to quantify the supply-chain level costs associated with the production of biomedical implants using Additive Manufacturing (AM) technologies, and developed the optimal deployment configuration of AM sites in the southeastern region of the United States for efficient and responsive fabrication of biomedical implants for use in hospitals and clinics in the region. Different from the existing studies that mainly focus on choosing between two extreme network configurations (one centralized location or many distributed locations) our hybrid approach is able to consider other configurations that are between the two ends of the spectrum where the optimal deployment decision usually lies. Unlike any other model in literature, ours is a two-stage formulation able to incorporate inventory decisions that inform the right amount of raw materials each location should order in the deployment configuration determination process. Given that the raw materials for the implants are expensive and not locally available, these inventory decisions are crucial and should be able to achieve a trade-off between having a large amount of raw materials which tie up capital and drives up cost but assure the on-demand promise of AM; and having few inventory which reduces inventory cost but risks increasing the lead time of AM and drastically reducing patient satisfaction.

(1) This study assumes that localized AM production of biomedical implants used in hospitals in the southeastern region of USA is feasible, without taking into account the demands of biomedical implants and hospitals that can perform similar procedures in other regions. However, the proposed continuous approximation model can be applied to a larger supply chain network that encompasses the entire country or account for other types of products, as long as the requisite hospital density data and demand for the remaining states or the information on other products are collected. The solutions of the larger scale cost model (i.e., the locations of AM facilities and order quantities) may only take a longer time to obtain using the

suggested algorithms by virtue of its scaling property. The model and algorithm proposed in this paper may be used as an analysis tool for decision makers to simulate and understand various network configuration options for AM deployment and choose the option that best suits their organizational objectives in terms of efficiency and responsiveness.

(2) We performed numerical experiments to analyze the effect of various network model parameters on the AM deployment and supply chain cost. We find that the demand level of the biomedical implants has the most significant effect on how many AM facilities should be located in the region and how distributed the deployment should be. Specifically, if other parameters are kept constant, doubling the demand, increases the number of AM facilities by more than 59%, thereby making the network more distributed, while the number reduces by up to 33% if the demand level is halved, making the network less distributed.

(3) Other factors such as the price and maintenance cost of AM machines, the labor cost of operating the machines and the unit transportation cost of an item per mile all affect the total supply chain network cost and deployment configuration of AM facilities. Reducing the fixed AM investment cost by 50% can result in an increase of up to 37% in the number of AM facilities established and reduce the total network cost by about $1.4 million or 0.8%.

(4) There is enormous cost saving in utilizing the proposed CA model to make the best AM deployment decision instead of using the extreme AM configuration options in literature. This cost saving advantage varies depending on the scenario of the supply chain parameters considered. Specifically, given the present demand data and supply

chain cost parameter values, we can achieve a saving of 7% of the total network cost by using the CA model instead of locating only one central AM facility to serve the entire region. The cost saving increases to 59% when compared with establishing an AM facility in every county in the region. The CA model records a ground-breaking saving of 71% of total network cost in a scenario where the demand of biomedical implants decrease by 50% and annual personnel cost doubles.

Future work is needed to improve the algorithm so that applying it to a network that covers the entire United States can yield a quick solution. We can modify the cost model to include uncertainties in the supply of raw materials or production rate of the AM machines to check what impact they will have on the AM deployment configuration decisions.

CHAPTER IV

AN ENHANCED SAMPLE AVERAGE APPROXIMATION METHOD FOR STOCHASTIC OPTIMIZATION

4.1 Introduction

Solving a large scale stochastic optimization problem is extremely challenging because of their inherent analytical complexities and high computational requirements ([73], [61], [140]). Sample Average Approximation (SAA) is a popular approach which is frequently employed to solve large scale stochastic optimization problems. In this method, the objective function value of the stochastic problem is unknown and approximated using a sample average estimate derived from a random sample ([2], [23], [30], [62], [125], [139]). SAA provides a straightforward framework which is amenable to parallel implementation and variance reduction techniques. Moreover, it possesses good convergence properties and well-developed statistical methods for validating solutions and conducting error analysis.

SAA has been successfully utilized to serve a wide range of applications, some of which include: reliability-based optimal design of engineering systems where the failure probabilities of highway bridges are replaced by corresponding Monte Carlo sampling estimates [126]; speech recognition optimization problem [28]; investment problem with conditional value at risk (CVaR) constraints [25]; portfolio selection and blending problems with chance-constraints [157]; stochastic knapsack problem to determine an optimum resource allocation strategy [73]; stochastic supply chain design problems with extremely large number of scenarios [136], and many others. The most significant challenge of using SAA confronted by the researchers in prior works is to choose the sample size for the algorithm. This is a critical step since it highly impacts the computational performance of the SAA algorithm. To address this challenge, a number of studies are conducted to determine the best scheme for choosing the sample size of the SAA algorithm. One stream of research focuses on keeping the sample size constant throughout the optimization process (e.g., [136], [156], [103]) . The major drawback of this approach is that it may lead to a bad sample path [61]. Another stream of research focuses on variable sample approach in which a schedule of sample sizes is used to solve the SAA problem (e.g., [125], [28], [61], [11], [40]). The general idea employed by the authors in variable sample scheme is to start the early iteration of the optimization algorithm with a small sample size and then gradually increase the sample size as the algorithm progresses. Note that starting with a small sample size may save some computational time; however, a large sample size eventually needs to be investigated to obtain a solution that is close to the true solution [99]. Therefore, all the methods discussed above may not perform well to solve stochastic discrete optimization problems. Although there is a theoretical sample size that can be used to compute sample sizes for discrete optimization problems (as shown in [73] and [61]), this estimate is too conservative for practical applications.

To address this challenge, this paper proposes a methodological approach to enhance the performance of the basic SAA by incorporating a dynamic clustering strategy within the algorithmic framework. In basic SAA, a small number of scenarios are generated in each iteration and the objective function is evaluated iteratively until the optimality gap falls below a certain threshold value. In our approach, a larger number of scenarios are considered as an initial sample size (much larger than the one used in basic SAA) and then clustering methods are employed to reduce this large sample size into small number of clusters. We assume that the average of each cluster is the most representative of all the samples in each cluster. We then represent those clusters as scenarios and use them to solve the SAA problem. Unlike prior studies where the sample size is either kept fixed or increased monotonically, our enhanced SAA approach provides the flexibility to either increase or decrease the sample size based on the computational performance obtained from previous iterations. This approach is then experimentally validated in the context of a facility location problem (**[FLP]**) with stochastic demand. We create different variants of the enhanced SAA algorithm (i.e., different clustering strategy, fixed clusters vs. dynamic clusters) and compare the computational performance of those variants with the basic SAA algorithm. Finally, we employ five different clustering techniques (e.g., K-means, K-means++, K-means||, Fuzzy C-means, and Mixed Integer Programming (MIP) based clustering techniques) and check how these clustering techniques affect the solution quality of the SAA algorithm.

The remainder of this paper is organized as follows. **Section 4.2** provides the literature review on SAA. **Section 4.3** introduces the enhanced SAA algorithm. **Section 4.4** conducts numerical experiments to verify the performance of the enhanced SAA algorithm. **Section 4.5** concludes this paper and discusses future research directions.

4.2 Literature review

We review the existing literatures related to SAA and categorize them into two major groups: (1) SAA with fixed sample size and (2) SAA with variable sample size.

4.2.1 SAA with fixed sample size

The first set of literature considers the basic SAA where the sample size remain fixed in all iterations. This approach is also referred to as *sample-path approximation* method ([56], [114]) or *stochastic counterpart* method ([128], [129], [138]) exploit the parallel implementation capability of the SAA to solve various two-stage stochastic linear programming problems with recourse. Kenyon and Morton [69] embed branch-and-cut inside the SAA to solve a stochastic vehicle routing problem under random travel and service times. Morton [99] develops an SAA procedure to solve a stochastic knapsack problem (SKP). Schütz, Tomasgard, and Ahmed [137] embed dual decomposition inside the SAA to solve a meat packing supply chain network designing problem. The authors investigate the effect of sample size on solution quality and find that increasing the sample size improves the solution quality of the SAA algorithm. Wang and Ahmed [157] use SAA to solve a conditional value-at-risk (CVaR) problem and find that the SAA solution is acceptable to the true CVaR problem with a probability of at least 97.7%.

Some other studies involving SAA implementations with fixed sample sizes are conducted by Kleywegt et al. [73], Verweij et al. [156], Santoso et al. [136] and Nemirovski et al. [103]. The major concurring theme among the studies in fixed sample SAA literature is that estimating the sample size in practice is not trivial and selecting the sample size involves two conflicting trade-offs: (i) larger sample sizes yield SAA solution comparable to the true solution and (ii) the computation effort required to solve the SAA problem often increases exponentially as the sample size increases. **Table 4.1** provides a summary of literature based on SAA with fixed sample size.

4.2.2 SAA with variable sample size

Later studies use variable sample size in SAA to solve stochastic optimization problems. Homem-De-Mello [61] first provides a variable-sample framework to solve a discrete stochastic optimization problem. The author shows that the sample size must grow at a certain rate to ensure convergence. Royset [125] proposes a closed-loop feedback optimal-control model to adaptively select sample sizes in variable sample average approximation (VSAA) algorithm to solve smooth stochastic programs (SSP). Although the method results in a sample size selection policy that appears to be robust to changing problem instances, it is not applicable to stochastic optimization problems with integer restrictions. Optimization problems that require integer solutions in their decision variables involve non-smooth functions which are not easily convertible to smooth functions for the application of the SAA method. Pasupathy [112] determines a balance choice of sample sizes and error tolerances in variable samples method of SAA where sample size refers to a measure of problem-generation effort and error tolerance is a measure of solution quality. Note that all the literature discussed above investigated problems in which SAA occurs only in the objective function.

Table 4.1 Summary of literature in SAA with fixed sample size

Ref.	Problem Type		Location of Sample Approximation		Sample type		Scenario Generation Strategy[a]	Application Area	Method	Limitations
	Constrained	Unconstrained	Objective	Constraints	*iid*	*non-iid*	Re-sampling			
(Linderoth et al. [85])	✓		✓			✓	✓	SOP[b] (MINLP[c])	L-shape two stage with recourse	Fixed Sample size
(Kenyon and Morton [69])	✓		✓		✓		✓	SOP (SVRP[d])	Branch and cut	Fixed Sample size
(Morton [99])	✓		✓		✓		✓	Stochastic knapsack problem	Fixed sample size at 30	Fixed Sample size
(Schütz et al. [137])	✓		✓		✓		✓	Supply chain design	Dual decomposition	Fixed Sample size
(Wang and Ahmed [157])	✓			✓	✓		✓	Portfolio selection	X	Fixed Sample size
(Verweij et al. [156])	✓		✓		✓		✓	Stochastic routing problems	Branch and cut	Fixed Sample size
(Santoso et al. [136])	✓		✓		✓		✓	Supply chain network design	Benders decomposition	Fixed Sample size at 20
(Nemirovski et al. [103])		✓	✓		✓		✓	Stochastic utility problem	X	Fixed Sample size

[a]No augmentation sampling study
[b]SOP: Stochastic optimization problem
[c]MINLP: Mixed integer non-linear problem
[d]SVRP: Stochastic vehicle routing problem

Another stream of research investigates problems in which SAA occurs in the constraints (e.g., [25], [163]). It is important to note that if the approximation occurs in the objective function then the major challenge relies on obtaining solutions that converge to the original problem. However, in cases where the approximation occurs in the constraints, i.e., in chance-constraints, one needs to ensure that the feasibility region of the approximating problem coincides with that of the original problem [25]. Branda [25] estimates the rate of convergence and sample size for lower bounds in SAA which ensures that the feasible solutions of the SAA are feasible for the original problem. Zhang et al. [163] develop a method for stochastic programs with complementary constraints where the equilibrium constraints can be replaced with smooth functions. Bastin et al. [16] implement variable sample size technique to estimate choice probabilities in solving unconstrained mixed logit models. Byrd et al. [28] develop a varying sample size based methodology to solve large scale machine learning problems. Similarly, a number of other related literatures such as Deng and Ferris [40], Krejić and Krklec [77], Krejic andJerinkic [76], Bastin et al. [16], Byrd et al. [28], and Bastin [15] study SAA with variable sample size to tackle different optimization problems with or without constraints. The literature for SAA with variable sample sizes is summarized in **Table 4.2**. Note that all the methods discussed above are not suitable for problems that have computationally expensive limit-state functions as they involve a large number of evaluations of such functions and their gradients.

Table 4.2 Summary of literature in SAA with variable sample size

Ref.	Problem Type		Location of Sample Approximation		Sample Size Sequence		Sample type		Scenario Generation Strategy		Application Area	Method	Limitations
	Constraints	Uncons Traints	Objective	Constraints	Incremental	Adaptive	*iid*	*non-iid*	Augmented	Re-sampling			
(Balaprakash et al. [11])		✓	✓		✓			✓		✓	Probabilistic TSP	Statistical t-test	Did not consider MINLP problems
(Bastin et al. [16])		✓	✓			✓	✓		✓		Logit Models	Parametric, trust-region context	Only unconstrained
(Bayraksan and Morton [18])	✓		✓		✓		✓			✓	SOP[a]	Parametric	Only increases
(Bayraksan and Morton [19])	✓		✓		✓		✓		✓	✓	SOP	Parametric	Not Adaptive
(Branda [25])	✓			✓				✓		✓	SOP (MINLP)	Convergence and H-calmness of constraints	Sample size only increases
(Byrd et al. [28])		✓	✓		✓		✓		✓		Speech recognition problem	Gradient-based (Variance of gradient)	Only unconstrained, only increasing size
(Chepuri and Homem-de-mello [30])	✓		✓			✓		✓		✓	SOP (SVRP[c])	CI Stat test, Cross Entropy	Not Adaptive
(Kleywegt et al. [73])	✓		✓		✓		✓				Stochastic knapsack problem	Optimality gap or variance of gap estimator	Only increasing, Not applied to MINLP
(Deng and Ferris [40])		✓	✓		✓		✓		Not specified		SOP (Quadratic functions)	Bayesian inference in trust region sufficient reduction	Non decreasing, Only unconstrained
(Homem-De-Mello [61])	✓		✓		✓		✓			✓	SOP (TSP[d])	Statistical t-test	Only increases
(Pasupathy [112])	✓		✓		✓		✓			✓	SRFP[b], SOP	Convergence Behavior	Not Adaptive
(Polak and Royset [115])	✓		✓		✓		✓		✓		SOP in structural design	Diagonalization scheme with auxiliary optimization problem	Only increasing, Not applied to MINLP
(Royset and Polak [126])	✓		✓		✓			✓		✓	Reliability-based Optimal design	Multiply by 5	Existence of function and gradient

Table 4.2 (continued)

(Royset and Szechtman [127])	✓		✓		✓		✓	Not specified	Various SOP	DP[e]	Only smooth SP's
(Zhang et al. [163])	✓		✓	✓	✓		✓	Not specified	SOP with complementary constraints	Multiply by 10	Constant multiple sample size
(Krejić and Krklec [77])		✓	✓			✓	✓	Maximum scenario generated at once	Linear regression models with noise	Parametric in line search framework.	Gradient of function must be known, unconstrained problem.
(Bastin [15])		✓	✓			✓	✓	✓	Logit Models	Parametric, trust-region context	Only unconstrained
(Krejic and Jerinkic [76])		✓	✓			✓	✓	Maximum scenario generated at once	Linear regression models with noise	Line search framework	Gradient should exist, unconstrained problem.

[a]SOP: Stochastic optimization problem
[b]SRFP: Stochastic root-finding problem
[c]SVRP: Stochastic vehicle routing problem
[d]TSP: Traveling salesman problem
[e]DP: Dynamic programming

To fill this gap in the literature, this paper utilizes different clustering techniques to dynamically adjust the scenario size of the SAA algorithm that generates a solution close to the true solution of the stochastic optimization problem. Until now, a limited number of studies consider scenario clustering to solve an optimization problem. Crainic, Hewitt, and Rei [35] propose a machine learning method to group scenarios of a progressive hedging algorithm and apply the approach in a stochastic network design problem. The authors further use clustering techniques inside a partial Benders decomposition algorithm to reduce the number of optimality and feasibility cuts generated by the algorithm. Escudero et al. [48] use scenario clustering inside a Lagrangean decomposition algorithm to produce high quality lower bounds for large scale multi-stage stochastic 0-1 problems. Our approach although relevant differs from the prior studies in that we apply scenario clustering to solve a large scale SAA problem. Moreover, our approach provides a simple framework that can be used to dynamically adjust the sample size of the SAA problem based on the results obtained from preliminary computations.

4.3 Methodology

This section first provides a brief introduction of the Sample Average Approximation (SAA) method (**Section 4.3.1**). We then highlight some of the limitations of the basic SAA method which pave the way for us to develop an enhanced Sample Average Approximation (**eSAA**) method. The **eSAA** method utilizes clustering techniques (e.g., K-means, K-means++, K-means||, Fuzzy C-means, and Mixed Integer Programming (MIP) based clustering techniques) and then adaptively controls the size of the samples by performing some statistical tests based on the computational performance from the previous iterations. The details of the **eSAA** method is discussed in **Section 4.3.2**. Let us now discuss the basic SAA method.

4.3.1 Sample average approximation (SAA)

The SAA is a Monte Carlo simulation–based approach to solve stochastic programming problems. The basic idea is simple indeed - a random sample is generated and the expected value function is approximated by the corresponding sample average function. The procedure is repeated several times until a stopping criterion is satisfied. The idea of using sample average approximations for solving stochastic programs has been studied extensively by various authors over the years. For example, the method was used to solve stochastic knapsack problems (e.g., [73]), stochastic routing problems (e.g., [156]), supply chain problems (e.g., [136]), investment problems (e.g., [111]), reliability-based problems (e.g., [126]), and many others.

To illustrate the concept of SAA, let us first investigate a general stochastic program of the following form:

$$\min\{\mathbb{E}[f(x,\omega)]: \mathrm{x} \in \boldsymbol{X}\} \tag{4.1}$$

where ω is a random vector with expectation $\mathbb{E}$ and a known statistical distribution p. The expectation $\mathbb{E}$ is with respect to p.

Let **X** denote the first-stage feasible set where $\mathbf{X} = \mathbf{R} \cap \{0, 1\}^n$ for some polyhedron **R** of dimension n and $\mathbf{\Omega}$ denote the set of scenarios. A special case of Equation (4.1) is the class of two-stage stochastic programming model which can be illustrated as follows:

$$\boldsymbol{z}^* = \min_{x \in \boldsymbol{X}} c^T x + \mathbb{E}_p[\mathcal{Q}(x, \xi(\omega))] \tag{4.2}$$

where

$$\mathcal{Q}\big(x, \xi(\omega)\big) = \min_{y \geq 0}\{q(\omega)^T y \mid Dy \geq h(\omega) - T(\omega)x\} \tag{4.3}$$

and *x* denotes the first-stage decisions which are required to be made prior to the realization of a scenario, ω ∈ **Ω,** and which is known when the second-stage recourse decisions *y* are made. The quantity $\mathcal{Q}\big(x, \xi(\omega)\big)$ represents the optimal value of the second-stage recourse problem and the parameters $\xi(\omega) = (q(\omega), h(\omega), T(\omega))$. Let, **Ω** contains a finite number of scenarios $\{\omega_1, \omega_2, \dots, \omega_{|\boldsymbol{\Omega}|}\}$with associated probabilities $\{p_n\}; n = 1,2, \dots, |\boldsymbol{\Omega}|$, then the expectation $\mathbb{E}[\mathcal{Q}(x, \xi(\omega))]$ can be evaluated as follows:

$$\mathbb{E}\big[\mathcal{Q}\big(x, \xi(\omega)\big)\big] = \sum_{n=1}^{|\boldsymbol{\Omega}|} p_n \mathcal{Q}(x, \xi(\omega_n)) \tag{4.4}$$

From Equation (4.4), it is clear that the number of scenarios grows exponentially with the size of the problem. To overcome this issue, an exterior sampling method is used to solve the deterministic equivalent problem of the problem specified by (4.2). The SAA method is an exterior sampling method in which a sample $\omega_1, \omega_2, \dots, \omega_N$ of **N** sample scenarios is generated from scenario set **Ω** according to the probability distribution *P* and then the expected value function $\mathbb{E}[\mathcal{Q}(x, \xi(\omega))]$ is approximated by the sample average function $\sum_{n=1}^{\boldsymbol{N}} \mathcal{Q}(x, \xi(\omega^n))/\boldsymbol{N}$. The Sample Average Approximation problem then becomes:

$$\boldsymbol{z^N} = \min_{x \in \boldsymbol{X}} c^T x + \frac{1}{\boldsymbol{N}} \sum_{n=1}^{\boldsymbol{N}} \mathcal{Q}(x, \xi(\omega^n)) \tag{4.5}$$

where $\mathbf{z^N}$ and $\hat{x}$ estimate the optimal value and solution of their true counterparts in the original stochastic program defined by Equation (4.2).

The steps involved in solving a stochastic problem using *Sample Average Approximation (SAA)* are given below:

Step 1: Generate **M** independent samples each of size **N** and solve the corresponding SAA:

$$\boldsymbol{z^N} = \min_{x \in \boldsymbol{X}} c^T x + \frac{1}{\boldsymbol{N}} \sum_{n=1}^{\boldsymbol{N}} \mathcal{Q}(x, \xi(\omega^n)) \tag{4.6}$$

Let $\boldsymbol{z_N^m}$ and $\boldsymbol{X_N^m}$ be the corresponding optimal solutions and an optimal values, respectively; m=1, 2, 3,…, **M**.

Step 2: Compute:

$$\bar{\boldsymbol{z}}_{\boldsymbol{M}}^{\boldsymbol{N}} = \frac{1}{\boldsymbol{M}} \sum_{m=1}^{\boldsymbol{M}} \boldsymbol{z_N^m} \tag{4.7}$$

$$\sigma_{z_{\boldsymbol{M}}^{\boldsymbol{N}}}^2 = \frac{1}{(\boldsymbol{M}-1)\boldsymbol{M}} \sum_{m=1}^{\boldsymbol{M}} \left(\boldsymbol{z_N^m} - \bar{\boldsymbol{z}}_{\boldsymbol{M}}^{\boldsymbol{N}}\right)^2 \tag{4.8}$$

The expected value of $\mathbf{z^N}$ is less than or equal to the optimal value **z*** of the true problem. Since $\bar{\boldsymbol{z}}_{\boldsymbol{M}}^{\boldsymbol{N}}$ is an unbiased estimator of $\mathbb{E}\left[\bar{\boldsymbol{z}}_{\boldsymbol{M}}^{\boldsymbol{N}}\right]$ and $\mathbb{E}\left[\bar{\boldsymbol{z}}_{\boldsymbol{M}}^{\boldsymbol{N}}\right] \leq \boldsymbol{z}^*$, we can say that $\bar{\boldsymbol{z}}_{\boldsymbol{M}}^{\boldsymbol{N}}$ provides a lower statistical bound for **z*** of the true problem and $\sigma_{\boldsymbol{V_M^N}}^2$ is an estimate of the variance of this estimator.

Step 3: Choose a feasible first-stage solution $\hat{x} \in \boldsymbol{X}$ of the true problem, e.g., one of the solutions from $\boldsymbol{X}_{\boldsymbol{N}}^{\boldsymbol{m}}$ and estimate the objective function value of the original problem (4.2) using a different sample $\boldsymbol{N'}$. The true objective function value is now given as:

$$\boldsymbol{z}^{\boldsymbol{N'}}(\hat{x}) = c^T\hat{x} + \frac{1}{\boldsymbol{N'}}\sum_{n=1}^{\boldsymbol{N'}} Q(\hat{x}, \xi(\omega^n)) \qquad 4.9)$$

where $\{\omega_1, \omega_2, \dots, \omega_{\boldsymbol{N'}}\}$ is a sample of size $\mathbf{N'}$. Typically, $\mathbf{N'}$ is chosen to be much larger than **N** i.e., $\mathbf{N'} \gg \mathbf{N}$. The estimator $\boldsymbol{z}^{\boldsymbol{N'}}(\hat{x})$ is an unbiased estimator of $c^T\hat{x} + \mathbb{E}[Q(\hat{x}, \xi(\omega))]$. Thus, for any feasible solution we have $\mathbb{E}[\boldsymbol{z}^{\boldsymbol{N'}}(\hat{x})] \geq \boldsymbol{z}^*$. The value of $\boldsymbol{z}^{\boldsymbol{N'}}(\hat{x})$ is updated in each iteration if the obtained value is less than the value of the previous iteration. The variance of this estimate can be expressed as:

$$\hat{\sigma}^2_{\boldsymbol{z}^{\boldsymbol{N'}}(\hat{x})} = \frac{1}{(\boldsymbol{N'}-1)\boldsymbol{N'}}\sum_{n=1}^{\boldsymbol{N'}} \left(c^T\hat{x} + Q\big(\hat{x}, \xi(\omega^n)\big) - \boldsymbol{z}^{\boldsymbol{N'}}(\hat{x})\right)^2 \qquad (4.10)$$

Step 4: Compute an estimate of the optimality gap of the solution $\hat{x}$ using the lower bound estimate and upper estimates by using the estimators calculated in **Steps 2** and **3**, respectively, as follows:

$$Gap_{\boldsymbol{N},\boldsymbol{M},\boldsymbol{N'}}(\hat{\boldsymbol{x}}) = \boldsymbol{z}^{\boldsymbol{N'}}(\hat{x}) - \bar{\boldsymbol{z}}_{\boldsymbol{M}}^{\boldsymbol{N}} \qquad (4.11)$$

The estimated variance of the gap is given by:

$$\sigma^2_{gap} = \hat{\sigma}^2_{\boldsymbol{z}^{\boldsymbol{N'}}(\hat{x})} + \sigma^2_{\boldsymbol{z}_{\boldsymbol{M}}^{\boldsymbol{N}}} \qquad (4.12)$$

The confidence interval for the optimality gap can be calculated as:

$$\boldsymbol{z}^{\boldsymbol{N'}}(\hat{x}) - \bar{\boldsymbol{z}}_{\boldsymbol{M}}^{\boldsymbol{N}} + z_\alpha\{\hat{\sigma}^2_{\boldsymbol{z}^{\boldsymbol{N'}}(\hat{x})} + \sigma^2_{\boldsymbol{z}_{\boldsymbol{M}}^{\boldsymbol{N}}}\}^{0.5} \qquad (4.13)$$

with $z_\alpha := \Phi^{-1}(1\text{-}\alpha)$, where $\Phi(\boldsymbol{z})$ is the cumulative distribution of the standard normal distribution.

Step 5: We now choose $\widehat{\boldsymbol{x}}^*$ as one optimal solution $\widehat{\boldsymbol{x}}^{\mathbf{1}}, \widehat{\boldsymbol{x}}^{\mathbf{2}}, \ldots, \widehat{\boldsymbol{x}}^{\boldsymbol{M}}$ which has the smallest objective value, i.e.,

$$\widehat{\boldsymbol{x}}^* \in \arg\min\left\{\boldsymbol{z}^{\boldsymbol{N}'}(\hat{x}) : \hat{x} \in \{\widehat{\boldsymbol{x}}^{\mathbf{1}}, \widehat{\boldsymbol{x}}^{\mathbf{2}}, \ldots, \widehat{\boldsymbol{x}}^{\boldsymbol{M}}\}\right\} \tag{4.14}$$

As described in **Step 1** of SAA, $\boldsymbol{z}_{\boldsymbol{N}}^{\boldsymbol{m}}$ and $\boldsymbol{X}_{\boldsymbol{N}}^{\boldsymbol{m}}$ are functions of the corresponding random sample. Under mild regularity conditions, it can be proved that as the sample size **N** increases, both $\boldsymbol{z}_{\boldsymbol{N}}^{\boldsymbol{m}}$ and $\boldsymbol{X}_{\boldsymbol{N}}^{\boldsymbol{m}}$ converge with probability one to their true counterparts. The convergence is captured in **Proposition 4.1** as follows:

Proposition 4.1: Let $\hat{\theta}_N$ and θ^* be the objective value of the SAA and true problem, respectively. We prove that $\hat{\theta}_N \to \theta^*$ and $D(\hat{x}_N, x^*) \to 0$ with probability 1 as $N \to \infty$, where $D(\hat{x}_N, x^*)$ is the difference between the optimal solution for the SAA problem and the optimal solution for the true problem.

Proof: The proof of this proposition is given by Kleywegt et al. [73]. ■

The analysis regarding convergence suggests that a reasonable and good approximate solution to the true problem can be obtained by solving an SAA problem with a modest sample size. In particular, suppose that the SAA problem is solved to an absolute optimality gap of $\delta \geq 0$ and let $\boldsymbol{\epsilon} > \delta$ and $\alpha \in (0,1)$. Then, a sample size of

$$\mathbf{N} > \frac{3\sigma_{max}^2}{(\epsilon - \delta)^2} \log\left(\frac{|\boldsymbol{X}|}{\alpha}\right) \tag{4.15}$$

ensures that the SAA solution by $\mathbf{X}_\mathbf{N}$ is a solution with an absolute optimality gap of $\boldsymbol{\epsilon}$ to the true problem with a probability of at least 1-α. Here σ_{max}^2 is a maximal variance of certain function differences (see [1] for details). This estimate has interesting consequences in terms of complexity of the problem. One of the main characteristics of Equation (4.15) is that **N** depends only logarithmically on the size of the feasible set **X** as well as on the tolerance probability α.

It appears that Equation (4.15) may be very conservative for practical estimates. Thus, one can choose the sample size **N** as a trade-off between the qualities of solution obtained from solving problem (4.6) and the computational complexity to solve it. Unfortunately, fixing a value of **N** is not very straightforward as it imposes complexity in solving **Step 1** of the SAA algorithm. Even though the introduction of SAA reduces the problem size considerably compared to the original problem (defined by (4.2)), we still have to solve a two-stage stochastic mixed integer problem with **N** scenarios which is computationally challenging as well as time-consuming. In particular, with large **N** the objective function of the SAA problem tends to be more accurate than the objective function of the true problem and thus expected to produce a tighter optimality gap. However, this increases computational complexity in solving the SAA problem which in some cases increases at least linearly and often exponentially as the size of **N** increases. On the other hand, a conservative **N** may lead to an ϵ-optimal solution to the true problem though the solution can be obtained at a reasonable time. Thus, choosing the right sample size **N** requires further investigation which motivates us to develop an enhanced Sample Average Approximation (**eSAA**) algorithm that dynamically adjust the sample size **N** based on the results from preliminary computations. It is noteworthy that the eSAA method can equally be applied when the stochastic programming problem requires all the decision variables to be continuous. In such a case, the problem becomes much easier to solve since there is no integer restrictions to solve the subproblems of the eSAA algorithm. The details of the **eSAA** algorithm is discussed in the next subsection.

4.3.2 Enhanced sample average approximation (eSAA)

In this study, we take a novel approach to obtaining samples and establishing sample size to be used in the SAA that are better representatives of the scenarios in the stochastic optimization problem. Specifically, we use some clustering algorithms (e.g., K-means, K-means++, K-means||, Fuzzy C-means, and Mixed Integer Programming (MIP) based clustering techniques) to group similar scenarios and obtain a sample size equal to the number of clusters. We then use this clustered scenarios to obtain a lower bound for our SAA problem which is indeed a lower bound for the true problem. Unlike other approaches in literature where the sample size is either increased or kept constant, our **eSAA** approach provides the opportunity to adaptively control the size of the samples. Based on the solution obtained after each iteration, we perform a *t*-test which guides us to adaptively increase or decrease the size of the samples **N** until the quality of the solution falls below an acceptable tolerance level. Moreover, the **eSAA** approach enables us to work with a bigger sample size ($\mathbf{N_K}$) compared to basic SAA (**N**), thereby increasing the chance of the approximation converging to the solution of the true problem.

To better illustrate our approach, let us consider a solution space $\mathbf{\Omega}$ which contains all the possible scenarios $\omega_1, \omega_2, \ldots, \omega_N$ generated in a stochastic program (shown in **Figure 4.1(a)**). In basic SAA, from this scenario pool, a small number of scenarios is taken as samples (say **N**) and the objective function is calculated iteratively until the optimality gap falls below a certain threshold value. However, in **eSAA** we group the scenarios in the form of a cluster where each cluster contains the scenarios that are most representative to that cluster (shown in **Figure 4.1(b)**). The number of scenarios in each cluster will now be reduced down to the number of scenarios (say $\mathbf{N_K}$) for the **eSAA** algorithm (shown in **Figure 4.1(c)**). Let $\mathbf{N_L}$ be the number of scenarios drawn from scenario space $\mathbf{\Omega}$ where $\mathbf{N_L} \gg \mathbf{N}$. We then partition sample $\mathbf{N_L}$ into a fixed number of clusters, say $\boldsymbol{k}$ clusters. Following the clustering, we take one sample from each cluster which represents the best from that given cluster and eventually reduced down to $\mathbf{N_K}$ number of clusters where $\mathbf{N_K} \ll \mathbf{N} \ll \mathbf{N_L}$. The expected value function $\mathbb{E}[\mathcal{Q}(x, \xi(\omega))]$ now can be approximated by the sample average function $\sum_{n=1}^{\boldsymbol{N_K}} \mathcal{Q}(x, \xi(\omega^n))/\boldsymbol{N_K}$. The Sample Average Approximation problem then becomes:

$$\boldsymbol{z}^{\boldsymbol{N_K}} = \min_{x \in \boldsymbol{X}} c^T x + \frac{1}{\boldsymbol{N_K}} \sum_{n=1}^{\boldsymbol{N_K}} \mathcal{Q}(x, \xi(\omega^n)) \tag{4.16}$$

where $\boldsymbol{z}^{\boldsymbol{N_K}}$ and $\hat{x}^K$ estimate the optimal value and solution of their true counterparts in the original stochastic program defined by Equation (4.2).

The steps involved in solving a stochastic problem using the enhanced Sample Average Approximation (**eSAA**) algorithm are illustrated below:

Step 1: Initialize, cluster size $\boldsymbol{k}$, step size $\boldsymbol{q_1}$ and $\boldsymbol{q_2}$ where $\boldsymbol{q_2} > \boldsymbol{q_1}$ and counter $\boldsymbol{g}$. Generate $\mathbf{M}$ independent samples each of size $\mathbf{N_L}$ where $\mathbf{N_L} \gg \mathbf{N}$. Use one of the clustering technique (e.g., K-means, K-means++, K-means||, Fuzzy C-means, and Mixed Integer Programming (MIP) based clustering techniques) described in **Section 4.3.2.1** to **4.3.2.4** to cluster $\mathbf{N_L}$ samples. The $\mathbf{N_L}$ samples can now be partitioned into $\boldsymbol{k}$ number of clusters and yields $\mathbf{N_K}$ number of scenarios where $\mathbf{N_K} \ll \mathbf{N}$. With $\mathbf{N_K}$ number of scenarios, we solve the following SAA problem:

$$\boldsymbol{z}^{\boldsymbol{N_K}} = \min_{x \in \boldsymbol{X}} c^T x + \frac{1}{\boldsymbol{N_K}} \sum_{n=1}^{\boldsymbol{N_K}} \mathcal{Q}(x, \xi(\omega^n)) \tag{4.17}$$

Let $\boldsymbol{z}_{\boldsymbol{N_K}}^{\boldsymbol{m}}$ and $\boldsymbol{X}_{\boldsymbol{N_K}}^{\boldsymbol{m}}$ be the corresponding optimal solutions and an optimal values, respectively; *m=1, 2, 3,…,* **M**.

Step 2: Compute:

$$\bar{\boldsymbol{z}}_{\boldsymbol{M}}^{\boldsymbol{N_K}} = \frac{1}{\boldsymbol{M}} \sum_{m=1}^{\boldsymbol{M}} \boldsymbol{z}_{\boldsymbol{N_K}}^{\boldsymbol{m}} \tag{4.18}$$

$$\sigma^2_{\boldsymbol{z}_{\boldsymbol{M}}^{\boldsymbol{N_K}}} = \frac{1}{(\boldsymbol{M}-1)\boldsymbol{M}} \sum_{m=1}^{\boldsymbol{M}} \left(\boldsymbol{z}_{\boldsymbol{N_K}}^{\boldsymbol{m}} - \bar{\boldsymbol{z}}_{\boldsymbol{M}}^{\boldsymbol{N_K}}\right)^2 \tag{4.19}$$

The expected value of $\boldsymbol{z}^{\boldsymbol{N_K}}$ is less than or equal to the optimal value **z*** of the true problem. Since $\bar{\boldsymbol{z}}_{\boldsymbol{M}}^{\boldsymbol{N_K}}$ is an unbiased estimator of $\mathbb{E}\left[\bar{\boldsymbol{z}}_{\boldsymbol{M}}^{\boldsymbol{N_K}}\right]$ and $\mathbb{E}\left[\bar{\boldsymbol{z}}_{\boldsymbol{M}}^{\boldsymbol{N_K}}\right] \leq \boldsymbol{z}^*$, we can say that $\bar{\boldsymbol{z}}_{\boldsymbol{M}}^{\boldsymbol{N_K}}$ provides a lower statistical bound for **z*** of the true problem and $\sigma^2_{\boldsymbol{V}_{\boldsymbol{M}}^{\boldsymbol{N_K}}}$ is an estimate of the variance of this estimator.

Step 3: Choose a feasible first-stage solution $\hat{x} \in \boldsymbol{X}$ of the true problem, e.g., one of the solutions from $\boldsymbol{X}_{\boldsymbol{N_K}}^{\boldsymbol{m}}$ and estimate the objective function value of the original problem (4.2) using a different sample $\mathbf{N'}$ where $\mathbf{N_K} \ll \mathbf{N} \ll \mathbf{N_L} \ll \mathbf{N'}$. The true objective function value is now given as follows:

$$\boldsymbol{z}^{\boldsymbol{N'}}(\hat{x}) = c^T \hat{x} + \frac{1}{\boldsymbol{N'}} \sum_{n=1}^{\boldsymbol{N'}} \mathcal{Q}(\hat{x}, \xi(\omega^n)) \tag{4.20}$$

where $\{\omega_1, \omega_2, \ldots, \omega_{N'}\}$ is a sample of size $\mathbf{N'}$. Typically, $\mathbf{N'}$ is chosen to be much larger than $\mathbf{N}$ i.e., $\mathbf{N'} \gg \mathbf{N}$. The estimator $\boldsymbol{z}^{\boldsymbol{N'}}(\hat{x})$ is an unbiased estimator of $c^T\hat{x} + \mathbb{E}[Q(\hat{x}, \xi(\omega))]$ and thus for any feasible solution we have that $\mathbb{E}[\boldsymbol{z}^{\boldsymbol{N'}}(\hat{x})] \geq \boldsymbol{z}^*$. The value of $\boldsymbol{z}^{\boldsymbol{N'}}(\hat{x})$ is updated in each iteration if the obtained value is less than the value of the previous iteration. The variance of this estimate can be expressed as:

$$\hat{\sigma}^2_{\boldsymbol{z}^{\boldsymbol{N'}}(\hat{\boldsymbol{x}})} = \frac{1}{(\boldsymbol{N'}-1)\boldsymbol{N'}} \sum_{n=1}^{\boldsymbol{N'}} \left(c^T\hat{x} + Q\big(\hat{x}, \xi(\omega^n)\big) - \boldsymbol{z}^{\boldsymbol{N'}}(\hat{x})\right)^2 \tag{4.21}$$

Step 4: Compute an estimate of the optimality gap of the solution $\hat{x}$ using the lower bound estimate and upper estimates by using the estimators calculated in **Steps 2** and **3**, respectively, as follows:

$$Gap_{\boldsymbol{N},\boldsymbol{M},\boldsymbol{N'}}(\hat{\boldsymbol{x}}) = \boldsymbol{z}^{\boldsymbol{N'}}(\hat{x}) - \bar{\boldsymbol{z}}_{\boldsymbol{M}}^{\boldsymbol{N_K}} \tag{4.22}$$

The estimated variance of the gap is given by:

$$\sigma^2_{gap} = \hat{\sigma}^2_{\boldsymbol{z}^{\boldsymbol{N'}}(\hat{\boldsymbol{x}})} + \sigma^2_{\boldsymbol{z}_{\boldsymbol{M}}^{\boldsymbol{N_K}}} \tag{4.23}$$

The confidence interval for the optimality gap can be calculated as:

$$\boldsymbol{z}^{\boldsymbol{N'}}(\hat{x}) - \bar{\boldsymbol{z}}_{\boldsymbol{M}}^{\boldsymbol{N_K}} + z_\alpha \{\hat{\sigma}^2_{\boldsymbol{z}^{\boldsymbol{N'}}(\hat{\boldsymbol{x}})} + \sigma^2_{\boldsymbol{z}_{\boldsymbol{M}}^{\boldsymbol{N_K}}}\}^{0.5} \tag{4.24}$$

with $z_\alpha := \Phi^{-1}(1\text{-}\alpha)$, where $\Phi(\boldsymbol{z})$ is the cumulative distribution of the standard normal distribution.

Step 5: If the optimality gap $(\boldsymbol{z}^{\boldsymbol{N}'}(\hat{x}) - \bar{\boldsymbol{z}}_{\boldsymbol{M}}^{\boldsymbol{N_K}})$ is less than or equal to the tolerance limit $(\boldsymbol{\epsilon})$, the approximated solution is assumed to converge to the true solution $\boldsymbol{z}^*$. Otherwise, do the following:

- Perform a paired *t*-test between present solution obtained at iteration *i* and iteration *i*-1 to test the hypothesis $H_0: \boldsymbol{z}_{\mathrm{i}}^{\boldsymbol{N}'}(\hat{x}) = \boldsymbol{z}_{\mathrm{i}-1}^{\boldsymbol{N}'}(\hat{x})$
- If the *p*-value of the test is large (say greater than or equal to 0.2), then set $\boldsymbol{k} \leftarrow \boldsymbol{k}$ and $\boldsymbol{g} \leftarrow \boldsymbol{g} + \mathbf{1}$. If **g** > **b** (say **b** = 2) then set $\boldsymbol{k} \leftarrow \boldsymbol{k} - \boldsymbol{q}_{\mathbf{1}}$ and go to **Step 1**.
- If the *p*-value of the test is sufficiently small (say smaller than 0.1) then set $\boldsymbol{k} \leftarrow \boldsymbol{k} + \boldsymbol{q}_{\mathbf{2}}$ and go to **Step 1**.

Step 6: We now choose $\widehat{\boldsymbol{x}}^*$as one optimal solution $\widehat{\boldsymbol{x}}_{\boldsymbol{k}}^{\mathbf{1}}, \widehat{\boldsymbol{x}}_{\boldsymbol{k}}^{\mathbf{2}}, \ldots, \widehat{\boldsymbol{x}}_{\boldsymbol{k}}^{\boldsymbol{M}}$ which has the smallest objective value, i.e.,

$$\widehat{\boldsymbol{x}}^* \in \arg\min\left\{\boldsymbol{z}^{\boldsymbol{N}'}(\hat{x}) : \hat{x} \in \left\{\widehat{\boldsymbol{x}}_{\boldsymbol{k}}^{\mathbf{1}}, \widehat{\boldsymbol{x}}_{\boldsymbol{k}}^{\mathbf{2}}, \ldots, \widehat{\boldsymbol{x}}_{\boldsymbol{k}}^{\boldsymbol{M}}\right\}\right\} \tag{4.25}$$

One of the salient features of our **eSAA** algorithm is that unlike other studies where we either fix the scenario size (e.g., [136], [156], [103], [99], [85], [69], [137], [157]) or driving one way to determine whether the number of clusters should be increased or not (e.g., [61]), our approach guides the scenario size **N** by either increasing or decreasing them based on the computational performance obtained from prior iterations. We have revised **Step 1** and **Step 5** of the basic sample average approximation algorithm (described in **Section 4.3.1**) where we cluster a large sample size $\mathbf{N_L}$ to start with an initial sample size $\mathbf{N_K}$ (discussed in **Step 1**) and perform a paired *t*-test to check if the objective function value at the current iteration is statistically different than the previous one (discussed in **Step 5**). Note that, a paired *t*-test is required in this case rather than an independent *t*-test, since the estimates $\boldsymbol{z}_{\mathrm{i}}^{\boldsymbol{N'}}(\hat{x})$ and $\boldsymbol{z}_{\mathrm{i-1}}^{\boldsymbol{N'}}(\hat{x})$ use the same random numbers. In what follows, we prove that:

(i) The solution obtained using the **eSAA** algorithm converges to the solution of the true problem (shown in **Proposition 4.2**).

(ii) The algorithm terminates in a finite number of iterations (shown in **Proposition 4.3**).

Proposition 4.2: Let $\hat{\theta}_{N_k}$ and θ^* be the objective value of the **eSAA** and true problem, respectively. We further define$D\left(\hat{x}_{N_k}, x^*\right)$ be the difference between the optimal solution for the **eSAA** problem and true problem. We then proof that $\hat{\theta}_{N_k} \to \theta^*$ and $D\left(\hat{x}_{N_k}, x^*\right) \to 0$ with probability 1 as $N_k \to \infty$.

Proof: Step 5 of the **eSAA** algorithm ensures that if the value of $\hat{\theta}_{N_k}$ does not converge to the true problem, then the size of $\boldsymbol{k'}$ increases through the expression $\boldsymbol{k'} \leftarrow \boldsymbol{k} + \boldsymbol{q_2}$, where $\boldsymbol{q_2}$ is a positive integer. In the worst case, if no improvements are found then the size of the cluster $\boldsymbol{k'}$ approaches to infinity i.e., $\boldsymbol{k'} \leftarrow \infty$. At this point $\hat{\theta}_{N_k} \to \theta^*$, which is guaranteed through **Proposition 4.1**. ■

Proposition 4.3: The **eSAA** algorithm terminates in a finite number of iterations.

Proof: The sample sizes $\boldsymbol{N_L}, \boldsymbol{N}, \boldsymbol{N_k}$ used in the **eSAA** algorithm are finite. Moreover, the feasibility region provided by *x* is finite. Since **Proposition 4.2** holds, we can deduce that **eSAA** algorithm will terminate in a finite number of iterations. ■

Some questions arise in the process of implementing our proposed **eSAA** algorithm such as: **(a)** Does clustering provide representative scenarios that yield comparable lower bounds as basic SAA? **(b)** Is there a saving in computational time for using clustering algorithm and representative scenarios in our approach versus using all the scenarios in SAA without clustering? In other words, does the saving in computation time due to the reduced number of scenarios offset the clustering time in our approach? We investigate these issues using numerical experiments in **Section 4.4**. Meanwhile, our methodology for creating groups or clusters of similar scenarios are inspired by a set of clustering methods*, i.e.,* K-means clustering, K-means++ clustering, K-means|| clustering, Fuzzy C-means clustering, and Mixed Integer Programming (MIP) clustering. We now present a brief description of all these clustering methodologies applied in our **eSAA** algorithm.

4.3.2.1 K-means clustering

K-means algorithm which is sometimes referred to as Lloyd's algorithm was proposed in 1957 by Stuart Lloyd [87]. K-means method is one of the most popular unsupervised learning algorithms that follow a simple, easy and relatively efficient way to classify a given data set into a certain number of clusters fixed a priori. It works in two phases. In the first phase, initial ***k*** centers are chosen at random. In the second phase, each point in the data set is assigned to the cluster containing the center that is nearest to it. At the end of this phase, the center value of each cluster is calculated, and depending upon the new values of centers, the second phase is repeated until the values of centers converge to the same value. The complexity of this algorithm is $O(nkl)$, where n is the number of data points, ***k*** is the number of clusters, and l is the number of iterations needed until convergence.

To explain K-means algorithm mathematically, let $\mathbf{X} = \{x_1,\ x_2, \dots, x_n\}$ be a set of points that has to be partitioned into $\boldsymbol{k}$ clusters. The objective is to assign a cluster to each data point in such a way that the positions $\mu_i, i = 1,2, \dots, \boldsymbol{k}$ of the clusters minimize the distance from the data points to the cluster. Essentially, K-means clustering solves:

$$arg\ min_r \sum_{i=1}^{\boldsymbol{k}} \sum_{x \in \boldsymbol{r}_i} d(x, \mu_i) \tag{4.26}$$

Here, $\boldsymbol{r_i}$ is the set of points that belongs to cluster *i*. The steps involved in K-means clustering algorithm are illustrated in **Algorithm 4.1**.

Algorithm 4.1: K-means clustering algorithm

1: $\mathbf{X} \leftarrow$ Set of data points
2: $\boldsymbol{k} \leftarrow$ Total number of clusters
3: Randomly select $\boldsymbol{k}$ cluster centers from **X**
4: $\mu_i \leftarrow \boldsymbol{k}$ cluster centers, where *i=1,2,…,k*
5: $\boldsymbol{r_i} \leftarrow$ set of points that belongs to cluster *i*, where *i=1,2,…,k*
6: Attribute the nearest cluster to each data point:
$$\boldsymbol{r_i} = \{j: d(x_i, \mu_i) \leq d(x_j, \mu_m),\ m \neq i, j = 1,2, \dots, n\}$$
7: Fix the position of each cluster to the mean of all points belonging to that cluster:
$$\mu_i = \frac{1}{|\boldsymbol{r_i}|} \sum_{j \in \boldsymbol{r_i}} x_{j,} \forall i$$
8: Repeat **Steps 6** and **7** until convergence.

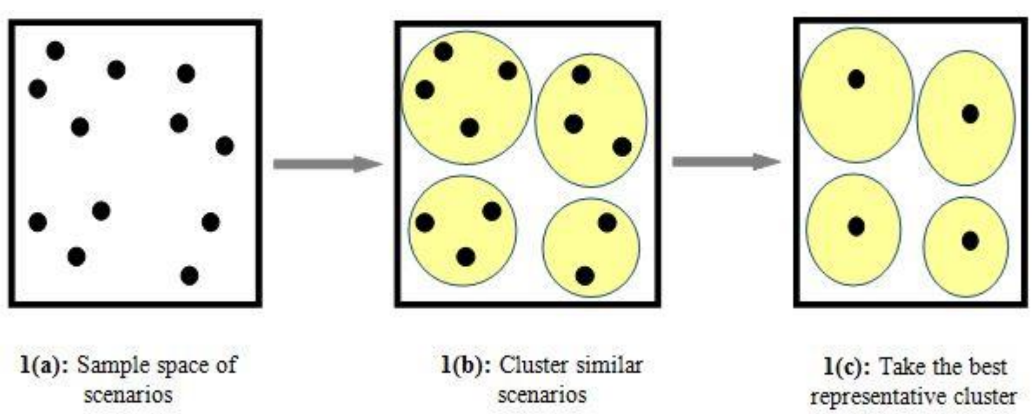


Figure 4.1 Pictorial representation of scenario aggregation performed in **eSSA**

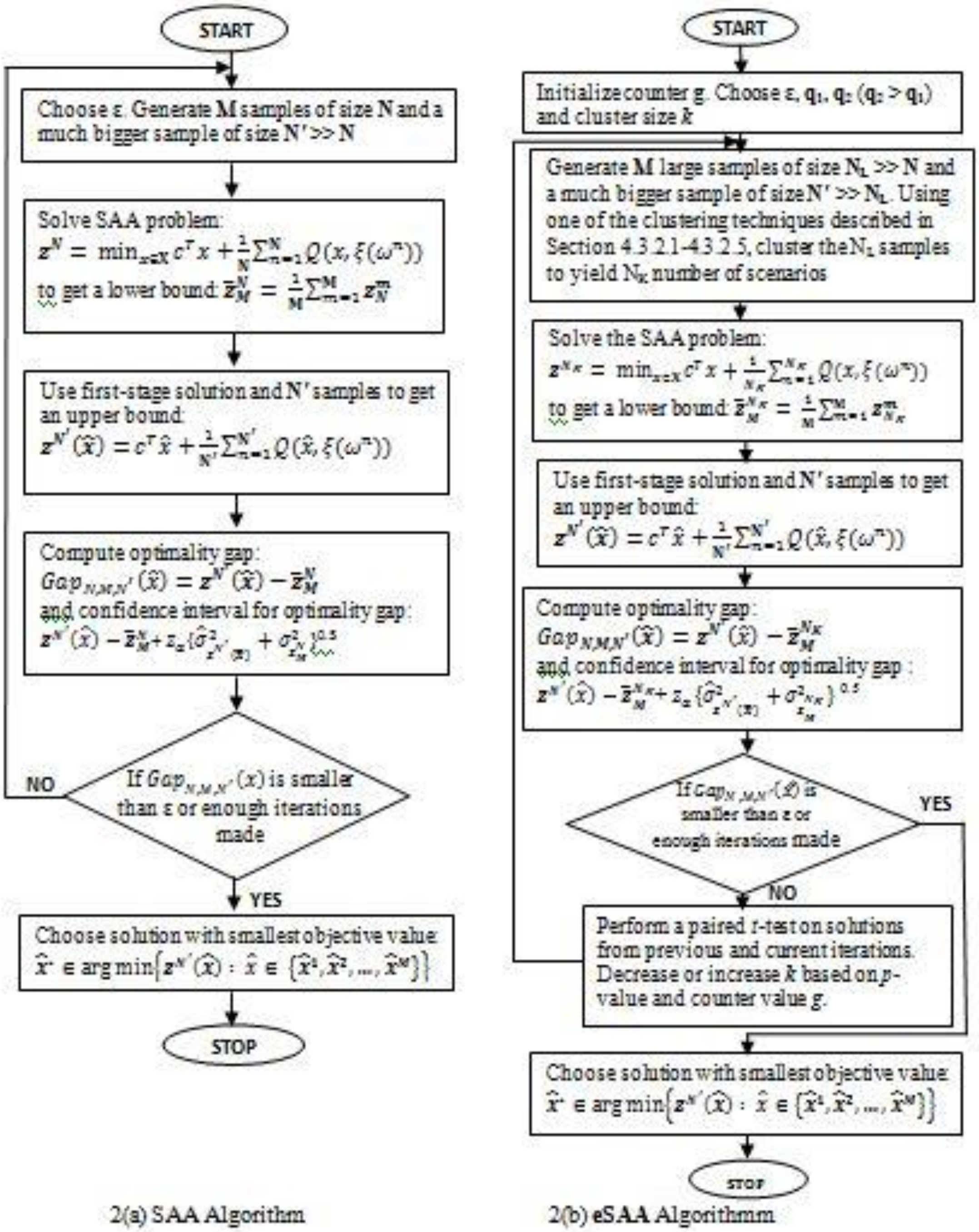


Figure 4.2 Comparison between SAA and **eSAA** algorithm

4.3.2.2 K-means++ clustering

In practice, the speed and simplicity of K-means clustering algorithm cannot be beat. Therefore, recent works have mainly focused on improving the initialization procedure. Deciding on a better way to initialize the clusters changes the performance of the Lloyd's iteration, both in terms of quality and convergence properties. Focusing on this direction, Ostrovsky et al. [109] and Arthur and Vassilvitskii [6] have proved that a simple procedure of selecting a good starting point can lead to good theoretical guarantees for the quality of the solution. They dubbed this method as K-means++ clustering algorithm. K-means++ method enhances the basic K-means clustering algorithm by implementing a better initialization approach in selecting the first ***k*** centers. Instead of randomly selecting the ***k*** centers, only one is randomly selected while the remaining *(**k** - 1)* centers are systematically selected with a probability proportional to its contribution to the overall error, given the previous selections. On a variety of datasets, K-means++ initialization obtains order of magnitude improvements over the random initialization of K-means clustering algorithm. K-means++ has been implemented in a wide range of applications such as defect prediction [110]. The pseudo code of K-means++ clustering method is shown in **Algorithm 4.2**.

Algorithm 4.2: K-means++ clustering algorithm

1: $\mathbf{X} \leftarrow$ Set of data points
2: $\boldsymbol{k} \leftarrow$ Total number of clusters
3: $\mu_1 \leftarrow$ sample a point randomly from **X**
4: $\boldsymbol{r_i} \leftarrow$ set of points that belong to cluster *i*, where *i=1,2,…,k*
5: **while** $|\mu_i| < \boldsymbol{k}$ **do**
6: sample $x \in \mathbf{X}$ with probability: $\frac{\arg\min_r \sum_{i=1}^{\boldsymbol{k}} \sum_{x \in \boldsymbol{r_i}} d(x,\mu)}{\arg\min_r \sum_{i=1}^{\boldsymbol{k}} \sum_{x \in \boldsymbol{r_i}} d(\boldsymbol{X},\mu)}$
7: $\mu \leftarrow \mu \cup \{x\}$
8: **end while**
9: Attribute the nearest cluster to each data point:
$$\boldsymbol{r_i} = \{j: d(x_i, \mu_i) \leq d(x_j, \mu_m),\ m \neq i, j = 1,2,\dots,n\}$$
10: Fix the position of each cluster to the mean of all points belonging to that cluster:
$$\mu_i = \frac{1}{|\boldsymbol{r_i}|} \sum_{j \in \boldsymbol{r_i}} x_j,\ \forall i$$
11: Repeat **Steps 9** and **10** until convergence.

4.3.2.3 K-means|| clustering

K-means algorithm chooses $\boldsymbol{k}$ centers in a single iteration following a specific distribution e.g., uniform distribution. On the other hand, K-means++ completes $\boldsymbol{k}$ iterations and selects one point in each iteration according to a non-uniform distribution. The superiority of K-means++ over K- means algorithm is primarily in constantly updating the non-uniform selection process. K-means parallel (K-means||) algorithm, developed by Bahmani et al. [10] combines the advantages of K-means and K-means++ in such a way that it takes fewer number of iterations and chooses more than one point in each iteration non-uniformly. In addition, K-means|| uses an oversampling factor *l* in its sampling points. This algorithm picks an initial center and computes Ψ as: $\Psi \coloneqq \arg\min_r \sum_{i=1}^{\boldsymbol{k}} \sum_{x \in \boldsymbol{r_i}} d(\boldsymbol{X}, \mu)$. Given a set of μ centers, in each of $O(log\psi)$ iterations this algorithm samples each *x* with a probability $\rho = \frac{l * \arg\min_r \sum_{i=1}^{\boldsymbol{k}} \sum_{x \in \boldsymbol{r_i}} d(x,\mu)}{\arg\min_r \sum_{i=1}^{\boldsymbol{k}} \sum_{x \in \boldsymbol{r_i}} d(\boldsymbol{X},\mu)}$ which is then added to μ. In order to reduce the number of centers, weights denoted by $\boldsymbol{w_x}$ are assigned to points in μ . These weighted points are then clustered to obtain the desired number of clusters. The structure of the algorithm lends itself for possible implementation in parallel systems. **Algorithm 4.3** demonstrates the steps of K-means|| clustering algorithm.

Algorithm 4.3: K-means|| clustering algorithm

1: **X** ← Set of data points
2: $\boldsymbol{k}$ ← Total number of clusters; l ← oversampling factor
3: μ ← sample a point randomly from **X**
4: $\boldsymbol{r_i}$ ← set of points that belong to cluster i, where $i=1,2,\dots,k$
5: $\Psi \leftarrow \arg\min_{r} \sum_{i=1}^{\boldsymbol{k}} \sum_{x\in \boldsymbol{r_i}} d(\boldsymbol{X},\mu)$
6: **for** $O(log\Psi)$ times **do**
7: μ' ← sample each point $x \in$ **X** with probability: $\rho = \frac{l* \arg\min_{r} \sum_{i=1}^{\boldsymbol{k}} \sum_{x\in \boldsymbol{r_i}} d(x,\mu)}{\arg\min_{r} \sum_{i=1}^{\boldsymbol{k}} \sum_{x\in \boldsymbol{r_i}} d(\boldsymbol{X},\mu)}$
8: $\mu \leftarrow \mu + \mu'$
9: **end for**
10: For $x \in \mu$, set $\boldsymbol{w_x}$ to be the number of points in **X** closer to x than any other point in μ
11: Attribute the nearest cluster to each data point:
$\boldsymbol{r_i} = \{j: d(x_i,\mu_i) \leq d(x_j,\mu_m),\ m \neq i, j = 1,2,\dots,n\}$
12: Fix the position of each cluster to the mean of all points belonging to that cluster:
$\mu_i = \frac{1}{|r_i|} \sum_{j\in \boldsymbol{r_i}} x_{j,} \forall i$
13: Repeat **Steps 11** and **12** until convergence.

4.3.2.4 Fuzzy C-means (FCM) clustering

One of the most widely used fuzzy clustering algorithms is the Fuzzy C-means (FCM) algorithm which was developed by James Bezdek in 1984 [22]. Fuzzy C-means is a clustering method which allows a data point to belong to two or more clusters. This algorithm works by assigning membership to each data point corresponding to each cluster center on the basis of the distance between the cluster centers and the data points. The data point that is closest to a cluster center has its membership towards this particular cluster center higher than any other data point. The summation of membership of a particular data point towards all the cluster centers is equal to one. The objective of the C-means algorithm is to minimize:

$$j_m = \sum_{i=1}^{\boldsymbol{N}} \sum_{j=1}^{\boldsymbol{c}} \mu_{ij}^m \left\| x_i - \boldsymbol{c_{jm}} \right\|^2 \tag{4.27}$$

Here, the fuzziness component or index is denoted by *m* which is any real number greater than 1. The total number of data points are denoted by **N** and **C** is the number of clusters. $\{x_i\}_{i \in \boldsymbol{N}}$ is the *i*-th measured data and $\boldsymbol{c_j}$ is the center of the *j*-th cluster. The degree of membership of x_i in cluster *j* is denoted by μ_{ij}.

This algorithm is carried out iteratively with the membership function and cluster centers updated after each iteration. The iteration will stop and the algorithm will terminate if $max_{ij} \left\| \boldsymbol{u}_{\boldsymbol{ij}}^{(\boldsymbol{k}+1)} - \boldsymbol{u}_{\boldsymbol{ij}}^{\boldsymbol{k}} \right\| \leq \boldsymbol{\epsilon}$, where the value of $\boldsymbol{\epsilon}$ may vary between 0 and 1. The pseudo code for Fuzzy C-means algorithm is outlined below in **Algorithm 4.4**:

Algorithm 4.4: Fuzzy C-means clustering algorithm

1: Randomly select cluster center
2: Initialize $U = [\boldsymbol{u_{ij}}]$ matrix, $U^{(0)}$
3: Calculate $\boldsymbol{u_{ij}}$ using:

$$\boldsymbol{u_{ij}} = \frac{1}{\sum_{\boldsymbol{k}=1}^{c} \left(\frac{\|x_i - \boldsymbol{c_j}\|}{\|x_i - \boldsymbol{c_k}\|} \right)^{2/(m-1)}}$$

4: Calculate centers vectors $C^{(\boldsymbol{k})}$=[$\boldsymbol{c_j}$] with $U^{(\boldsymbol{k})}$:

$$\boldsymbol{c_j} = \frac{\sum_{i=1}^{N} \mu_{ij}^{m} x_j}{\sum_{i=1}^{N} \mu_{ij}^{m}}$$

5: Update $U^{\boldsymbol{k}}, U^{(\boldsymbol{k}+1)}$:

$$\boldsymbol{u_{ij}} = \frac{1}{\sum_{\boldsymbol{k}=1}^{c} \left(\frac{\|x_i - \boldsymbol{c_j}\|}{\|x_i - \boldsymbol{c_k}\|} \right)^{2/(m-1)}}$$

6: If ($||U^{(\boldsymbol{k}+1)} - U^{\boldsymbol{k}}|| \leq \boldsymbol{\epsilon}$) or minimum value of j is achieved, **STOP** the algorithm. Otherwise repeat from **Step 2**.

Proposition 4.4 proves the validity of the lower bound provided by the clustering approach based on cluster size $\boldsymbol{k}$.

Proposition 4.4: Let $\boldsymbol{z}^*$ be the optimal solution of a true problem defined by (4.2). Let an approximate solution $(\boldsymbol{x}_{\mathbf{N}'}^*, \boldsymbol{z}_{\mathbf{N}'}^*)$ be obtained by solving $\mathbf{N}'$ sampled realizations of problem (4.2)'s stochastic parameter. Moreover, let $(\boldsymbol{x}_{\mathbf{N}}^*, \boldsymbol{z}_{\mathbf{N}}^*)$ be the solution obtained by solving problem (4.2) with $\mathbf{N}$ realizations where $\mathbf{N} \gg \mathbf{N}'$. Then, we prove the following:

- The expectation of $\boldsymbol{z}_{\boldsymbol{N}'}^*$ is a lower bound on $\boldsymbol{z}^*$ and $\boldsymbol{z}_{\boldsymbol{N}}^*$ provides an improved lower bound.
- If we form $\boldsymbol{C}$ clusters from the samples in the $\mathbf{N}'$ realizations, the solution $(\boldsymbol{x}_{\boldsymbol{C}}^*, \boldsymbol{z}_{\boldsymbol{C}}^*)$ obtained by using the centroids of the $\boldsymbol{C}$ clusters also provides a valid lower bound on $\boldsymbol{z}^*$ which improves as $\boldsymbol{C}$ increases.

Proof: Let $\boldsymbol{\xi} = \{\xi_1, \xi_2, \dots \xi_{\mathbf{N}}, \xi_{\mathbf{N+1}}\}$ be a set of data elements to be grouped into $\boldsymbol{C}$ clusters. Let, $\boldsymbol{u_{ij}}$, $(i = 1,2, \dots, \mathbf{N}+1; j = 1,2, \dots, \mathbf{C})$ be the degree of membership of data ξ_i in cluster *j* evaluated in fuzzy C-means as: $\boldsymbol{u_{ij}} = \frac{1}{\sum_{\mathbf{k}=1}^{\mathbf{C}} \left(\frac{\|\xi_i - \boldsymbol{c_j}\|}{\|\xi_i - \boldsymbol{c_k}\|}\right)^{2/(m-1)}}$, with $m > 1$ being the fuzziness exponent; $\boldsymbol{c_j} = \frac{\sum_{i=1}^{\mathbf{N+1}} \mu_{ij}^m \xi_i}{\sum_{i=1}^{\mathbf{N+1}} \mu_{ij}^m}$ the center of cluster *j*; $\|\xi_i - \boldsymbol{c_j}\|$ the distance from point *i* to current cluster *j*; and $\|\xi_i - \boldsymbol{c_k}\|$ the distance from point *i* to other clusters $\boldsymbol{k}$.

At the convergence of the clustering algorithm, it is obvious that $p_1 = \sum_{j=1}^{\boldsymbol{C}} \boldsymbol{u_{ij}} = 1 \; \forall i \in \boldsymbol{\xi}$ and $p_2 = \sum_{j=1}^{\boldsymbol{C}} (\boldsymbol{u_{ij}})^2 \leq 1 \; \forall i \in \boldsymbol{\xi}$**.** Without loss of generality, let us assume that the elements in ξ are distinct, i.e., $\xi_1 \neq \xi_2 \neq \xi_{\mathbf{N}} \neq \xi_{\mathbf{N+1}}$. If $\boldsymbol{C} = \mathbf{N}+1$, in other words, we are required to group the data into **N**+*1* clusters, it's trivial to show that $\boldsymbol{u_{ij}} = \begin{cases} 1 \; for \;\; j = \boldsymbol{k} \\ 0 \; otherwise \end{cases} \; \forall i \in \xi$. This means that only one element occurs in each cluster $\boldsymbol{k}$.
Moreover, in this case $p_2 = p_1 = 1$.

$$\min_{x \in \mathbf{X}} \mathbb{E} f(x, \xi_i) = \min_{x \in \mathbf{X}} \left(\mathbb{E} \frac{1}{\mathbf{N}+1} \sum_i^{\mathbf{N+1}} f(x, \xi_i) \right)$$
$$\geq \mathbb{E} \min_{x \in X} \left(\frac{1}{\mathbf{N}+1} \sum_i^{\mathbf{N+1}} f(x, \xi_i) \right)$$

Thus,

$$\mathbb{E}(\boldsymbol{z}_{\boldsymbol{N+1}}^*) = \mathbb{E} \min_{x \in \mathbf{X}} \left(\frac{1}{\mathbf{N}+1} \sum_i^{\mathbf{N+1}} f(x, \xi_i) \right) \leq \boldsymbol{z}^*$$

which is a valid lower bound.

For a cluster size $\boldsymbol{C} = \mathbf{N}'$ where $\mathbf{N}' < \mathbf{N}+1$, $p_2 \leq 1 \; \forall i \in \xi$. Using $\boldsymbol{\xi} = \{\xi_1, \xi_2, \dots \xi_{\mathbf{N}'}, \xi_{\mathbf{N}'+1}\}$ to define $\boldsymbol{z}_{\mathbf{N}'}^*$ and $\boldsymbol{z}_{\mathbf{N}'+\mathbf{1}}^*$:

$$\mathbb{E}(\boldsymbol{z}^*_{\boldsymbol{N'}+\boldsymbol{1}}) = \mathbb{E}\ \min_{x\in\mathbf{X}}\left(\frac{1}{\mathbf{N'}+1}\sum_{i}^{\mathbf{N'}+1} f(x,\xi_i)\right)$$

$$= \mathbb{E}\ \min_{x\in\mathbf{X}}\left(\frac{1}{\mathbf{N'}+1}\sum_{i}^{\mathbf{N'}+1}\frac{1}{\mathbf{N'}}\sum_{j\neq i}^{\mathbf{N'}+1} f(x,\xi_j)\right)$$

$$\geq \frac{1}{\mathbf{N'}+1}\sum_{i}^{\mathbf{N'}+1}\mathbb{E}\ \min_{x\in\mathbf{X}}\frac{1}{\mathbf{N'}}\sum_{j\neq i}^{\mathbf{N'}+1} f(x,\xi_j)$$

$$= \mathbb{E}(\boldsymbol{z}^*_{\boldsymbol{N'}})$$

which implies a better lower bound. ■

4.3.2.5 Mathematical programming-based clustering

We now present a mathematical formulation of mixed integer programming (MIP) model for the clustering phenomenon. This formulation was proposed by Sağlam, Salman, Sayın, and Türkay [133] but similar type of formulations were developed previously by Brusco [26] and Rao [119].

Consider a data set of *n* points where *n* ∈ **N** with *m* dimensions. We want to achieve ***k*** number of exclusive clusters where ***k*** ∈ **K** and is known a priori. The main objective of this formulation is to find the optimal division or partition of this data set into ***k*** clusters. In this model, $\mathbf{D} \coloneqq \{D_l\}_{l\in\boldsymbol{K}}$ and D_{max} are defined as the diameter of cluster *l* and the maximum diameter among the desired clusters, respectively. The parameter d_{ij} denotes the distance between two data points $i \in \mathbf{N}$ and $j \in \mathbf{N}$. $\mathbf{X} \coloneqq \{x_{il}\}_{i\in\mathbf{N},l\in\boldsymbol{K}}$ is a binary variable that takes the value 1 if *i* is assigned to cluster *l* and 0 otherwise. The objective of the model is to minimize D_{max}. With this, the clustering problem can be formulated as a MIP problem as shown below:

Minimize D_{max} (4.28)

$$D_l \geq d_{ij} x_{il} x_{jl} \quad \forall i \in \mathbf{N}, j \in \mathbf{N}, l \in \mathbf{K} \tag{4.29}$$

$$\sum_{l=1}^{K} x_{il} = 1 \quad \forall i \in \mathbf{N} \tag{4.30}$$

$$D_{max} \geq D_l \quad \forall l \in \mathbf{K} \tag{4.31}$$

$$x_{il} \in \{0,1\} \quad \forall i \in \mathbf{N}, l \in \mathbf{K} \tag{4.32}$$

$$D_l \geq 0 \quad \forall l \in \mathbf{K} \tag{4.33}$$

Constraints (4.29) indicate that the diameter of the cluster is at least equal to the maximum distance between any two arbitrary data points in the same cluster. Constraints (4.30) indicate the exclusivity of the clusters meaning each data point will only be assigned to only one cluster. Constraints (4.31) along with the objective function denote that D_{max} is equal to the maximum diameter and greater than any other cluster diameters. Constraints (4.32) are binary constraints and constraints (4.33) are non-negativity constraints.

The expression $x_{il}x_{jl}$ in constraints (4.29) is the product of two binary decision variables with the value of 0 or 1. This makes the above model a non-convex bi-linear mixed integer programming (MIP) model. Thus, even with a small set of data points the above model is hard to solve in a reasonable amount of time. The following technique linearizes constraints (4.29) without increasing the size of the formulation:

$$D_l \geq d_{ij}(x_{il} + x_{jl} - 1) \quad \forall i \in \mathbf{N}, j \in \mathbf{N}, l \in \mathbf{K} \tag{4.34}$$

Constraints (4.34) indicate that data points *i* and *j* are assigned to cluster *l* and the diameter of the cluster has to be at least as long as the distance between $i \in \mathbf{N}$ and $j \in \mathbf{N}$. In constraints (4.34), if one or both of the decision variables i.e., x_{il} and x_{jl} are equal to zero, it will make the constraints redundant. If and only if both the decision variables are equal to 1, then constraints (4.34) will be active.

4.4 Numerical study

In this section, we investigate the performance of our proposed enhanced sample average approximation (**eSAA**) approach using (1) A classical facility location problem (**[FLP]**) with stochastic demands (2) A single-sink transportation problem (**[SSP]**) and (3) A supply transportation problem (**[STP]**). **[SSP]** and **[STP]**, formulated by Maggioni et al. [88] and Maggioni et al. [89], respectively. The purpose of these tests is to investigate the robustness of using the **eSAA** approach as well as study the effects of problem parameters, such as the number of scenarios and cluster size on the performance of the method. The result will also increase the prospect of using the approach as an alternative to the continuous approximation approach utilized in Chapter III in solving the AM deployment configuration problem. However, we first start by providing an overview of the **[FLP]** and then discuss the computational performance of solving **[FLP]** with our **eSAA** algorithm.

4.4.1 Facility location problem

The facility location problem (**[FLP]**) is a classical combinatorial optimization problem of determining the number and location of facilities (e.g., factories, warehouses, schools) and assigning customers to them (e.g., depots, retail outlets, students) so as to minimize the overall system cost. The facility location problem can be either capacitated or uncapacitated. In a capacitated facility location problem (CFLP), there is a limit on the number of customers each facility can serve or amount of products that it can produce. In an uncapacitated facility location problem (UFLP), an arbitrary number of customers can be served by a facility since there is no limit to the amount of products that it can produce.

Pioneering works on facility location problem can be attributed to Kuehn and Hamburger [79] and Balinski [12]. Since then, the problems have been extensively studied with many exact and heuristic solution approaches. For example, Erlenkotter [46], Galvão and Raggi [52], Ardjmand et al. [5], Posta et al. [117], and Monabbati and Kakhki [97] discussed different solution approaches to solve UFLP. Similarly, new models and algorithms are developed (e.g., Akinc and Khumawala [3], Barceló and Casanovas [13], Jacobsen [66], Rahmaniani and Ghaderi [118], and Küçükdeniz et al. [78]) to solve CFLP. The classical facility location problems are extended by many researchers over the years to consider economies of scale (e.g., Van Roy [154], Feldman et al. [50], and Trappey et al. [149]), increasing production costs (e.g., Harkness and ReVelle [58] and Dogan [42]) and concave costs (e.g., Soland [144], Dupont [44], and Saif and Elhedhli [134]) in the modeling formulation. These works are applied to determine the optimal location of facilities for manufacturing systems, energy production and distribution systems, servers for computer internet communication networks, ambulance locations for emergency services, hospitals for health-care services, and academic institutions. Facility location problems with stochastic demand are *NP*-hard problems ([93], [102]); therefore, solving large instances of the problem is a challenging task. This motivates us to use stochastic facility location problem as a test case to check and validate the performance of our enhanced sample average approximation (**eSAA**) algorithm.

We now give a mathematical formulation of the capacitated **[FLP]**. The problem can be stated simply as follows. We are given a set of candidate facility locations **J** with installing cost ψ_j and supply capacity S_j $\forall j \in \mathbf{J}$. We are also given a set of warehouse locations $k \in \mathbf{K}$ with stochastic demands $d_{k\omega}$. The cost of shipping one unit of product from each plant location $j \in \mathbf{J}$ to customer/warehouse location $k \in \mathbf{K}$ is denoted by c_{jk}. There is a unit penalty cost associated with not meeting the demand at warehouse facilities which is denoted by β_k. We assume that there are fixed number of scenarios $|\mathbf{\Omega}|$ and the probability associated with each scenario is denoted by ρ_ω.

The first-stage decision variables $\mathbf{Y} \coloneqq \{Y_j\}_{j \in J}$ decide the location to open the facilities i.e.,

$$Y_j = \begin{cases} 1 \text{ if a palnt is opened at location } j \\ 0 \text{ otherwise} \end{cases}$$

The second-stage decision variables $\mathbf{X} \coloneqq \{X_{jk\omega}\}_{j \in \mathbf{J}, k \in \mathbf{K}, \omega \in \mathbf{\Omega}}$ decide the amount of product shipped from plant $j \in \mathbf{J}$ to warehouse $k \in \mathbf{K}$ under scenario $\omega \in \mathbf{\Omega}$ and $\boldsymbol{Z} \coloneqq \{Z_{k\omega}\}_{k \in \mathbf{K}, \omega \in \mathbf{\Omega}}$ decide the unsatisfied demand at warehouse $k \in \mathbf{K}$ under scenario $\omega \in \mathbf{\Omega}$. The aim is to minimize the first-stage and expected value of the second-stage costs. With this, we now formulate the following two-stage mixed-integer linear programming (MILP) formulation **[FLP]** as shown below:

$$[\mathbf{FLP}]\ Minimize\ \sum_{j \in \mathbf{J}} \psi_j Y_j + \sum_{\omega \in \mathbf{\Omega}} \rho_\omega \mathbb{E}(Y, \omega) \tag{4.35}$$

subject to

$$Y_j \in \{0,1\} \quad \forall\ j \in \mathbf{J} \tag{4.36}$$

with $\mathbb{E}(Y, \omega)$ being the solution of the following second-stage problem:

$$\mathbb{E}(Y, \omega) = Minimize\ \sum_{j \in \mathbf{J}} \sum_{k \in \mathbf{K}} c_{ij} X_{jk\omega} + \sum_{k \in \mathbf{K}} \beta_k Z_{k\omega} \tag{4.37}$$

$\sum_{j\in\mathbf{J}} X_{jk\omega} + Z_{k\omega} = d_{k\omega}\ \forall k \in \mathbf{K}, \omega \in \mathbf{\Omega}$ (4.38)

$\sum_{k\in\mathbf{K}} X_{jk\omega} \leq S_j Y_j\ \forall j \in \mathbf{J}, \omega \in \mathbf{\Omega}$ (4.39)

$X_{jk\omega} \geq 0\ \forall j \in \mathbf{J}, k \in \mathbf{K}, \omega \in \mathbf{\Omega}$ (4.40)

$Z_{k\omega} \geq 0\ \forall k \in \mathbf{K}, \omega \in \mathbf{\Omega}$ (4.41)

The objective function minimizes total cost of the system including first-stage cost (e.g., investment cost of opening plants) and second-stage costs (e.g., transportation and shortage costs) under a set of possible scenarios. More specifically, the first term of the objective function represents the total set-up cost of locating the plants. The second term is the total cost of transporting products from plants to warehouses and the last term in the objective function is the cost associated with not meeting demand at the warehouses.

Constraints (4.38) indicate that the demand at warehouse $k \in \mathbf{K}$ is fulfilled in all scenarios either by the regular network or through external sources. Constraints (4.39) indicate that the amount of product transported from each plant $j \in \mathbf{J}$ is limited by the supply capacity S_j. Finally, Constraints (4.40) and (4.41) are the standard non-negativity constraints.

4.4.2 Analyzing the performance of solution algorithms

This section presents our computational experience in solving model **[FLP]** using the algorithms proposed in **Section 4.3**. To help the readers follow our approaches, we have used the following notations to represent the algorithms:

- **[SAA]:** Basic sample average approximation algorithm (described in **Section 4.3.1**)
- **[eSAA(D)]:** Enhanced sample average approximation algorithm (described in **Section 4.3.2**)
- **[eSAA(F)]:** Enhanced sample average approximation algorithm with fixed cluster size (e.g., same as **[eSAA(D)]** but the cluster size is kept constant throughout all the iterations)

The algorithms presented above are implemented in Python using GUROBI optimization solver *(http://www.gurobi.com/)* on a desktop with Intel Core i7 3.60 GHz processor and 16.0 GB RAM. The algorithms are terminated when at least one of the following condition is met: (a) the optimality gap (i.e., ϵ = |UB − LB|/UB) falls below a tolerance threshold value, $\epsilon = 0.001$; or (b) the maximum time limit $time^{max}$= 10,800 (in CPU seconds) is reached; or (c) the maximum number of iteration $iter^{max}$ = 100 is reached. The size of the equivalent deterministic problem of model **[FLP]** is presented in **Table 4.3**.

Table 4.3 Problem size of the test instances

Instances	|**J**|	|**K**|	Binary Variables	Continuous Variables	Total Variables	No. of Constraints
S1	10	10	10	110	120	20
S2	30	30	30	930	960	60
S3	50	50	50	2550	2600	100
S4	70	70	70	4970	5040	140
S5	100	100	100	10,100	10,200	200
S6	120	120	120	14,520	14,640	240

The first set of experiments (shown in **Tables 4.4 – 4.9**) show the computational performance in solving **[eSAA(F)]** and **[eSAA(D)]** against **[SAA]**. K-means++ clustering strategy is chosen to be implemented in both **[eSAA(F)]** and **[eSAA(D)]** for this first set of experiments. We consider 6 problem instances which is shown in **Table 4.3**. Additionally, we have tested the performance of the enhancement techniques under both normal and uniform distribution. Under each instance a total of 6 sample sizes are considered, i.e., **N** = {100, 200, 300, 400, 500}. For each sample, we experimented with two sets of replications, **M** = {5, 10}. Note that, we do not present the results obtained from GUROBI. This is because GUROBI takes more time than **[SAA]**, **[eSAA(F)]**, and **[eSAA(D)]** even for smaller instances and smaller sample sizes and goes out of memory if one or both of them increase. In all of our experimental results, if the algorithms are solved in less than the stopping criteria ϵ then we highlighted the algorithm which gave the smallest running time. Otherwise, if such a quality solution is not found within the maximum time or iteration limit then the algorithm with the smallest optimality gap is highlighted. For the first set of experiments with uniform distribution, the results indicate that both **[eSAA(F)]** and **[eSAA(D)]** perform significantly better than **[SAA]** for all instances. All the problems are solved within pre-specified optimality/tolerance gap within the specified time limit. More specifically, **[eSAA(D)]** is on average 8.4% faster than **[eSAA(F)]** and 688% faster than **[SAA]**. Simultaneously, computation time of [**eSAA(F)]** is on average 626% faster than **[SAA].** Furthermore, **[eSAA(D)]** drops the average optimality gap to 0.018% compared to 0.02% and 0.033% of **[eSAA(F)]** and **[SAA]**, respectively. We observe the same trend while performing the first set of experiments with normal distribution. **[eSAA(D)]** algorithm has found to be superior compared to the other two counterparts in terms of computation time and solution quality. On average, **[eSAA(D)]** is 9.4% faster than **[eSAA(F)]** and 712% faster than **[SAA]**. Additionally, the quality of solution is found to be better with **[eSAA(D)]** having an average optimality gap of 0.016% compared to 0.025% and 0.036% in **[eSAA(F)]** and **[SAA]**, respectively.

Table 4.4 Performance comparison between **[SAA], [eSAA(F)]**, and **[eSAA(D)]** (Instance **S1**)

		[SAA]			**[eSAA(F)]**			**[eSAA(D)]**		
N	**M**	**ϵ** (%)	Time (sec)	Iter	**ϵ** (%)	Time (sec)	Iter	**ϵ** (%)	Time (sec)	Iter
Uniform distribution										
100	5	0.00	2.7	3.6	0.06	1.4	1.0	0.00	**1.1**	1.3
	10	0.02	3.3	2.5	0.04	3.0	1.2	0.01	**2.7**	1.6
200	5	0.00	4.4	1.9	0.00	**1.9**	1.2	0.02	2.1	1.2
	10	0.01	5.4	1.2	0.01	4.2	1.0	0.00	**3.4**	1.1
300	5	0.00	6.6	2.6	0.07	3.1	1.6	0.01	**2.9**	1.0
	10	0.02	8.1	2.1	0.02	6.5	1.0	0.01	**5.9**	1.2
400	5	0.02	9.3	2.5	0.02	2.5	1.0	0.01	**2.0**	1.2
	10	0.01	11.0	1.6	0.01	4.8	1.0	0.02	**4.1**	1.0
500	5	0.04	12.0	1.3	0.01	**4.7**	1.4	0.02	5.1	1.1
	10	0.03	15.0	1.8	0.04	10.0	1.3	0.01	**8.1**	1.3
Avg.		0.02	7.7	2.1	0.03	4.2	1.1	0.01	**3.7**	1.2
Normal distribution										
100	5	0.01	2.7	2.3	0.02	**1.3**	1.6	0.02	**1.3**	1.6
	10	0.02	3.3	2.1	0.04	3.1	2.1	0.01	**2.6**	1.1
200	5	0.00	4.4	2.9	0.03	**1.8**	1.6	0.01	2.2	1.3
	10	0.04	5.4	1.5	0.02	4.4	1.1	0.02	**3.5**	1.2
300	5	0.01	6.6	2.5	0.00	3.2	1.9	0.00	**2.7**	1.5
	10	0.00	8.1	1.6	0.02	6.7	1.1	0.00	**5.8**	1.4
400	5	0.02	9.3	2.9	0.00	2.3	1.5	0.01	**2.2**	1.1
	10	0.02	11.0	1.7	0.01	4.6	1.1	0.01	**4.3**	1.0
500	5	0.01	12.0	1.6	0.01	**4.9**	1.3	0.00	5.2	1.0
	10	0.00	16.0	1.6	0.02	8.8	1.2	0.01	**7.7**	1.0
Avg.		0.01	7.9	2.07	0.02	4.1	1.4	0.01	**3.8**	1.2

Table 4.5 Performance comparison between **[SAA]**, **[eSAA(F)]**, and **[eSAA(D)** (Instance **S2**)

		[SAA]			**[eSAA(F)]**			**[eSAA(D)]**		
N	**M**	ϵ (%)	Time (sec)	Iter	ϵ (%)	Time (sec)	Iter	ϵ (%)	Time (sec)	Iter
Uniform distribution										
100	5	0.05	41.0	4.2	0.05	14.0	1.0	0.00	**11.0**	1.1
	10	0.02	52.0	3.5	0.02	27.0	1.6	0.05	**25.0**	1.0
200	5	0.02	83.0	4.1	0.09	25.0	1.4	0.01	**20.0**	1.2
	10	0.05	104	3.0	0.00	52.0	1.2	0.02	**44.0**	1.0
300	5	0.03	140	4.2	0.01	36.0	1.6	0.02	**32.0**	1.5
	10	0.04	169	4.1	0.01	68.0	1.2	0.01	**58.0**	1.0
400	5	0.05	212	2.9	0.07	**43.0**	1.4	0.02	46.0	1.3
	10	0.04	259	2.1	0.01	**77.0**	1.6	0.01	81.0	1.3
500	5	0.03	294	2.5	0.06	75.0	1.8	0.02	**66.0**	1.1
	10	0.06	362	2.0	0.01	165	1.5	0.01	**163**	1.0
Avg.		0.04	171	3.2	0.03	58	1.4	0.02	**55**	1.1
Normal distribution										
100	5	0.02	44.0	4.1	0.01	15.0	1.6	0.02	**10.0**	1.0
	10	0.01	55.0	4.2	0.01	26.0	1.2	0.01	**25.0**	1.0
200	5	0.05	78.0	3.2	0.03	26.0	2.1	0.02	**21.0**	1.1
	10	0.03	97.0	2.0	0.05	55.0	1.3	0.01	**41.0**	1.2
300	5	0.02	154	2.3	0.02	35.0	2.5	0.02	**33.0**	1.0
	10	0.04	179	1.6	0.02	73.0	1.4	0.04	**53.0**	1.2
400	5	0.08	200	1.5	0.01	**45.0**	1.6	0.00	49.0	1.3
	10	0.07	280	2.2	0.03	83.0	1.0	0.01	**79.0**	1.2
500	5	0.06	306	1.6	0.01	70.0	1.9	0.00	**69.0**	1.0
	10	0.01	369	1.1	0.02	**166**	1.0	0.01	178	1.3
Avg.		0.04	176	2.3	0.02	59	1.5	0.01	**56**	1.1

Table 4.6 Performance comparison between **[SAA], [eSAA(F)]**, and **[eSAA(D)]** (Instance **S3**)

		[SAA]			**[eSAA(F)]**			**[eSAA(D)]**		
N	**M**	**ϵ** (%)	Time (sec)	Iter	**ϵ** (%)	Time (sec)	Iter	**ϵ** (%)	Time (sec)	Iter
Uniform distribution										
100	5	0.03	165	4.1	0.09	**44.0**	3.5	0.00	47.0	2.2
	10	0.04	208	3.2	0.02	75.0	3.4	0.00	**60.0**	2.1
200	5	0.03	349	5.9	0.07	68.0	3.6	0.04	**55.0**	1.6
	10	0.05	426	2.1	0.00	114	2.9	0.01	**103**	1.1
300	5	0.03	613	1.9	0.06	**82.0**	3.5	0.02	90.0	1.0
	10	0.03	742	2.3	0.02	139	2.5	0.04	**113**	1.2
400	5	0.02	899	1.5	0.01	78.0	3.4	0.02	**74.0**	1.5
	10	0.06	1124	1.2	0.01	133	2.4	0.03	**120**	1.2
500	5	0.00	1340	2.9	0.01	164	1.0	0.01	**133**	1.1
	10	0.05	1635	2.1	0 .00	271	1.0	0.00	**233**	1.3
Avg.		0.03	750	2.7	0.03	117	2.7	0.02	**103**	1.4
Normal distribution										
100	5	0.05	151	3.4	0.05	**41.0**	2.5	0.02	45.0	1.2
	10	0.08	205	3.3	0.02	68.0	2.1	0.00	**66.0**	1.4
200	5	0.01	377	3.3	0.04	70.0	4.2	0.04	**53.0**	1.5
	10	0.02	397	3.1	0.02	122	2.2	0.02	**97.0**	1.1
300	5	0.05	592	2.6	0.00	**81.0**	4.6	0.01	83.0	1.2
	10	0.04	753	2.4	0.02	145	4.3	0.00	**107**	1.5
400	5	0.02	913	3.2	0.01	**72.0**	2.2	0.01	79.0	1.2
	10	0.06	1212	3.2	0.02	144	4.1	0.02	**118**	1.6
500	5	0.04	1287	2.6	0.02	177	1.2	0.04	**123**	1.4
	10	0.02	1668	2.4	0.03	248	1.2	0.00	**214**	1.2
Avg.		0.04	756	2.9	0.02	117	2.8	0.02	**99.0**	1.3

Table 4.7 Performance comparison between **[SAA], [eSAA(F)]**, and **[eSAA(D)]** (Instance **S4**)

		[SAA]			**[eSAA(F)]**			**[eSAA(D)]**		
N	**M**	ϵ (%)	Time (sec)	Iter	ϵ (%)	Time (sec)	Iter	ϵ (%)	Time (sec)	Iter
Uniform distribution										
100	5	0.02	410	5.1	0.02	**76.0**	7.2	0.00	82.0	1.6
	10	0.06	774	4.7	0.02	137	6.4	0.00	**111**	1.2
200	5	0.02	928	5.2	0.01	67.0	6.0	0.03	**54.0**	2.2
	10	0.02	1935	3.0	0.00	115	6.2	0.02	**104**	1.9
300	5	0.03	1799	3.6	0.03	**112**	6.1	0.02	123	2.6
	10	0.00	3561	3.8	0.00	194	5.7	0.00	**157**	2.1
400	5	0.02	3153	4.1	0.02	131	5.0	0.02	**124**	2.2
	10	0.05	5893	2.4	0.03	250	5.1	0.01	**225**	2.0
500	5	0.02	4246	2.2	0.01	164	5.2	0.02	**133**	1.4
	10	0.02	9146	2.0	0.01	287	4.0	0.01	**247**	1.5
Avg.		0.03	3185	3.6	0.02	153	5.7	0.01	**136**	1.8
Normal distribution										
100	5	0.05	397	4.2	0.05	**76.0**	3.2	0.02	85.0	1.5
	10	0.02	787	2.1	0.04	141	2.8	0.01	**116**	1.6
200	5	0.06	910	4.3	0.04	67.0	3.6	0.03	**58.0**	2.3
	10	0.04	1969	4.2	0.02	114	2.0	0.01	**106**	1.1
300	5	0.05	1805	2.0	0.06	**121**	2.6	0.06	131	1.2
	10	0.04	3738	2.6	0.01	189	2.4	0.01	**147**	1.6
400	5	0.02	3430	1.8	0.00	123	1.6	0.03	**114**	1.5
	10	0.06	6073	2.1	0.05	231	1.2	0.02	**221**	1.4
500	5	0.04	4353	2.0	0.03	178	2.5	0.01	**145**	1.9
	10	0.01	9036	1.2	0.01	291	2.1	0.03	**226**	2.0
Avg.		0.04	3250	2.6	0.03	153	2.4	0.02	**135**	1.6

Table 4.8 Performance comparison between **[SAA], [eSAA(F)]**, and **[eSAA(D)]** (Instance **S5**)

		[SAA]			**[eSAA(F)]**			**[eSAA(D)]**		
N	**M**	ϵ (%)	Time (sec)	Iter	ϵ (%)	Time (sec)	Iter	ϵ (%)	Time (sec)	Iter
		Uniform distribution								
100	5	0.04	881	4.2	0.03	204	3.3	0.01	**188**	1.9
	10	0.06	1749	4.1	0.04	386	2.9	0.05	**309**	1.0
200	5	0.04	2190	3.8	0.01	292	5.2	0.01	**248**	1.6
	10	0.02	4857	3.3	0.06	555	4.8	0.03	**500**	1.6
300	5	0.09	4084	3.9	0.02	433	3.2	0.01	**372**	2.1
	10	0.04	8475	3.5	0 .02	**823**	1.5	0.06	889	1.1
400	5	0.08	7031	3.6	0.03	**449**	2.2	0.02	471	1.3
	10	0.09	14615	3.1	0.06	858	1.9	0.02	**755**	2.0
500	5	0.04	9299	3.0	0.05	452	2.0	0.01	**366**	1.6
	10	0.02	22865	2.2	0 .01	814	1.9	0.02	**806**	1.7
Avg.		0.05	7605	3.4	0.03	527	2.9	0.02	**490**	1.6
		Normal distribution								
100	5	0.00	890	4.0	0.05	211	3.2	0.02	**198**	1.6
	10	0.08	1724	4.3	0.04	351	2.2	0.05	**327**	2.1
200	5	0.06	1973	4.0	0.05	288	3.6	0.04	**228**	1.3
	10	0.07	4506	3.6	0.06	557	3.1	0.02	**460**	1.0
300	5	0.03	3845	4.1	0.01	423	2.9	0.01	**405**	1.5
	10	0.05	9124	4.3	0.02	**815**	2.5	0.01	967	1.4
400	5	0.06	7327	3.1	0.03	**492**	2.6	0.01	508	1.9
	10	0.08	13826	2.5	0.05	820	2.5	0.03	**698**	1.4
500	5	0.09	9736	2.3	0.04	472	2.6	0.01	**384**	1.5
	10	0.07	24789	2.1	0.07	**755**	3.2	0.02	864	1.1
Avg.		0.06	7774	3.4	0.04	518	2.8	0.02	**504**	1.5

Table 4.9 Performance comparison between **[SAA]**, **[eSAA(F)]**, and **[eSAA(D)]** (Instance **S6**)

		[SAA]			[eSAA(F)]			[eSAA(D)]		
N	M	ϵ (%)	Time (sec)	Iter	ϵ (%)	Time (sec)	Iter	ϵ (%)	Time (sec)	Iter
Uniform distribution										
100	5	0.06	2978	4.1	0.01	2464	7.2	0.01	**1996**	1.6
	10	0.03	5720	5.7	0.03	5691	6.4	0.02	**4610**	1.2
200	5	0.02	7556	5.2	0.01	2548	6.0	0.03	**2293**	2.2
	10	0.01	16902	3.0	0.03	**5859**	6.2	0.04	6445	1.9
300	5	0.04	14252	3.6	0.02	2541	6.1	0.05	**2058**	2.6
	10	0.03	26782	3.8	0.04	5894	5.7	0.01	**5599**	2.1
400	5	0.02	23554	4.1	0.02	2618	5.0	0.02	**2356**	2.2
	10	0.02	50274	2.4	0.03	6041	5.1	0.05	**4893**	2.0
500	5	0.01	30779	2.2	0.00	2674	5.2	0.03	**2300**	1.4
	10	0.06	75226	2.0	0.02	**6202**	4.0	0.05	6698	1.5
Avg.		0.03	25402	3.6	0.02	4253	5.7	0.03	**3925**	1.8
Normal distribution										
100	5	0.01	2742	4.3	0.01	2682	2.0	0.00	**2046**	1.9
	10	0.02	6083	5.1	0.03	6065	1.6	0.01	**4303**	1.4
200	5	0.03	6928	5.4	0.01	2678	2.2	0.03	**2317**	2.3
	10	0.04	18282	4.1	0.03	**6020**	1.6	0.01	6975	1.5
300	5	0.05	15030	3.9	0.02	2627	2.9	0.04	**1857**	1.9
	10	0.01	26420	3.1	0.04	6442	1.1	0.03	**5680**	2.0
400	5	0.02	21894	3.8	0.02	2513	2.3	0.02	**2309**	1.2
	10	0.05	53615	2.4	0.03	5686	1.2	0.02	**4637**	1.0
500	5	0.03	31021	2.3	0.00	2735	1.6	0.01	**2091**	1.5
	10	0.05	79285	2.0	0.02	**5689**	1.5	0.06	6725	1.1
Avg.		0.03	26130	3.6	0.02	4314	1.8	0.02	**3894**	1.5

The second set of experiments (**Table 4.10 – 4.15**) report the impact of introducing dynamicity in **[eSAA(D)]** over **[eSAA(F)]** under different clustering techniques such as, K-means, K-means++, K-means||, and C-means clustering. To perform these tests, we kept the sample size fixed for all experiments i.e., **N′** = 1,000. The results indicate that incorporating dynamicity substantially improves the performance of the enhanced sample average approximation algorithm. Furthermore, it is observed that both algorithms are capable of solving all the problem instances within pre-specified optimality gap and time limit. It has been proven to be true under both normal and uniform distribution. Under uniform distribution, algorithm **[eSAA(D)]** is on average

12.7% faster than algorithm **[eSAA(F)]** whereas the number increases to 21.1% for normal distribution. For all instances, **[eSAA(D)]** has given faster solution than **[eSAA(F)].** More specifically, for smaller instances (instances **S1**-**S4**) both [**eSAA(F)]** and **[eSAA(D)]** algorithms with *k*-means clustering have given better result in terms of computational time; however, for larger instances (instance **S5** and **S6**) **[eSAA(F)]** and **[eSAA(D)]** with K-means|| clustering have given better results. Although, both **[eSAA(D)]** and [**eSAA(F)]** terminate with an $\boldsymbol{\varepsilon}$-optimal solution, the quality of solution produced by **[eSAA(D)]** is constantly higher for all instances. Note that the experimental results show same trends for both the uniform and normal distribution.

Table 4.10 Performance comparison between [**eSAA(F)]** and **[eSAA(D)]** (Instance **S1**)

N	M	[eSAA(F)] K-means ϵ (%)	K-means Time (sec)	K-means Iter	K -means++ ϵ (%)	K -means++ Time (sec)	K -means++ Iter	K-means ǁ ϵ (%)	K-means ǁ Time (sec)	K-means ǁ Iter	C-means ϵ (%)	C-means Time (sec)	C-means Iter	[eSAA(D)] K-means ϵ (%)	K-means Time (sec)	K-means Iter	K-means ++ ϵ (%)	K-means ++ Time (sec)	K-means ++ Iter	K-means ǁ ϵ (%)	K-means ǁ Time (sec)	K-means ǁ Iter	C-means ϵ (%)	C-means Time (sec)	C-means Iter
Uniform distribution																									
100	5	0.07	2.0	3.5	0.06	1.4	1.0	0.06	2.4	2.8	0.04	4.9	2.7	0.08	1.6	4.5	0.00	**1.1**	1.3	0.02	2.6	3.2	0.05	5.3	1.3
	10	0.04	4.4	2.9	0.04	3.0	1.2	0..09	5.2	1.4	0.08	9.3	1.8	0.01	3.6	3.6	0.01	**2.7**	1.6	0.04	5.6	1.4	0.02	7.5	1.1
200	5	0.03	1.6	2.6	0.00	1.9	1.2	0.01	4.7	2.3	0.07	6.8	2.3	0.04	**1.4**	3.1	0.02	2.1	1.2	0.07	3.8	2.3	0.02	5.5	2.0
	10	0.07	**3.4**	1.7	0.01	4.2	1.0	0.02	10.0	1.4	0.08	14.6	2.0	0.04	3.7	3.0	0.00	**3.4**	1.1	0.03	8.1	2.1	0.03	13.0	1.4
300	5	0.08	2.7	1.5	0.07	3.1	1.6	0.06	6.0	1.9	0.04	10.6	1.8	0.00	**2.2**	3.4	0.01	2.9	1.0	0.04	5.4	2.9	0.04	12.0	1.4
	10	0.05	5.1	1.0	0.02	6.5	1.0	0.04	13.0	1.3	0.04	22.8	1.2	0.00	**4.8**	2.4	0.01	5.9	1.2	0.03	14.0	1.0	0.02	18.0	1.1
400	5	0.06	3.0	2.4	0.02	2.5	1.0	0.06	9.7	1.3	0.05	13.7	1.5	0.01	2.7	2.3	0.01	**2.0**	1.2	0.05	7.9	1.2	0.05	13.0	1.0
	10	0.04	6.5	2.0	0.01	4.8	1.0	0.04	20.0	1.4	0.04	30.2	1.0	0.01	5.3	1.2	0.02	**4.1**	1.0	0.05	19.0	1.2	0.00	27.0	1.0
500	5	0.07	3.2	2.0	0.01	4.7	1.4	0.07	13.0	1.2	0.03	15.5	1.4	0.02	**2.8**	2.0	0.02	5.1	1.1	0.00	12.0	1.1	0.01	13.0	1.1
	10	0.04	**6.9**	1.5	0.04	10	1.3	0.03	25.0	1.0	0.02	32.6	1.0	0.02	7.5	1.1	0.01	8.1	1.3	0.05	20.0	1.4	0.01	28.0	1.0
Avg.		0.05	3.9	2.1	0.03	4.2	1.1	0.05	11	1.6	0.05	16.0	1.7	0.02	**3.6**	2.7	0.01	3.7	1.2	0.04	9.9	1.8	0.03	14.0	1.1
Normal distribution																									
100	5	0.04	2.4	2.1	0.02	**1.3**	1.6	0.05	2.6	2.7	0.05	4.7	2.4	0.02	1.7	4.9	0.02	**1.3**	1.6	0.04	2.5	2.2	0.01	5.2	2.4
	10	0.04	5.4	1.2	0.04	3.1	2.1	0.04	5.3	1.9	0.04	9.2	2.3	0.01	3.5	3.1	0.01	**2.6**	1.1	0.02	5.8	1.4	0.02	7.6	1.2
200	5	0.06	1.7	2.1	0.03	1.8	1.6	0.07	4.5	1.8	0.03	6.4	2.4	0.01	**1.5**	3.3	0.01	2.2	1.3	0.05	3.6	2.3	0.01	5.7	2.3
	10	0.03	3.7	1.1	0.02	4.4	1.1	0.04	10.1	1.6	0.06	14.6	1.4	0.02	3.9	2.4	0.02	**3.5**	1.2	0.03	8.2	2.1	0.03	14.0	1.1
300	5	0.04	2.9	1.2	0.00	3.2	1.9	0.06	6.0	1.4	0.09	9.2	1.7	0.00	**2.1**	3.4	0.00	2.7	1.5	0.04	5.2	2.6	0.04	12.0	1.4
	10	0.04	5.4	1.0	0.02	6.7	1.1	0.04	14.0	1.0	0.05	20.8	1.2	0.01	**4.6**	2.1	0.00	5.8	1.4	0.03	13.0	1.1	0.03	19.0	1.0
400	5	0.08	3.3	2.3	0.00	2.3	1.5	0.06	9.6	1.3	0.09	13.4	1.7	0.06	2.8	3.0	0.01	**2.2**	1.1	0.03	7.7	1.3	0.05	12.0	1.4
	10	0.04	6.9	2.0	0.01	**4.6**	1.1	0.03	19.0	1.2	0.08	33.2	1.0	0.03	5.1	2.2	0.01	4.3	1.0	0.06	18.0	1.2	0.01	28.0	1.0
500	5	0.04	3.5	3.1	0.01	4.9	1.3	0.07	14.0	1.2	0.03	14.5	1.3	0.02	**2.6**	1.9	0.00	5.2	1.0	0.05	13.0	1.1	0.01	13.0	1.2
	10	0.03	**6.8**	1.2	0.02	8.8	1.2	0.04	23.0	1.3	0.02	32.1	1.1	0.00	7.7	1.1	0.01	7.7	1.0	0.03	18.0	1.0	0.02	28.0	1.0
Avg.		0.04	4.2	1.7	.017	4.1	1.4	0.05	10.8	1.5	0.05	15.8	1.6	0.01	**3.55**	2.7	0.01	3.8	1.2	0.04	9.5	1.6	0.02	14.5	1.4

Table 4.11 Performance comparison between [**eSAA(F)]** and **[eSAA(D)]** (Instance **S2**)

N	M	[ESAA (F)]												[ESAA (D)]											
		K-means			K-means ++			K-means ‖			C-means			K-means			K-means ++			K-means ‖			C-means		
		ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter
Uniform distribution																									
100	5	0.09	10.0	3.1	0.05	14.0	1.0	0.08	30.0	2.4	0.09	17.0	2.6	0.01	**9.0**	4.5	0.00	11.0	1.1	0.03	28.0	3.4	0.02	14.0	1.9
	10	0.05	21.0	2.2	0.02	27.0	1.6	0.05	66.0	1.3	0.06	30.0	1.5	0.03	**17.0**	3.6	0.05	25.0	1.0	0.01	53.0	1.3	0.00	27.0	2.3
200	5	0.01	11.0	2.1	0.09	25.0	1.4	0.01	23.0	2.1	0.04	26.0	2.1	0.02	**10.0**	3.1	0.01	20.0	1.2	0.04	20.0	1.2	0.03	28.0	2.6
	10	0.06	20.0	1.9	0.00	52.0	1.2	0.02	44.0	1.8	0.07	57.0	2.0	0.04	**16.0**	3.0	0.02	44.0	1.0	0.01	40.0	1.1	0.03	50.0	1.5
300	5	0.09	12.0	1.1	0.01	36.0	1.6	0.06	31.0	1.4	0.06	37.0	1.6	0.00	**10.0**	3.4	0.02	32.0	1.5	0.04	27.0	1.3	0.02	37.0	1.4
	10	0.04	21.0	1.0	0.01	68.0	1.2	0.03	65.0	1.3	0.04	72.0	1.1	0.03	**19.0**	2.4	0.01	58.0	1.0	0.00	70.0	1.0	0.03	66.0	1.1
400	5	0.06	14.0	2.6	0.07	43.0	1.4	0.06	41.0	1.0	0.01	47.0	1.2	0.02	**12.0**	2.3	0.02	46.0	1.3	0.03	43.0	1.6	0.05	40.0	1.2
	10	0.09	**31.0**	2.0	0.01	77.0	1.6	0.01	77.0	1.4	0.04	98.0	1.0	0.01	33.0	1.2	0.01	81.0	1.3	0.00	68.0	1.0	0.00	84.0	1.0
500	5	0.07	16.0	3.1	0.06	75.0	1.8	0.07	65.0	1.2	0.03	59.0	1.6	0.02	**17.0**	2.0	0.02	66.0	1.1	0.02	53.0	1.5	0.01	62.0	1.4
	10	0.04	33.0	1.5	0.01	165	1.5	0.03	117	1.1	0.02	112	1.0	0.02	**29.0**	1.1	0.01	163	1.0	0.01	116	1.0	0.04	91.0	1.2
Avg.		0.06	19.0	2.1	0.03	58.0	1.4	0.04	56.0	1.5	0.05	56.0	1.6	0.02	**17.0**	2.7	0.02	55.0	1.1	0.02	52.0	1.4	0.02	50.0	1.6
Normal distribution																									
100	5	0.06	**9.0**	3	0.01	15.0	1.6	0.08	32.0	2.4	0.04	18.0	2.5	0.02	**9.0**	4.9	0.02	10.0	1.0	0.06	27.0	2.6	0.01	15.0	2.5
	10	0.04	22.0	2.1	0.01	26.0	1.2	0.04	70.0	1.0	0.04	33.0	2.4	0.04	**16.0**	3.1	0.01	25.0	1.0	0.02	55.0	1.0	0.02	25.0	1.2
200	5	0.05	**10.0**	2	0.03	26.0	2.1	0.06	23.0	1.8	0.04	24.0	2.4	0.01	11.0	3.3	0.02	21.0	1.1	0.00	20.0	1.7	0.01	28.0	2.5
	10	0.03	18.0	2.1	0.05	55.0	1.3	0.04	44.0	1.6	0.06	61.0	1.9	0.02	**15.0**	2.4	0.01	41.0	1.2	0.03	37.0	1.0	0.03	53.0	1.1
300	5	0.04	12.0	1.2	0.02	35.0	2.5	0.05	34.0	1.4	0.08	35.0	1.9	0.00	**11.0**	3.4	0.02	33.0	1.0	0.00	29.0	1.9	0.03	34.0	1.4
	10	0.04	21.0	1.1	0.02	73.0	1.4	0.04	59.0	1.1	0.05	69.0	1.0	0.04	**19.0**	2.1	0.04	53.0	1.2	0.03	67.0	1.2	0.03	64.0	1.0
400	5	0.06	**13.0**	2.6	0.01	45.0	1.6	0.06	40.0	1.6	0.09	46.0	1.6	0.06	**13.0**	3.0	0.00	49.0	1.3	0.00	39.0	1.5	0.05	40.0	1.5
	10	0.04	**30.0**	2.1	0.03	83.0	1.0	0.02	80.0	1.2	0.07	91.0	1.0	0.06	32.0	2.2	0.01	79.0	1.2	0.04	65.0	1.0	0.00	78.0	1.0
500	5	0.04	**17.0**	3.1	0.01	70.0	1.9	0.07	60.0	1.4	0.03	58.0	1.3	0.04	18.0	1.9	0.00	69.0	1.0	0.02	53.0	1.3	0.05	66.0	1.2
	10	0.03	33.0	1.4	0.02	166	1.0	0.03	124	1.3	0.01	107	1.0	0.01	**31.0**	1.1	0.01	178	1.3	0.00	124	1.0	0.01	89.0	1.0
Avg.		0.04	19	2.1	0.02	59.0	1.5	0.05	57.0	1.5	0.05	54.0	1.7	0.03	**18.0**	2.7	0.01	56.0	1.1	0.02	52.0	1.4	0.02	49.0	1.4

Table 4.12 Performance comparison between [**eSAA(F)]** and **[eSAA(D)]** (Instance **S3**)

N	M	[ESAA (F)]												[ESAA (D)]											
		K-means			K-means ++			K-means ‖			C-means			K-means			K-means ++			K-means ‖			C-means		
		ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter
Uniform distribution																									
100	5	0.01	**38.0**	3.5	0.09	44.0	3.5	0.08	54.0	2.6	0.08	**38.0**	1.8	0.04	41.0	4.2	0.00	47.0	2.2	0.02	44.0	3.6	0.02	41.0	1.5
	10	0.02	63.0	3.1	0.02	75.0	3.4	0.04	89.0	1.1	0.05	64.0	1.1	0.03	68.0	3.1	0.00	**60.0**	2.1	0.01	72.0	1.2	0.02	68.0	1.1
200	5	0.07	44.0	3.2	0.07	68.0	3.6	0.07	68.0	1.9	0.03	56.0	2.4	0.02	**36.0**	3.4	0.04	55.0	1.6	0.07	61.0	1.1	0.03	62.0	2.1
	10	0.06	75.0	3.0	0.00	114	2.9	0.05	116	1.2	0.09	95.0	2.0	0.04	**61.0**	3.0	0.01	103	1.1	0.01	128	1.2	0.03	77.0	1.3
300	5	0.04	54.0	3.0	0.06	82.0	3.5	0.04	72.0	1.3	0.04	72.0	1.6	0.00	**49.0**	3.5	0.02	90.0	1.0	0.04	58.0	1.3	0.02	68.0	1.4
	10	0.05	**91.0**	2.8	0.02	139	2.5	0.04	120	1.0	0.05	118	1.7	0.02	100	2.9	0.04	113	1.2	0.00	114	1.0	0.05	106	1.1
400	5	0.03	66.0	3.3	0.01	78.0	3.4	0.03	92.0	1.0	0.04	92.0	1.1	0.02	**53.0**	2.1	0.02	74.0	1.5	0.03	83.0	1.3	0.05	75.0	1.2
	10	0.04	111	2.2	0.01	133	2.4	0.05	157	1.4	0.07	153	1.0	0.04	**105**	1.2	0.03	120	1.2	0.00	127	1.0	0.00	132	1.0
500	5	0.00	85.0	2.0	0.01	164	1.0	0.05	166	1.2	0.01	113	1.3	0.02	**77.0**	2.1	0.01	133	1.1	0.02	143	1.4	0.01	122	1.2
	10	0.04	140	1.1	0.00	271	1.0	0.06	281	1.6	0.04	191	1.0	0.02	**113**	1.1	0.00	233	1.3	0.06	303	1.0	0.04	155	1.0
Avg.		0.04	77.0	2.7	0.03	117	2.7	0.05	122	1.4	0.05	99.0	1.5	0.03	**70.0**	2.7	0.02	103	1.4	0.03	113	1.4	0.03	89.0	1.3
Normal distribution																									
100	5	0.04	40.0	4.4	0.05	41.0	2.5	0.03	51.0	2.4	0.06	35.0	2.5	0.02	38.0	4.9	0.02	45.0	1.2	0.04	43.0	2.4	0.01	**31.0**	2.5
	10	0.04	**58.0**	3.1	0.02	68.0	2.1	0.05	96.0	1.0	0.04	70.0	2.4	0.04	67.0	3.1	0.00	66.0	1.4	0.02	76.0	1.0	0.02	61.0	1.2
200	5	0.04	48.0	3.1	0.04	70.0	4.2	0.09	73.0	1.8	0.04	60.0	2.4	0.01	**39.0**	3.3	0.04	53.0	1.5	0.02	66.0	1.6	0.01	66.0	2.5
	10	0.03	81.0	3.0	0.02	122	2.2	0.06	126	1.6	0.06	87.0	1.9	0.02	**60.0**	2.4	0.02	97.0	1.1	0.03	137	1.0	0.03	80.0	1.1
300	5	0.01	56.0	3.6	0.00	81.0	4.6	0.04	75.0	1.4	0.05	75.0	1.9	0.00	**45.0**	3.4	0.01	83.0	1.2	0.00	53.0	1.6	0.04	67.0	1.4
	10	0.04	**96.0**	2.8	0.02	145	4.3	0.03	119	1.1	0.05	129	1.0	0.04	108	2.1	0.00	107	1.5	0.03	103	1.2	0.03	113	1.0
400	5	0.05	68.0	3.3	0.01	72.0	2.2	0.04	90.0	1.6	0.05	98.0	1.6	0.06	**52.0**	3.0	0.01	79.0	1.2	0.00	89.0	1.5	0.05	77.0	1.5
	10	0.01	108	2.2	0.02	144	4.1	0.07	167	1.2	0.07	162	1.0	0.06	**98.0**	2.2	0.02	118	1.6	0.06	122	1.0	0.00	120	1.0
500	5	0.04	91.0	2.5	0.02	177	1.2	0.07	152	1.4	0.03	112	1.3	0.04	**70.0**	1.9	0.04	123	1.4	0.02	137	1.3	0.08	116	1.2
	10	0.01	154	1.4	0.03	248	1.2	0.05	268	1.3	0.04	208	1.0	0.01	**119**	1.1	0.00	214	1.2	0.00	283	1.0	0.01	140	1.0
Avg.		0.03	80.0	2.9	0.02	117	2.8	0.05	122	1.5	0.05	104	1.7	0.03	**70.0**	2.7	0.02	99.0	1.3	0.02	111	1.4	0.03	87.0	1.4

Table 4.13 Performance comparison between [**eSAA(F)]** and **[eSAA(D)]** (Instance **S4**)

N	M	[ESAA (F)]												[ESAA (D)]											
		K-means			K-means ++			K-means ||			C-means			K-means			K-means ++			K-means ||			C-means		
		ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter
Uniform distribution																									
100	5	0.06	**75.0**	4.1	0.02	76.0	7.2	0.09	110	2.4	0.04	153	1.5	0.03	81.0	4.0	0.00	82.0	1.6	0.04	89.0	2.6	0.05	124	1.9
	10	0.05	128	4.0	0.02	137	6.4	0.04	190	1.2	0.05	267	1.4	0.05	138	3.1	0.00	**111**	1.2	0.04	154	1.0	0.02	240	1.1
200	5	0.01	85.0	3.7	0.01	67.0	6.0	0.09	154	1.8	0.03	270	2.1	0.01	69.0	3.4	0.03	**54.0**	2.2	0.07	139	1.4	0.03	297	2.1
	10	0.06	147	3.1	0.00	115	6.2	0.05	263	1.1	0.06	467	2.0	0.06	119	3.1	0.02	**104**	1.9	0.03	289	1.0	0.03	378	1.4
300	5	0.00	96.0	3.5	0.03	112	6.1	0.04	159	1.4	0.04	403	1.6	0.00	**86.0**	3.5	0.02	123	2.6	0.04	129	1.4	0.04	383	1.4
	10	0.01	172	3.1	0.00	194	5.7	0.03	304	1.0	0.05	769	1.1	0.01	189	2.9	0.00	**157**	2.1	0.03	289	1.0	0.05	692	1.1
400	5	0.07	123	3.1	0.02	131	5.0	0.03	201	1.0	0.05	541	1.2	0.02	**100**	2.4	0.02	124	2.2	0.03	181	1.3	0.05	438	1.2
	10	0.04	215	2.2	0.03	250	5.1	0.05	362	1.5	0.05	925	1.0	0.04	**204**	2.2	0.01	225	2.0	0.05	293	1.0	0.00	796	1.0
500	5	0.02	149	2.1	0.01	164	5.2	0.07	316	1.2	0.01	700	1.0	0.02	134	2.1	0.02	**133**	1.4	0.02	272	1.2	0.01	756	1.2
	10	0.05	284	1.3	0.01	287	4.0	0.06	553	1.6	0.04	1260	1.0	0.02	**230**	1.1	0.01	247	1.5	0.06	597	1.0	0.04	1021	1.0
Avg.		0.04	147	3.0	0.02	153	5.7	0.06	**261**	1.4	0.04	576	1.4	0.03	**135**	2.8	0.01	136	1.8	0.04	243	1.3	0.03	513	1.3
Normal distribution																									
100	5	0.05	**75.0**	4.1	0.05	76.0	3.2	0.03	104	2.1	0.04	163	2.5	0.02	85	4.0	0.02	85	1.5	0.04	95	2.5	0.09	113	2.9
	10	0.04	131	3.8	0.04	141	2.8	0.04	195	1.0	0.04	290	2.4	0.03	134	3.4	0.01	**116**	1.6	0.02	154	1.3	0.02	225	1.2
200	5	0.01	90.0	3.4	0.04	67.0	3.6	0.09	154	1.7	0.03	262	2.4	0.01	66	3.3	0.03	**58**	2.3	0.05	145	1.5	0.01	270	2.5
	10	0.03	138	3.0	0.02	114	2.0	0.04	270	1.6	0.06	465	1.9	0.03	114	2.5	0.01	**106**	1.1	0.03	308	1.0	0.03	382	1.1
300	5	0.01	101	3.1	0.06	121	2.6	0.04	152	1.4	0.02	372	1.8	0.00	**78**	3.1	0.06	131	1.2	0.01	140	1.6	0.04	360	1.4
	10	0.04	164	2.8	0.01	189	2.4	0.03	319	1.1	0.05	825	1.1	0.04	179	2.8	0.01	**147**	1.6	0.03	277	1.0	0.03	668	1.1
400	5	0.05	132	3.0	0.00	**123**	1.6	0.04	208	1.0	0.05	530	1.4	0.05	**106**	3.0	0.03	114	1.5	0.03	182	1.5	0.05	434	1.5
	10	0.04	231	2.2	0.05	**231**	1.2	0.05	391	1.2	0.06	855	1.0	0.06	**184**	2.2	0.02	221	1.4	0.06	318	1.0	0.00	800	1.0
500	5	0.04	161	2.1	0.03	178	2.5	0.07	289	1.4	0.08	742	1.2	0.02	**134**	2.0	0.01	145	1.9	0.02	297	1.1	0.01	750	1.4
	10	0.01	298	1.4	0.01	**291**	2.1	0.05	512	1.1	0.04	1350	1.0	0.01	**224**	1.1	0.03	226	2.0	0.06	627	1.0	0.01	1053	1.1
Avg.		0.03	152	2.9	0.03	153	2.4	0.05	259	1.4	0.05	585	1.7	0.03	**130**	2.7	0.02	135	1.6	0.04	254	1.4	0.03	506	1.5

Table 4.14 Performance comparison between [**eSAA(F)**] and [**eSAA(D)**] (Instance **S5**)

N	M	[ESAA (F)]												[ESAA (D)]											
		K-means			K-means ++			K-means ‖			C-means			K-means			K-means ++			K-means ‖			C-means		
		ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter
Uniform distribution																									
100	5	0.09	714	5.3	0.03	204	3.3	0.08	223	3.2	0	314	1.6	0.01	571	5.5	0.01	188	1.9	0.05	**181**	3.4	0.02	311	1.4
	10	0.05	1357	5.2	0.04	386	2.9	0.05	424	4.4	0.05	599	1.3	0.05	1221	5.0	0.05	**309**	1.0	0.05	390	1.4	0.05	485	1.2
200	5	0.08	1298	5.2	0.01	292	5.2	0.06	262	2.4	0.06	573	1.2	0.01	1402	4.2	0.01	248	1.6	0.06	**210**	2.3	0.06	527	1.2
	10	0.03	2479	3.9	0.06	555	4.8	0.06	498	2.1	0.06	1083	1.1	0.03	2182	2.9	0.03	500	1.6	0.06	**424**	2.0	0.04	866	1.1
300	5	0.07	1710	4.8	0.02	433	3.2	0.07	322	2.9	0.01	816	1.2	0.01	1693	3.8	0.01	372	2.1	0.08	**290**	2.9	0.01	694	1.3
	10	0.05	3078	3.0	0.02	823	1.5	0.05	609	1.2	0.01	1550	1.0	0.06	2832	3.0	0.06	889	1.1	0.04	**524**	1.0	0.01	1395	1.0
400	5	0.02	2095	3.9	0.03	449	2.2	0.02	**409**	1.8	0	1037	1.2	0.02	1783	2.8	0.02	471	1.3	0.02	442	1.3	0.0	892	1.2
	10	0.04	3981	2.8	0.06	858	1.9	0.04	**736**	1.5	0.02	1981	1.0	0.02	3424	2.4	0.02	**755**	2.0	0.04	773	1.2	0.02	2139	1.2
500	5	0.07	2271	2.6	0.05	452	2.0	0.03	461	1.4	0.02	1057	1.0	0.01	2385	2.1	0.01	**366**	1.6	0.03	406	1.1	0.01	1110	1.2
	10	0.01	4292	2.3	0.01	814	1.9	0.08	830	1.1	0.06	1903	1.0	0.02	3477	1.3	0.02	**806**	1.7	0.01	822	1.1	0.03	1675	1.0
Avg.		0.05	2328	3.9	0.03	527	2.9	0.05	477	2.2	0.03	1091	1.2	0.02	2097	3.3	0.02	490	1.6	0.04	**446**	1.8	0.03	1009	1.2
Normal distribution																									
100	5	0.08	754	4.8	0.05	211	3.2	0.09	206	3.0	0.01	298	1.9	0.05	579	4.5	0.02	198	1.6	0.04	**180**	2.4	0.04	285	1.7
	10	0.03	1476	4.1	0.04	351	2.2	0.05	392	1.9	0.05	555	2.3	0.01	1100	4.0	0.05	**327**	2.1	0.05	417	1.4	0.05	470	1.3
200	5	0.07	1220	4.6	0.05	288	3.6	0.04	254	2.1	0.03	590	1.9	0.07	1391	4.9	0.04	228	1.3	0.06	**195**	2.3	0.0	504	1.2
	10	0.05	2703	3.5	0.06	557	3.1	0.06	495	2.0	0.04	989	1.4	0.04	2318	3.0	0.02	460	1.0	0.06	**414**	2.1	0.05	813	1.1
300	5	0.02	1703	4.7	0.01	423	2.9	0.07	309	2.3	0.01	835	1.2	0.02	1707	3.8	0.01	405	1.5	0.07	**309**	2.8	0.01	746	1.2
	10	0.05	3355	3.3	0.02	815	2.5	0.03	640	1.6	0.01	1457	1.0	0.05	2798	3.2	0.01	967	1.4	0.04	**506**	1.0	0.01	1256	1.0
400	5	0.06.	1949	3.8	0.03	492	2.6	0.02	**417**	1.9	0.02	1125	1.0	0.03.	1698	2.6	0.01	508	1.9	0.02	430	1.3	0.0	961	1.3
	10	0.04	4355	2.4	0.05	820	2.5	0.02	**698**	1.1	0.02	2179	1.0	0.04	3277	1.5	0.03	**698**	1.4	0.04	821	1.2	0.02	2285	1.3
500	5	0.04	2232	2.5	0.04	472	2.6	0.03	439	1.6	0.02	1138	1.0	0.01	2568	1.5	0.01	**384**	1.5	0.02	414	1.1	0.01	1021	1.2
	10	0.01	3912	2.1	0.07	**755**	3.2	0.08	**810**	1.0	0.07	2078	1.0	0.00	3526	2.1	0.02	864	1.1	0.02	811	1.0	0.0	1610	1.1
Avg.		0.04	2366	3.6	0.04	518	2.8	0.05	466	1.9	0.03	1124	1.4	0.03	2096	3.1	0.02	504	1.5	0.04	**450**	1.7	0.02	995	1.2

Table 4.15 Performance comparison between [**eSAA(F)]** and **[eSAA(D)]** (Instance **S6**)

N	M	[ESAA (F)]												[ESAA (D)]											
		K-means			K-means ++			K-means ‖			C-means			K-means			K-means ++			K-means ‖			C-means		
		ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter	ϵ (%)	Time	Iter
Uniform distribution																									
100	5	0.05	2352	5.9	0.01	2464	7.2	0.03	2598	6.9	0.02	2576	8.2	0.02	**1905**	5.7	0.01	1996	1.6	0.01	2601	6.1	0.02	2782	7.1
	10	0.04	5411	5.4	0.03	5691	6.4	0.03	5565	7.3	0.04	5922	7.9	0.04	4870	5.1	0.02	4610	1.2	0.01	**4507**	5.3	0.01	6396	5.4
200	5	0.06	2394	6.2	0.01	2548	6.0	0.02	2499	6.5	0.02	3136	7.5	0.03	2633	6.0	0.03	2293	2.2	0.02	**2024**	6.5	0.01	2540	6.7
	10	0.03	5530	6.0	0.03	5859	6.2	0.03	5747	5.2	0.01	7245	6.9	0.03	**4479**	4.2	0.04	6445	1.9	0.03	5172	4.2	0.01	5868	5.4
300	5	0.06	2667	5.8	0.02	2541	6.1	0.01	2548	5.9	0.00	3542	7.5	0.04	2534	4.4	0.05	**2058**	2.6	0.00	2802	5.9	0.00	3188	6.5
	10	0.02	6181	5.1	0.04	5894	5.7	0.02	5887	5.1	0.04	8218	7.1	0.02	5563	4.0	0.01	5599	2.1	0.02	**4768**	5.5	0.01	9040	5.1
400	5	0.01	2765	4.1	0.02	2618	5.0	0.02	2569	5.8	0.00	3654	5.6	0.01	**2240**	4.1	0.02	2356	2.2	0.00	2440	5.8	0.01	2960	6.4
	10	0.02	6412	4.9	0.03	6041	5.1	0.01	5957	5.4	0.03	8442	5.4	0.03	5514	2.9	0.05	**4893**	2.0	0.01	5361	6.0	0.03	8020	6.5
500	5	0.04	2807	5.6	0.00	2674	5.2	0.02	2670	5.0	0.01	4123	4.8	0.00	3032	3.6	0.03	2300	1.4	0.02	**2162**	4.0	0.01	3711	3.9
	10	0.01	6482	3.3	0.02	6202	4.0	0.00	6100	4.1	0.00	9569	4.1	0.01	5250	2.3	0.05	6698	1.5	0.00	**5246**	3.3	0.02	7751	3.3
Avg.		0.03	4300	5.2	0.02	4253	5.7	0.02	4214	5.7	0.02	5643	6.5	0.02	3802	4.2	0.03	3925	1.8	0.01	**3708**	5.3	0.01	5226	5.6
Normal distribution																									
100	5	0.04	2493	5.7	0.01	2682	2.0	0.02	2312	7.1	0.01	2758	8.4	0.03	**1877**	5.2	0.00	2046	1.9	0.01	2525	7.3	0.03	2888	6.2
	10	0.04	5681	5.1	0.03	6065	1.6	0.05	5253	7.3	0.04	6129	7.3	0.02	4785	4.9	0.01	**4303**	1.4	0.04	4625	7.0	0.02	6352	6.4
200	5	0.06	2319	6.4	0.01	2678	2.2	0.06	2608	6.5	0.05	3321	7.5	0.03	2759	6.1	0.03	2317	2.3	0.06	**2200**	6.1	0.01	2497	5.7
	10	0.03	5377	5.9	0.03	6020	1.6	0.04	5835	5.2	0.01	6643	6.1	0.04	**4299**	5.5	0.01	6975	1.5	0.04	4944	5.3	0.01	6280	5.1
300	5	0.04	2734	5.4	0.02	2627	2.9	0.03	2392	5.9	0.01	3503	7.4	0.02	2522	4.1	0.04	**1857**	1.9	0.00	2972	5.4	0.01	3359	5.9
	10	0.02	5777	5.1	0.04	6442	1.1	0.04	6352	5.1	0.04	8815	7.0	0.01	5080	4.0	0.03	5680	2.0	0.04	**4541**	4.9	0.01	9776	4.0
400	5	0.01	2524	4.6	0.02	2513	2.3	0.02	2490	5.8	0.02	3328	5.4	0.02	**2157**	4.6	0.02	2309	1.2	0.02	2205	5.7	0.02	2856	5.4
	10	0.01	7044	4.5	0.03	5686	1.2	0.01	5651	5.4	0.03	9027	5.4	0.03	5492	3.1	0.02	**4637**	1.0	0.01	5340	5.1	0.03	8173	3.5
500	5	0.05	2898	4.3	0.00	2735	1.6	0.02	2690	5.0	0.02	4438	4.9	0.00	2978	3.2	0.01	**2091**	1.5	0.05	2222	5.2	0.01	3902	3.9
	10	0.01	5884	3.3	0.02	5689	1.5	0.01	5521	4.1	0.00	8687	4.5	0.00	4771	2.1	0.06	6725	1.1	0.00	**5019**	4.2	0.01	8165	3.1
Avg.		0.03	4273	5	0.02	4314	1.8	0.03	4110	5.7	0.02	5665	6.4	0.02	3672	4.3	0.02	**3894**	1.5	0.03	3659	5.6	0.02	5425	4.9

Our computational experiences with experimental sets 1 and 2 indicate that as the sample size increases it adds more complexity in solving algorithm **[SAA]** compared to **[eSAA(F)]** and **[eSAA(D)].** For instances, as the sample size (**N**) increases from 100 to 500 the average computational time in solving **[SAA]** increases up to 1546% compared to 443% and 397% in **[eSAA(F)]** and **[eSAA(D)]**, respectively. Note that this computation benefits are achieved in both **[eSAA(F)]** and **[eSAA(D)]** algorithms without sacrificing any solution qualities.

To better illustrate the effect of sample size **N** and replication number **M** on computation time, we solve our stochastic **[FLP]** instance **S4** by varying the sample size **N** (shown in **Figure 4.3**) and **M** (shown in **Figure 4.4**) in **[SAA]** and **[eSAA(D)]**. The results in **Figure 4.3** show that while the solution time increases steadily with **N** in **[SAA],** the increase is not steady in **[eSAA(D)]**. Fuzzy C-means provides the lowest savings while *K-means*++ and K-means produce the highest savings in computation time for the instance we considered. The poor computational performance from fuzzy C-means may be due to the time it takes in computing the degree of membership of every data in multiple clusters. In **Figure 4.4** we vary the number of replications from 10 to 50 and observe that the solution time increases with the number of replications. Note that in both experiments an MIP clustering technique is employed to solve **[eSAA(F)]**. The poor performance of the MIP clustering technique may be attributed due to the enormous time taken to solve the *NP*-hard formulation of the clustering problem and thus may not be worthy to use for relatively large sample size scenarios.

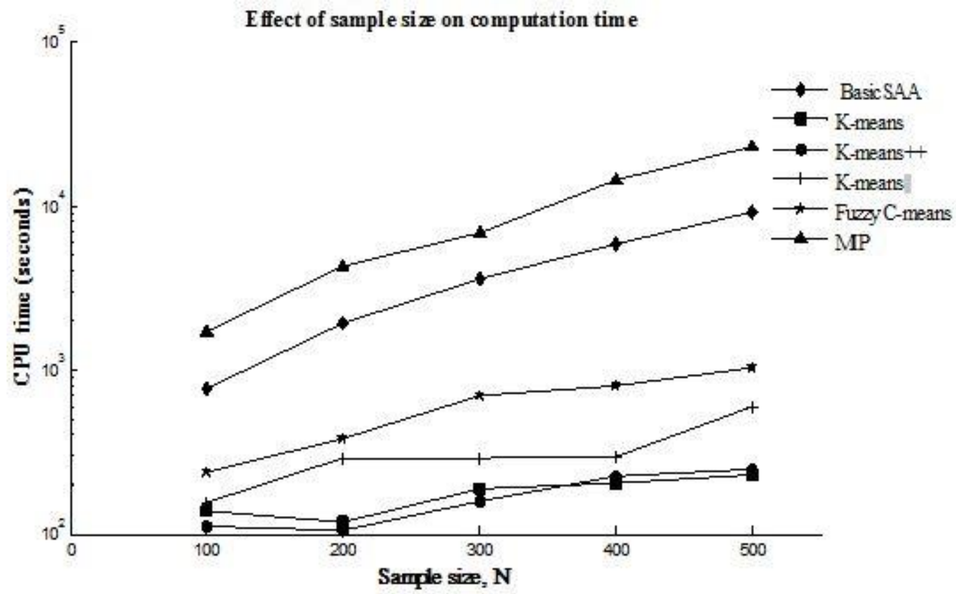


Figure 4.3 Effect of sample size on computation time

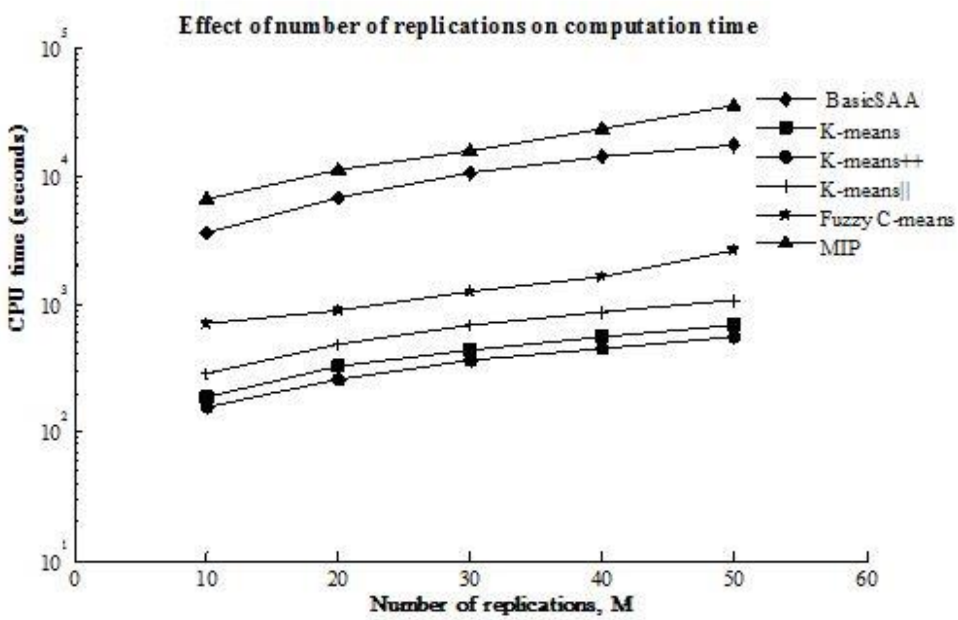


Figure 4.4 Effect of number of replications on computation time

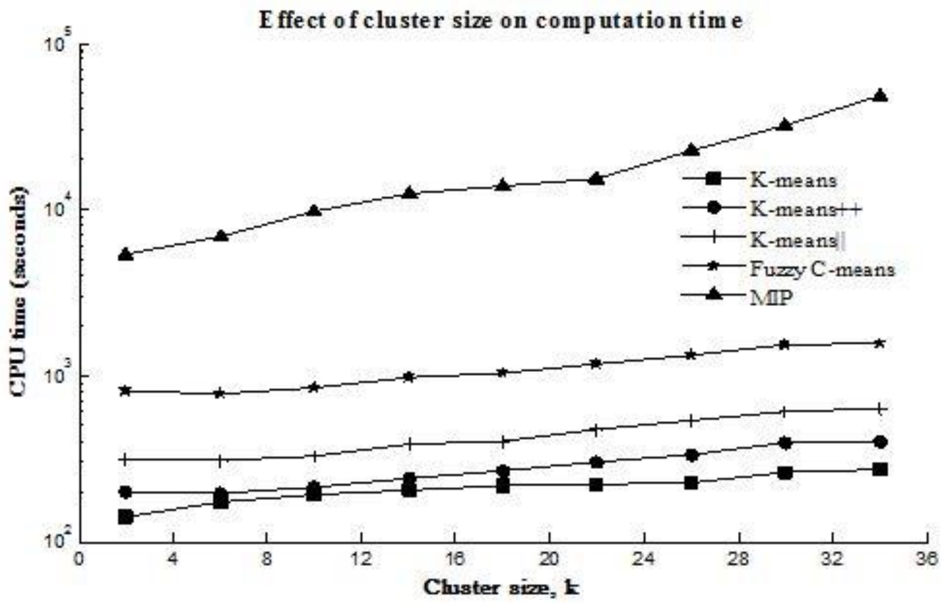


Figure 4.5 Effect of cluster size on computation time

4.4.3 Single-sink transportation problem ([SSP])

Maggioni et al. [88] propose a *single-sink transportation problem* (**[SSP]**) where the authors investigate the production capacity of the suppliers under uncertain customer demand. Details about the problem description along with the formulation can be obtained from Maggioni et al. [88]; however, we now introduce the formulation along with a short description of the problem. In this problem, the authors assume that a single warehouse is the only destination location. An external source is assumed to be responsible for leasing the vehicles. The supply capacity of this external source is assumed to be enough to supply any number of vehicles required. However, the vehicles must be booked in advance before the realization of demand at the warehouse. After the realization of demand, booking of vehicles can be cancelled with a cancellation fee which denoted by α. If the demand at warehouse exceeds the supply capacity of the supply plants, the residual amount is purchased from another source at a higher price, β. The objective of this problem is to determine for each supplier the number of vehicles to book in advance to minimize the total costs, given by the sum of the transportation costs and penalty costs. **Table 4.16** introduces the notations used in this formulation.

Table 4.16 Notations and symbols in **[SSP]** formulation

Notation	Explanation
Sets	
I	Set of suppliers
Ω	Set of scenarios
Parameters	
c_i	Unit transportation cost of supplier $i \in I$
p_i	Unit production cost of supplier $i \in I$
β	Penalty cost
q	Vehicle capacity
g	Maximum capacity that can be booked
h	Initial inventory level at the customer
l_{max}	Storage capacity at the customer
p^{ω}	Probability of scenario $\omega \in \Omega$
a_i	Supply capacity of supplier $i \in I$ in scenario $\omega \in \Omega$
d^{ω}	Customer demand at scenario $\omega \in \Omega$
A	Cancellation fee
Decision variables	
x_i	Number of vehicles booked from supplier $i \in I$
z_i^{ω}	Number of vehicles actually used from supplier $i \in I$ in scenario $\omega \in \Omega$
r^{ω}	Penalty amount in scenario $\omega \in \Omega$

Now, the two-stage stochastic model becomes

$$[\boldsymbol{SSP}]: Minimize\ \ q\sum_{i=1}^{I} c_i x_i + \sum_{\omega=1}^{\Omega} p^{\omega}\left[\beta r^{\omega} - (1-\alpha) q \sum_{i=1}^{I} c_i (x_i - z_i^{\omega})\right]$$

subject to

$$q\textstyle\sum_{i=1}^{I} x_i \ \leq \ g \qquad (4.42)$$

$$h + \; q \sum_{i=1}^{I} z_i^{\omega} + r^{\omega} - d^{\omega} \;\; \geq \;\; 0 \;\; \forall \omega \in \Omega \tag{4.43}$$

$$h + \; q \sum_{i=1}^{I} z_i^{\omega} + r^{\omega} - d^{\omega} \;\; \leq \;\; l_{max} \;\; \forall \omega \in \Omega \tag{4.44}$$

$$z_i^{\omega} \;\; \leq \;\; x_i \;\; \forall i \in I, \omega \in \Omega \tag{4.45}$$

$$q z_i^{\omega} \;\; \leq \;\; a_i \;\; \forall i \in I, \omega \in \Omega \tag{4.46}$$

$$r^{\omega} \;\; \geq \;\; 0 \;\; \forall \omega \in \Omega \tag{4.47}$$

$$x_i \;\; \in \;\; \mathbb{Z}^{+} \;\; \forall i \in I, \omega \in \Omega \tag{4.48}$$

$$z_i^{\omega} \;\; \in \;\; \mathbb{Z}^{+} \;\; \forall i \in I, \omega \in \Omega \tag{4.49}$$

Constraint (4.42) ensures that the total number of booked vehicles from supplier $i \in I$ to the customer is not greater than $\frac{g}{q}$. Constraints (4.43) and (4.44) ensure that second-stage storage level is between 0 and l_{max}. Constraints (4.45) guarantee that the total number of vehicles serving supplier $i \in I$ is at most equal to the number of vehicles booked in advance under scenario $\in \Omega$, Constraints (4.46) indicate that the quantity of product delivered from supplier $i \in I$ does not exceed production capacity a_i under scenario $\omega \in \Omega$. Constraints (4.47) are continuous variables whereas constraints (4.48) and (4.49) are integer variables.

We now use the data provided by Maggioni et al. [88] to generate three instances (reported in **Table 4.17**) to solve problem **[SSP]** using the algorithms proposed in **Section 4.3.2**.

Table 4.17 Deterministic equivalent of test instances for problem **[SSP]**

Instance	$\|I\|$	Integer Variables	Continuous Variables	Total Variables	No. of Constraints
SSP1	50	100	1	101	104
SSP2	100	200	1	201	204
SSP3	200	400	1	401	404

Table 4.18 presents the experimental results in solving problem **[SSP]** using algorithms **[SAA]**, **[eSAA(F)]** and **[eSAA(D)]** on the three problem instances reported in **Table 4.17**. The results are in alignment with the results discussed previously for **[FLP]** and it is observed that all the problems are solved within a pre-specified tolerance gap under the specified time limit. Results indicate that both **[eSAA(F)]** and **[eSAA(D)]** outperform **[SAA]** in terms of solution quality and running time for all the test instances reported in **Table 4.17**. On average, **[eSAA(D)]** and **[eSAA(F)]** are approximately 217% and 205% faster than **[SAA]** algorithm, respectively.

Table 4.18 Results for **[SAA]**, **[eSAA(F)]**, and **[eSAA(D)]** in problem **[SSP]**

Problem Instance	**N**	**M**	**[SAA]** ϵ (%)	Time (sec)	Iter	**[eSAA(F)]** ϵ (%)	Time (sec)	Iter	**[eSAA(D)]** ϵ (%)	Time (sec)	Iter
SSP1	100	5	0.05	3.8	2.1	0.02	**2.6**	1.4	0.03	2.7	1.0
		10	0.01	5.1	5.0	0.04	**2.8**	2.0	0.01	**2.8**	1.0
	200	5	0.01	5.3	3.3	0.02	**2.8**	2.2	0.02	**2.8**	1.0
		10	0.03	8.0	5.2	0.03	3.0	3.0	0.01	**2.9**	1.0
	300	5	0.02	6.9	2.7	0.01	**2.9**	1.6	0.02	3.1	1.0
		10	0.02	11.4	1.4	0.02	3.7	2.2	0.07	**3.2**	1.0
	400	5	0.01	8.8	1.1	0.01	**3.1**	1.6	0.01	3.2	1.0
		10	0.02	14.9	1.3	0.05	6.5	1.2	0.03	**3.7**	1.0
	500	5	0.06	9.0	2.0	0.02	**3.4**	3.4	0.01	4.0	1.0
		10	0.01	15.5	1.8	0.01	8.3	3.0	0.02	**5.6**	1.0
	Avg.		0.02	8.9	2.6	0.02	3.9	2.2	0.02	**3.4**	1.0
SSP2	100	5	0.08	7.7	2.0	0.07	**5.2**	1.4	0.04	**5.2**	1.0
		10	0.03	10.8	1.6	0.02	7.1	1.1	0.05	**6.9**	1.0
	200	5	0.01	10.7	1.3	0.09	**5.4**	1.2	0.02	**5.4**	1.0
		10	0.05	18.1	1.4	0.03	7.6	1.7	0.01	**7.5**	1.0
	300	5	0.03	14.2	1.9	0.01	5.7	3.0	0.07	**5.6**	1.0
		10	0.06	25.3	1.3	0.01	8.0	1.5	0.01	**7.9**	1.0
	400	5	0.01	18.0	2.7	0.07	5.9	1.8	0.08	**5.8**	1.0
		10	0.09	34.0	1.2	0.02	8.5	1.2	0.01	**8.5**	1.0
	500	5	0.03	21.5	1.5	0.06	6.6	3.0	0.06	**6.2**	1.0
		10	0.06	40.7	1.4	0.01	9.1	1.6	0.02	**9.0**	1.0
	Avg.		0.05	20.1	1.6	0.04	6.9	1.8	0.04	**6.8**	1.0
SSP3	100	5	0.04	15.1	1.2	0.09	10.8	2.0	0.01	**10.1**	1.0
		10	0.05	20.7	2.6	0.01	11.1	1.4	0.07	**10.7**	1.0
	200	5	0.02	21.9	2.4	0.06	**10.8**	1.8	0.04	**10.8**	1.0
		10	0.06	33.7	3.1	0.01	11.2	1.2	0.02	**11.0**	1.0
	300	5	0.01	29.2	3.3	0.06	**10.9**	1.2	0.01	**10.9**	1.0
		10	0.04	48.1	1.6	0.03	11.6	1.1	0.04	**11.5**	1.0
	400	5	0.01	36.5	1.9	0.01	11.2	2.2	0.08	**11.1**	1.0
		10	0.06	62.8	1.3	0.04	12.3	1.0	0.03	**12.1**	1.0
	500	5	0.08	43.5	1.8	0.05	**11.4**	1.0	0.05	**11.4**	1.0
		10	0.05	76.5	1.2	0.01	12.7	1.0	0.01	**12.6**	1.0
	Avg.		0.04	38.8	2.0	0.04	11.4	1.4	0.04	**11.2**	1.0

4.4.4 Supply transportation problem ([STP])

Maggioni et al. [89] propose a *supply transportation problem* (**[STP]**) where the authors investigate a transportation problem related to gypsum replenishment for a cement producer under customer demand uncertainty. The details of the problem description along with the formulation can be obtained from Maggioni et al. [89]; however, we now introduce the formulation along with a short description of the problem. In this problem, a total of 24 suppliers, each having several plants serve the need of 15 warehouses of the same customer. Shipments are performed by capacitated vehicles whereas the booking of these vehicles has to be done in advance prior to a realization of a customer demand. Similar to the *single-sink transportation problem* (**[SSP]**), booking of vehicles can be cancelled after the realization of demand. Thus, a penalty cost will be imposed for not fulfilling the customer demand by the suppliers. The objective is to determine the number of vehicles to book at the beginning of each week to replenish gypsum at all cement factories of the producer to minimize the total cost, given by the sum of the transportation costs and penalty cost incurred due to purchasing from external suppliers in extreme situations. **Table 4.19** introduces the notations used in the formulation of **[STP]**.

Table 4.19 Notations and symbols in **[STP]** formulation

Notation	Explanation
Sets	
S	Set of suppliers
I_s	Set of plant locations of supplier $s \in S$
D	Set of warehouse locations
Ω	Set of scenarios
Parameters	
t_{id}	Unit transportation cost of plant $i \in I_s, s \in S$ to warehouse $d \in D$
b_d	Penalty cost for assigning a vehicle to warehouse $d \in D$
Q	Vehicle capacity
g_d	Maximum capacity that can be booked for warehouse $d \in D$
g_s	Maximum requirement capacity of supplier $s \in S$
a_s	Minimum requirement capacity of supplier $s \in S$
l_{max}	Storage capacity at the warehouses
α	Discount
p^{ω}	Probability of scenario $\omega \in \Omega$
d_d^{ω}	Customer demand at warehouse $d \in D$ in scenario $\omega \in \Omega$
Decision variables	
x_{id}	Number of vehicles booked from supplier $i \in I_s$ to warehouse $d \in D$
z_{id}^{ω}	Number of vehicles actually used from supplier $i \in I_s$ to warehouse $d \in D$ in scenario $\omega \in \Omega$
r_d^{ω}	Number of extra vehicles used from external sources for warehouse $d \in D$ in scenario $\omega \in \Omega$

Now, the two-stage stochastic model becomes

$$[\mathbf{STP}]\ \text{Minimize}\ q\sum_{s=1}^{S}\sum_{i=1}^{I_s}\sum_{d=1}^{D} t_{id}x_{id} + \sum_{\omega=1}^{\Omega} p^{\omega}[\sum_{d=1}^{D} q\, b_d r_d^{\omega} - \alpha q \sum_{s=1}^{S}\sum_{i=1}^{I_s}\sum_{d=1}^{D} t_{id}(x_{id} - z_{id}^{\omega})]$$

subject to

$$q \sum_{s=1}^{S} \sum_{i=1}^{I_s} x_{id} \leq g_d \quad \forall \ d \in D \tag{4.50}$$

$$0 \leq l_d^0 + q\left(\sum_{s=1}^{S} \sum_{i=1}^{I_s} z_{id}^{\omega} r_d^{\omega}\right) - d_d^{\omega} \leq l_{max} \quad \geq \ 0 \ \forall \, d \in D, \omega \in \Omega \tag{4.51}$$

$$z_{id}^{\omega} \leq x_{id} \ \ \forall \, i \ \in I_s, s \in \mathrm{S}, \mathrm{d} \in D, \omega \in \Omega \tag{4.52}$$

$$a_s \leq l_d^0 + q\left(\sum_{i=1}^{I_s} \sum_{d=1}^{D} z_{id}^{\omega}\right) \leq g_s \ \ \forall \ s \in S, \omega \in \Omega \tag{4.53}$$

$$z_{id}^{\omega} \ \in \ \mathbb{Z}^+ \ \ \forall \, i \ \in I_s, d \in D, \omega \in \Omega \tag{4.54}$$

$$r_d^{\omega} \ \in \ \mathbb{Z}^+ \ \ \forall \, i \ \in I_s, d \in D, \omega \in \Omega \tag{4.55}$$

$$x_{id} \ \in \ \mathbb{Z}^+ \ \ \forall \, i \ \in I_s, d \in D, \omega \in \Omega \tag{4.56}$$

Constraints (4.50) ensure that for each warehouse $d \in D$, the total number of booked vehicles from the suppliers to the warehouses does not exceed ($\frac{g_d}{\mathrm{q}}$). Constraints (4.51) indicate that the storage level of warehouses $d \in D$ is between 0 and l_{max}. Constraints (4.52) guarantee that the number of vehicles used by the suppliers is at most equal to the number of vehicles booked in advance. Constraints (4.53) indicate that for all suppliers $s \in \mathrm{S}$, the volume of products transported to warehouses $d \in D$ by the used vehicles is at least a_s and at most g_s. Constraints (4.54), (4.55), and (4.56) are integer constraints.

We now use the data provided by Maggioni et al. [89] to generate three instances (reported **Table 4.20**) to solve **[STP]** using the algorithms proposed in **Section 4.3.2**.

Table 4.20 Deterministic equivalent of test instances for problem **[STP]**

Instance	$\lvert I_s \rvert$	Integer Variables	No. of Constraints
STP1	5	165	774
STP2	10	315	1494
STP3	15	455	2214

Table 4.21 presents the experimental results obtained from solving problem **[STP]** using algorithms **[SAA]**, **[eSAA(F)]**, and **[eSAA(D)]** on the three problem instances reported in **Table 4.20**. Yet again, the results are consistent with the results discussed previously for **[FLP]** and **[STP]**. It is observed that on average, **[eSAA(D)]** and **[eSAA(F)]** are 2235% and 1655% faster than **[SAA]**, respectively. Moreover, the average optimality gap produced by **[eSAA(D)]** and **[eSAA(F)]** are 33.0% and 9.1% better than that from **[SAA]**, respectively. In summary, the results obtained by using **[eSAA(F)]** and **[eSAA(D)]** to solve **[SSP]** and **[STP]** repeat the promising trends observed from solving **[FLP]** within our experimental range.

Table 4.21 Results for **[SAA]**, **[eSAA(F)]**, and **[eSAA(D)]** in problem **[STP]**

Problem instance	N	M	[SAA]			[eSAA(F)]			[eSAA(D)]		
			ϵ (%)	Time (sec)	Iter	ϵ (%)	Time (sec)	Iter	ϵ (%)	Time (sec)	Iter
STP1	100	5	0.03	148	4.2	0.03	**21**	3.3	0.01	24	1.5
		10	0.06	279	3.5	0.08	**35**	2.9	0.01	36	1.6
	200	5	0.03	334	4.1	0.02	**29**	3.7	0.04	31	2.3
		10	0.07	697	2.1	0.01	**39**	2.1	0.03	42	1.2
	300	5	0.04	648	2.6	0.04	39	2.7	0.03	**38**	1.3
		10	0.01	1282	2.8	0.01	61	2.5	0.01	**49**	1.4
	400	5	0.03	1135	3.2	0.03	41	1.7	0.07	**39**	1.6
		10	0.06	2121	1.3	0.04	78	1.3	0.02	**70**	1.4
	500	5	0.03	1529	1.1	0.02	51	2.6	0.03	**41**	1.8
		10	0.03	3293	1.0	0.07	90	2.2	0.02	**77**	2.1
	Avg.		0.04	1147	2.6	0.04	48	2.5	0.03	**45**	1.6
STP2	100	5	0.08	393	4.3	0.02	74	3.4	0.01	**71**	2
		10	0.05	741	4.2	0.04	123	3.1	0.04	**111**	1.1
	200	5	0.03	889	3.9	0.01	102	5.3	0.01	**97**	1.7
		10	0.01	1853	3.4	0.05	137	4.9	0.08	**131**	1.6
	300	5	0.08	1723	4.1	0.02	140	3.3	0.01	**119**	2.2
		10	0.03	3410	3.6	0.09	215	1.6	0.05	**152**	1.1
	400	5	0.07	3019	3.7	0.08	145	2.3	0.03	**120**	1.4
		10	0.08	5643	3.2	0.05	277	2	0.03	**218**	2.1
	500	5	0.03	4066	3.1	0.04	182	2.1	0.01	**129**	1.7
		10	0.01	8758	2.3	0.01	318	2	0.02	**239**	1.8
	Avg.		0.05	3050	3.6	0.04	171	3	0.03	**139**	1.7
STP3	100	5	0.05	942	4.2	0.02	189	6.1	0.02	**154**	1.4
		10	0.02	1779	5.8	0.03	314	5.4	0.01	**234**	1.1
	200	5	0.01	2133	5.3	0.01	261	5.0	0.04	**203**	2.0
		10	0.01	4447	3.1	0.02	350	5.1	0.06	**274**	1.8
	300	5	0.03	4135	3.7	0.01	356	5.3	0.05	**250**	2.4
		10	0.02	8184	3.9	0.04	548	4.7	0.01	**319**	1.9
	400	5	0.02	7246	4.2	0.07	370	4.0	0.03	**252**	2.1
		10	0.08	13544	2.5	0.03	706	4.1	0.04	**457**	1.8
	500	5	0.01	9758	2.3	0.01	463	4.3	0.02	**270**	1.2
		10	0.05	21020	2.1	0.03	811	3.2	0.04	**502**	1.3
	Avg.		0.03	7319	3.7	0.03	437	4.7	0.03	**292**	1.7

4.5 Conclusions

This study proposes a methodological approach to enhance the performance of the basic SAA by incorporating dynamic clustering strategy within the algorithmic framework. This approach is then experimentally validated in the context of a stochastic facility location problem. We created different variants of the enhanced sample average approximation algorithm (i.e., different clustering strategy, fixed clusters vs. dynamic clusters) and the compare the computational performance of those variants with the basic SAA algorithm. Computational performance indicates that both enhanced SAA with fixed clustering size and dynamic clustering size are capable of tackling large scenario sets and offers high quality solutions constantly in a reasonable amount of time. It is observed that on average enhanced SAA with fixed clustering size and dynamic clustering size solves [**FLP**] almost 631% and 699% faster than the basic SAA algorithm. Moreover, we observe that there is no single winner among the clustering techniques to solve all the problem instances of the enhanced SAA algorithm. For instance, *k*-means has outperformed others in solving instances from **S1** to **S4** whereas k-means|| has provided superior results in solving large scale problem instances, i.e., **S5** and **S6**. Enhanced SAA incorporating fuzzy C-means gives the worst result among all the clustering techniques; however, the integration still outperforms the basic SAA algorithm in terms of computation time and solution quality.

In summary, the contributions of this paper to the literature are manifold. First, our method provides the flexibility to start with any sample size and then dynamically adjusting the size based on prior computational performances to ensure convergence of the algorithm. Second, we incorporated different clustering strategies inside SAA to obtain a valid lower bound and improves the performance of basic SAA algorithm. Finally, we tested our algorithm in a classical facility location problem to determine the effectiveness of using our approach in a stochastic network framework.

This work can be extended in several directions. First of all, we can apply the technique to the AM feasibility problem in Chapter II as well as the AM deployment problem in Chapter III formulated as a mixed integer programming problem. Our method can also be used to solve other optimization problems such as two-stage chance-constrained problems and progressive hedging based optimization problems. Additionally, efforts are required to develop advanced clustering strategies inside our proposed methodology to further improve the performance of the algorithm. These issues will be addressed in future studies.

CHAPTER V

CONCLUSIONS AND FUTURE WORK

5.1 Conclusions

The adoption of additive manufacturing for fabricating biomedical implants at hospitals provides many potential benefits which include opportunity to receive more patient-specific, customized parts with faster response, a lower inventory level, and reduced delivery costs. Our study shows that a mathematical model that captures both process-level and system-level costs helps to make better economic decisions on the feasibility of AM technology in the manufacture of biomedical implants. A key cost parameter, the ratio between unit production costs of AM and TM (ATR) indicates the point at which the adoption of AM makes an economic sense in the fabrication of biomedical implants. Using the state of Mississippi as a test bed, when ATR < 3.5, our study suggest a harmonious implementation of AM and TM production in which case the demand of biomedical implants may be filled using both AM and TM facilities depending on the required product lead time, locations of patients, capacity of the AM facilities. Another key parameter is the urgency of the product. When a biomedical implant is needed in a short time window (e.g., in a life-or-death situation), TM suppliers may not have the parts with specific features (e.g., dimensions, shapes, etc.) in stock, and may require an additional lengthy customization process. In this case, AM may be a viable option because of the short response time and the capability of mass customization, irrespective of the high cost.

In order to reap the full benefits of AM technology, the deployment configuration of AM facilities is an important issue that one needs to take into consideration given the high cost of AM machines. Moreover, a model that recognizes the high cost of raw materials used in manufacturing biomedical implants while making inventory decisions in solving the AM deployment problem provides a more realistic solution. Our proposed continuous approximation (CA) cost model quantifies the supply-chain network costs associated with the production of biomedical implants using AM technologies, and provides the optimal deployment configuration of AM sites in the southeastern region of the United States for efficient and responsive fabrication of biomedical implants for use in hospitals and clinics in the region. Utilizing the proposed CA model in making AM deployment decision instead of the extreme AM configuration options in literature results in enormous saving in cost. We can achieve a saving of 7% of the total network cost by using the CA model instead of locating only one central AM facility to serve the entire region. The saving increases to 59% when compared with establishing an AM facility in every county in the region. The CA model records a ground-breaking saving of 71% of total network cost in a scenario where the demand of biomedical implants decrease by 50% and annual personnel cost doubles.

Results from our extensive numerical experiments show the demand level of the biomedical implants has the most significant effect on how many AM facilities should be located in the region and how distributed the deployment should be. Specifically, if other parameters are kept constant, doubling the demand, increases the number of AM facilities by more than 59%, thereby making the network more distributed, while the number reduces by up to 33% if the demand level is halved, making the network less distributed. Other factors such as the price and maintenance cost of AM machines, the labor cost of operating the machines and the unit transportation cost of an item per mile all affect the total supply chain network cost and deployment configuration of AM facilities. Reducing the fixed AM investment cost by 50% can result in an increase of up to 37% in the number of AM facilities established and reduce the total network cost by about $1.4 million or 0.8%.

Our proposed enhanced sample average approximation (eSAA) technique provides a methodological approach that incorporates clustering and statistical tests in an optimization procedure to achieve faster solution convergence time than the basic sample average approximation approach. The eSAA with fixed clustering size and dynamic clustering size solves our test stochastic facility location problem up to 631% and 699% faster than the basic SAA technique.

5.2 Future work

It will be interesting to see the application of our models and techniques beyond healthcare to solve AM- related decision problems in other areas such as automobile, aviation and energy production equipment. In such a study, one can account for the cost analysis of assemblies. AM allows for the production of multiple parts simultaneously in the same build, making it possible to produce an entire product. TM often includes production of parts at multiple locations, where an inventory of each part might be stored. The parts are shipped to a facility where they are assembled into a product. AM has the potential to replace some of these steps for some products, as this process might allow for the production of the entire assembly. This would reduce the need to maintain large inventories for each part of one product. It also reduces the transportation of parts produced at varying locations and reduces the need for just-in-time delivery.

We can extend our proposed eSAA technique of Chapter IV to solve the AM feasibility problem in Chapter II as well as the AM deployment problem in Chapter III formulated as a mixed integer programming problem, especially when the network is scaled up to include the entire USA. We can also apply the method to solve other optimization problems such as two-stage chance-constrained problems and progressive hedging based optimization problems. Additionally, efforts are required to develop advanced clustering strategies inside our proposed methodology to further improve the performance of the algorithm.

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