Sequential decision making and simulation-optimization for the design of complex engineering systems

by

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DEDICATION

I dedicate my dissertation work to my wonderful friend and wife, Maryam and my mother, my father, and my brother for devoting themselves to my life, for their unconditional love and support. Thanks for your endless support in this long trip.

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ABSTRACT

In this dissertation, we create a novel simulation-based design platform to determine the optimal design of engineered systems. We develop resilient, reliable, and flexible design solutions that account for system uncertainties within the optimization algorithm. The purpose of this dissertation is to study simulationoptimization and sequential decision-making strategies for the design of complex engineering systems. Simulation optimization and sequential decision-making frameworks are developed in order to optimize the design of complex engineering systems in four different studies: designing a resilient wind turbine system for risk-averse decision-makers, improving the reliable design of airfield concrete pavement, incorporating flexibility into the design of a hybrid renewable energy system, and finding the optimal policy for the design of engineering systems using reinforcement learning. In chapter 2, a framework is developed to incorporate risk aversion into a firm's design decisions for a resilient wind turbine system. In chapter 3, a reliabilitybased design optimization framework is developed for airfield concrete pavement design. Chapter 4 presents a multi-stage simulation-optimization algorithm for the flexible design of a hybrid renewable energy system. In chapter 5, a new framework is developed to find the optimal policy for the design of engineering systems operating under uncertainty.

CHAPTER 1. INTRODUCTION

1.1 Overview

The advent of computing technology has given people the ability to solve complex mathematical models. Computer simulations can rapidly solve equations that are difficult to solve analytically and can explore thousands of scenarios in a short amount of time. Tens of thousands of replications of Monte Carlo simulation can often be run in mere seconds, and from those replications, metrics such as the average value of output parameters can be estimated with good precision.

In the context of this thesis, a simulation is used to solve a mathematical model representing a system and to evaluate the behavior of the system given input variables (Carson and Maria, 1997). When simulations are used to inform decisions, running thousands of replications for each possible alternative in the set of feasible decisions will often enable an appropriate comparison among the alternatives. Randomness in the simulation implies that one replication of the simulation given a specific alternative will return an output value that in general will change for each replication. According to the strong law of large numbers, the average of all output values will tend to towards the expected value of the output as the number of replications goes toward infinity.

If the simulation is complex, if the number of decision variables is large, and/or if at least one of the decision variables is a continuous variable, conducting thousands of replications for each feasible alternative may not be realistic. Simulation optimization seeks to identify the optimal alternative that maximizes or minimizes a decision maker's objective (e.g., expected value of an output) when the objective is evaluated via simulation (Powell and Ryzhov, 2012; Fu, 2002; Amaran et al., 2016). Simulation optimization can encapsulate several methodologies including gradient based search methods, Bayesian methods, stochastic optimization, heuristic methods (such as genetic algorithm and simulated annealing), and ranking and selection (Carson and Maria, 1997). Carson and Maria (1997) and Fu et al. (2015) provide excellent overview of these methods.

Simulation optimization techniques may be essential for many engineering problems, especially since the outcome of many design decisions are generated via simulation (Prasetio, 2003). This thesis combines Monte Carlo simulations of engineering design problems with a Bayesian optimization algorithm (Brochu et al., 2010; Calandra et al., 2016, 2014; Snoek et al., 2012) to find the optimal engineering system design. The Bayesian optimization algorithm uses simulation to create a surrogate model of the objective function and exploits it in order to identify decision variables in the feasible solution space to sample in the simulation (Lizotte, 2008a). Bayesian optimization is an iterative process where the output of the algorithm (an alternative) is an input into a Monte Carlo simulation to evaluate the objective function, and the simulation output is used by the Bayesian optimization algorithm to generate the next alternative. It initially estimates the objective function using samples of the decision variables and fits a multivariate normal prior over the samples. The algorithm creates a posterior distribution based on that prior and the likelihood that is generated by using the Monte Carlo simulation to evaluate the objective function for an alternative. The Bayesian optimization algorithm uses the posterior distribution to identify the next alternative to sample in the simulation based on trade-off function between the expected value of the objection function (exploitation) and the variation or uncertainty around the objective function (exploration) for each alternative. This process iterates until the improvement in the output of the simulation model is less than a predefined threshold. This thesis uses the Random Embedding Bayesian Optimization (REMBO) developed by (Wang et al., 2013b).

Simulation optimization algorithms, including Bayesian optimization, have some limitations. First, a summary statistic such as the average value from a simulation model is used as an input to the optimization algorithm. The algorithm optimizes this summary statistic, which is a point estimate (e.g., expected profit), without really considering the entire empirical distribution of the output. Another limitation of using simulation optimization is that since conducting an infinite number of replications is impossible, the simulation only provides an estimate of that summary statistic to be optimized. For simulations that take a relatively long time to run, the number of replications may not be enough to accurately estimate the objection function. Due to the randomness in both the simulation and the Bayesian optimization algorithm, the solution identified as the best may not truly be the optimal decision.

Despite these limitations, simulation optimization and Bayesian optimization algorithms have been shown to perform quite well in optimizing objective functions evaluated via simulation (Azimi et al., 2010). This thesis develops simulation optimization frameworks to identify optimal solutions for engineering design problems. Simulation optimization and sequential decision-making frameworks are developed in order to optimize the design of complex engineering systems in four different studies: (i) designing a resilient system for risk-averse decision-makers with an application to wind turbines, (ii) improving the reliable design of airfield concrete pavement, (iii) incorporating flexibility into the design of a hybrid renewable energy system (HRES), and (iv) using reinforcement learning for dynamic engineering design decisions.

1.2 Overview of Design Optimization for Resilience for Risk-Averse Firms

Managers of engineered systems are faced with the challenge of assessing uncertainties and the cost of failure as they attempt to design systems that will be more robust to adverse events (Rockafellar and Royset, 2015). The high frequency of disruptive events such as natural hazards, technological failures, and humaninduced incidents encourages firms to cope with these events with predefined plans (Torabi et al., 2016; Henry and Ramirez-Marquez, 2012). A framework that incorporates resilience into the early design stage can help designers identify the best solutions for these future adverse events (Anderies, 2014). Resilience helps a system maintain its performance above a failure limit and recover if the system's performance falls below that limit. Resilience should be built into engineered systems like wind turbines (Schiel et al., 2017) and solar energy panels (Esteban and Portugal-Pereira, 2014) to prevent failure or facilitate their restoration in the case of failure.

The resilience of a system under time-dependent adverse conditions can be assessed by modeling the degradation and recovery of the system's components. Youn et al. (2011) define and measure resilience as a combination of reliability and the ability to recover from failure. MacKenzie and Hu (2018a) establish a framework to enable designers to incorporate this resilience metric into an engineering design by including parameters for resilience (redundancy, robustness, rapidity, recoverability) as design decisions that impact the profit during the system's lifecycle. The paper uses Bayesian optimization to identify design parameters that maximize the expected profit of designing and fielding a system.

Chapter 2 expands on MacKenzie and Hu (2018a) by analyzing how a decision maker's risk attitude should impact the design of resilient engineered systems. A risk-averse utility function can help in the early stage of design by capturing the risk attitude of decision makers as they consider the trade-offs among initial costs, resilience, and future profits. Although maximizing expected utility is increasingly being proposed as a valuable method to account for uncertainty and risk in engineering design (Hazelrigg, 1998; Malak et al., 2015; Thurston, 2001), developing a utility function to assess the future impact of failure in order to inform design decisions represents a novel contribution in engineering design optimization routine for resilience. The use of VAR has only appeared sparsely in the engineering design literature (Hassan et al., 2005; Mohammadi, 2014). The Bayesian optimization algorithm is utilized to find the optimal design of the components of the engineering system.

This research on designing for resilience advances the engineering design discipline by modeling the firm's appetite for risk within the context of designing a system that can fail due to degradation in the presence of adverse events and can respond to and recover from failure. Connecting resilience to a firm's utility function or via the VAR metric will allow the firm to determine how resilient a system should be during the early design stage. The results of the research show that in order to make the system more resilient, risk-averse firms should pay more in design costs to prevent catastrophic costs of failure. In this case, the system is less likely to fail due to the high resilience of its physical components.

Further research could explore to what extent the expected utility model and the expected profit model with a VAR constraint provide similar results. Since the VAR constraint only considers extreme losses (less than 5%) and the utility function captures the entire distribution, there may be certain types of uncertainty in which the results are slightly different. Machine learning algorithms could also be employed to learn from and make predictions on the parameters of complex engineered systems. They may facilitate our understanding of how design characteristics impact system resilience.

1.3 Overview of Simulation Optimization for Airfield Pavement Design

In chapter 3, a reliability-based design optimization framework is developed for the airfield concrete pavement design. Airport pavements are designed over many years to withstand repeated traffic loading imposed by a broad range of aircraft types over many years, to resist the abrasive action of traffic, and to endure deterioration induced by adverse weather conditions and other influences in a cost-effective manner. Prior research in pavement design optimization includes deterministic optimization of lifecycle costs and benefits of pavement (Santos and Ferreira, 2011; Mikolaj et al., 2017) and a genetic algorithm to optimize building costs for highway pavement (Hadi and Arfiadi, 2001).

The current software developed by the Federal Aviation Administration for airport runway design is called FAARFIELD (FAA, 2016). Since this mode of design is implemented based on some initial assumed inputs, obtaining an optimum design for a given traffic and environmental loading and design age is an iterative process to find the best possible design. However, it takes considerable amount of time to perform this iterative process using the 3-D Finite Element-based FAARFIELD software.

The design optimization methods developed in the literature find the optimal design either by considering fixed values for some uncertain parameters or considering a limited number of scenarios for the uncertain parameters. A new framework is needed to incorporate thousands of scenarios for uncertain parameters to design pavement in such a way that the pavement can operate under different and varying conditions in future. The objective of chapter 3 is to develop a new design methodology called Simulation Optimization for Airfield Rigid Pavement (SOARP). SOARP is a comprehensive reliability-based simulation-optimization framework. This framework empowers the designers to consider a large number of scenarios for designing airfield concrete pavement with various reliability levels. The novelty of this study and its primary difference with FAARFIELD's design methods and other methods in the literature lie in its use of simulation optimization while generating thousands of scenarios for the uncertain parameters to find the optimal design of the airfield pavement. The optimization algorithm is aimed at minimizing design cost while using a reliability constraint to keep pavement fatigue failure under an allowable amount. The design optimization framework is developed to find the optimal design for multiple design lives and reliability levels. This study includes aircraft traffic consisting of a B747-8, a B787-8, an A340-500 opt, and an A340-600 opt. In this study, an Artificial Neural Network is employed to replicate FEAFAA/NIKE3D-FAA pavement-response solution. The design optimization framework is optimized for multiple values of design life (20, 25, and 30 years) and multiple reliability levels (0.5, 0.8, 0.9, and 0.95). The results show that the expected design cost and optimal total thickness increase as the reliability level and design life increase. This research can help the designer to find the optimal design for pavement considering many future uncertainties.

Current research assumes that the initial system design will perform over many years of design and the initial design may not change in future. However, future research can study how the initial pavement design can be modified or altered based on the future uncertainties (for example, annual airplane departures). This will give the designers the ability to modify the initial design in the future based on different realizations of uncertain parameters.

This is a collaborative research with Adel Rezaei Tarahomi, Iowa State University Civil Engineering Department former PhD student. Dr. Rezaei Tarahomi is an expert on the field of airfield concrete pavement design. In this research, he developed the ANN model and I developed the simulation optimization framework.

1.4 Overview of Optimizing the Flexible Design of Hybrid Renewable Energy Systems

Engineered systems may operate in unstable environments, and new applications for engineered systems may arise in the future. Understanding the potential for new applications and different environments under which a system will operate is important in engineering design. A design that looks promising now may not be successful in the future because the operating conditions or demand for a product may change.

Since engineered systems frequently face unpredictable environments, these systems may be designed with the capability to respond to future changes (Saleh et al., 2003). Flexibility in design enables the designers to review the initial design in the future and provides them with the option to take actions to modify the system (Cardin, 2014; Cardin et al., 2015).

Determining the value of flexibility for engineered systems may rely on real options analysis (Shi and Min, 2014; Kucuksayacigil and Min, 2018; Ajak and Topal, 2015; Binder et al., 2017) and/or a multi-stage

stochastic model (Cardin et al., 2017). Papers that evaluate the flexibility for engineered systems (Cardin et al., 2017; Hu et al., 2018; Hu and Cardin, 2015) generally assume that the model can be easily evaluated for any input decision. This assumption may not work for cases where the objective function is estimated via a simulation in which it is not computationally efficient to evaluate the model output for every input. Related to flexibility in engineering systems is the decision about whether or not to expand capacity of the system. Multiple papers have solved optimization problems for capacity expansion with uncertainty (Khodaei et al., 2010; Hajipour et al., 2015; Gil et al., 2014).

Engineered systems, especially large-scale infrastructure, may also operate for long time. A decisionmaking framework is needed to incorporate both long-range uncertainties and the computationally expensive simulations. Chapter 4 optimizes the design of an HRES when the objective function is evaluated using Monte Carlo simulation that incorporates uncertainties over a long period of time (i.e., a 20-year lifespan in this study). The mathematical model for the HRES comes from Kaviani et al. (2009), Sharafi and ELMekkawy (2014), and Khalilnejad et al. (2018). For instance, Kaviani et al. (2009) optimize the design of an HRES without considering the uncertainty of wind speed, solar irradiation, and demand. In those studies, the initial design of the system is fixed during the long-term planning horizon and cannot be changed in the future.

Two models are developed to optimize the system design. The first model uses the Bayesian optimization algorithm that considers 10,000 possible future scenarios, and the design variables are selected to minimize the expected discounted cost. In this model, the initial design of the HRES is fixed and unchanged during the planning horizon. The second model is a design with flexibility model to allow the decision makers to review the initial design in the future and expand the capacity of the system depending on the realization of uncertain demand.

The uniqueness of this chapter is that it assesses the value of flexibility in engineered systems that require computationally expensive simulations to evaluate the objective function, and a model optimizes the design of such systems under uncertain parameters. A multi-stage flexibility algorithm is proposed to find the optimal capacity expansion for the components of the HRES over a 20-year planning horizon. The optimization algorithm measures the value of flexibility by comparing the expected lifecycle cost with flexibility to the expected lifecycle cost without flexibility. The results show that adding flexibility to the design significantly reduces the design cost for the HRES.

The method outlined in this chapter differs from the previous literature because the method simulates thousands of scenarios with the uncertain parameters to identify the optimal engineering system design. Traditional stochastic programming approaches for flexibility usually consider a limited number of scenarios within their optimization algorithms (Cardin et al., 2017; Hu et al., 2018; Hu and Cardin, 2015). The flexible design algorithm in this chapter classifies the scenarios into different categories which allows the optimization algorithm to consider thousands of scenarios without being subject to the curse of dimensionality.

Two limitations of Chapter 4 are the algorithm's classification of scenarios and the algorithm requires that decisions are made at predetermined points in time. Chapter 5 seeks to overcome these limitations by exploring each scenario by itself and enabling future decisions about the engineered system to be made at many more points in time. The application of the flexibility or capacity expansion algorithm to the HRES is reasonable, but the simulation of the power generation system is created at a macro-level. The model assumes the system generates power to meet demand within the state of California and ignores transmission constraints and individual geographic demand and supply points. The overarching framework assumes that it is feasible to modify the design or expand capacity in the future, which may not be realistic for all engineered systems. The optimal design may also change if the time period is different or other parameters (e.g., materials, operations and maintenance requirements) change over time.

1.5 Overview of Deep Reinforcement Learning for Dynamic Decision Making under Uncertainty

Chapter 4 identifies a flexible design by classifying thousands of scenarios into a few categories However, engineering systems should be designed such that the initial design can be altered or modified for any possible scenario of the uncertain parameters in the future (e.g., 10,000 scenarios of uncertain parameters). Solving such a sequential decision problem using simulation is challenging (Frazier, 2010). The field of stochastic programming contains many methods designed to solve multi-stage stochastic problems. Scenario-based methods like scenario generation and reduction are popular methods in stochastic optimization (Dupačová et al., 2003). Growe-Kuska et al. (2003) propose algorithms for reducing the number scenarios and constructing scenario trees that approximate the random data processes of multi-stage dynamic decision models under uncertainty in the electricity power sector. Decomposition methods are also used to solve multi-stage stochastic (Rebennack, 2016).

Due to the curse of dimensionality, solving dynamic programming problem with a continuous state space for problems in which the objective function is evaluated via simulation will likely require heuristics and/or scenario reduction approaches. Learning algorithms such as reinforcement learning do not require decision makers to solve as many optimization problems. Reinforcement learning is a learning algorithm to control a system in order to maximize some numerical value (Szepesvári, 2010). In reinforcement learning, a decision maker or agent interacts with and explores the environment to gradually develop an optimal policy that will make the best decision for any state in the environment (Mnih et al., 2015).

Chapter 5 proposes a framework to find the optimal design of an engineering system using a Deep Qlearning algorithm when the system's performance is evaluated with a Monte Carlo simulation and multiple sources of uncertainty exist over the planning horizon. The combination of a multi-stage engineering decision making problem, a Monte Carlo simulation, and reinforcement learning (Deep Q-learning algorithm) represents a unique contribution in engineering design. A decision maker can use reinforcement learning to find the optimal policy for a multi-stage stochastic problem and learn the optimal policy by running the simulation and evaluating the objective function for thousands of random scenarios. Since this framework can incorporate many different types of simulation models with any type of uncertainty, no assumption is needed for the distribution of the uncertain parameters.

The proposed algorithm is applied to two illustrative engineering design problems. The first example contains a linear objective function and one source of uncertainty. The second example contains a nonlinear objective function and two sources of uncertainty. Multiple configurations of the problem are discussed to show how the proposed methodology is capable of identifying the optimal policy under different uncertain conditions. The objective function and the constraints for both of these problems are evaluated with a Monte Carlo simulation where the objective function's value can change due to variability in the simulation.

Although the examples presented in chapter 5 provide an illustration of how the Deep-Q learning algorithm can be applied to engineering design problems, the examples are relatively simple. Future research can apply the framework in this thesis to a real engineering design problem, which will provide more insight into the potential benefits as well as drawbacks of this approach. Also, the performance of the proposed algorithm can be tested against other multi-stage stochastic optimization methods to compare the quality of the solutions and time it takes to find the optimal solution. The framework developed for dynamic decision making under uncertainty can be modified to include continuous decision variables as well.

1.6 Summary of Contribution

These studies in this thesis present simulations of the performance of an engineered system with different resilient, reliable, and flexible characteristics. The simulations allow decision makers to analyze the impact of those characteristics on the performance of the system. Since the optimization model requires a Monte Carlo simulation to evaluate the objective function, a Bayesian optimization algorithm is used to find the optimal design in chapters 2-4. The Bayesian optimization algorithm is used to identify the optimal combination of continuous design variables while the performance of the engineering system is evaluated with a Monte Carlo simulation model. Chapter 5 also uses a Monte Carlo simulation, but a deep Q-learning algorithm is employed to identify the optimal decisions over time.

The contribution of this thesis is to propose decision-making frameworks for engineering design problems that use Monte Carlo simulation. This research seeks to fill the gap in engineering system design by proposing static and sequential decision-making frameworks that use simulation optimization techniques to optimize a design. The purpose of this dissertation is to study simulation optimization and sequential decision-making strategies for the design of complex engineering systems. This dissertation presents simulation-based design platforms to determine the optimal design of engineered systems. I develop resilient, reliable, and flexible design solutions that account for system uncertainties within the optimization algorithm. The frameworks enable the designers of the engineering systems to make decisions under uncertainty while creating or revising those systems.

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CHAPTER 2. DESIGN OPTIMIZATION FOR RESILIENCE FOR RISK-AVERSE FIRMS

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Abstract

Designers should try to design systems that are resilient to adverse conditions during a system's lifetime. The resilience of a system under time-dependent adverse conditions can be assessed by modeling the degradation and recovery of the system's components. Decision makers in a firm should attempt to find the optimal design to make the system resilient to the various adverse conditions. A risk-neutral firm maximizes the expected profit gained from fielding the system, but a risk-averse firm may sacrifice some profit in order to avoid failure from these adverse conditions. The uniqueness of this paper lies in its model of a design firm's risk aversion with a utility function or Value-at-Risk (VAR) and its use of that model to identify the optimal resilient design for the risk-averse firm. These risk-averse decisionmaking methods are applied to a design firm determining the resilience of a new engineered system. This paper significantly advances the engineering design discipline by modeling the firm's appetite for risk within the context of designing a system that can fail due to degradation in the presence of adverse events and can respond to and recover from failure. Since the optimization model requires a complex Monte Carlo simulation to evaluate the objective function, we use a ranking and selection method and Bayesian optimization to find the optimal design. This paper incorporates the design of the wind turbine and the reliability and restoration of the turbine's components for both risk-neutral and risk-averse decision makers. The results show that in order to make the system more resilient, risk-averse firms should pay a larger design cost to prevent catastrophic costs of failure. In this case, the system is less likely to fail due to the high resilience of its physical components.

2.1 Introduction

Decision makers should try to understand uncertainty in the early design and account for it within their engineering design process (Callaghan and Lewis, 2000). A firm should seek to understand how an early system design will evolve over time and impact the performance of the system (Nikolaidis, 2007). Although complex engineering such as wind turbines, electric power systems, and airplanes systems have different functionality and operations, they can all suffer from disruptions and face various types of uncertainty during their operation and lifetime. The potential effects of adverse events on highly complex systems are more uncertain because complex systems comprise many interdependent components and subsystems. The frequency of these events may increase as the system ages and result in less reliable systems (Bar-Yam, 2003). For example, a survey of failures in the wind power energy system (Anderies, 2014) finds that a wind turbine failed 402 times per year, on average, in Sweden from 1997 to 2005.

Managers of engineered systems are faced with the challenge of assessing these uncertainties and the cost of failure as they attempt to design systems that will be more robust to adverse events (Rockafellar and Royset, 2015). The high frequency of disruptive events such as natural hazards, technological failures, and human-induced incidents encourages firms to cope with these events with predefined plans (Torabi et al., 2016; Henry and Ramirez-Marquez, 2012). A framework that incorporates resilience into the early design stage can help designers identify the best solutions for these future adverse events (Anderies, 2014). Traditional risk management systems help decision makers identify and analyze the risks and mitigate the system-wide effects of adverse events after the system is designed or fielded (Linkov et al., 2014; Torabi et al., 2016). A design-for-resilience framework attempts to integrate plans for redundancy, robustness, response, and recovery into the design process (Linkov et al., 2014).

Resilience appears in different domains from ecological systems to psychological, infrastructure, networks, and enterprises (e.g. (Ayyub, 2014; Carpenter et al., 2001; Tierney and Bruneau, 2007; Rosenkrantz et al., 2009; Hosseini et al., 2016)). These domains may use different definitions of resilience, but a simple and widespread definition is that resilience is the ability of a system to withstand and recover from a disruption (Ayyub, 2014). Resilience helps a system maintain its performance above a failure limit and recover if the system's performance falls below that limit. Resilience becomes essential to a system analysis approach to maintain the performance of the system above the failure limit (Henry and Ramirez-Marquez, 2012). Integrating resilience into system design is needed to address the complex and challenging uncertainties and properly cope with adverse events (Linkov et al., 2014). Resilience should be built into complex engineered systems like wind turbines (Schiel et al., 2017) and solar energy panels (Esteban and Portugal-Pereira, 2014) to prevent failure or facilitate their restoration in the case of failure.

Despite the growing interest in resilience, engineering resilience is still a relatively new concept in the area of design (Henry and Ramirez-Marquez, 2012; Yodo and Wang, 2016; Reed et al., 2009; Todini, 2000). Bruneau et al. (Bruneau et al., 2003) define resilience as a measure of robustness, rapidity, resourcefulness, and redundancy, and their metric for resilience is the area underneath the performance curve ("the resilience triangle"). Other metrics for resilience change over time as the system is disrupted and then recovers (Henry and Ramirez-Marquez, 2012). The resilience model is often used to evaluate different protection or recovery strategies (Barker et al., 2013; Pant et al., 2014; Baroud et al., 2014) or to determine which assets to protect (Alderson et al., 2013). However, less work has incorporated resilience into engineering design decision making. Recently, Youn et al. (Youn et al., 2011) define resilience as a function of reliability and restoration in order to aid in the design of more resilient systems.

Analyzing system design may identify the most critical components that influence system performance and reliability (Barker et al., 2013). Resilience analysis assesses the robustness of these components to adverse conditions and their ability to be repaired or restored after an adverse event. Since system components degrade over time, these components may become vulnerable to adverse conditions. MacKenzie and Hu (MacKenzie and Hu, 2018a) use the resilience metric from Youn et al. (Youn et al., 2011) to model the performance of a complex system by considering adverse conditions during the lifetime of the system. Their model optimizes the resilient design for a firm who seeks to maximize its expected profit. A design firm may be risk averse, however, which means that the firm may prefer to avoid significant monetary losses even if it means not pursuing uncertain monetary gains (Rockafellar and Royset, 2015). In the area of design, a risk-averse firm is willing to spend more initially to design a more reliable or resilient system because the higher initial investment will avoid catastrophic and costly failures in the future. The uniqueness of this paper and its primary difference with (MacKenzie and Hu, 2018a) lie in its modeling of a design firm's risk aversion via the use of a utility function or with a risk measure such as Value-at-Risk (VAR) and its use of that model to identify the optimal resilient design for the risk-averse firm. Risk-averse decision makers should prefer to build a more resilient system even if that means a smaller expected profit.

This paper makes several unique contributions. We analyze how the risk attitude of the decision makers in engineering design should impact system resilience. A risk-averse utility function can help in the early stage of design by capturing the risk attitude of decision makers as they consider the trade-offs among initial costs, resilience, and future profits. Although maximizing expected utility is increasingly being proposed as a valuable method to account for uncertainty and risk in engineering design (Hazelrigg, 1998; Malak et al., 2015; Thurston, 2001), developing a utility function to assess the future impact of failure in order to inform design decisions represents a novel contribution in engineering design. This paper is also the first paper to incorporate the financial risk measure VAR into an engineering design optimization routine for resilience. The use of VAR has only appeared sparsely in the engineering design literature (Hassan et al., 2005; Mohammadi, 2014). Furthermore, Sequential Monte Carlo Simulation is used to simulate the degradation and the actions to restore the performance of the system. Bayesian optimization algorithm is utilized to find the optimal design of the components of the engineering system.

This paper presents a model to simulate the performance of an engineered system with different resilience characteristics to enable the decision makers to analyze the impact of those characteristics on the performance of the system. Different types of adverse conditions may cause the system to degrade, which impacts the system's resilience. A firm can use the simulated time-dependent resilience analysis to make design decisions while using either the utility function or VAR to represent its risk attitude.

We illustrate our developed framework with three applications to understand how system resilience is impacted by the risk attitude of the decision maker. In order to analyze the effect of risk aversion on the design features of the system, a simple example with one subsystem and the optimal design for different risk averse decision makers is discussed. The second example is an extension of the example in (MacKenzie and Hu, 2018a) in order to compare the results of a risk-averse design with the result of a risk-neutral design. Another significant difference with (MacKenzie and Hu, 2018a) is an application to the design of a wind turbine. This paper incorporates the design of the wind turbine and the reliability and restoration

of the turbine's components for both risk-neutral and risk-averse decision makers. This paper significantly advances the engineering design discipline by modeling the firm's appetite for risk within the context of designing a system that can fail due to degradation in the presence of adverse events and can respond to and recover from failure. Connecting resilience to a firm's utility function or via a VAR metric will provide the firms with the ability to understand how resilient a system should be during the early design stage.

The rest of the paper is as follows. Section 2.2 describes the decision-making framework for resilience and demonstrates how this framework is extended to expected utility and VAR. Section 2.3 applies the risk-averse design-for-resilience framework to three examples (one example with a single subsystem an example with three subsystems, and a wind turbine). Finally, Section 2.4 provides concluding remarks and directions for further research.

2.2 Decision Making for Resilience

The following section outlines the decision-making framework for resilience. Following (MacKenzie and Hu, 2018a), the analysis of time-dependent system resilience is first presented with a model for the firm's cost and profit. The second subsection describes how to incorporate a risk-averse utility function, and the third subsection describes the use of the VAR metric in the decision-making model. The fourth and fifth subsections describe the solution algorithm and the Bayesian optimization routine to identify the optimal design characteristics.

2.2.1 System Resilience, Cost, and Profit

Reliability refers to the ability of the system to maintain its performance above the failure limit under stated conditions for a given period of time (Modarres et al., 2016), but resilience also incorporates restoration in terms of how a system can be restored to an adequate performance above its failure limit after an adverse event occurs. This paper uses the definition of resilience from Youn et al. (Youn et al., 2011), where resilience is the sum of reliability and restoration. A non-resilient engineered system will not recover from severe and gradual adverse events. Reliability and restoration should work together to enhance the system's resilience. Resilience can be quantitatively measured as:

$$\psi = R + \rho(1 - R) \tag{2.1}$$

where reliability *R* is the probability the system has not failed and restoration ρ is the probability of a successful recovery action given that the system has failed (Youn et al., 2011). Thus, resilience ψ is the probability the system is operating. MacKenzie and Hu (MacKenzie and Hu, 2018a) present a framework for measuring and quantifying resilience under time-dependent adverse conditions. This subsection summarizes their decision-making model for an expected-value (or risk-neutral) decision maker.

Simulating the system performance with different design characteristics enables the decision makers to analyze the impact of those characteristics on the performance of the system. Sequential Monte Carlo Simulation (MCS) can be used to simulate the degradation and the actions to restore the performance of the system. MCS enables the decision makers to analyze the stochastic behavior of degradation and restoration. The system performance can be measured beginning with the initial state of the system plus the degradation over time and the random occurrence of adverse events. A sequential MCS computes the time-dependent resilience of the system in Eq. (2.1) based on the performance, degradation, failure, and restoration of the system's subsystems or components.

Different types of adverse conditions may degrade the system performance, and the accumulation of degradation eventually causes system failure. The behavior of the system performance is assessed under randomly varying adverse conditions. Within the MCS, the system performance relies on the performance of all the subsystems and their components. Algorithm 1 outlines the simulation for the degradation and restoration of a single component. For a single simulation trajectory *j*, where j = 1, 2, ..., N, $s^{j}(t)$ indicates if the component is operating at time t ($s^{j}(t) = 0$), has failed without beginning to recover ($s^{j}(t) = 1$), or is recovering ($s^{j}(t) = 2$) at time *t*. The performance of a component at time *t*, $G^{j}(t)$, is a function of the component's performance at time t - 1, $G^{j}(t - 1)$, and a degradation function $f(Q, \mu_{\beta}, \alpha, \tau)$, where we assume that $\alpha = 0.008$ and $\tau = 1.5$ (line 6). The degradation function follows a log-sigmoid function and depends on the mean robustness design μ_{β} and the severity of the adverse event *Q*. The severity of the adverse condition Q (such as wear-out and lightning strikes) follows a normal distribution with a predefined mean and standard deviation.

Algorithm 1 Performance simulation for each component

- 1: Assumptions: Initial system state is normal (s = 0); states, 0:normal, 1:response, 2:recovery
- 2: Inputs: Random adverse event (*Q*), mean of robustness (μ_{β}), response (μ_{rp}) and recovery (μ_{rc}) times, performance after recovery ($G_{rc} = 0.8$), failure limit ($\underline{G} = 0.2$)

3: while t < T do

for $j \leftarrow 1$ to N do 4: if $s^{j}(t) == 0$ or $s^{j}(t) == 1$ then 5: $G^{j}(t) \leftarrow G^{j}(t-1) - f(\mathcal{Q},\mu_{\beta},\alpha,\tau)$ where $f(\mathcal{Q},\mu_{\beta},\alpha,\tau) = \frac{\alpha}{1+e^{-\tau(\mathcal{Q}+\mu_{\beta})}}$ 6: else 7: $G^{j}(t) \leftarrow G^{j}(t-1) + (G_{rc} - G^{j}_{re})/\mu_{rc}$ 8: end if 9: 10: end for $Update^* s^j(t)$ 11: $t \leftarrow t + 1$ 12: 13: end while 14: *Update*^{*} $s^{j}(t)$:

15: Counted time after failure = t_f 16: Counted time after response is initiated = t_r 17: if $G^j(t) > \underline{G}$ then 18: $s^j(t) \leftarrow 0$ 19: else if $G^j(t) < \underline{G} \& t_f \leq S_{rp}^{**}$ then 20: $s^j(t) \leftarrow 1$ 21: else if $G^j(t) < \underline{G} \& t_f > S_{rp} \& t_r \leq S_{rc}^{***}$ then 22: $s^j(t) \leftarrow 2$ 23: end if 24: ** S_{rp} is a random sample from $N(\mu_{rp}, \sigma^2)$ 25: *** S_{rc} is a random sample from $N(\mu_{rc}, \sigma^2)$ 26: Outputs: Component performance (*G*) for all trajectories (*N*) and simulation time (*T*)



Figure 2.1: Simulation trajectories of component

Restoration consists of two different parts: response and recovery. When component performance degrades below the failure limit \underline{G} , as in lines 19-20 of Algorithm 1, the response plans is initiated and can be characterized by the rapidity of response to failure. After responding to the adverse condition (lines 21-22), the component could be recovered from the effects of adverse events. The parameters S_{rp} and S_{rc} in lines 24 and 25 are randomly selected from response and recovery probability distribution functions and reflect the time to respond and recover in a single trajectory. Response and recovery times follow normal probability distributions with means of μ_{rp} and μ_{rc} , respectively, and a constant standard deviation. Line 8 of Algorithm 1 indicates how the component recovers after its performance has degraded below the failure limit. The parameter G_{rc} is the performance to which the component is restored and G_{re}^{j} is the component's performance in trajectory j when the recovery plan is initiated.

Figure 2.1 depicts N = 1000 simulated trajectories of a component's performance based on Algorithm 1 where the mean robustness $\mu_{\beta} = -7$, the mean response time $\mu_{rp} = 1$, and the mean recovery time $\mu_{rc} = 9$. The figure shows that the performance trajectories degrade below the failure limit three times on average and it takes approximately 10 weeks on average to restore performance.

The system's resilience can be measured using the simulated trajectories of the performance of all of the components. A subsystem is a group of identical components operating in parallel to reflect redundancy. A subsystem is considered operating if at least one of its components is greater than the failure limit. A subsystem is in a failed state if all of its components are less than the failure limit. The operation of the system then depends on the functioning of the individual subsystems. If the subsystems operate in series,

the system is operating only if all of its subsystems are operating. If the subsystems operate in parallel, the system is in a failed state only if all of the subsystems are in a failed state. The parameter $\hat{\Re}_j(t)$ is an indicator variable that represents if the system is in an operating ($\hat{\Re}_j(t) = 1$) or failed ($\hat{\Re}_j(t) = 0$) state at time *t* based on simulation trajectory *j* for each of the components in the system. If the there are *N* simulation trajectories, the system resilience at time *t*, $\psi(t)$ can be estimated as

$$\Psi(t) = \frac{1}{N} \sum_{j=1}^{N} \hat{\Re}_j(t).$$
(2.2)

Thus, $\psi(t)$ is a number between 0 and 1 representing the simulated probability that the system is operating. The static resilience metric from Eq. (2.1) is now a time-dependent resilience metric.

Designing a more resilient system should increase the system's operating time and decrease the number and durations of failures. That will help increase the firm's operating profit because it can avoid costly repairs after the system is fielded. However, designing and building a more resilient system may also increase the firm's design and production costs.

The design cost of the system consists of two major parts: the cost of designing the components for each subsystem and the cost of installing each component in each subsystem. We assume there are M total subsystems. Eq. (2.3) depicts the design cost where $c_{design,i}(d^{(i)})$ is the design cost for subsystem i, i = 1, 2, ..., M given design decisions $d^{(i)}$ and where $p_i m_i$ is the installation cost of installing m_i components in subsystem i each with an installation cost of p_i :

$$C_{design}(d) = \sum_{i=1}^{M} \left(c_{design,i}(d^{(i)}) + p_i m_i \right)$$
(2.3)

where $C_{design}(d)$ is the total design cost as a function of the design decision variables d.

After the system is fielded, the firm should earn an operating profit (which could be negative). The operating profit function at time t, $\pi\left(\hat{\Re}_{j}(t), \omega(t)\right)$, is a function of whether the system is functioning or not (i.e., $\hat{\Re}_{j}(t)$) and a vector of other parameters $\omega(t)$ that indicate the firm's revenue and cost at time t based on whether or not the system is functioning. The total discounted profit $x_{j}(d)$ for the firm for a simulated trajectory j given a design decision d is:

$$x_j(d) = \int_0^T \lambda^t \pi\left(\hat{\Re}_j(t), \omega(t)\right) dt - C_{design}(d)$$
(2.4)

where *T* is the length of time the system is fielded and $\lambda \leq 1$ is the discount factor.

Robustness, time to respond, and time to recovery form a random vector for each component. The means of these variables in addition to the redundancy of each subsystem are the design variables of the system. For example, robustness is assumed to be normally distributed with a mean of μ_{β} and a constant variance. For a design with mean robustness equal to μ_{β} , a random number from the normal distribution with mean μ_{β} will be selected as the robustness and used in one trajectory simulation. In order to evaluate the total discounted profit considering a specific design of the system ($\mu_{\beta}, \mu_{rp}, \mu_{rc}$), *N* random numbers will be selected from the distribution of each of the decision variables (i.e., robustness, response and recovery times). Interested readers are referred to MacKenzie and Hu (MacKenzie and Hu, 2018a) for further details on the system resilience and profit models.

2.2.2 Expected Utility Model

MacKenzie and Hu (MacKenzie and Hu, 2018a) optimize the prior design decision-making model for a risk-neutral firm who wants to maximize its expected profit. However, a firm may be risk averse and be willing to spend more in design costs in order to avoid really large and costly failures in the future. This is especially true if the firm considers potential catastrophic costs of failure due to adverse events. A riskaverse utility function can reflect a decision maker's preference over risk and be used to find the optimal design features in the system design phase (Callaghan and Lewis, 2000). Here, risk refers to losing money or generating less profit due to large repair costs and costly failures. Resilience refers to the ability of an engineering system to withstand and recover from disruptions. A risk-averse decision maker would likely be willing to spend more now in order to design a more resilient system because a more resilient system would have fewer catastrophic failures.

Decision theory explains that risk aversion can be properly modeled with a concave utility function U(x) over the firm's profit x (Rabin, 2013). A typical risk-averse utility function is exponential utility which assumes constant absolute risk aversion. Constant absolute risk aversion indicates that a decision maker's



Figure 2.2: Utility functions for different risk attitudes

risk attitude does not change as the dollar amounts change. The exponential utility as a function of the firm's profit x is

$$U(x) = 1 - \exp(-\gamma x) \tag{2.5}$$

where $\gamma > 0$ is the degree of risk aversion for the firm. If $\gamma \rightarrow 0$, the decision maker is risk neutral, and the exponential utility function reduces to a linear function. As γ increases, the decision maker is becoming more risk averse as exhibited by an increasingly concave utility function. If $\gamma \rightarrow \infty$, the decision maker is extremely risk averse and will choose the alternative that minimizes his or her worst outcome. Figure 2.2 depicts the exponential utility function for different values of γ , in which the firm's profit is on the order of thousands of dollars, which corresponds to the applications in Section 3.

The sequential MCS produces component performance trajectories that can be used to calculate the profit using Eq. (2.4). The profit from trajectory j in Eq. (2.4) is an input into the firm's utility function in Eq. (2.5). The objective function, i.e, expected utility, is calculated via Eq. (2.6) by averaging over the profits gained from N simulation trajectories. The risk-averse firm will select the design variables d in order to maximize its expected utility EU(d):

$$\begin{array}{l} \underset{d \in D}{\text{maximize } EU(d) = 1 - \frac{1}{N} \sum_{j=1}^{N} \exp\left(-\gamma x_j(d)\right) \\ = 1 - \frac{1}{N} \sum_{j=1}^{N} \exp\left(-\gamma \left[\int\limits_{0}^{T} \lambda^t \pi\left(\hat{\Re}_j(t), \boldsymbol{\omega}(t)\right) dt - C_{design}(d)\right]\right) \end{array}$$
(2.6)

where *N* represents the number of trajectories in the MCS and *D* represents the feasible set of design alternatives.

Utility as given in Eq. (2.5) is an interval scale in which the utilities provide a degree of relative difference between design decisions but no absolute difference. Consequently, it is often preferable to provide results that translates expected utility into units of dollars. The certainty equivalent (*CE*) of decision represents how much money a person would accept that makes him or her indifferent between the *CE* and a risky, or uncertain, investment. The *CE* for a firm provides the same ordering as expected utility because *CE* can be calculated as the inverse of the utility function (Ben-Tal and Teboulle, 2007). The *CE* of a design decision *d* is calculated from the expected utility equation in Eq. (2.6):

$$CE(d) = -\frac{1}{\gamma} \log\left(1 - EU(d)\right)$$
(2.7)

If a firm becomes more risk averse (i.e., if γ increases), the firm's CE(d) will decrease because the firm is willing to receive less profit for certain in order to avoid more risky situations. The risk-averse utility function incorporates a firm's willingness to trade off between expected profit and the risk of losing money.

Within engineering design, utility theory has been used to facilitate design decisions (e.g. (Fernandez et al., 2001; Thurston, 1991; Babuscia and Cheung, 2014)). Fernandez et al. (Fernandez et al., 2001) apply utility theory to identify appropriate manufacturing technology to select design characteristics, and Nikolaidis (Nikolaidis, 2007) incorporates reliability within a utility function for design. Utility functions may also be used in design decision making in order to evaluate trade-offs among multiple criteria (Pahl and Beitz, 1984).

2.2.3 Expected Profit with VAR

Although expected utility provides a theoretically sound method to make decisions with uncertainty, firms may be hesitant to rely on a utility function, which may appear obtuse to some decision makers. Also, the assumption of constant absolute risk aversion that underpins the exponential utility function may not be valid, and a decision maker's tolerance for risk often changes as his or her initial wealth changes. Another method to incorporate risk aversion into a firm's decision-making process is through the use of VAR. VAR is defined as the largest profit x_{VAR} such that there is a q probability that the profit is less than or equal to x_{VAR} , or {max $x : P(X \le x) \le q$ } where X is the uncertain profit (MacKenzie, 2014).

Since the probability q that determines VAR is usually set to a rather low value (e.g., q = 0.05 or 0.01), VAR focuses a firm's attention on rather extreme losses. Since the firm's profit continues to be evaluated via MCS, the firm will seek to maximize its expected profit while ensuring that its VAR constraint x_{VAR} is not violated:

$$\underset{d \in D}{\text{maximize}} \ \frac{1}{N} \sum_{j=1}^{N} x_j(d)$$

$$\text{subject to} \ \frac{1}{N} \sum_{j=1}^{N} I(x_j(d) \le x_{VAR}) \le q$$

$$(2.8)$$

where the constraint represents the simulated probability that the profit is less than or equal to VAR. The indicator function $I(x_j(d) \le x_{VAR})$ equals 1 if the profit of a simulated trajectory is less than or equal to x_{VAR} and equal 0 if the profit is greater than x_{VAR} . The firm determines both x_{VAR} and the probability q before optimizing the problem in (2.8).

VAR provides a firm with a method to assess the risk of extreme losses. Since designing a new system can require a significant up-front investment for future, yet uncertain, profits, a firm can use VAR to assess the riskiness of a design. The design-for-resilience model with VAR requires that the firm specify a probability q and profit x_{VAR} such that the firm would not accept any design alternative d where the probability that the profit is less than x_{VAR} is greater than q. A firm seeks to maximize the expected profit subject to the VAR constraint. This limits the risk exposure of a firm through the use of VAR.
VAR has typically been used as a financial risk measure in investment science (Acerbi and Tasche, 2002; Giesecke et al., 2008), but its use has spread to other company decisions. Some researchers have proposed VAR within the engineering design field to evaluate different design options. For instance, Hassan et al. (Hassan et al., 2005) apply VAR to compare different design solutions for flexibility in engineering design. VAR describes the loss that can occur over a given period of time due to exposure to risks. If the firm is constrained to ensure that the probability that its profit is less than the predetermined value of VAR, then it is likely to make design decisions to avoid the most extreme losses (Basak and Shapiro, 2001).

2.2.4 Solution Algorithm

Both the expected utility decision and the expected profit subject to a VAR constraint require optimizing over the set of design variables. In order to find the best solution in engineering design, optimization approaches should explore the design space to identify the optimal design while considering the decision maker's risk attitude (Papageorgiou et al., 2016). Evaluating all of the design alternatives is not always feasible due to limited resources (Huang et al., 2015). The randomness and uncertainty in parameters bring further challenges to estimating the expected profit or utility of the design. A simulation optimization approach can determine the optimal design for both risk-averse decision-making frameworks. Simulation optimization is a broad-based term for stochastic optimization problems in which the objective function is evaluated via simulation (Powell and Ryzhov, 2012; Fu, 2002). Simulation optimization (Fu et al.,) can encapsulate several methodologies including ranking and selection methods for discrete optimization, response surface methodologies (Kleijnen, 1998; Baş and Boyacı, 2007; Öktem et al., 2005), nested partitions (Shi et al., 1999; Shi and Ólafsson, 2000), random search methods (Lu et al., 2013; Plett, 2006), and Bayesian methods (Mockus, 1994; Jones et al., 1998; Streltsov and Vakili, 1999; Jones, 2001). Developing methods to efficiently select the design parameters for mixed-integer stochastic programming for simulation optimization is a critical challenge for determining the optimal design for resilience.

MacKenzie and Hu (MacKenzie and Hu, 2018a) provide a two-stage simulation optimization method to maximize a firm's expected profit when the design decision variables include both discrete and continuous variables. The first stage employs a ranking and selection method in order to identify the optimal discrete

Algorithm 2 Calculate expected profit with VAR constraint

for j = 1 : N do if $x_j(d) - x_{VAR} \ge 0$ then $\Upsilon_j = 1$ else $\Upsilon_j = 0$ end if end for if $\sum_{j=1}^{N} \Upsilon_j \ge (1-q)N$ then $EV(d) = \frac{1}{N} \sum_{j=1}^{N} x_j(d)$ else EV(d) = 0end if

variables while considering the continuous decision variables as random variables. For each possible combination of discrete decision variables, the sample mean of profit (or utility) is calculated based on the MCS. The second stage fixes the optimal discrete variables and then uses a Bayesian optimization algorithm to identify the optimal combination of the continuous design decision variables. This paper uses the Random Embedding Bayesian Optimization (REMBO) developed by Wang et al. (Wang et al., 2013c, 2016b) to implement the Bayesian optimization algorithm. The implementation procedure of Bayesian optimization algorithm is discussed in subsection 2.2.5.

Simulating expected utility is straightforward and the expected utility function in Eq. (2.6) is used as the objective function. Identifying the optimal design alternatives that maximize the firm's expected profit while satisfying the VAR constraint requires a restriction that the model would not generate a profit less than x_{VAR} in more than 100*q* percent of the simulations. Existing approaches to optimize a function with a chance constraint (e.g. (Ahmed and Shapiro, 2008; Pagnoncelli et al., 2009)) are not applicable to the simulation optimization approach necessary for this paper. Algorithm 2 depicts the modification to the simulation optimization algorithm described above in order to calculate the expected profit subject to a VAR constraint. In the algorithm, the expected value for a design decision EV(d) equals 0 if the number of simulations in which the profit is less than x_{VAR} is more than *qN* where *N* is the total number of trajectories. Since the resilience analysis simulation is a complex process that includes time-consuming and complicated simulations, the analysis over different parameters is done in parallel to reduce the time of the simulation and optimization process. This helps us to reduce the computational time by 75 percent as the computer can use its four cores simultaneously.

2.2.5 Bayesian Optimization Algorithm

Since designers may have little knowledge about the dynamics in the simulation model, traditional optimization algorithms that require either first-order (i.e., gradient) or second-order (i.e., Hessian) information may be invalid. Bayesian optimization can effectively utilize the input-output relationship of a black-box oracle (e.g., the input-output generated from a simulation) to estimate the optimal parameters. Bayesian optimization provides a method to find the optimal design without using the first- or second-order information.

The prior and acquisition functions are the two major ingredients of the Bayesian optimization algorithm. As is typical with Bayesian optimization, we choose a Gaussian process as the prior function. The objective function f, such as the expected utility from Eq. (2.6) or expected profit from Eq. (2.8), is approximated with a multivariate normal probability distribution function with a mean of zero and a covariance matrix K. Algorithm 6 shows the pseudo-code of the Bayesian optimization algorithm. After simulating ydesign alternatives to estimate $f_{1:y}$ —the expected profits or expected utilities at the y design alternatives the posterior mean and variance of a new design alternative d' can be calculated. The set $\Delta_y = \{d_{1:y}, f_{1:y}\}$ contains the y design alternatives and the corresponding expected profits or expected utilities assessed via simulation.

Since the objective function at the new design alternative d' is unknown, it is assumed that

$$f'|\Delta_{\mathbf{v}}, d' \sim N(\mu(d'|\Delta_{\mathbf{v}}), \sigma^2(d'|\Delta_{\mathbf{v}}))$$
(2.9)

where $\mu(d'|\Delta_y)$ is the posterior predictive mean and $\sigma^2(d'|\Delta_y)$ is the posterior predictive variance given the simulated *y* alternatives. The Sherman-Morrison-Woodbury formula is used in line 4 of Algorithm 6 to calculate the posterior mean and variance for a new design alternative *d*':

$$\mu(d'|\Delta_{y}) = k(d', d_{1:y})K(d_{1:y}, d_{1:y})^{-1}f_{1:y}$$

$$\sigma^{2}(d'|\Delta_{y}) = k(d', d') - k(d', d_{1:y})K(d_{1:y}, d_{1:y})^{-1}k(d_{1:y}, d')$$
(2.10)

where $K(d_{1:y}, d_{1:y})$ is the covariance matrix for the *y* design alternatives that are simulated to estimate the expected profit or utility, $k(d', d_{1:y})$ is the covariance of the *y* design variables and the new point d', and k(d', d') is the variance of design point d'. The covariance between two variables d_i and d_j can be calculated with the Gaussian kernel function:

$$k(d_i, d_j) = \exp(-\frac{1}{2}(d_i - d_j)^T diag(\theta)^{-2}(d_i - d_j))$$
(2.11)

where the vector θ describes the relative importance of each design variable. The kernel function shows how similar an alternative d_i is to the alternative d_j . Eq. (3.7) is used to assess the posterior means and variances for any given unknown design alternative.

Line 3 of Algorithm 6 identifies the next design alternative d_{y+1} to simulate by maximizing the acquisition function $u(d|\Delta_y)$:

$$u(d|\Delta_{\mathbf{y}}) = E(\max\{0, f_{\mathbf{y}+1}(d) - f(d^{+})\}|\Delta_{\mathbf{y}})$$
(2.12)

where $d^+ = \arg \max_{d \in \{d_{1:y}\}} f(d)$ and the distribution for f_{y+1} follows Eq. (2.9). Maximizing this acquisition function indicates the algorithm is seeking to maximize both the posterior mean and variance. Maximizing the acquisition function represents a trade-off between exploration and exploitation. When the algorithm chooses to exploit, it increases the likelihood of finding the design alternative that results in the lower expected cost. However, when it explores the solution space it chooses to simulate a design alternative with a larger uncertainty (Brochu et al., 2010). Choosing to simulate a design alternative with a large mean increases the likelihood of finding the design alternative that results in the greatest expected profit or utility. A design alternative with a large variance indicates significant uncertainty exists with that particular alternative. It is desirable to reduce that uncertainty by simulating that design alternative. The process continues until the maximum number of iterations *Y* is reached. Algorithm 3 Implementation procedure of Bayesian optimization.

- 1: for $y \leftarrow 1$ to Y do
- 2: Calculate $\mu(d'|\Delta_y)$ and $\sigma^2(d'|\Delta_y)$
- 3: Find d_{y+1} by optimizing the acquisition function $u: d_{y+1} = \arg \max_{d \in D} u(d|\Delta_y)$
- 4: Use Monte Carlo simulation to calculate $f(d_{y+1})$
- 5: Augment data points $\Delta_{y+1} = \Delta_y \bigcup \{ (d_{y+1}, f(d_{y+1})) \}$
- 6: **end for**
- 7: $d^* = \arg \max u(d' | \Delta_y)$
- 8: Output: d^* : Optimal continuous design variables (mean robustness, mean response time, and mean recovery time for each subsystem)

The Bayesian optimization algorithm has become a powerful approach to solve a variety of optimization problems where traditional optimization algorithms are ineffective and weak (Gardner et al., 2014). For instance, it is widely used to optimize the hyperparameters of machine learning models such as support vector machines or deep neural networks (Klein et al., 2016). By doing hyperparameter optimization, the Bayesian optimization algorithm is able to achieve higher boost in accuracy of prediction in reasonable time compared to other optimization algorithms such as grid search, random search, gradient-based, and evolutionary algorithms (Thornton et al., 2013; Calandra et al., 2016, 2014; Snoek et al., 2012). Figure 2.3 shows step by step procedure to find the optimal design given the simulation of the system performance, resilience, and design optimization. Our methodology starts with the initial design of the components of the system's resilience is measured using the simulated trajectories of the performance of all of the components. Based on the time-dependent resilience, the expected profit for the design is calculated. The Bayesian optimization algorithm is used to find the next design variables and update the decision variables in order to maximize the expected utility or expected profit under VAR. This process iterates until it finds the optimal components design.

2.3 Illustrative Examples

Designing a resilient engineered system requires designing and selecting physical components in a way that the system can operate and is unlikely to fail. We illustrate our developed framework with an application



Figure 2.3: Flow chart illustrating design optimization for resilience for risk averse firms

to understand how system resilience is impacted by the risk attitude of the decision maker. Two examples illustrating the risk-averse decision-making design-for-resilience framework will be presented. The first example consists of one subsystem, and the second example consists of three subsystems. The simpler one-subsystem example is developed in order to better illustrate how risk aversion impacts the choice of design characteristics. An application to the design of a wind turbine is discussed in subsection 2.3.3.

Similar to (MacKenzie and Hu, 2018a), the design variables comprise the redundancy, robustness, time to respond, and time to recover for each subsystem. Redundancy and robustness enhance the reliability of the system, and the times to respond and restore the system if failure occurs comprise restoration. Thus,



Figure 2.4: Engineered system with one subsystem and redundant components

these four characteristics determine the resilience of the system. Redundancy describes the number of the components that can function if the primary component fails. Robustness describes the ability of the system to withstand an adverse event in order to prevent failure. If a failure occurs, the time to respond is the time until the system begins to be repaired. The time to recover is the time when the system begins to be repaired until it finishes being repaired.

2.3.1 One-Subsystem Example

The one subsystem contains *m* components operating in parallel. Each component has the exact same design characteristics, and each additional component is considered a redundant component. Thus, there are m-1 redundant components. The firm selects the mean robustness for the component μ_{β} , the mean time to respond μ_{rp} , and the mean time to recover μ_{rc} . The parameters μ_{rp} and μ_{rc} are measured in units of time. The parameter $\mu_{\beta} < 0$ is the mean of the fragility curve of the component determined by a log-sigmoid function as described in Section 2. More robustness indicates that μ_{β} is less negative. Figure 2.4 depicts a diagram for the system.

The design cost for the component increases as the number of components increases, the component's robustness increases, and its time to respond and recover decreases. Eq. (2.13) provides the design cost parameters for Eq. (2.3) where $d = (m, \mu_{\beta}, \mu_{rp}, \mu_{rc})$:

$$C_{design}(m,\mu_{\beta},\mu_{rp},\mu_{rc}) = 208|\mu_{\beta}| + 2392/\mu_{rp} + 2392/\mu_{rc} + pm$$
(2.13)

The mean robustness can vary between -20 and -1; the mean response time can vary between 1 and 10; and the mean recovery time can vary between 1 and 50. Eq. (2.13) shows as the robustness of the components increase cost of design linearly increases. However, the cost of design decreases while the response and recovery times increases. This shows building a system with very robust components and very quick response and recovery times can impose high cost to the system.

The operating profit at time t is $\pi \left(\hat{\Re}_j(t), \omega(t) \right) = \omega_1 \hat{\Re}_j(t) - \omega_2 (1 - \hat{\Re}_j(t))$ where $\omega(t) = (\omega_1, \omega_2)$ remains constant for all time t. The parameter $\omega_1 = 40$ is the firm's positive operating profit when the system is functioning. The parameter $\omega_2 = 20$ is the firm's cost when the system is not functioning. The system is functioning if the performance is greater than or equal to $\underline{G} = 0.2$. The time value of the money in Eq. (2.4) is represented by $\lambda = 0.999$. The total lifetime of the system is T = 300 cycles.

In order to find the optimal design of the system, the expected utility model depicted in Eq. (2.6) is maximized. Table 2.1 depicts the expected utility results for four values of γ for this system given the above input numbers. A risk-neutral firm who maximizes its expected profit should choose 2 components (or 1 redundant component). The mean robustness is at its absolute minimum $\mu_{\beta} = -1$ and the mean response and recovery time are closer to their maximum values than their minimum values. By designing a system with 1 redundant component and largely neglecting the other design characteristics, the risk-neutral firm maximizes its expected profit. It achieves a resilience level of 0.945, which may suggest the system is not very resilient. It is in a failed state approximately 5 percent of the time. However, it is too costly to increase the resilience of the system for a firm who desires to maximize its expected profit.

The increasing γ indicates increasing risk aversion. A more risk-averse firm should add an additional redundant component (when $\gamma \ge 5 \times 10^{-4}$), and it should design a slightly more robust component ($\mu_{\beta} = -1.3$). The mean response time decreases to $\mu_{rp} = 4.3$ and the mean recovery time decreases to $\mu_{rc} = 5.7$ for a very risk-averse firm.

This example illustrates that a risk-averse firm should be willing to pay more to design a more resilient system. The design cost doubles from 704 to 1396 as the firm changes from a risk-neutral to a very risk-

	$\gamma = 0$ (expected profit model)	$\gamma = 1 \times 10^{-4}$	$\gamma = 5 \times 10^{-4}$	$\gamma = 4 \times 10^{-3}$
Number of components	2	2	3	3
Mean of robustness	-1	-1	-1	-1.3
Mean of response time	7.5	5.2	3.84	4.3
Mean of recovery time	31.0	14.4	20.3	5.7
Expected profit	1423	1385	1296	1025
Standard deviation of profit	65	70	50	40
Resilience	94.5%	96.9%	97.8%	98.2%
Design cost	704	934	1098	1396

Table 2.1: The optimal design characteristics of the one-subsystem example

averse decision maker. The resilience of the system increases from 0.945 to 0.982, and the firm's expected profit decreases from 1423 in the risk-neutral case to 1025 in the very risk-averse case. A more risk-averse firm should be willing to sacrifice more expected profit in order to design a more resilient system because the firm is more fearful of lost profits or very costly failures due to the non-resilient system.

2.3.2 Three-Subsystems Example

The one-subsystem example illustrates clear trade-offs among design cost, resilience, and expected profit, but most systems have many more than one subsystem. The second example, which is derived from (MacKenzie and Hu, 2018a) for an aircraft control actuator, is more complex with three subsystems. The three subsystems are in series, meaning that the system is functioning only if each subsystem is operating correctly. The results due to risk aversion are not as straightforward as the one-subsystem example, but useful insights can still be generated.

Subsystem *i* has m_i components in parallel, and each component in a subsystem has the same design characteristics: mean robustness $\mu_{\beta}^{(i)}$, mean time to respond $\mu_{rp}^{(i)}$, and mean time to recover $\mu_{rc}^{(i)}$. As with the previous illustration, the mean robustness can vary between -20 and -1; the mean response time can vary between 1 and 10; and the mean recovery time can vary between 1 and 50. There are $m_i - 1$ redundant components in subsystem *i*. Eq. (2.14) depicts the design cost for subsystem *i*, $c_{design,i} \left(\mu_{\beta}^{(i)}, \mu_{rp}^{(i)}, \mu_{rc}^{(i)} \right)$ as a function of the three design characteristics:

Table 2.2: Design cost parameters of the three-subsystems example

Subsystem <i>i</i>	p_i	ζ_{1i}	ζ_{2i}	ζ_{3i}	ρ_{1i}	ρ_{2i}	ρ_{3i}
1	50	80	100	60	0.2	0.1	0.1
2	200	70	40	20	0.2	0.1	0.1
3	75	60	80	40	0.2	0.1	0.1

$$c_{design,i}\left(\mu_{\beta}^{(i)},\mu_{rp}^{(i)},\mu_{rc}^{(i)}\right) = \zeta_{1i}\left(\exp\left(\rho_{1i}\mu_{\beta}^{(i)}\right) - 1\right) + \zeta_{2i}\exp\left(-\rho_{2i}\mu_{rp}^{(i)}\right) + \zeta_{3i}\exp\left(-\rho_{3i}\mu_{rc}^{(i)}\right)$$
(2.14)

where ζ_{1i} , ζ_{2i} , ζ_{3i} , ρ_{1i} , ρ_{2i} , and ρ_{3i} are parameters in the cost function. Eq. (2.14) shows that the exponential cost function for design implies increasing marginal costs as the design characteristic continues to improve. Table 2.2 shows the parameters of the cost function, and p_i is the per-component installation cost for component *i*.

As with the one-subsystem example, the operating profit at time *t* is $\pi \left(\hat{\Re}_j(t), \omega(t) \right) = \omega_1 \hat{\Re}_j(t) - \omega_2(1 - \hat{\Re}_j(t))$ where $\omega(t) = (\omega_1, \omega_2)$ remains constant for all time *t*. The parameter $\omega_1 = 30$ is the firm's positive operating profit for a functioning system and $\omega_2 = 20$ is the firm's cost for a failed system. The system is functioning if the performance is greater than or equal to $\underline{G} = 0.2$, and $\lambda = 0.999$. The total lifetime of the system is T = 300 cycles.

The first step of the proposed algorithm utilizes the ranking and selection algorithm to identify the system redundancy level m_i for each of the three subsystems. In the second stage, the continuous decision variables (i.e. mean robustness, mean time to respond, and mean time to recovery) are calculated via the Bayesian optimization algorithm to find the optimal design characteristic of each subsystem. One trial of the Bayesian optimization algorithm takes approximately 91 seconds. Five hundred runs are conducted to ensure the algorithm finds the true maximum. The total run time with a core i7-4770 CPU is approximately 12 hours.

2.3.2.1 Results of Expected Utility Model

In order to find the optimal design of the three-subsystems example, first, the expected utility model in Eq. (2.6) is maximized. Table 2.3 depicts the results for several values of γ . If the firm is risk neutral

	Subsystem i	$\gamma = 0$	$\gamma = 1 \times$	$\gamma = 2 \times$	$\gamma = 3 \times$	$\gamma = 5 \times$	$\gamma = 1 \times$
		(expected	10 ⁻⁴	10 ⁻⁴	10 ⁻⁴	10 ⁻⁴	10 ⁻³
		profit					
		model)					
Number of	Subsystem 1	3	3	3	3	3	3
components	Subsystem 2	1	1	1	1	1	1
components	Subsystem 3	2	2	2	2	2	2
Moon of	Subsystem 1	-1	-1	-1	-1.1	-1	-1
robustness	Subsystem 2	-12.9	-12.9	-14.5	-14.3	-15.4	-14.9
Tobustiless	Subsystem 3	-1	-1	-1.3	-1	-1	-1
Maan of	Subsystem 1	1.2	1.1	1	1.1	1.3	1
	Subsystem 2	1.6	9.9	1.4	1.2	9.8	1.2
response time	Subsystem 3	1	2.3	1	1	1	1.1
Moon of	Subsystem 1	29	5.1	48	49.8	6	1.4
	Subsystem 2	50	46.2	50	12.4	50	49.3
recovery time	Subsystem 3	41.8	3.6	3.7	1	4.6	1.2
Expected		3970	3964	3935	3932	3918	3906
profit							
Standard		118	101	103	107	100	104
deviation of							
profit							
Resilience		97.7%	98.1%	98.2%	98.2%	98.4%	98.8%
Design cost		918	985	1006	1021	1055	1136

Table 2.3: The optimal design characteristics of the three-subsystems example for the expected utility model

(i.e., $\gamma = 0$), the first, second, and third subsystems should be built with three, one, and two components, respectively. According to Table 2.2, the cost of adding redundancy for the second subsystem is almost three times greater than that of the third subsystem and four times greater than that of the first subsystem. It is not profitable to add redundancy in the second subsystem. Instead of adding redundancy, the risk-neutral firm should design the component in the second subsystem with more robustness than those in the other two subsystems to prevent failure.

As the firm becomes more risk averse (i.e., γ increases), the firm should design slightly more robust components and decrease the response and recovery times. The number of components remains constant for all values of risk aversion. A more risk-averse firm should design a more resilient system, but it is more cost effective to achieve that higher resilience by increasing the robustness or decreasing the response and recovery times rather than by increasing the redundancy. The firm should not increase the resilience by paying more to build extra components in each subsystem. Since the cost of building extra components is high, the model does not recommend increasing redundancy beyond what is recommended in the risk-neutral case.

The mean absolute value of robustness of the second subsystem increases from 12.9 to 14.9 as the firm becomes very risk averse ($\gamma = 10^{-3}$). The mean robustness for the first and third subsystems remains very small as the firm becomes very risk averse. Instead, the restoration time (the mean of the recovery time plus the mean of the response time) of the first subsystem decreases from 30.2 to 2.4. The restoration time of the second subsystem slightly decreases from 51.6 to 50.5. Finally, the restoration time of the third subsystem significantly decreases from 42.8 to 2.3.

As depicted in Table 2.3, the resilience and expected profit depend on the firm's degree of risk aversion. As a firm becomes more risk averse, it should pay more for design cost in order to increase the resilience of the system. If the firm is risk neutral, the resilience is 0.977. If the firm is very risk averse ($\gamma = 10^{-3}$), the resilience is 0.988. The expected profit decreases from 3970 to 3906. The expected profit, design cost, and resilience do not change significantly for the different risk averse cases because the risk-neutral firm should already build a quite resilient system. It is very costly to increase the system's resilience to more than 0.99, which is not desirable even if the firm is very risk averse.

2.3.2.2 Results of Expected Profit with VAR

The three-subsystem example is also optimized using the VAR constraint by solving the optimization problem in (2.8). Figure 2.5 depicts the simulated distribution of the firm's profit given the optimal design for a risk-neutral firm who is maximizing its expected profit. The probability that profit is less than 3000 is 0.006 and the probability that the profit is between 3000 and 4200 is 0.994. The probability that the firm's profit exceeds 3600 is 0.881. Given this distribution, four different values for x_{VAR} are chosen (3000, 3300, 3500, and 3600) for this analysis, and q = 0.05. The algorithm described in Section 3 is followed with the VAR constraint. The ranking and selection method chooses the number of components for each subsystem, and the Bayesian optimization algorithm identifies the design features (mean robustness, mean



Figure 2.5: Histogram of profit given the optimal design for maximizing expected profit

time to respond, and mean time to recovery) for each component. An increasing x_{VAR} indicates a more risk-averse firm, which incentivizes the firm to design a more resilient system.

Table 2.4 depicts the results of a firm who maximizes its expected profit subject to the VAR constraint. The results are similar to those of the expected utility model. The number of components should not change as the VAR constraint increases, but the second subsystem should be designed with more robustness (the absolute value of the mean robustness increases from 12.9 to 16.1). The firm should design the first and third subsystems so that the mean recovery time decreases from 29 to 15.9 and from 41.8 to 1.2 for each subsystem, respectively, as VAR increases. The resilience of the system increases from 0.977 to 0.987, and the firm's expected profit decreases from 3970 to 3919.

2.3.2.3 Comparison of Results of Expected Utility and Expected Profit with VAR Models

The design-for-resilience illustration with three subsystems has been modeled with an expected utility and a VAR model. The two approaches reach similar results through different methods. The VAR model seeks to maximize the firm's expected profit but increasingly constraints the set of feasible designs as the VAR metric increases. The expected utility model does not insert additional constraints but the degree of

		Expected	$x_{VAR} = 3000$	$x_{VAR} = 3300$	$x_{VAR} = 3500$	$x_{VAR} = 3600$
		profit model				
Number of	Subsystem 1	3	3	3	3	3
components	Subsystem 2	1	1	1	1	1
components	Subsystem 3	2	2	2	2	2
Mean of	Subsystem 1	-1	-1	-1	-1.1	-1.1
robustnoss	Subsystem 2	-12.9	-13.1	-13.3	-14.4	-16.1
Tobustiless	Subsystem 3	-1	-1	-1	-1.33	-1.5
Moon of	Subsystem 1	1.2	1	1.3	1.2	1
response time	Subsystem 2	1.6	10	10	7.9	4.9
response time	Subsystem 3	1	1.7	1.2	1	1
Mean of	Subsystem 1	29	50	6	3.3	15.9
recovery time	Subsystem 2	50	3.9	3.2	49.5	47.1
recovery time	Subsystem 3	41.8	1	4.2	1	1.2
Expected		3970	3967	3953	3946	3919
profit						
Standard		115	110	108	103	100
deviation of						
profit						
Resilience		97.7%	98.1%	98.4%	98.7%	98.7%
Design cost		918	976	1023	1069	1080

Table 2.4: The optimal design characteristics of the three-subsystems example for expected profit with VAR

risk aversion as measured by γ increasingly makes low profits very undesirable. The firm is becoming more risk averse either by increasing x_{VAR} or by increasing γ .

2.3.3 Wind Turbine System

A wind turbine is a clean renewable source of energy. In 2014, the global total wind energy capacity was approximately 370,000 MW (Lei and Sandborn, 2016). A wind turbine needs to be reliable in the face of different adverse events (such as wear-out, lightning strike, icing, and a control system malfunction) which may degrade the turbine's performance and or cause failure in its subsystems (Tazi et al., 2017; Spinato et al., 2009). It is crucial to build a resilient wind turbine so that it provides an uninterrupted supply of electricity. In some places like Iowa, where 36% of the state's electricity comes from wind, the supply of electricity is very dependent on wind turbine operations. We apply the design-for-resilience framework to analyze the effect of the decision maker's risk attitude in the design characteristics of wind turbine.



Figure 2.6: Major components of the wind turbine

The wind turbine consists of multiple subsystems, which are connected in series, as shown in Figure 2.6. The subsystems are the rotor, gearbox, generator, brakes and hydraulics, and electronics and grid, and $i = 1, 2, \dots, 5$. This turbine can generate 2 MW of electricity per hour.

Constructing the design cost function is an important step in estimating the profit and resilience of the operating system. Eq. (2.15) depicts the proposed design cost function for each subsystem of the wind turbine:

$$c_{design,i}(\mu_{\beta}^{(i)},\mu_{rp}^{(i)},\mu_{rc}^{(i)}) = 168(\kappa_{1i}\exp(-0.1\mu_{\beta}^{(i)}-1) + \kappa_{2i}\exp(-0.2\mu_{rp}^{(i)}) + \kappa_{3i}\exp(-0.2\mu_{rc}^{(i)})) \times 10^{4}$$
(2.15)

Table 2.5 shows the maintenance costs of the five turbine subsystems (Sheng, 2013; Einarsson, 2016), which are used to estimate κ_{1i} , κ_{2i} , and κ_{3i} . The parameter κ_{1i} is estimated using the inverse of expected time to failure of subsystem *i*. It is assumed that increasing the robustness of a subsystem with a smaller expected time to failure will be more expensive than increasing the robustness of a subsystem with a greater expected time to failure. According to the U.S. Energy Information Administration (EIA,), the average consumer price of electricity is approximately \$150 for 1 MWh. For a 2 MW wind turbine, the lost revenue from not functioning during one hour is \$300. As shown in Table 2.5, the ratio of response cost to response time is used to estimate κ_{2i} , and the ratio of repair cost to repair time is used to estimate κ_{3i} . These parameters are standardized in the interval of [0,1] to align the costs on the similar scales. Table 2.6 depicts the design cost

Subsystem	Repair	Repair	Response	Expected	Response cost	Repair cost /
	cost (\$)	time (hr)	time (hr)	time to	/ response time	repair time
				failure (yr)		
Rotor	36000	204	8	5	37.5	176
Gearbox	30000	230	5	11	60	130
Generator	9000	95	6	10	50	94
Brakes and	2500	73	4	6.5	75	34
Hydraulics						
Electrical	30300	20	6	1.6	50	100
and Grid						

Table 2.5: Wind turbine subsystems data (Sheng (2013); Einarsson (2016))

Table 2.6: Design cost coefficients for the wind turbine system

Subsystem	κ_{1i}	κ_{2i}	κ_{3i}
Rotor	0.17	0.14	0.33
Gearbox	0.08	0.22	0.24
Generator	0.09	0.18	0.18
Brakes and Hydraulics	0.13	0.27	0.06
Electrical and Grid	0.54	0.18	0.19

coefficients for the wind turbine system. We assume that adding redundant components such as a second rotor or gearbox is not feasible for this example.

The decision variables, mean robustness, mean response time, and mean recovery time, are constrained within the optimization routine. The mean robustness $\mu_{\beta}^{(i)}$ varies between -20 and -1; the mean response time $\mu_{rp}^{(i)}$ varies between 0 and 7 days, and the mean recovery time $\mu_{rc}^{(i)}$ varies between 0 and 14 days for each subsystem. Similar to the prior examples, the operating profit at time *t* is $\pi\left(\hat{\Re}_{j}(t), \omega(t)\right) = \omega_{1}\hat{\Re}_{j}(t) - \omega_{2}(1-\hat{\Re}_{j}(t))$ where $\omega_{1} = 300 \times 24 \times 7 = \$50,400$ is the profit from selling 2 MW of electricity per hour in one week and $\omega_{2} = 100 \times 24 \times 7 = \$16,800$ is the cost of a failed system in a week, where \$100 is the hourly labor cost. The performance of each component of the wind turbine system is simulated using N = 1000 trajectories of performance during T = 700 weeks of simulation. The time step in the simulation is one week, and the total lifetime of the wind turbine is T = 700 weeks. It is assumed that the failure limit is equal (e.g., 0.2) for all the components of the subsystems. However, future research can address considering different failure limits for the components of engineering systems.

The design-for-resilience model with expected utility is solved for three risk attitudes: a risk-neutral attitude ($\gamma = 0$), a slightly risk-averse attitude ($\gamma = 10^{-5}$), and a very risk-averse attitude ($\gamma = 10^{-4}$). As there is no redundancy in the wind turbine system, the continuous decision variables (i.e., mean robustness, mean time to respond, and mean time to recovery) are calculated via the Bayesian optimization algorithm to find the optimal design characteristics for each subsystem. When a subsystem fails due to an adverse event, the maintenance team should respond to the event and begin recovering or repairing the subsystem.

The design variables of the components of the wind turbine system are optimized using Eq. (2.6). Table 2.7 shows the optimal design for resilience for the three different risk attitudes. As the designer becomes more risk averse (i.e., γ increases), the designer should design more robust subsystems that also enable quicker response and recovery times. The mean absolute value of robustness for each subsystem increases as the designer becomes more risk averse. The restoration time (the mean of the recovery time plus the mean of the response time) for each subsystem also changes due to risk aversion. For instance, the restoration time of the gearbox decreases from 19.1 to 10 days as risk aversion increases. However, the restoration time for the rotor increases from 17.1 to 17.8 days as risk aversion increases. Since a more risk-averse designer should design a more robust rotor that is less likely to fail, the restoration time is less important for the rotor.

Figures 2.7a and 2.7b depict the performance trajectories of each of the wind turbine's subsystems for the risk-neutral and very risk-averse cases. The performance trajectories are based on the sequential MCS in Algorithm 1 given the optimal values for the decision variables. These random trajectories were used to estimate the system resilience curves in Figures 2.8a and 2.8b based on Eq. (2.2). In the risk neutral case, the electrical and grid and generator components fail more than the other components and have the most variability than the other components when those failures will occur. Although the frequency of failures for these components is optimal for a design firm who wishes to maximize its expected profit, designers may conclude these failures occur more frequently than they would like. They could increase the robustness of these components in order to reduce the number of failures. If the designers are comfortable with the frequency of those failures, they can use the simulation trajectories to forecast when failures are likely to occur and plan to respond and replace or repair those components at those time periods.

	Subsystem <i>i</i>	$\gamma = 0$ (ex-	$\gamma = 10^{-5}$	$\gamma = 10^{-4}$
		pected profit		
		model)		
	Rotor	-10.8	-13.8	-17.4
Mean of	Gearbox	-12.1	-18.9	-18.7
robustness	Generator	-1	-12.8	-14.1
Tobustiless	Brakes and Hy-	-10.9	-11.8	-15.2
	draulics			
	Electrical and Grid	-1	-1.7	-7.3
	Rotor	4.7	1.9	5.8
Mean of	Gearbox	6.5	3.9	6
response time	Generator	4.4	2	1.5
(days)	Brakes and Hy-	7	4.1	5.6
	draulics			
	Electrical and Grid	7	4.2	4.5
	Rotor	12.4	13.9	12
Mean of	Gearbox	12.6	6.5	8.5
recovery time	Generator	4.8	13.5	7.9
(days)	Brakes and Hy-	7.4	3.5	3.1
	draulics			
	Electrical and Grid	12.1	2	6.5
Expected profit		\$22.9 million	\$22.6 million	\$22.5 million
Standard devia-		\$90 thousand	\$12 thousand	\$5 thousand
tion of profit				
Resilience		0.96	0.97	0.98
Design cost		\$1.47 million	\$2 million	\$2.3 million

Table 2.7: The optimal design characteristics of the wind turbine for the expected utility model

Figure 2.7b shows that the rotor and gearbox are built to be very robust in the very risk-averse case, therefore they never fail in the simulation periods. The generator only fails once in the very risk-averse case; however, it fails frequently in the risk-neutral case. Figures 2.8a and 2.8b show that the system's design is more resilient in the very risk-averse case compared to the risk-neutral case.

As depicted in Table 2.7, the resilience and expected profit depend on the firm's degree of risk aversion. As a firm becomes more risk averse, it should pay a larger design cost in order to design and build a more resilient wind turbine. The firm's expected profit decreases from \$22.9 million to \$22.5 million as it becomes more risk averse. The firm's expected profit decreases by approximately 2% as it increases the



Figure 2.7: Simulation trajectories for the optimal design of wind turbine system

turbine's resilience. The design cost increases from \$1.47 million to \$2.3 million, and the wind turbine's resilience increases from 0.96 to 0.98.

2.4 Conclusion

This paper provides a framework to incorporate risk aversion into a firm's design decisions for a resilient engineered system. The resilience of the system is a function of the system's reliability and its restoration after failure. Following the work of MacKenzie and Hu (MacKenzie and Hu, 2018a), we use the redundancy, robustness, response, and recovery of the system (i.e. the design characteristics of the system) to measure the system's resilience to adverse events. The firm's risk attitude may incentivize the firm to design a more resilient system even if that means higher design costs and less expected profit. Two models to capture a firm's risk aversion are presented: an expected utility model and an expected profit with VAR constraint.

The use of exponential utility and VAR metric represents unique contributions to the design of more resilient systems. The illustrative examples demonstrate how risk aversion should influence a firm to design a more resilient system. In the simple one-subsystem example, a more risk-averse firm should add an additional redundant component and design a component that is easier to repair and restore. The more complex



Figure 2.8: Resilience curve for the wind turbine system

three-subsystem example has less significant changes in the design characteristics, but risk aversion should influence the firm to increase the robustness of one subsystem and decrease the response and recovery times of the other two subsystems. The expected utility model and the expected profit with a VAR constraint model return similar results in the illustrative example. The wind turbine example demonstrates more explicitly how the design-for-resilience framework with risk aversion can be applied to a real engineered system. As the firm or designer becomes more risk averse, the designer should focus on making the wind turbine more robust in order to decrease the likelihood of failure.

Applying the Bayesian optimization algorithm alongside the sequential Monte Carlo simulation enables the designers to find the optimal characteristics of the engineered system for both risk-neutral and risk-averse decision makers. We analyze how the risk attitude of the decision maker should impact system resilience. This approach can help in the early stage of design by capturing the risk attitude of decision makers as they consider the trade-offs among the initial costs, resilience, and future profits. The results show that studying the trade-offs between risk aversion and risk neutrality is important to find the robustness of the components and response and recovery times, as the design features for resilience changes when we incorporate risk attitude within the design framework.

Further applications could explore to what extent the expected utility model and the expected profit model with a VAR constraint provide similar results. Since the VAR constraint only considers extreme losses (less than 5%) and the utility function captures the entire distribution, there may be certain types of uncertainty in which the results are slightly different. Future research can measure the effect of CVAR in the design for resilience and compare it to the VAR results. Machine learning algorithms can be employed to learn from and make predictions on the parameters of complex engineered systems. They may facilitate our understanding of how design characteristics impact system resilience.

2.5 References

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CHAPTER 3. SOARP: SIMULATION OPTIMIZATION FOR AIRFIELD RIGID PAVEMENT DESIGN

A paper submitted to International Journal of Pavement Engineering

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Abstract

The current state-of-the-art airfield concrete pavement design is accomplished using FAARFIELD software developed and released by the U.S. Federal Aviation Administration (FAA). Since this mode of design is implemented based on some initial assumed inputs, obtaining an optimum design for a given traffic and environmental loading and design age is an iterative process to find the best possible design. However, it takes considerable amount of time to perform this iterative process using the 3-D Finite Element (FE) based FAARFIELD software. To overcome this challenge, a more efficient methodology, Simulation Optimization for Airfield Rigid Pavement (SOARP), is proposed. SOARP relies on artificial neural network (ANN) models combined with a design optimization framework to determine the optimal design of airfield rigid pavement, and this optimal design should perform satisfactorily for different values of uncertain parameters. SOARP is implemented for various reliability levels and design lives for the airfield rigid pavement. In addition, the pavement thickness designed by SOARP and FAARFIELD are compared for various flexural strength and reliability levels. The results show that SOARP either results in more reliable or less expensive pavement designs.

3.1 Introduction

Airport pavements are designed over many years to withstand repeated traffic loading imposed by a broad entire range of aircraft types over many years, to resist the abrasive action of traffic, and to endure deterioration induced by adverse weather conditions (e.g., extreme hot or cold weather) and other influences in a cost-effective manner. For rigid airport pavement design, the Federal Aviation Administrative (FAA) uses three-dimensional finite- element (3D-FE) procedures for rigid airport pavement design, as implemented in the FAA Rigid and Flexible Iterative Elastic Layer Design (FAARFIELD) program (FAA, 2016). The iterative processes encountered in rigid pavement thickness design based on 3D-FE solution exhibit long and unpredictable run times, especially when the number of slabs is increased and top-down cracking is considered (Rezaei-Tarahomi et al., 2017a; Kaya et al., 2017).

Although there are many features affecting pavement performance, typical airfield rigid pavement design processes in FAARFIELD use a trial-and-error approach to find optimum slab size (joint spacing), joint stiffness, temperature-induced initial curling, and predefined load location, using a trial-and -error approach. Since it is also not practical to determine the optimum design solution from an exhaustive set of all acceptable designs using this approach (Gaurav et al., 2011), some practical alternatives are needed to expand the airfield rigid pavement design beyond the current restricted approach, making design calculation computationally-tractable, agile, and comprehensive. To achieve this goal, this study proposes a novel approach utilizing Artificial Neural Networks (ANN) along with an optimization technique for airfield rigid pavement design, recognizing that there have been previous studies utilizing predictive models (e.g., ANN) or optimization methods in pavement design and rehabilitation problems to make pavement engineering practices versatile and practical.

Santos and Ferreira (2011) presented a deterministic pavement-design optimization model that considers pavement performance, construction costs, maintenance and rehabilitation costs in the model, assuming deterministic values for all model parameters. Mikolaj et al. (2017) optimized a rehabilitation plan featuring cost-benefit analysis to maximize life-cycle length of pavement constructed with asphalt concrete materials. Hadi and Arfiadi (2001) used a genetic algorithm to optimize pavement building costs of rigid highway pavement. Mamlouk et al. (2000) developed a project-level optimization model for flexible pavements whose design variables were initial pavement thickness, overlay thickness, and overlay timing used to minimize highway agency and user costs.

Engineering design problems typically have multiple variables, and there is often uncertainty around these variables (Li et al., 2019). Monte Carlo simulation is often used to explore the design output given design parameters (Sadoughi et al., 2018). Some studies in the pavement design area have considered that

simulation evaluates the effects of different design inputs on the desired output (Timm and Newcomb, 2006; Noshadravan et al., 2013; Lee and Ibbs, 2005). For example, Timm and Newcomb (2006) developed a Monte Carlo simulation framework for asphalt to conduct a probabilistic analysis of pavement reaction to loading and to evaluate the resulting damage. In their proposed framework, to meet the damage criteria, random samples were generated from probability distributions of asphalt layer thickness, loading configurations, and material properties, and sequences of new random numbers were generated from the input parameters until the level of damage is less than a threshold value. Their proposed frameworks lack an optimization model that could lead to an exact or near-exact solution.

Design of new and rehabilitated pavements involves many uncertainties, variabilities, and approximations. Generally, reliability refers to the ability of the system to perform above a safety limit under various sources of uncertainty (MacKenzie and Hu, 2018b). In pavement design, reliability can be defined as the probability that pavement performance would remain within an allowable range during the design life (Dinegdae et al., 2018). A reliability-based pavement design can properly incorporate the uncertainty and variability to make an effective design (ARA, 2003; Dalla Valle, 2015). The American Association of State Highway and Transportation Officials (AASHTO) mechanistic empirical pavement design guide (MEPDG) considers the reliability of pavement sections in the design (Dinegdae et al., 2018). Dinegdae et al. (2018) evaluated pavement reliability analysis by incorporating response surface methods. They developed a twocomponent reliability analysis methodology to evaluate the reliability of fatigue cracking failure in actual field pavements. Their study shows how the influence of different design input variables can be captured within a reliability analysis framework. Retherford and McDonald (2010) investigated potential reliability methods and discussed their advantages and disadvantages in the mechanistic empirical design approach to pavement design.

A number of studies applied reliability in the pavement design optimization. Sanchez-Silva et al. (2005) presented a model for reliability cost-based optimization of asphalt pavement structures that considered asphalt-surface fatigue damage and the degradation of granular materials by repetitive loading cycles. They also combined reliability-based design optimization with long-term pavement-maintenance policy. Gaurav et al. (2011) minimized asphalt-pavement design costs using a surrogate-based optimization approach. They

considered design reliability in the model via the use of chance constraints, and the design variables were the asphalt-concrete base, and sub-base thicknesses. They considered deterministic values for model parameters such as Granular base, Granular sub-base, and sub-grade. By considering different reliability levels in pavement design optimization, decision makers can determine an optimal design that considers expected design costs or choose a design that meets their degree of risk aversion.

The objective of this study is to develop a novel design methodology called Simulation Optimization for Airfield Rigid Pavement (SOARP). SOARP is a comprehensive reliability-based simulation-optimization framework benefiting from artificial intelligence for critical stress responses prediction for the airfield concrete design. The optimal design can be identified more quickly than with other methods. This framework empowers the designers to consider large number of scenarios for designing airfield concrete pavement. This study proposes SOARP for decision makers involved in the design of airport concrete to achieve various reliability levels. The novelty of this study and its primary difference with FAARFIELD's design methods lie in its use of ANN to predict critical responses. Another difference is to conduct airfield concrete pavement design with using Monte Carlo simulation and Bayesian optimization under different reliability levels.

3.2 ANN-based Bayesian Optimization Framework

Figure 5.1 shows the whole procedures of the SOARP Framework. The framework is aimed at minimizing the design cost while the fatigue failure of the pavement is kept under the allowable amount by a reliability constraint. The cost function (objective function) represents the total cost of the design thickness of the Portland cement concrete (PCC) slab, base layer, and subbase layer. The reliability constraint limits structural fatigue life of the pavement to an allowable load repetition-to-failure using the cumulative damage factor (CDF). The CDF calculation follows the same method used in FAARFIELD (Brill, 2010; Kawa, 2012; FAA, 2016). Unlike FAARFIELD, an ANN is used instead of finite element analysis to determine the critical response. SOARP employs ANNs as analysis engine for replicating critical stress responses associated with cracking which is used for calculating the CDF of the pavement. Using an ANN in this framework enables performing large number of simulations without interruptions induced by time-consuming analysis and complex calculations. The following subsections describe the approaches, models, and the mathematics employed for design optimization including CDF calculations, reliability constraint, objective function, ANN models development, and Bayesian optimization algorithm.



Figure 3.1: Flow chart of SOARP steps

3.2.1 Mathematical Model

1. Randomly generate *N* samples from the distributions of uncertain parameters: Gear loading angle (θ_g) , Loading location on the slab (*X* and *Y*), temperature gradient, thermal coefficient, PCC slab cost, base layer cost, and subbase layer cost.

Calculate critical bottom tensile stress using the trained ANN models for the airplanes (see section 3.2.2).

3. Calculate cumulative damage factor (FAA, 2016) for each airplane using the design variables (PCC slab thickness (d_1) , base layer thickness (d_2) , and subbase layer thickness (d_3)) by the optimization algorithm:

$$CDF = \frac{(\text{Annual Departure}) \times (\text{Life in Years})}{(\text{Pass/Coverage}) \times (\text{Coverage to Design Failure})}$$
(3.1)

To calculate the pass to coverage ratio (P/C), coverage to pass (C/P) is calculated using Eq. (3.2). For rigid pavements, the pavement surface is divided into 81 longitudinal strips (10 inch strips at lateral distance between -400 and 400 in.), and the C/P ratio is computed for each offset. For each offset i, $(C/P)_i$ is computed using the following probability equation:

$$(C/P)_i = \sum_{k=1}^{N_t} P\left[\left(x_i - \frac{w}{2}\right) \le x_k \le \left(x_i + \frac{w}{2}\right)\right]$$
(3.2)

where N_t is the number of tires on the landing gear, x_i is lateral distance from a longitudinal reference line (e.g., runway or taxiway centerline) to the midpoint of strip i, x_k is the lateral distance from the same reference line to the centerline of tire k, and w is the tire width (Kawa, 2012). Coverage to design failure (C) can then be obtained by solving Eq. (3.3) (Brill, 2010):

$$DF = \left[\frac{F'_{s}bd}{(1-\alpha)(d-b) + F'_{s}b}\right] \times \log C$$

$$+ \left[\frac{(1-\alpha)(ad-bc) + F'_{s}bc}{(1-\alpha)(d-b) + F'_{s}b}\right]$$
(3.3)

where the design factor $DF = R/\sigma$ and $\alpha = SCI/100$. *R* is the flexural strength of the PCC and σ is the analytical stress obtained by ANN critical response models. For new rigid pavements, a structural condition index (*SCI*) of 80 is the FAA definition of structural failure, consistent with the condition that 50 percent of slabs in the traffic area exhibit a structural crack (FAA, 2016). The parameter values of Eq. (3.3) from Brill and Kawa (2017) are:

$$F'_{s} = 1$$

$$b = d = 0.160$$

$$a = 0.760 + 2.543 \times 10^{-5} (E - 4500)$$

$$c = 0.857 + 2.314 \times 10^{-5} (E - 4500)$$
(3.4)

where *E* is the subgrade modulus considered to be 20,000 psi. To calculate the cumulative CDF (CCDF), the *CDF* values for all airplanes in the traffic mix load are summed for each of the 80 strips, after which the peak value of the *CCDF* is represented as *TCDF* (Eq. (3.5)). Figure 3.2 shows the CCDF and CDF calculated by Eq. (3.1) for each airplane.

$$CCDF_{s} = \sum_{k=1}^{4} CDF_{ks} \forall s = \{1, 2, ..., 80\}$$

$$TCDF = \max_{s} CCDF_{s}$$
(3.5)



Figure 3.2: CCDF and CDF for each airplane.

4. Solve the optimization problem and use Monte Carlo simulation to determine the expected design cost, while ensuring that the reliability constraint is not violated:

$$\underset{d \in D}{\text{minimize}} \frac{1}{N} \sum_{j=1}^{N} \sum_{q=1}^{Q} C_{jq} d_{q}$$
(3.6)
subject to $P(TCDF \le T) \ge \Re$

The first part of Eq. (3.6) represents the expected design cost considering N simulations, where C_{jq} is the cost of design for design variable d in simulation j. D represents the feasible set of design alternatives. Since several of the parameters are uncertain, Monte Carlo simulation can be used to calculate the cost function, with the expected cost of design calculated as the average after N different simulations. The second part of Eq. (3.6) shows the reliability constraint representing the simulated probability that *TCDF* is less than or

equal to *T* (e.g., 1.05), where *T* is the TCDF threshold. The decision maker establishes reliability level \Re (e.g., 0.95) before optimizing the problem using Eq. (3.6). For a design to be reliable the TCDF should be less than the threshold (*T*) \Re % of times. This framework allows the design to fail fewer than $(1 - \Re)$ % of the time. If *TCDF* > *T* then the pavement will fail before reaching its design life, but it would be too costly to build or design a system that would never fail during its operation.

The Bayesian optimization algorithm is used to solve this problem. The algorithm procedure and the optimization termination criteria are elaborated in detail in subsection 3.2.3.

3.2.2 Artificial Neural Networks

Rezaei Tarahomi et al. (2017); Rezaei-Tarahomi et al. (2017b); Rezaei Tarahomi et al. (2018, 2019b) and Kaya et al. (2017, , 2018) developed ANN-based response models predicting the critical stress associated with top-down and bottom-up cracking in rigid airfield pavements. Their study was part of a research study sponsored by the Federal Aviation Administrative (FAA). The models were trained using ANN algorithms for each type of aircraft under a variety of mechanical loading only and combined mechanical and temperature induced loading circumstances. In order to train the ANN models, data sets were generated by implementing hundreds of thousands three-dimensional finite element (3D FE) simulations of nine-slab airfield rigid pavements using NIKE3D-FAA. The data set consists of the pavement characteristics and associated maximum pavement stress responses. The ANN was trained to predict the critical responses by using the pavement properties inputs. Various ANN architectures (one and two hidden layers with varying number of neurons) and training algorithms were tried and tested. The optimum models were selected for each aircraft. Figure 3.3 shows a two-layer ANN architecture used by Rezaei Tarahomi et al. (2018, 2019b,b) for combined loading condition.

Rezaei Tarahomi et al. (2017, 2018, 2019b) showed that employing ANN in the current FAA design process can be beneficial by performing rapid analysis and reducing computer run time for multiple-slab simulation to a matter of seconds. Incorporating ANN surrogate response models into the pavement design process can therefore significantly enhance efficiency of the design process by reducing the iteration time for calculation of critical stresses for each type of aircraft in a mixed-aircraft traffic loading scenario. Using



Figure 3.3: Two-layer ANN model architecture for simultaneous temperature- and mechanical-loading cases.

rapid-response ANN models can also help expand current design method beyond those compromising the currently used one-slab model involving limited-loading circumstances.

Before incorporating such alternative models into the current FAA design process, they must be tested and validated. Rezaei Tarahomi et al. (2017, 2018, 2019b,a) assessed ANN models accuracy in analyzing airfield concrete pavement using various testing, independent testing, and sensitivity testing data sets. The accuracy metrics demonstrated promising predictions for training and testing and confirmed a good fit and a lack of memorization of the predictors-output relationship. In addition, this study is presenting SOARP method which employs the trained ANN models along with the FAA's airfield concrete pavement design. This method enables finding the optimum thickness for each pavement's layer by using the ANN-predicted critical stress. Moreover, it is implemented in a case study and then validated by comparing SOARP method with FAARFIELD.

3.2.3 Optimization Algorithm

In this study, the expected cost of design is minimized under different reliability levels. To calculate the objective function and determine an optimal design, the ANN model is used in each simulation scenario. ANNs are complex black-box functions whose outputs provide little information about functional forms because there is often no simple relationship between network weights and model properties (Zhang et al., 2018). The first or second order information of the highly nonlinear simulation model is hard to estimate.

Hence, the traditional optimization algorithms such as gradient descent which uses the first order information of the objective function is not applicable to solve the problem. The Bayesian optimization is able to achieve accurate results in reasonable time compared to other optimization algorithms such as random search and evolutionary algorithms (Thornton et al., 2013). This algorithm outperforms other global optimization algorithms on challenging optimization problems (Snoek et al., 2012).

Bayesian optimization algorithm can effectively model input-output relationships of a black-box model. The inputs of the model are the design variables and the outputs are the design costs evaluated with the Monte Carlo simulation. As the procedure to calculate the design is complex and consist of uncertain parameters, the design cost can only be evaluated with the Monte Carlo simulation. Considering uncertainty in the parameters in the pavement design frameworks requires the use of computationally expensive simulations to evaluate and calculate the objective function. Bayesian optimization generates candidate designs and inserts them into the model and then evaluates the resulting objective function to minimize expected cost. This algorithm constitutes a powerful method for finding the optimal design d^* .

The Bayesian optimization algorithm creates a surrogate model for the objective function and exploits it in order to find the next evaluation points in the feasible solution space (Lizotte, 2008a). The Gaussian process is a powerful prior distribution for functions; therefore, we select it as the prior over the objective function (Snoek et al., 2012). Bayesian optimization estimates the objective function using *J* samples of the design variables *d*. The algorithm fits a multivariate normal prior over the *J* samples. The prior has a mean of 0 and the covariance matrix *K*. After simulating *J* design alternatives to estimate $f_{1:J}$ —the expected cost of the *J* design alternatives—the posterior predictive mean and variance of a new design alternative d' can be calculated using the Sherman-Woodbury-Morrison formula:

$$\mu(d'|d_{1:J}) = k(d', d_{1:J})K(d_{1:J}, d_{1:J})^{-1}f_{1:J}$$
(3.7)

$$\sigma^{2}(d'|d_{1:J}) = k(d',d') - k(d',d_{1:J})K(d_{1:J},d_{1:J})^{-1}f_{1:J}$$
(3.8)

where $d_{1:J}$ is the *J* previously evaluated thicknesses used to predict the next point. The objective function at the new design alternative d' has the following form:

$$f(d'|d_{1:J}) \sim N\left(\mu(d'|d_{1:J}), \sigma^2(d'|d_{1:J})\right)$$
(3.9)
Algorithm 4 Implementation procedure of Bayesian optimization.

- 1: **for** i = 1 to *I* **do**
- 2: Calculate $\mu(d'|d_{1:J})$ and $\sigma^2(d'|d_{1:J})$
- 3: Find d_{J+1} by optimizing the acquisition function $u(d'|d_{1:J}) = E(\max\{0, f_{J+1}(d) f(d^+)\}|d_{1:J})$
- 4: Use Monte Carlo simulation to calculate $f(d_{J+1})$
- 5: Augment data points $S_{J+1} = S_J \bigcup \{ (d_{J+1}, f(d_{J+1})) \}$
- 6: **end for**
- 7: $d^* = \arg \max f(d_{1:J})$

8: Output: d^* : Optimal design variables (slab, base, and subbase thickness)

Bayesian optimization selects the J + 1 design variable by maximizing the following utility (i.e., acquisition) function:

$$u(d'|S_{1:J}) = E(\max\{0, f_{J+1}(d) - f(d^+)\}|S_{1:J})$$
(3.10)

where $d^+ = \arg \max_{d \in \{d_{1:J}\}} f(d)$ is the current best design that results in the smallest expected design cost based on *J* evaluated alternatives. The set $S_J = \{d_{1:J}, f_{1:J}\}$ contains *J* design alternatives and their corresponding expected costs assessed via simulation. Maximizing the acquisition function represents a trade-off between exploration and exploitation. When the algorithm chooses to exploit, it seeks to sample in solution spaces close to designs that already generate small expected costs. However, when it explores the solution space it chooses to simulate a design alternative with a larger uncertainty (Brochu et al., 2010). This procedure iterates until there is very little improvement in the objective function or the maximum number of iterations *I* is reached (i.e, termination criteria) (Frazier, 2018; Klein et al., 2016). Algorithm 6 describes the Bayesian optimization procedure. The implementation procedure is adopted from the Random Embedding Bayesian Optimization (REMBO) algorithm developed by Wang et al. (2013b).

3.3 Pavement Design Optimization Case Study

The case study described in this section involved design of a nine-slab concrete pavement with base and subbase layers on top of a subgrade. Aircraft traffic assumed in this study included a B747-8, a B787-8, an A340-500 opt, and an A340-600 opt with 3,000, 3,000, 1,500, and 1,500 annual departures, respectively.

Inputs		Value		
PCC Slab	Modulus (Psi)	$3.0 imes 10^6$		
	Poisson Ratio	0.15		
Base	Modulus (Psi)	$5.0 imes 10^{5}$		
	Poisson Ratio	0.2		
Granular Subbase	Modulus (Psi)	$7.5 imes 10^{4}$		
	Poisson Ratio	0.35		
Subgrade	Modulus (Psi)	$2.0 imes10^4$		
	Poisson Ratio	0.4		
Slab Dimension (ft	.)	20 imes 20		
Loading Angle θ_g		<i>Uniform</i> (5, 85)		
Loading Position X	K	<i>Triangular</i> (0.47, 0.85, 1)		
Loading Position Y	7	<i>Triangular</i> (0, 0.4, 0.5)		
Temperature Gradi	ent (°F/in.)	<i>Normal</i> $(0, 0.65^2)$		
Thermal Coefficier	nt (1/°F)	$5.1 imes 10^{-6}$		
Equivalent Joint St	iffness (Psi/in)	$1.0 imes 10^5$		
Concrete Strength	(Psi)	650		
PCC Cost (6") (\$/\$	Sq. Yd.)	Uniform (55, 80)		
Base Layer Cost (6	5") (\$/Sq. Yd.)	Uniform (20, 30)		
Subbase layer Cost	t (6") (\$/Sq. Yd.)	Uniform (9.5, 14.5)		

Table 3.1: Input values of Case study

The costs used for this case study were those for designing an airport in Des Moines, Iowa. Table 3.1 describes the parameters of the model along with the values used in the case study.

Based on the probabilistic distributions of uncertain parameters, 10,000 samples (sufficient for pavement design (Timm and Newcomb, 2006)) are generated using Monte Carlo simulation. Samples generated by the Monte Carlo simulation are then entered into the ANN models to estimate the critical stress in the PCC slab.

The distribution of *TCDF* is estimated from 10,000 simulations of the inputs. If the design variables generated by algorithm 6 ensure that the reliability constraint is met, the expected cost would be recorded for that design (Eq. (3.6)), and this process is iterated until the optimization termination criteria has been met.

Table 3.2 shows the optimal design for different design life and reliability levels. For lives of 20, 25, and 30 years, a higher level of reliability is associated with thicker concrete pavement structure and consequent

higher expected cost. For example, for a 20-year design life and 50% reliability, the total thickness is 38.3 in, while for 95% reliability it is 49.4 in., reflecting a 25% increase in the expected design cost. Figure 3.4 illustrates the rising trend in expected cost when the design life increases from 20 to 30 years and the reliability level increases from 50% to 95%.

Design		Т	hicknes	Expected		
Life	Reliability	Slab	Base	Subbase	Cost	
	0.50	15.8	16.5	6.0	\$11,446	
	0.80	15.5	21.9	6.0	\$12,310	
20	0.90	15.2	24.6	6.0	\$12,642	
	0.95	13.4	30.0	6.0	\$12,784	
25	0.50	15.9	16.2	6.0	\$11,479	
	0.80	15.4	22.2	6.0	\$12,335	
	0.90	14.6	26.7	6.0	\$12,742	
	0.95	13.6	30.0	6.0	\$12,853	
30	0.50	15.9	16.7	6.0	\$11,565	
	0.80	14.9	24.1	6.0	\$12,422	
	0.90	15.2	25.1	6.0	\$12,765	
	0.95	13.7	30.0	6.0	\$12,951	

Table 3.2: Optimal thicknesses for different design lives and reliability levels

Figure 3.5 shows the TCDF distribution (for 10,000 different combinations of inputs) of the optimal designs for a 20-year design life at various reliability levels. For example, the 0.95-reliability plot implies that, for 10,000 simulations, 9,500 of the designs meet the reliability constraint (TCDF <= 1.05). The pavement structures with the calculated optimum thicknesses withstand applied traffic and environmental loading during a 20-year design life without reaching the maximum fatigue damage level caused by the loading.

Figure 3.6 shows the distribution of the cost for the optimal design of the concrete pavement for 95% reliability and design life of 20 years. The figure shows that there is approximately a 90% probability that the design cost will be between \$10,951 and \$14,612 per 20×20 ft.² slab.



Figure 3.4: Expected cost variation for different reliability level and design life



Figure 3.5: The distribution of TCDF value for optimal design of 20 years design life.

3.3.1 Sensitivity Analysis

The sensitivity of the pavement thickness design to the PCC and subgrade elastic modulus variation will be demonstrated in this section. Although PCC and subgrade modulus were both considered constant, they are very effective in determining the responses and consequent design outcomes.

3.3.1.1 Sensitivity of total thickness to PCC flexural strength

Figure 3.7 is presented to illustrate the designed total thickness including PCC thickness (d_1) , base layer thickness (d_2) , and subbase layer thickness (d_3) for different PCC flexural strength values. In addition, Figure 3.7 displays the expected cost variation for various optimal design of SOARP obtained for different flexural strength. The figures show that increasing the strength of the PCC slab results in lower expected



Figure 3.6: Cost distribution of optimal design for reliability = 0.95 and design life = 20

cost and total thickness $(d_1 + d_2 + d_3)$ for the optimal designs. For example, increasing the flexural strength from 650 to 800 psi reduces the expected cost of a 20 × 20 ft slab from \$16,230 to \$11,760.



Figure 3.7: Sensitivity analysis for PCC slab elastic modulus

3.3.1.2 Sensitivity of PCC thickness to subgrade elastic modulus

Figure 3.8 displays the optimum PCC thickness variation for various subgrade modulus. Figure 3.8 shows that increasing the subgrade strength will decrease the optimum PCC thickness, leading to the conclusion that stronger subgrades can afford to have thinner PCC slabs on them to be protected from load-induced deterioration. Also Figure 3.8 shows decrease of the expected cost when subgrade elastic modulus increases. In this study, variation of the subgrade modulus directly affects on critical stress occurred in the PCC slab. Higher elastic modulus results in lower critical stress and consequently lower required thickness.



Figure 3.8: Sensitivity analysis for subgrade elastic modulus

3.3.2 Design with FAARFIELD vs SOARP

This section compares results from SOARP framework with those from the FAARFIELD design. FAARFIELD receives design inputs and determines the PCC slab thickness that results in CDF = 1 for a given design life and traffic mix. FAARFIELD considers the critical condition of edge loading when determining the PCC slab thickness. However, SOARP considers 10,000 scenarios for the uncertain parameters and considers them all in the process of optimizing the thickness leading to consideration of many critical or non-critical conditions either in simulation or optimization. The proposed design has considered all possible conditions that could possibly affect the pavement.

The SOARP method is used to calculate the optimal PCC slab, base, and subbase thickness for different levels of flexural strength of the PCC. These thickness values for the base and subbase layers are used in FAARFIELD to calculate the slab thickness while assuming the same traffic loading mix, layer properties, and design life. Figure 3.9 shows FAARFIELD's design for R = 700 psi and reliability = 50% for a given base and subbase thickness determined with SOARP. Figure 3.10 compares the slab thickness calculated by FAARFIELD to that found by SOARP when the flexural strength of the PCC slab is changed.

Figures 3.10a and 3.10b display the PCC thickness corresponding to reliabilities of 50% and 95%, respectively. For a reliability of 50%, FAARFIELD's designed PCC thicknesses is higher than those of SOARP's results except for R = 800. For a reliability of 95%, SOARP's optimal PCC thicknesses are higher than FAARFIELD's designed thicknesses. This suggests that if FAARFIELD's designed slab thickness is used in SOARP's framework the obtained reliability would likely be more than 50% and less than 95%.



Figure 3.9: FAARFIELD software.

For example, when FAARFIELD's designed thickness of $d_1 = 15.9$ ($d_2 = 19$ and $d_3 = 6$) is used in 10,000 simulations of the SOARP, nearly 63% of them resulted in *TCDF* <= 1.05, corresponding to reliability of 0.63 (see figure 3.10a). Also, when FAARFIELD's designed slab thickness of $d_1 = 11.5$ ($d_2 = 30$ and $d_3 = 21$) is used for SOARP simulation, 70% of the simulations resulted in *TCDF* <= 1.05 (reliability = 0.7) (see figure 3.10b). It is indicating that FAARFIELD either recommends a more expensive design when there is a 50% reliability or it recommends a design that does not achieve the 95% reliability. As the reliability increases, SOARP design tends to result in thicker PCC slabs than for FAARFIELD, and that the FAARFIELD's designed thickness very likely cannot withstand all of assumed conditions generated within the uncertain variables' ranges.

FAARFIELD does not include all the factors and uncertainty that SOARP considers. Also FAARFIELD does not optimize over all three design parameters, but SOARP optimizes all three design parameters. By using ANN response models along with the Bayesian simulation optimization, the proposed SOARP method attempts to overcome some of the limitations from which current design methods suffer.

3.4 Conclusions

This study describes the development of a comprehensive reliability-based simulation-optimization framework for finding the optimal design of airfield concrete pavement consisting of a nine-slab concrete pavement with base and subbase layers atop a subgrade. This study includes aircraft traffic consisting of a B747-8, a B787-8, an A340-500 opt, and an A340-600 opt. Thousands of scenarios were generated to simu-



Figure 3.10: Comparison of FAARFIELD results and the SOARP method given different flexural strength of the PCC

late real-world conditions for long-term usage of the assumed airfield. The design optimization was aimed at minimizing design cost while using a reliability constraint to keep pavement fatigue failure under an allowable amount. In this study ANNs were employed to replicate FEAFAA/NIKE3D-FAA pavement-response solution. Replicating critical stress responses associated with airfield rigid pavement cracking would significantly make the design process more efficient by reducing total iteration time for calculation of critical responses for each type of aircraft in mixed-aircraft traffic loading.

The design optimization framework was optimized for multiple values of design life (20, 25, and 30 years) and multiple reliability levels (0.5, 0.8, 0.9, and 0.95). The results show that the expected design cost and optimal total thickness produced by 10,000 simulations of the inputs increased while the reliability level and design life increased. For a 80% reliability level and a 20-year design life, the expected cost is \$12,310 per slab for a total thickness of 43.4, while for a 95% reliability level and 30-year design life, the total thickness is 49.7 in. It should be noted that by considering thousands of scenarios with uncertain inputs (e.g., loading position of the aircraft), and by estimating the critical stress level using ANN, the pavement structure with the calculated optimum thicknesses should withstand applied traffic and environmental loading during its design life without reaching the maximum fatigue damage level caused by the loading.

We also compared the optimal design found by SOARP with a FAARFIELD design that assumes default thicknesses for the base and subbase layers and then finds slab thickness using iteration, continuing the process until the CDF value becomes 1. In the SOARP framework, we first generated thousands of scenarios of pavement structure and loading conditions and calculated CDF values and an estimation of their distribution. By considering the uncertainty of inputs in CDF calculation, a designer can simulate possible potential critical conditions. The results show that SOARP either results in more reliable or less expensive pavement designs.

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CHAPTER 4. OPTIMIZING THE FLEXIBLE DESIGN OF HYBRID RENEWABLE ENERGY SYSTEMS

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Abstract

Engineered systems often operate in unstable environments, and new applications for engineered systems may arise in the future. Understanding the potential for new applications and different environments under which a system will operate is important in engineering design. The goal of this study is to optimize the design of a hybrid renewable energy system to deliver electricity under highly uncertain demand. This research explores designing the hybrid system while taking into account uncertainties over a long period of time (i.e., 20 years in this study). The objective is to minimize the expected discounted cost of the hybrid renewable energy system during the next 20 years. A design solution may also be flexible, which means that the design can be adapted or modified in the future to meet new scenarios. This paper incorporates flexibility into engineering design under long-range uncertainty when the objective function is evaluated via a Monte Carlo simulation. The value of flexibility is measured by comparing the cost without flexibility and cost with flexibility. The hybrid renewable energy system design is solved in order to satisfy demand for electricity in California from 2017-2036.

4.1 Introduction

Traditional engineering design assumes that customers and the public know what they want with a high degree of certainty and that requirements will not change over time. The new system will operate in a stable environment in which the regulations, technologies, demographics, and usage patterns will not change De Neufville and Scholtes (2011). However, a design may not be successful in the future because the operating conditions or demand for a product may change. For example, an automobile company may design and manufacture cars based on the current fuel price without considering the long-term uncertainty

in the fuel price Kang et al. (2016). The demand for this company's products may decrease in the future if its cars are not fuel efficient. Many engineered systems and products may also be used in ways that were not originally intended by the designers. For example, the Global Positioning System (GPS) was originally developed for military use, but a countless number of commercial devices rely on the GPS today. The developers failed to design the original GPS with the capability to extend to these non-military uses De Neufville and Scholtes (2011).

Since engineered systems constantly face changes and unpredictability in their environments, these systems should be designed with the capability to respond to future changes Saleh et al. (2003). Flexibility in design enables the designers to review the initial design in the future and provides them with the option to take actions to review and modify the system. Designers should take into account the future uncertainties in the initial design of the system, and they should consider designing engineered systems that are flexible to the future conditions. Abandoning the system permanently or expanding the capacity to handle more demand in the future are examples of flexibility in engineering design Cardin (2014). Studies show that a flexible design can reduce the costs of design by 10-30% in comparison to the standard design Cardin et al. (2015).

A flexible design usually gives designers or the firm the ability to easily modify the design in order to respond to changing circumstances such as increasing or decreasing demand Saleh et al. (2003). In recent years, flexibility has been considered in a number of fields from architecture to software design MacKinnon (1968); Fox and Yeh (2000); Amram et al. (1998); Raouf and Ben-Daya (1995); Highsmith (2013). Engineering system design can be viewed as a decision-making process, but complexity and uncertainty makes decision making for systems design challenging Zhang et al. (2011). Designers need to understand the costs and benefits of designing a flexible system (or, the value of flexibility) in order to determine if they should pursue a flexible design.

Determining the value of flexibility presents challenges for complex engineered systems. Since an engineered system can face various types of uncertainties during the life cycle of the system, the designers may want to consider multiple strategies for flexibility Cardin et al. (2017). Real options analysis (ROA) incorporates flexibility into the design and deals with future uncertainty by borrowing concepts from options

analysis in investment science. Shi and Min (2014) analyze an ROA model for product remanufacturing and derive the remanufacturing cost threshold at which the remanufacturing option should be exercised. The ROA approach facilitates the process of assessing the value of flexibility of investments in physical assets under uncertainty, based on financial options theory Mun (2002). One challenge of ROA is that its assumptions often rely on financial markets rather than on engineered systems.

Generally, methods for ROA in design can be divided into three categories: analytical methods (e.g., Black-Scholes model), the binomial lattice model, and Monte Carlo simulation. The Black-Scholes model is a continuous time Markov chain model in which the states and the time are assumed to be continuous. The binomial lattice model is a discrete time Markov chain in which both time and states are discrete. Ajak and Topal (2015) apply ROA in design and decision making at the mine operational level. The real options problem is solved using the binomial lattice model and applying decision tree analysis. Kucuksayacigil and Min (2018) develop an ROA framework that calculates the valuation for a transmission option to expand the network while modeling demand as a geometric Brownian motion process. Binder et al. (2017) apply ROA in the design of energy systems. They measure the value of flexibility with a simple decision rule of comparing the expected utility of net present value of the flexible and inflexible designs. A Monte Carlo simulation method draws random numbers from probability distributions of uncertain parameters and creates different scenarios using the random numbers to compute the objective function. Fletcher et al. (2017) classify multiple uncertainty sources to evaluate flexible design. They use Monte Carlo simulation to evaluate multiple flexible designs in building a water infrastructure in Melbourne, Australia.

Cardin et al. (2017) develop a multistage stochastic model to incorporate flexibility (i.e., capacity expansion) into engineering system design. The goal is to select the appropriate capacity expansion strategy to maximize the expected total profit. Decision rules which are based on heuristic-triggering mechanisms determine when it is appropriate to exercise the flexibility. Their approach generates only 40 sample paths from the total set of uncertain scenarios to include in the optimization problem. Hu et al. (2018) propose an approach to design a flexible waste-to-energy system based on decision rules and a differential evolution algorithm. The objective of their paper is to find the optimal decisions (i.e., capacity expansion) that maximize the discounted expected profit of the system under uncertainty. Their meta-heuristic optimization

method can find approximate solutions for the capacity expansion problem. Hu and Cardin (2015) propose a methodology to identify opportunities to embed flexibility for the waste-to-energy system. A Bayesian network is used to model complex interdependencies between the system elements and infer the probability distributions of unobserved uncertain parameters. A Monte Carlo simulation is used to estimate the net present value of the system for the design with and without flexibility. The value of flexibility is calculated based on the difference between the net present values. These papers Cardin et al. (2017); Hu et al. (2018); Hu and Cardin (2015) assume that the model can be easily evaluated for any input decision. This assumption does not work for cases where the objective function is estimated with a complex simulation in which it is not computationally efficient to evaluate the model output for multiple inputs.

The method outlined in this paper differs from the previous literature because our method simulates thousands of scenarios with all of the uncertain parameters to identify the optimal engineering system design. Traditional stochastic programming approaches for flexibility only consider a limited number of scenarios within their optimization algorithm. The flexible design algorithm in this paper classifies the scenarios into different categories which allows the optimization algorithm to consider thousands of scenarios without being subject to the curse of dimensionality.

Engineering system design may require optimizing high-dimensional, computationally expensive objective functions under long-range uncertainties. Two examples include the wing design of a high-speed aircraft in the aerospace industry Koch et al. (1999) and the crash worthiness design in the automotive industry Gu (2001). Designing with many parameters involves optimizing an objective function in high-dimensional space. The evaluation of the objective function often requires the use of a computationally expensive simulation model. High-dimensional design problems typically have discrete and continuous variables, and there is often uncertainty around these problems. Monte Carlo simulation is often used to explore the design output given design parameters and while considering the uncertainty.

Engineered systems, especially large-scale infrastructure, may operate for long time. Thus, a decisionmaking framework is needed to incorporate both long-range uncertainties and the computationally expensive simulations. This paper optimizes the design of a hybrid renewable energy system (HRES) when the objective function is evaluated using Monte Carlo simulation that incorporates uncertainties over a long period of time (i.e., a 20-year lifespan in this study). Two models are developed to optimize the system design. The first model uses a simulation optimization algorithm that considers 10,000 possible future scenarios, and the design variables are selected that minimize the expected discounted cost. In this model, the initial design of the HRES will be fixed and unchanged during the planning horizon. The second model is a design with flexibility model to allow the decision makers to review the initial design in the future and modify the design depending on the realization of the uncertainty.

The uniqueness of this paper is that it measures the value of flexibility in complex engineered systems that require using computationally expensive simulations to evaluate the objective function, and the paper develops a model to optimize the design of such systems under highly uncertain parameters. Our study is the first to use simulation optimization to identify a flexible design for an HRES. In this study, a multi-stage flexibility algorithm is proposed to find the optimal capacity expansion for the components of the HRES over a 20-year planning horizon. The mathematical model is modified to identify the flexible design by considering multiple stages of decision making to minimize the expected cost of design. The optimization algorithm measures the value of flexibility by comparing the value of design with flexibility to the value of design without flexibility. A new algorithm is presented that finds the optimal capacity expansion amount to respond to future uncertainties relating to complex engineered systems.

The rest of the paper is organized as follows. In section 5.3, the decision-making framework—to include the structure of the HRES, the model for flexibility, and the simulation optimization routine—is discussed in detail. Section 4.3 applies the proposed flexibility algorithm and the simulation optimization method to a real-world case study. Finally, section 4.4 provides concluding remarks and directions for further research.

4.2 Decision-Making Framework

4.2.1 Hybrid Renewable Energy Systems

The environmental effects of fossil fuel are encouraging greater usage of renewable energy to meet rising energy demand. The high cost of renewable energy technologies is one of the main challenges to greater use of renewable energy sources. To overcome these challenges, renewable energy sources can be integrated to meet the energy demand of a given area. There are different types of HRES such as biomass-wind-fuel cell, photovoltaic-wind-battery, and photovoltaic-wind-battery-fuel cell Deshmukh and Deshmukh (2008). The HRES that we consider consists of photovoltaic (solar panel), wind turbine, battery, electrolyzer, hydrogen tank, and fuel cell.

The mathematical model for the HRES comes from Kaviani et al. (2009); Sharafi and ELMekkawy (2014); Khalilnejad et al. (2018). For instance, Kaviani et al. (2009) optimize the design of HRES without considering the uncertainty of wind speed, solar irradiation, and demand. Kaviani et al. (2009) state that incorporating the uncertainty of these parameters in the HRES model requires the use of "computationally intensive and time consuming algorithms like Monte Carlo simulations." In those studies, the initial design of the system is fixed during the long-term planning horizon and cannot be changed in the future. This assumption makes their models less applicable to an unpredictable and changing future. Incorporating the flexible design in which the initial design of the HRES can be modified in the future and modeling complex uncertainties represent an important advancement in understanding how to best design renewable energy systems.

The solar panel and wind turbine work to generate electricity to satisfy demand. If the generation from solar and wind exceeds demand, then the surplus amount is stored in the battery for the future. If the battery's capacity is exceeded, any excess energy is converted to hydrogen by the electrolyzer and stored in the hydrogen tank. The fuel cell can convert the hydrogen to electricity. The battery and fuel cell will be utilized if the solar and wind generation fail to satisfy demand in a given period. If the wind, solar, and battery sources of energy cannot fulfill demand, the fuel cell can convert the stored hydrogen to electricity. Energy storage systems (i.e., the battery and hydrogen tank) are included in the model to overcome the mismatch between the electricity demand and supply Sadati et al. (2015). If the combination of all of these sources cannot satisfy demand, diesel fuel can be used to meet the remaining demand. Figure 4.1 depicts the energy flow inside the HRES.



Figure 4.1: The energy flow of hybrid renewable energy system

4.2.1.1 Solar Panel

The solar photovoltaic (PV) panel is a device that converts the solar irradiation into electricity using solar cells. It can play an important role in generating energy in regions that receive a large amount of sunlight. The hourly output power of the PV panel E_t^{pv} is calculated as:

$$E_t^{pv} = \eta^{pv} \cdot SI_t \cdot A^{pv} \tag{4.1}$$

where η^{pv} is the efficiency of the PV panel, SI_t indicates the solar irradiation on the surface of the panel at time *t*, and A^{pv} represents the area of the solar panel.

4.2.1.2 Wind Turbine

Wind turbines convert kinetic energy from the wind into the electrical energy. The output power of the wind turbine E^{wg} is calculated as:

$$E_{t}^{wg} = \begin{cases} 0.5C_{p}\rho A^{wg}u_{t}^{3}, & \text{if } u_{c} < u < u_{r} \\ 0.5C_{p}\rho A^{wg}u_{r}^{3}, & \text{if } u_{r} < u < u_{f} \\ 0, & \text{otherwise} \end{cases}$$
(4.2)

where C_p is the power coefficient, ρ is the air density, and A^{wg} is the area of the rotor, u, u_c , u_r , and u_f are the wind velocity, cut-in wind velocity, the rated wind velocity, and the cut-off wind speed, respectively Dufo-López and Bernal-Agustín (2008).

4.2.1.3 Battery

If the total amount of wind and solar power exceeds demand, then the battery will be charged. Otherwise, the battery is discharged to fulfill the unmet demand. The battery state of charge at time $t S_t^{bat}$ is:

$$S_t^{bat} = \begin{cases} S_{t-1}^{bat} - \eta_{bat}^d \times D_t^{bat} / cap_{bat}, & \text{if } D_t > E_t^{wg} + E_t^{pv} \\ \\ S_t^{bat} - \eta_{bat}^c \times E_t^{bat} / cap_{bat}, & \text{if } D_t < E_t^{wg} + E_t^{pv} \end{cases}$$

$$(4.3)$$

where η_{bat}^c represents the efficiency of the battery if it is charging, η_{bat}^d when it is discharging, and cap_{bat} depicts the capacity of the battery. The battery is charging when the amount of electricity generated from solar panels and wind turbines is greater than the demand at that period. Otherwise, the battery will be discharged. $E_t^{bat}(D_t^{bat})$ is the amount of energy that goes into (out of) the battery at time *t*. The battery can be charged until it reaches S_{max}^{bat} , and it can be discharged until it reaches S_{min}^{bat} . Thus, $S_t^{bat} < S_t^{bat} < S_{max}^{bat}$.

4.2.1.4 Electrolyzer

The electrolyzer converts electricity into hydrogen Khalilnejad et al. (2018). It is directly connected to the hydrogen tank. When the battery is full and a surplus amount of electricity generated by wind and solar exists, the electrolyzer converts the surplus electricity to hydrogen. The amount of energy generated by the

electrolyzer to be stored in the hydrogen tank E_{el} is calculated as:

$$E_{t}^{el} = \begin{cases} \eta^{el} (E_{t}^{wg} + E_{t}^{pv} + E_{t}^{bat} - D_{t}), & \text{if } D_{t} > E_{t}^{wg} + E_{t}^{pv} + E_{t}^{bat} \\ & \& S_{t}^{bat} = S_{max}^{bat} \\ 0, & otherwise \end{cases}$$
(4.4)

where η^{el} is the electrolyzer's efficiency in converting electricity to hydrogen. D_t is the demand for the electricity at time *t*.

4.2.1.5 Hydrogen Tank

The hydrogen tank stores the energy produced by electrolyzer. The amount of energy in the hydrogen tank increases when the electrolyzer supplies the hydrogen tank with hydrogen, and the amount of energy in the tank decreases when the fuel cell consumes energy. The amount of energy in the tank at time $t E_t^{tank}$ is:

$$E_t^{tank} = E_{t-1}^{tank} + E_t^{el} - E_t^{fc}$$
(4.5)

where E_t^{fc} is the amount of energy generated by the fuel cell at time t.

4.2.1.6 Fuel Cell

The fuel cell is a device that converts chemical energy into electricity. It can be used as a source of energy to generate electricity. The amount of electricity or energy generated by the fuel cell E_t^{fc} is:

$$E_{t}^{fc} = \begin{cases} \eta^{fc} \min[D_{t} - (E_{t}^{wg} + E_{t}^{pv} + E_{t}^{bat}), & \text{if } D_{t} < E_{t}^{wg} + E_{t}^{pv} \\ \eta^{tank} E_{t}^{tank})] & + E_{t}^{bat} \& S_{t}^{bat} = S_{min}^{bat} \\ 0, & otherwise \end{cases}$$
(4.6)

where η^{fc} and η^{tank} are the efficiencies of the fuel cell and hydrogen tank, respectively. The fuel cell is utilized when the demand for electricity is greater than the total amount of energy generated by solar panel, wind turbine, and battery and the battery is fully discharged.

4.2.1.7 Diesel Generator

The diesel generator is used as the emergency source of power to satisfy any demand that cannot be met by the renewable sources. The amount of energy needed by the diesel generator at time $t E_t^{ds}$ is calculated as:

$$E_{t}^{ds} = \begin{cases} \frac{1}{\eta^{ds}} [D_{t} - (E_{t}^{wg} + E_{t}^{pv} + E_{t}^{pv} + E_{t}^{bat} + E_{t}^{fc})], & \text{if } D_{t} > (E_{t}^{wg} + E_{t}^{pv} + E_{t}^{bat} + E_{t}^{fc}) \\ 0, & \text{otherwise} \end{cases}$$
(4.7)

where η^{ds} is the efficiency of the diesel generator.

4.2.2 Cost model of HRES

The objective is to minimize the discounted life-cycle cost of the HRES. The cost function consists of four parts: investment, operations and maintenance, replacement, and diesel fuel costs. The total cost of the HRES depends on the size or capacity of each component (i.e., the decision variables). The investment cost *INV* occurs at the beginning of system operation. The operations and maintenance cost *OP* occurs in each period during the system's life cycle. Since the system needs to be maintained properly, replacement costs *REP* occurs when any of the components of the HRES requires replacement. The diesel fuel costs *FC* represents the cost of purchasing diesel fuel to satisfy demand. If the total amount of supply by HRES at period *t* is less than the demand, then the shortage amount will be fulfilled by purchasing diesel from the market. The model ignores the power transmission cost between system components and also from the supply to the demand location. The model is a simplified version of the real HRES system where there should be multiple system components at different locations.

The parameters c_i^{inv} , c_i^{om} , and c_i^{rep} are the investment, operations and maintenance, and replacement costs for the *i*th design component. The I = 6 design components of the HRES are: the PV panel, the wind turbine, the battery, the electrolyzer, the hydrogen tank, and the fuel cell. Each component has an energy capacity cap_i . The number of times the *i*th component will be replaced is R_i . L_i is lifetime of component *i*. The planning-time horizon has *T* total periods, and λ represents the interest rate. The parameter c_{ds} is the diesel cost. Eqs. (4.8-4.12) provide the formula for calculating the life-cycle cost and its four cost components. Eq. (4.8) shows the total cost of the system when operating for the *T* periods. Eq. (4.9) shows the investment cost. Eq. (4.10) displays the annual cost of operations and maintenance which is converted to the present value. Eq. (4.11) shows the present value of the cost to replace the system's components at the end of their lifetime. Eq. (4.12) calculates the present value of the fuel cost when the renewable energy sources cannot fulfill demand.

$$cost = INV + OP + REP + FC \tag{4.8}$$

$$INV = \sum_{i=1}^{I} c_i^{inv} cap_i \tag{4.9}$$

$$OP = \sum_{i=1}^{I} c_i^{om} \frac{(1+\lambda)^T - 1}{\lambda (1+\lambda)^T} cap_i$$
(4.10)

$$REP = \sum_{i=1}^{I} \sum_{r=1}^{R_i} c_i^{rep} \frac{1}{(1+\lambda)^{L_i \times r}} cap_i$$
(4.11)

$$FC = c_{ds} \sum_{t=1}^{T} \frac{1}{(1+\lambda)^t} E_{ds,t}$$
(4.12)

Complexity and dynamics inside the hybrid renewable energy system require the use of Monte Carlo simulation to calculate the cost function. Monte Carlo simulation is used to propagate the parameter uncertainties to the uncertainty in the life-cycle cost. The expected cost of design is calculated as the average after *N* different simulations.

The decision variables for designing the HRES are the capacity of each component, cap_i . The energy generated by each component at time t, E_t^{pv} , E_t^{wg} , E_t^{bat} , E_t^{el} , E_t^{tank} , and E_t^{fc} , must not exceed the chosen capacity for each component cap_i . Each component also has a maximum capacity, cap_i^{max} , so that

$$E_t^i \le cap_i \ \forall i = 1, \dots, I, \ t = 1, \dots, T$$
 (4.13)

and

$$0 \le cap_i \le cap_i^{max} \ \forall i = 1, \dots, I \tag{4.14}$$

where E_t^i represents the energy generated by component *i* at time *t*.

The design decision maker should choose to minimize the expected discounted life-cycle cost of the HRES by choosing the capacity of each component and ensuring the constraints in Eqs. (4.13) and (4.14) be satisfied.

4.2.3 Flexibility Modeling

A flexible design may differ from an optimal design because the optimal design will be optimal for a probability-weighted combination of scenarios and the flexible design will allow for different designs, each of which depends on the realization of individual scenarios. In the design without flexibility, the decision maker would design the HRES based on all of the future demand and cost simulations from the current time to the end of planning horizon. However, in the design with flexibility, the designers have the option to modify the design and decide whether or not to expand the capacities of the HRES if it is needed to generate more electricity to meet increasing future demand.

Many articles have studied capacity expansion problem Wu et al. (2005); Smith (1979); Prueitt and Park (1997); Philip and Liittschwager (1979); Karsak and ÖZOGUL (2002); Berretta and Mobasheri (1972); Ammons and McGinnis (1985); Wang et al. (2009); Khodaei et al. (2010); Hajipour et al. (2015); Gil et al. (2014); Cardin et al. (2017); Hu et al. (2018); Hu and Cardin (2015). For example, Wang et al. (2009) use game theory and bi-level optimization to find amount to capacity expansion amount under an incomplete information for the competitors in the energy market. Khodaei et al. (2010) develop a mixed-integer linear programming optimization model to solve the capacity expansion problem. Hajipour et al. (2015) develop a stochastic program based on a Monte Carlo approach to find the optimal capacity for the components of the Microgrid system with wind farms and energy storage. Gil et al. (2014) apply mixed-integer linear programming optimization model to solve the capacity expansion problem with one source of uncertainty. Cardin et al. (2017), Hu et al. (2018), and Hu and Cardin (2015) study how to find the flexible design by expanding the capacity of the waste-to-energy system.

The procedure of design for flexibility when the objective function should be evaluated with the computationally expensive simulations cannot be done rolling back from the end of simulation and exercising the options at each period of time. In this case, the model should be optimized for each of N simulations, which is usually large (10,000 simulations or more), and for each period in the planning time horizon, T. Solving the optimization model will suffer from the curse of dimensionality. In the proposed algorithm for design for flexibility (see algorithm 5), we discretize the continuous HRES problem and consider a multi-stage decision making process for flexible design. The decision maker has the option to expand the capacity of each component during each review of system. For example, the decision to expand the capacity of each component of the HRES could occur every 5 years.

The proposed algorithm starts by optimizing the model (i.e., Eqs. (4.1-4.14)) during the first T_1 periods (e.g., $T_1 = 10$ years) by taking into account all of the *N* future scenarios from time 0 to T_1 (lines 2-4 in algorithm 5). The initial optimal design will be used as an input into the design modification stages. At time T_1 , the first decision for the capacity expansion will be made. The future scenarios from the first design modification period to the next review of the system (periods T_1 to T_2) are divided into K_2 different categorized into low, medium, and high demand during periods T_1 to T_2 . Given the initial optimal design, the algorithm optimizes the additional capacity by minimizing the expected cost for each of the K_2 categories from T_1 to T_2 . At the end of stage 2, there will be K_2 different designs and expected costs (lines 5-10).

At stage 3, given the initial optimal design and each of the K_2 different additional categories, the expected cost will be minimized by optimizing Eqs. (4.1-4.14). The future scenarios from the second design modification period to the next review of the system (periods T_2 to T_3) are divided into K_3 different categories (e.g., low, medium, and high demand). Given the initial optimal design and each optimal expansion amounts of stage 2, the algorithm optimizes the additional capacities by minimizing the expected cost for each of the K_3 categories from periods T_2 to T_3 . In stage 3, there will be K_2K_3 different additional capacities. There will be K_3 optimal additional capacities for each of K_2 expansion amounts at stage 2 (lines 11-19). This process will continue *S* times where *S* is the number of modification stages.

At stage S + 1, given the initial optimal design and all additional capacities in the previous *S* design stages, the expected cost will be minimized by optimizing Eqs. (4.1-4.14). The demand from stage S + 1 of the design modification period to the end of planning horizon is divided into K_{S+1} different regions. Given the initial optimal design and each of the optimal expansion amounts of all previous *S* stages, the algorithm optimizes the additional capacities by minimizing the expected cost for each of the K_{S+1} categories from T_S to *T*. In stage S + 1, there will be $\prod_{s=1}^{S} K_{s+1}$ optimal additional capacities for each K_{S+1} expansion amounts at stage S + 1 (lines 21-31 of algorithm 5). At each decision-making stage, the capacities of the components can be increased to fulfill demand for the upcoming planning periods.

Algorithm 5 Multi-stage flexibility modeling

- 1: Inputs: N future scenarios of demand for t = (0,T), S number of design stages where each design stage occurs at discrete times $0, T_1, T_2, \ldots, T$.
- 2: Stage 1
- 3: Solve Eqs. (4.1-4.14) and find optimal design for N scenarios from $t = (0:T_1)$
- 4: Outputs: $E[cost^1]$ and cap¹
- 5: *Stage 2*
- 6: Inputs: N future demand scenarios from time T_1 to T_2 described as $D^{T_1:T_2}$ and cap¹
- 7: for $k_2 \leftarrow 1$ to K_2 do
- 8: Solve Eqs. (4.1-4.14) and find the optimal additional capacity $|D = {}^*D_{k_2}^{T_1:T_2}$
- 9: end for
- 10: Outputs: K_2 different $E[cost^{1,k_2}]$ and cap^{1,k_2}
- 11: Stage 3
- 12: Inputs: N future demand scenarios from time T_2 to T_3 described as $D^{T_2:T_3}$, cap¹, and K_2 different cap^{1,k₂}
- 13: **for** $k_3 \leftarrow 1$ to K_3 **do**
- 14: **for** $k_2 \leftarrow 1$ to K_2 **do**
- 15: Solve Eqs. (4.1-4.14) and find optimal additional capacity $|D = D_{k_3}^{T_2:T_3}$
- 16: **end for**
- 17: end for
- 18: Outputs: K_2K_3 different $E[cost^{1,k_2,k_3}]$ and **cap**^{1,k_2,k_3}
- 19: *Stage S+1*
- 20: Inputs: *N* future demand scenarios from time T_S to *T* described as $D^{T_S:T}$, **cap**¹, K_2 different **cap**^{1,k2}, K_2K_3 different **cap**^{1,k2,k3}, ..., $K_2K_3...K_S$ different **cap**^{1,k2,k3}, ..., K_3K_3 , K_3K_3 ,
- 21: for $k_{s+1} \leftarrow 1$ to K_{S+1} do
- 22: **for** $k_s \leftarrow 1$ to K_s **do**
- 23: ••.
- 24: **for** $k_2 \leftarrow 1$ to K_2 **do**
- 25: Solve Eqs. (4.1-4.14) and find optimal additional capacity $|D = D_{k_r}^{T_s \cdot T}$
- 26: end for
- 27: **end for**
- 28: end for
- 29: Outputs: $\prod_{n=1}^{S} K_{s+1}$ different $E[cost^{1,k_2,k_3,...,k_{S+1}}]$ and **cap**^{1,k_2,k_3,...,k_{S+1}}
- 30: ${}^{*}D_{k_{2}}^{T_{1}:T_{2}}$ is demand (D) from T_{1} to T_{2} in which the value of D at time T_{1} is within the region k_{2}

The total expected cost of the flexible design *ECF* is the sum of the initial expected cost $E[cost^1]$ and average capacity expansion costs from stage 1 to stage S + 1, which are discounted by the interest rate λ . Since the number of different decisions to expand capacities in stage *s* is $\prod_{s'=1}^{s} K_{s'+1}$, the expected cost in stage *s* for category $k_s = 1, \ldots, K_s$ is denoted as $E[cost^{1,k_2,k_3,\ldots,k_s}]$. The total expected cost of flexible design is shown in Eq. (4.15). Eq. (4.15) assumes that each of the k_s categories in design stage *s* occurs with equal probability. If one category is more likely than another category, Eq. (4.15) can be modified to include the specific probability of each category.

$$ECF = E[cost^{1}] + \frac{1}{K_{2}} \frac{1}{(1+\lambda)^{T_{1}}} \sum_{k_{2}=1}^{K_{2}} E[cost^{1,k_{2}}] + \frac{1}{K_{2}K_{3}} \frac{1}{(1+\lambda)^{T_{2}}} \sum_{k_{2}=1}^{K_{2}} \sum_{k_{3}=1}^{K_{3}} E[cost^{1,k_{2},k_{3}}] + \dots + \frac{1}{\prod_{s=1}^{S} K_{s+1}} \frac{1}{(1+\lambda)^{T_{s}}} \sum_{k_{2}=1}^{K_{2}} \sum_{k_{3}=1}^{K_{3}} \dots \sum_{k_{s+1}=1}^{K_{s+1}} E[cost^{1,k_{2},\dots,k_{s+1}}]$$
(4.15)

The proposed algorithm for flexibility is able to find the flexible design for an arbitrary number of categories. However, increasing the number of categories and design stages may make solving the decision impractical. A four-stage problem with 10 categories at each stage requires solving 1+10+100+1000 = 1111 optimization problems. However, a four-stage problem with three categories only requires solving 1+3+9+27 = 40 optimization problems, which is much more practical to solve.

4.2.4 Optimization Algorithm

Black-box functions (e.g., f) provide system output for specified values of system inputs, and there typically exists little information about the properties of f. The optimization of a black-box system is referred to as black-box optimization. Black-box optimization algorithms optimize the objective function fthrough a query of the value of f(x) for a point x, but they cannot make any assumptions on the analytic form of f Chen et al. (2018).

Bayesian optimization is a method to utilize the input-output relationship of the black-box systems. Many design decisions are evaluated using complex simulation models, and having tools that can optimize the design using such simulations is important for many practical engineering problems. To optimize such models, the key challenge is that the designer has little knowledge about how the objective function changes with respect to changes in the design decision variables. Such difficulty makes many traditional algorithms that require either first-order (i.e., gradient) or second-order (i.e., Hessian) information invalid. Bayesian optimization algorithms can effectively solve problems that seek to integrate optimization into simulation analysis Shahriari et al. (2016). Further details about Bayesian optimization is discussed in Martinez-Cantin (2014).

The decision variable $cap = [cap_{pv}, cap_{wg}, cap_{bat}, cap_{el}, cap_{tank}, cap_{fc}]$ is a vector composed of the capacities of all of the components of the HRES (i.e., solar panel, wind turbine, battery, electrolyzer, fuel tank, and fuel cell). The Bayesian optimization algorithm evaluates the objective function without using any first-order or second-order information. The algorithm constructs a surrogate model for the objective function and exploits the surrogate model to find the next evaluation points in the feasible solution space Lizotte (2008b). A surrogate model is used since the objective function cannot be directly calculated. The surrogate model helps us to estimate the black-box function by constructing an approximate model. The prior and acquisition functions are the two major ingredients of the Bayesian optimization algorithm. We choose the Gaussian process as the prior over the objective function depicted in Eq. (4.8) as it is a powerful prior distribution for functions Snoek et al. (2012). The objective function is approximated with a multivariate normal probability distribution function. The predictive distribution for the unobserved values of the objective function for the unobserved values of the objective function for the component of the surface
$$p(f^{new}|\mathbf{cap}^{new}, f(\mathbf{cap}_{1:n}), \mathbf{cap}_{1:n}) = N(f^*|\mu(\mathbf{cap}^*|\mathbf{cap}_{1:n}), \sigma^2(\mathbf{cap}^*|\mathbf{cap}_{1:n}))$$
(4.16)

$$\mu(\operatorname{cap}^*|\operatorname{cap}_{1:n}) = Cov(\operatorname{cap}^*, \operatorname{cap}_{1:n})Cov(\operatorname{cap}_{1:n}, \operatorname{cap}_{1:n})^{-1}f(\operatorname{cap}_{1:n})$$
(4.17)

$$\sigma^{2}(\mathbf{cap}^{*}|\mathbf{cap}_{1:n}) = Cov(\mathbf{cap}^{*},\mathbf{cap}^{*}) - Cov(\mathbf{cap}^{*},\mathbf{cap}_{1:n})Cov(\mathbf{cap}_{1:n},\mathbf{cap}_{1:n})^{-1}Cov(\mathbf{cap}^{*},\mathbf{cap}_{1:n})^{T} \quad (4.18)$$

where $cap_{1:n}$ is the *n* previously evaluated capacities used to predict the next point, $Cov(cap_{1:n}, cap_{1:n})$ is the covariance matrix for the *n* design alternatives that are simulated to estimate the objective function, $Cov(cap^*, cap_{1:n})$ is the covariance of the *n* design variables and the new capacity cap^* to be evaluated, $\mu(\mathbf{cap}^*|\mathbf{cap}_{1:n})$ is the posterior predictive mean, and $\sigma^2(\mathbf{cap}^*|\mathbf{cap}_{1:n})$ is the posterior predictive variance. The Gaussian radial basis function kernel is used to calculate the covariance between two capacities **cap** and **cap**':

$$Cov(\mathbf{cap}, \mathbf{cap}') = \exp\left(\frac{||\mathbf{cap} - \mathbf{cap}'||^2}{2\gamma^2}\right)$$
 (4.19)

where γ is a free parameter which will be tuned in the optimization. The current best capacity that results in the smallest expected cost based on *n* evaluated design alternatives is denoted as $\mathbf{cap}_{best} = \operatorname{argmin}_{\mathbf{cap}_{1:n}} f(\mathbf{cap}_{1:n})$. The objective function evaluation (i.e., expected discounted cost) corresponding to \mathbf{cap}_{best} is $f(\mathbf{cap}_{best})$. The next alternative to sample in the simulation is found by maximizing the acquisition function which is the expected improvement *EI* over the current best Mockus et al. (1978).

$$EI(\mathbf{cap}^*|\mathbf{cap}_{1:n}) = (\mu(\mathbf{cap}^*|\mathbf{cap}_{1:n}) - f(\mathbf{cap}_{best}))\Phi(Z) + \sigma(\mathbf{cap}^*|\mathbf{cap}_{1:n})\Phi(Z)$$
(4.20)

where $Z = \frac{\mu(\operatorname{cap}^*|\operatorname{cap}_{1:n}) - f(\operatorname{cap}_{best})}{\sigma(\operatorname{cap}^*|\operatorname{cap}_{1:n})}$ and $\Phi(\cdot)$ denotes the cumulative standard normal distribution function. Algorithm 6 shows a step by step procedure of the Bayesian optimization. We use the Random Embedding Bayesian Optimization (REMBO) developed Wang et al. (2013b) to implement the Bayesian optimization algorithm.

Algorithm 6 Implementation procedure of Bayesian optimization.

- 1: Choose an appropriate acquisition function and prior over the objective function
- 2: Find the posterior over the objective function given some observations
- 3: Use the posterior and an appropriate acquisition function to take the next evaluation points
- 4: Augment data points

4.3 Application

In this section, the design of HRES is optimized to deliver electricity for the state of California under highly uncertain demand. The planning horizon is 20 years (from 2017 to 2036) and each period is 1 month. It is assumed that the hourly solar irradiation is normally distributed with a mean of $0.5 \ kwh/m^2$ and a standard deviation of 0.1. The wind velocity is normally distributed with a mean of $5 \ m/h$ and standard deviation of 1. Random numbers from the distribution of the solar irradiation and wind speed are selected

Component	Lifetime (years)		c_i^{inv}			c_i^{rep}			c_i^{om}	
	low	mode	high	low	mode	high	low	mode	high	
Wind	10	25	30	5	7	9	5	6	7.5	20
Solar	10	20	25	1.5	2.5	3	1.2	2	2.5	75
Battery	1	5	7	1.5	2	2.2	1.3	1.5	2.1	20
Electrolyzer	5	10	13	1	2	3	0.9	1.5	2	25
Fuel Tank	10	20	25	0.8	1.3	1.5	0.8	1.2	1.3	15
Fuel Cell	0.7	1.7	2.7	1	3	4	1.9	2.5	3	172

Table 4.1: The cost (in millions of \$ per 1 MW) and lifetime parameters of the components of the HRES (Sharafi and ELMekkawy (2014))

and included in the simulation of the dynamics of the system. The interest rate, λ , is 2% per year. It is assumed that the efficiency of the PV panel is $\eta^{pv} = 0.15$. The power coefficient of wind turbine is $C_p = 0.59$, and air density is $\rho = 1.225$. The cut-in wind, rated wind velocities, and cut-off wind speed are $u_c = 3.5$ m/h, $u_r = 14$ m/h, $u_f = 25$ m/h, respectively. The application assumes that the maximum and minimum state of battery are $S_{max}^{bat} = 1$ and $S_{min}^{bat} = 0.2$. The efficiency of the electrolyzer, fuel cell, hydrogen tank, and diesel generator are $\eta^{el} = 0.6$, $\eta^{fc} = 0.6$, $\eta^{tank} = 0.95$ and $\eta^{ds} = 0.95$, respectively.

The investment and replacement cost parameters follow triangular distributions. Table 4.1 shows the investment, maintenance, and replacement cost parameters and the lifetime of the components for the HRES. The cost function parameters come from Sharafi and ELMekkawy (2014).

A simulation-optimization approach is used in order to find the optimal design for the HRES. As described in Section II, each component in the HRES has a relatively complicated dynamic, and calculating the system costs depends on several uncertainties including demand, solar irradiation, wind speed, and component costs and lifetimes. Thus, the HRES model is evaluated with a Monte Carlo simulation. The output of the simulation determines the objective function values that enter into the Bayesian optimization algorithm to identify the optimal design. The goal is to minimize the expected cost function that results from the interaction among the components of the HRES as both supply and demand fluctuate over a time span of 20 years. The Monte Carlo simulation enables the decision maker to analyze the stochastic behavior of the HRES.

4.3.1 Demand Forecast

Renewable energy systems are designed for long-term usage. Therefore, it is necessary to establish these sources of electricity generation considering possible future scenarios which will substantially impact the design. Uncertainty in the future demand will impact the design of the HRES, and forecasting demand is required for the control of power systems Taylor (2003). Good demand forecasting is an essential prerequisite of an energy system study for the capacity expansion planning. Since future demand will be uncertain, incorporating that uncertainty into the forecasting model will help the system manage load efficiently Akay and Atak (2007); Sadati et al. (2018). One of the goals of this paper is to investigate how the long-range demand uncertainty impacts the design of the HRES.

Demand for electricity is serially autocorrelated, which suggests that a time series model may be appropriate. We choose the Auto Regressive Integrated Moving Average (ARIMA) Arima (1976). ARIMA is a well-known model for time series analysis. In time series forecasting, the goal is to predict a series that typically is not deterministic but rather contains a random component. The ARIMA model is a linear combination of past observed data points (here demand for electricity) and errors to produce a forecast Yuan et al. (2017); De Felice et al. (2013). This method is widely used in the literature to forecast demand for electricity De Felice et al. (2013); Conejo et al. (2005); Jakaša et al. (2011); Zhou et al. (2006); Tan et al. (2010); Zhou et al. (2004); Che and Wang (2010). The general form of ARIMA(p,d,q) forecasts the future based on the following:

$$(1 - \sum_{i=1}^{p} \mathcal{O}_{i} \mathfrak{I}_{i})(1 - \mathfrak{I})^{d} D_{t} = (1 + \sum_{i=1}^{q} \theta_{i} \mathfrak{I}^{i}) \varepsilon_{t}$$

$$(4.21)$$

where *p* is the lag order, *d* is the degree of differencing, *q* is the order of the moving average, \Im is the lag operator, \wp is the autoregressive operator represented as a polynomial in the lag operator, and θ is the moving-average operator represented as a polynomial in the lag operator. The forecast variable D_t is the demand for electricity at time *t*, and ε_t is a normally distributed error with mean zero. The *arima* function in MATLAB software mat () is used to generate the ARIMA model for electricity demand using historical data of monthly electricity demand for California from 2001 to 2016 Administration ().



Figure 4.2: Simulation of electricity demand for California, 2017-2036

Since many different events could occur over 20 years that would have a large impact on electricity demand in California, we consider a large amount of uncertainty in the future electricity demand in California. The error term ε_t follows a Gaussian distribution with the mean of 0, and we assume a variance of 20,000.

Monte Carlo simulation is used to generate 10,000 simulated paths of demand by sampling from ε_t for t = 1, 2, ..., 240 months and applying the ARIMA model. Figure 4.2 shows the historical monthly demand and the generated scenarios for electricity demand for 20 years. For the first five years of planning (2017-2021), the simulated demand scenarios exhibit less uncertainty where 90% of the monthly demand is contained within the interval of [1.81, 2.15] million kwh. From 2021 to the end of the planning horizon (i.e., 2036), the uncertainty in demand accumulates which leads to a wide variety of demand paths in the future. Although the demand uncertainty is very large at the end of planning horizon, 90% of the monthly demand at the end of 2036 is contained within the interval of [1.67, 3.97] million kwh. Modeling the demand with large uncertainty that covers 20 years into the future enables designers to consider extreme demand scenarios, which may not be very likely but may still need to be considered in policy planning. Such a large uncertainty can help motivate the need for flexibility in capacity planning.

4.3.2 Design without flexibility

In the Monte Carlo simulation of the time series model, 10,000 scenarios are generated for modeling the demand for the next 20 years. The model is solved with 10,000 samples from uncertain parameters

Plant	Optimal Capacity (GW)	Percentage (%)
Solar panel	392	70
Wind turbine	146	/8
Battery	89	17
Electrolyzer	1041	-
Hydrogen tank	3221	-
Fuel cell	138	4
Diesel	-	>1

Table 4.2: The optimal design of the HRES for design without flexibility

(demand, cost coefficients, wind speed, and solar irradiation) for 240 months (2017-2036). The simulation optimization algorithm uses Eqs. (4.1-4.14) to identify the design alternative that minimizes the expected discounted cost. In design without flexibility, the system is designed at the beginning of the system operation in 2017 and will not be modified in the future.

Table 4.2 shows the optimal results for design without flexibility. The optimal capacities represent the nominal capacity of the components. The actual capacity of each component is the nominal capacity multiplied by the efficiency. For instance, the solar panel is built with 392 GW nominal capacity; however, the actual capacity is $0.15 \times 392 = 58.8$ GW.

The results show that 78% of the demand during the 10,000 simulations from 2017-2036 are fulfilled with solar and wind generation. These two components supply the majority of demand. Since the amount of energy generated by these two sources exceed the demand for many time periods, the surplus amount of energy will be conserved in the battery for future use. When the battery is full, the electrolyzer converts the energy into hydrogen, which is stored in the hydrogen tank and will be converted to electricity by the fuel cell. For instance, based on one of the 10,000 simulations (e.g., Figure 4.3a), the amount of energy generated by wind and solar almost always exceeds demand during the entire 20 years. There are a few instances in that simulation when solar and wind generation is low that energy from the battery is used.

The results show that the battery and fuel cell satisfy 17% and 4% of the demand, respectively. The HRES requires diesel to meet approximately 1% of the demand. The optimal design of the HRES fulfills more than 99% of the electricity with the renewable sources. The expected discounted cost of the design is \$40.66 trillion, which includes a \$9.56 trillion investment cost, \$21.66 trillion in operations and maintenance



(a) Demand fulfillment in simulation with (b) Demand fulfillment in simulation with(c) Demand fulfillment in simulation with constant demand decreasing demand

Figure 4.3: Demand fulfillment for three random demand scenarios

costs, \$9.4 trillion in replacement costs, \$40 billion in fuel costs. The large life-cycle cost is due to needing to build huge components for the HRES system. Fulfilling the total demand for electricity in the state of California with HRES requires a large amount of investment and maintenance cost. A study shows that tens of trillions of dollars are needed to achieve California's 80% greenhouse gas reduction target in 2050 by constructing renewable energy systems Yang et al. (2015).

Figures 4.3a, 4.3b, and 4.3c show three random simulations to illustrate how demand is fulfilled with different sources of energy in different simulations. In some cases (Figures 4.3a and 4.3c), the electricity generated by solar and wind exceeds the demand most of the time. The battery stores the surplus electricity and is used to satisfy demand a small proportion of the time in these two simulations. Figure 4.3b illustrates that in some scenarios solar and wind generation cannot fulfill the increasing demand in the future. Although the battery helps to satisfy some of the demand, most of the surplus energy generated from years 2017-2031 is stored in the hydrogen tank. The fuel cell converts the hydrogen to electricity and satisfies much of the shortfall in demand from 2031-2034. In 2035, the hydrogen tank is depleted and the fuel cell is unable to provide any more electricity. Diesel fuel is required it meet demand in 2035-2036.

To evaluate the effect of the number of simulation replications, the expected cost of the optimal design is calculated for different numbers of replications. The 95% confidence interval over the expected cost is [39.5, 41.0] for 100 replications, [40.0, 40.9] for 1000 replications, and [40.4, 40.8] for 10,000 replications. Ten thousand replications thus provides a narrower confidence interval within an appropriate computational time. Including more than 10,000 replications would drastically increase the computation time without reducing



Figure 4.4: Parallel coordinates plot for design without flexibility

the variation in the objective function. Ten thousand replications is sufficient to estimate the objective function in the Monte Carlo simulation.

Design decision making involves making trade-offs among many design variables and attributes. Determining how to make those trade-offs may be difficult in complex engineered systems Miller et al. (2014). Optimization helps the decision maker to find the optimal design that offers the best trade-off among all possible design alternatives. Each design alternative can lead to a different expected cost. To better visualize the trade space, parallel coordinate plots can show design alternatives with respect to different attributes and design variables Miller et al. (2014). The set of feasible alternatives from the objective space is projected on the parallel coordinate plot in Figure 4.4. The plot illustrates how the 50 different combinations of design variables impact the expected cost. The 50 combinations are the 50 best results of the optimization algorithm. It shows the sensitivity of the objective function to each decision variable. The optimal design is represented by the black line. The red line is the second best solution with an expected cost of \$46.25 trillion among those 50 best solutions in the model. This figure shows the complexity of the HRES model. If the value for each variable changes, a large difference in the expected cost may be seen. For instance, if the solar panel's capacity is 176 GW and the wind turbine's capacity is 312 GW, then more capacity is needed for the fuel cell (691 GW) with an expected cost of \$85.27 trillion.

4.3.3 Design with flexibility

The design with flexibility strategy requires a smaller initial investment than the design without flexibility. This strategy defers additional costs to the future and takes advantage of the time value of money Cardin (2014). A flexible design usually gives designers or the company the ability to easily modify the design in order to respond to changing circumstances. In this section, the value of flexibility will be measured by comparing the expected discounted cost of designing with flexibility and the expected discounted cost of designing without flexibility. Algorithm 5 identifies a flexible design alternative by factoring in the cost of modifying the design in the future.

4.3.3.1 Case 1: One stage flexibility modeling

Two different cases for the flexible design are developed. In the first case, one additional stage for the design modification is considered and S = 1 and $T_1 = 10$. In stage 1, the initial design and expected discounted cost considers the uncertain demand profiles for 2017-2026. The results of this first stage decision making show that the initial optimal design of the components of the HRES have less capacity compared to the optimal solution in the design without flexibility model (see Table 4.3).

The initial optimal design from 2017-2026 serves as an input to decision making in stage 2, which covers 2027-2036. The stage 2 decision making considers three different demand profiles (i.e., $K_2 = 3$). If demand in month 120, the last month in year 2026, is less than 2.02 million kwh, the demand is considered low. If demand in month 120 is greater than 2.02 million kwh and less than 2.27 million kwh, the demand is considered medium. If demand in month 120 is greater than 2.02 million kwh and less than 2.27 million kwh, the demand is considered high. Each of these demand profiles occur in 33% of the simulations. Given the initial optimal design, the Bayesian optimization determines if additional capacity for the HRES should be constructed if demand is low, if demand is medium, and if demand is high. Stage 2 contains three different sets of design variables and three different expected discounted costs, one for each demand profile. The average expansion costs are calculated as the expected cost of additional capacity at stage 2. The total expected cost of flexible design is calculated using Eq. (4.15).

Table 4.3 shows the optimal design for the HRES with flexibility with a possible design modification in 2027. Although the wind turbines should initially be constructed with a relatively small capacity in order to avoid unnecessary capacity during the first 10 years, the decision maker should expand the capacity of the wind turbines and the battery in the high or medium demand profiles. Since the wind turbines should be expanded, more battery capacity is needed to store the surplus amounts of energy. The results also show that in the low demand profile, the capacity of the HRES should not be expanded. Diesel should be purchased from the market to supply electricity if demand increases in years 2027-2036. Table 4.3 shows that the optimization algorithm chooses the solar panel with a higher initial capacity compared to the wind turbine; however, in the second stage, the algorithm finds that the wind turbine should be expanded and the solar panel should be operating for the next 10 years with the initial capacity.

The results show that the initial expected cost in stage 1 (\$20.55 trillion) is almost half of the expected cost of design without flexibility (\$40.66 trillion). However, this initial low capacity design will be expanded in the medium and high demand scenarios which increases the expected cost beyond just the stage 1 cost. The total expected cost of design with flexibility for case 1 is \$27.22 trillion. The design with flexibility enables the system to defer the additional cost of investment and replacement to the future, avoid the operation and maintenance cost of the full deployment for the first 10 years of operation, and take advantage of the time value of money. The value of flexibility is the difference between the expected cost of design with flexibility and the expected design without flexibility. In this case, the value of flexibility is \$13.44 = \$40.66 - \$27.22 trillion, a 33% percent reduction in cost.

4.3.3.2 Case 2: Two stage flexibility modeling

The second case assumes that the design can be modified twice, once in year 2027 and once in year 2032 ($T_1 = 10$, $T_2 = 15$). Similar to the first case, there are three different regions in each stage of the design modification (i.e., $K_2 = K_3 = 3$). Based on Algorithm 5, at stage 2, three models should be solved for 3 different ranges of demand for low, medium, and high demand profiles. The definitions of the demand profiles in 2027 are equivalent to those in case 1.
Component	Initial design (Cigo watt)	Stage 2			
Component	minital design (Olga watt)	High demand	Medium Demand	Low Demand	
Solar panel	263	0	0	0	
Wind turbine	31	128	98	0	
Battery	17	54	39	0	
Electrolyzer	230	0	0	0	
Hydrogen tank	616	0	0	0	
Fuel cell	68	0	0	0	
Expected Cost (\$ trillion)	20.55	12.22	7.63	7.08	
Total Cost (\$ trillion)	27.22				
Value of flexibility (\$ trillion)	13.44				

Table 4.3: The optimal design of the HRES with flexibility for the 1 stage case

The initial optimal design from 2017-2026 serves as an input to decision making in stage 2, which covers 2027-2031. Given the initial optimal design, the Bayesian optimization determines if additional capacity for the HRES should be constructed if demand is low, if demand is medium, and if demand is high. Stage 2 contains three different sets of design variables and three different expected discounted costs, one for each demand profile. The stage 3 decision making also considers low, medium, and high demand profiles. Low demand in month 180 is less than 2.20 million kwh, medium demand is between 2.20 and 2.63 million kwh, and high demand is greater than 2.63 million kwh.

The initial optimal design from 2017-2026 and optimal additional capacities for the three different demand profiles in stage 2 serve as the inputs to decision making in stage 3, which covers 2032-2036. Given the initial optimal design, the Bayesian optimization determines if additional capacity for the HRES should be constructed at 2032 for the following 9 scenarios: high demand in both stages 2 and 3, high demand at stage 3 and medium demand at stage 2, high demand at stage 3 and low demand at stage 2, medium demand at stage 3 and high demand at stage 2, medium demand in both stages 2 and 3, medium demand at stage 3 and low demand at stage 2, low demand at stage 3 and high demand at stage 2, low demand at stage 3 and medium demand at stage 2, and low demand in both stages 2 and 3.

The average expansion cost is calculated as the expected cost of additional capacity at stage 2 plus the expected cost of additional capacity at stage 3. The total expected cost of the flexible design is calculated using Eq. (4.15). Table 4.4 shows the optimal design for the HRES with design flexibility in 2027 and

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Componen	, Initial	Stage 2			Stage 3 given high or medium demand in stage 2			Stage 3 given low demand in stage 2		
design		High	Medium	Low	High	Medium	Low	High	Medium	Low
		demand	demand	demand	demand	demand	demand	demand	demand	demand
Solar	263	0	0	0	0	0	0	0	0	0
panel										
Wind	31	62	62	0	0	0	0	106	107	0
turbine										
Battery	17	25	25	0	50	0	0	47	56	0
Electrolyze	r230	0	0	0	0	0	0	0	0	0
Hydrogen	616	0	0	0	0	0	211	0	0	0
tank										
Fuel cell	68	0	0	0	0	0	0	0	0	0
Cost (\$	20.55	6.11	3.33	3.19	6.38	4.72	0.41	7.5	4.3	2.91
trillion)										
Total	26.52									
Cost (\$										
trillion)										
Value	14.14									
of flexi-										
bility(\$										
trillion)										

Table 4.4: The optimal design of the HRES with flexibility in design for the two stages case

2032. Similar to case 1, the initial design of the system will satisfy demand for 2017-2026 considering all of the 10,000 simulations for demand. The initial optimal design is the same as in case 1. In 2027, the capacity of the wind turbines and battery are expanded for the high and medium demand profiles, but not as much as in case 1. In case 2, the total capacity in 2027 should fulfill demand from 2027-2031, but in case 1, it is necessary to expand capacity to meet demand from 2027-2036. If demand is low in stage 2, none of the system components' capacities will be expanded, which is similar to the case 1. Instead, the needed electricity will be purchased from the market with diesel.

Given the initial design in stage 1 and the decisions about expanding capacity in stage 2, the additional capacity is optimized for high, medium, and low demand profiles for 2032-2036. The capacity expansion amounts at stage 2 are the same for the medium and high demand profiles in 2027-2031 (see Table 4.4), and the planning for stage 3 given medium demand in stage 2 is the same as the planning for stage 3 given high demand in stage 2. Additional capacity for the battery should be added for high demand profiles in stage 3. If demand is high or medium in stage 2 and low in stage 3, the capacity of the hydrogen tank should be expanded. In these scenarios, the total amount of energy generated by the wind turbine and solar panel exceeds demand, and the surplus amount should be reserved in the hydrogen tank.

There should be no expansion in stage 2 if demand is low. If demand remains low in stage 3, there should not be any expansion either. If demand is high or medium in stage 3, the decision maker should add additional capacity to the wind turbine and the battery. The capacity increases for high and medium demand in stage 3 are very similar.

4.3.3.3 Value of flexibility

In the first case of designing with flexibility, less capacity is needed for the first 10 years operation because demand does not increase significantly. If demand is high or medium in month 120, the designer should choose to increase the capacity of the wind turbine and battery. In case 2, the initial capacity should be similarly expanded for the wind turbine and battery if demand is high or medium in stage 2. Differences occur between the two cases because case 2 has an additional stage to plan for in years 2032-2036. If demand is high or medium in stage 2 and low in stage 3, the capacity of the hydrogen tank should be expanded to have more space for the excess amount of energy generated. If demand is low in stage 2 and high or medium in stage 3, the capacity of the battery and wind turbine should be expanded to meet the rising demand because no expansion occurred in stage 2.

The expected discounted cost of design with flexibility for case 2 is \$26.52 trillion which is less than the expected cost in case 1. In case 2, the designers have two options to exercise, one in 2027 and one in 2032. Delaying a decision on expanding capacity to 2032 allows the designers to take advantage of the time value of money.

Figure 4.5 shows that the expected cost decreases as more design modifications are included. In reality, there may be an increase in the initial investment cost that will allow the designers to easily expand capacity in the future. If that increase in the initial investment cost to enable the possible design modification in the future is less than \$13.44 trillion for the one-stage modification or \$14.14 trillion for the two-stage modification, then the designer should spend the money to have that option available to him or her in the future. These two values show the value of adding flexibility to the design of HRES.

Flexibility usually requires an upfront cost in order to be able to pursue the flexible alternatives. However, our methodology calculates the expected cost of design with flexibility. The difference between the expected costs of the design with flexibility and without flexibility is the maximum amount that the designer should pay to have a flexible option. This article only studies one type of flexibility modeling (i.e., capacity expansion) for the HRES. Future research can study other flexibility modeling ideas such as abandoning the system permanently or switching design configurations Cardin et al. (2015).



Figure 4.5: The expected cost vs. design modification stages of the HRES

4.4 Conclusion

This paper has presented a method to incorporate the demand uncertainty into the flexible design of an HRES. The HRES is composed of six components: solar panel, wind turbine, battery, electrolyzer, hydrogen tank, and fuel cell. The electricity demand data for California for over a 20-year period is simulated with an ARIMA time series model. The Bayesian optimization algorithm identifies the optimal design of the HRES by minimizing the expected discounted cost considering the demand for electricity for California and other uncertain cost parameters over 20 years. A flexible design allows the designers to modify the initial design in the future. A design with flexibility is conducted in two cases: a single design modification and two opportunities to modify the design. The results show that a single design modification 10 years after system deployment reduces the system's expected discounted cost by 33%. Including a second design modification would reduce the expected cost by an additional 3%.

This paper makes an important contribution to the literature of flexible design by measuring the value of flexibility in a complex engineered systems which require the use of computationally expensive simulations to evaluate the objective function. The model optimizes the design of engineered system by using probability distributions to forecast highly uncertain demand 20 years into the future. A multi-stage flexibility

modeling algorithm is developed to evaluate the value of flexibility. The algorithm is tested considering three categories at each stage. Future studies could further analyze and find the optimal number of divisions at each stage.

Future research could also include the time to exercise an option as a decision variable. For example, Kucuksayacigil and Min (2017) use ROA to find the optimal time to enlarge a ship after the ship is designed. If simulation optimization is required to optimize over many periods, such as 240 months, it is time consuming and even impossible with today's CPUs to optimize the mathematical model 240 times rolling back from the end for the 10,000 simulations. A heuristic model could be developed to find the optimal time to review the initial design of HRES.

The proposed algorithm for flexibility in design can be applied to any complex engineered system such as jet engines design and self-driving cars. These complex engineered systems require optimizing highdimensional, computationally expensive objective functions in a highly uncertain environment. Our proposed algorithm can potentially help designers to design complex engineered systems flexible to future uncertain situations.

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CHAPTER 5. DEEP REINFORCEMENT LEARNING FOR DYNAMIC DECISION MAKING UNDER UNCERTAINTY

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Abstract

Engineering systems operate in an unstable and uncertain environment. Engineering system design can be viewed as a decision-making process where complexity and uncertainty makes decision making for systems design challenging. In this paper, we proposed a framework to find the optimal design of an engineering system using Deep Q-learning algorithm when it is evaluated with a Monte Carlo simulation and it faces with multiple sources of uncertainties during the planning horizon. This study proposes a solution to find the sequence of decisions that can optimize the output of a simulation of an engineering system under thousands of scenarios for the uncertain parameters.

5.1 Introduction

Designing engineered systems such as energy systems and transportation systems may be challenging. These systems often operate for a long period of time under varying conditions. When the system is designed, there may be large amounts of uncertainty about the future, which makes decisions about how best to design the system difficult (Cardin et al., 2017). Designers design the system based on the best available information at the time of the decision, and they should also account for future uncertainties in the initial design of the system. The initial design may or may not change as the future evolves and conditions change. For example, power plant designers should consider uncertainties in the price and demand for electricity, but they may also want the ability to change the initial design based on the evolution of price and demand and other conditions (e.g., technology for renewable energy sources) in the future. Engineering system design can be viewed as a decision-making process, but complexity and uncertainty make decision making for systems design challenging (Zhang et al., 2011).

If a designer plans to modify the design, add capacity, or alter the system in the future, then the design decision is a multi-stage decision problem. The problem is frequently stochastic because of uncertainties in the future conditions. Designers often solve multi-stage stochastic optimization problems to find the optimal design of the system and how that design should be modified under different conditions in the future (Cardin, 2014). The initial design may periodically change in the future based on the evolution of the system. If designers neglect to account for uncertain conditions in the future, then modifying the initial design may be very costly in the future. Sequential decision problems occur in a range of engineering real-world problems such as robot control (Kent et al., 2018; Mihaylova et al., 2002; Parker and Zhang, 2009), power plant design (Carazas and Souza, 2010; Meigounpoory et al., 2008), and supply chain management (Fattahi and Govindan, 2018; Shabani and Sowlati, 2016b; Nickel et al., 2012). Real-world problems include parameters that are unknown at the time a decision should be made (Shapiro and Philpott, 2007).

Evaluating engineering system design often requires the use of a large-scale and computationally expensive simulation model. For example, designing power plants (Amin, 2011), architectural design (Goldstein and Khan, 2017), and mechanical systems (Goldstein et al., 2018; Berquist et al., 2017) may require the use of complex simulations to evaluate the performance of the system and the effect of multiple sources of uncertainty in the design (Shabani and Sowlati, 2016a). Computing the optimal policy for a system whose objective function is evaluated via a simulation in sequential settings is challenging (Frazier, 2010). Using dynamic programming to find the global optimal solution to this type of problem is difficult. The curse of dimensionality will arise, and solving the dynamic programming problem with a continuous state space for problems in which the objective function is evaluated via simulation will likely require heuristics and/or scenario reduction approaches. Solving the exact backward dynamic programming problem requires the evaluation of almost all of the non-optimal solutions of time *t* at time t - 1. For example, if problem contains 4 stages with a a thousand possible realizations of an uncertainty, the decision maker would need to solve 1000^4 optimization problems if a forward approximate dynamic programming is used (Shapiro and Nemirovski, 2005).

Learning algorithms such as reinforcement learning do not require decision makers to solve as many optimization problems. Reinforcement learning is a learning algorithm to control a system so as to maximize

some numerical value which represents a long-term goal (Szepesvári, 2010). In reinforcement learning, a decision maker or agent interacts with and explores the environment to gradually develop an optimal policy that will make the best decision for any state in the environment (Mnih et al., 2015).

Reinforcement learning has been successfully applied to a range of challenging problems such as robotics (Lillicrap et al., 2015), playing Go (Silver et al., 2016), and competitive video games (Hester et al., 2017; Gu et al., 2016). Reinforcement learning algorithms such as Deep Q-learning (Mnih et al., 2015) and Deep Deterministic Policy Gradient (Lillicrap et al., 2015) have achieved great success for sequential decision-making problems involving high dimensional inputs such as Atari games (Lyu, 2019). The goal of reinforcement learning is to learn good policies for sequential decision problems by optimizing a cumulative future reward (Van Hasselt et al., 2016). In this paper, we incorporate a Deep Q-learning algorithm in order to solve multi-stage stochastic problem for the engineering system where the objective function and constraints are evaluated with the Monte Carlo simulation. The decision maker interacts with and learns from a stochastic and uncertain environment in order to find the best policy to optimize the objective function (e.g., profit or cost).

The goal of this paper is to propose a framework to identify the optimal decision for an engineering system when the objective function is evaluated with Monte Carlo simulations. A decision maker can use reinforcement learning to find the optimal policy for a multi-stage stochastic problem without solving numerous optimization problems and instead learn the optimal policy by running the simulation and evaluating the objective function. Since this framework can incorporate many different types of simulation models with any type of uncertainty, no assumption is needed for the distribution of the uncertain parameters.

The uniqueness of this paper is that our proposed framework uses a Deep Q-learning to find the optimal design of an engineering system when the performance of the system is evaluated with a Monte Carlo simulation and multiple sources of uncertainty influence the performance and desirability of the system. The proposed methodology learns the optimal policy by interacting with the environment via simulation instead of by solving many optimization problems.

5.2 Literature Review

The field of stochastic programming contains many methods designed to solve multi-stage stochastic problems. Scenario-based methods like scenario generation and reduction are popular methods in stochastic optimization (Dupačová et al., 2003). These methods approximate the underlying probability distribution of the uncertain parameters. If the number of scenarios increases, it may be necessary to reduce the number of scenarios using heuristic methods. Due to computational complexity and time limitations, the probability distributions are approximated by a model with a reduced set of scenarios (Römisch, 2009; Growe-Kuska et al., 2003; Heitsch and Römisch, 2009). Growe-Kuska et al. (2003) propose algorithms for reducing the number scenarios and constructing scenario trees that approximate the random data processes of multistage dynamic decision models under uncertainty in the electricity power sector. Hu and Li (2019) propose an algorithm to reduce the number of scenarios based on the concept of correlation loss. They optimize two objectives: minimizing the correlation loss before and after scenario reduction and maximizing the similarity between the original scenario set and the reduced scenario set. The main drawbacks of the scenario reduction techniques are that the number of scenarios is a user-defined parameter, and the set of scenarios is an approximation and may not represent all possible combinations of the uncertain parameters (Wang et al., 2016a). Decomposition methods are also used to solve multi-stage stochastic problems. They are used primarily for large-scale stochastic optimization problems. They decompose the original problem into small tractable sub-problems by relaxing coupling constraints (Vigerske, 2013). Nested Benders decomposition is one of the popular methods to solve stochastic programs when the problem can be decomposed into smaller components, each of which can be solved independently and then reintegrated to solve the original problem (Murphy, 2013). This algorithm has been widely used to solve engineering design problems in the power network and energy systems (Soares et al., 2017; Gebreslassie et al., 2012), manufacturing (Chu and You, 2013), and supply chain (Keyvanshokooh et al., 2016; Santoso et al., 2005). Rebennack (2016) combines stochastic dual dynamic programming and the scenario tree framework in order to incorporate different types of uncertainties. Sherali and Fraticelli (2002) modify Benders decomposition method by using a Reformulation-Linearization Technique and lift-and-project cuts to solve discrete optimization problems. Boland et al. (2016) develop Proximity Search Benders decomposition which emphasizes high-quality, but not necessarily optimal solutions.

Several random search methods have been developed to solve multi-stage stochastic methods such as pure adaptive search (Patel et al., 1989) and accelerated random search (Ombach, 2014; Appel et al., 2004). Evolutionary algorithms such as genetics algorithm, differential evolution, and simulated annealing are also used to solve multi-stage stochastic programming problems in engineering (Dutta et al., 2017; Zohrevand et al., 2016; Zheng et al., 2019).

A significant number of papers solve engineering system design problems under uncertainty that evolves over time. Zhang and Babovic (2011) propose a simulation-based real option valuation for the design of an engineering system. They find the optimal and flexible design by considering a discrete and limited number of scenarios in their proposed evolutionary algorithm. Marques et al. (2015) identify the optimal design by only considering 8 possible future scenarios in the design of a water distribution network. Power and Reid (2018) use a real options decision framework to increase the performance of firms using regression models. Cheah and Liu (2006) use a Monte Carlo simulation of a discounted cash flow model to find the flexible design of the infrastructure projects. Mak and Shen (2009) apply a two-stage integer stochastic programming formulation to optimize the design of a manufacturing system under demand uncertainty. In the first stage, the demand of each product is known, however, in the second it is assumed that the demand follows a probability distribution. The optimal design is found considering 20 products and small number of scenarios for demand uncertainty. Postponing some decisions at the planning stage can lead to a large reduction in costs. Research show that postponing decisions at the planning stage can lead to a large reduction in investment cost and a significant increase in profits, especially for expensive flexible system design (Biller et al., 2006).

Several researchers use simulation optimization for engineering design when no closed-form formula exists for the objective function and/or constraints. Simulation optimization identifies the optimal solution for a problem where the objective function and constraints are evaluated through simulation (Amaran et al., 2016). For example, Damodaram and Zechman (2013) use simulation optimization to identify and explore watershed management plans. Fong et al. (2011) use simulation optimization to design solar-thermal refrig-

eration systems in which Monte Carlo simulation calculates the objective function (energy consumption). MacKenzie and Hu (2019) develop a simulation optimization framework to maximize expected profit for designing resilience in engineered systems. Giahi et al. (2020) use a Bayesian optimization algorithm to find the optimal design of engineering systems for risk-averse decision makers. Li et al. (2019) develop a novel simulation optimization framework to optimize the design of engineered systems to minimize the design cost while satisfying reliability requirements. This technique is widely used in the literature to solve the static engineering design problem. However, many design problems are dynamic, and uncertainty changes over time. These problems require solving multi-stage dynamic stochastic problem.

Reinforcement learning seeks to maximize the cumulative future reward. The goal of decision maker is to learn an optimal policy to maximize the cumulative return. The Deep Q-learning algorithm can avoid the curse of dimensionality that appears in the stochastic dynamic programming. Instead, the decision maker will learn how to make a decision at each stage based on the environmental conditions and simulated results. The proposed framework can benefit the decision-making process for the design of engineering systems where there are many possible scenarios for uncertainties and the objective function and constraints are evaluated with a Monte Carlo simulation. The proposed framework can solve a dynamic decision problem where a sequence of decisions are made over time.

5.3 Decision-Making Framework

Multi-stage stochastic programs are a well-recognized model for sequential decision making conditioned on information revealed at different points in time called stages (Pantuso and Boomsma, 2019). A linear multi-stage stochastic program takes the following form:

$$\max f(x,\xi) = c_{1}(\xi_{1})x_{1} + E\sum_{t=2}^{T} c_{t}(\xi_{t})x_{t}$$

subject to $\sum_{\tau=1}^{t} A_{t\tau}(\xi_{t})x_{\tau} \le b_{t}(\xi_{t}), t = 1..., T$
 $x_{t} \in X_{t}, t = 1..., T$ (5.1)

where t = 1, ..., T are stages, $\xi := (\xi_1, ..., \xi_T)$ is a stochastic process defined on some probability space, and $x := (x_1, ..., x_T)$ is the collection of decisions. The function $f(x, \xi)$ is a linear objective function for the planning time T, $c_t(\xi_t)$ is the per-unit reward at time t, $A_{t\tau}(\xi_t)$ is a vector of coefficients, and $b_t(\xi_t)$ is a constraint at time t. The stocastic program in (5.1) requires that decisions x_t is a function of the history of decisions until t - 1, and that alternatives are members of the feasibility set X_t . In many practical applications, ξ is discrete, possibly by assumption (Pantuso and Boomsma, 2019). As stated in (Shapiro and Nemirovski, 2005), there are some challenges regarding this problem: probability distributions either cannot be accurately estimated or change over time and the evaluation of the expected value function involves calculating multivariate integrals. A finite discretization of the random data enables the solution to be calculated in the form of summation.

Solving multi-stage linear stochastic programming problems when the number of stages and the number of scenarios are large is very challenging. This problem is even more difficult when the functions are non-linear. The functions are non-linear for many engineering design problems that rely on simulation. The non-linear problem introduced in (5.2) can be used to formulate a multi-stage stochastic program when the objective function is evaluated via a simulation.

$$\max f(x,\xi) = g(x_1,\xi_1) + E \sum_{t=2}^{T} g(\xi_t, x_t)$$

subject to $h(\xi_t, x_t) \le b_t(\xi_t), t = 1..., T$
 $x_t \in X_t, t = 1..., T$ (5.2)

where $g(x_t, \xi_t)$ or g_t is a non-linear objective function from time t to t + 1, $h(\xi_t, x_t)$ is a non-linear constraint at time t. The value of objective function and constraints at any time are evaluated with Monte Carlo simulations. In this paper, we solve the problem in (5.2) when x_t is a discrete variable and we maximize the expected value of an objective function (e.g., profit).

5.3.1 Q-Learning

In this paper, the decision maker of the reinforcement learning algorithm also refers to the designer of the engineering system. Reinforcement learning maximizes the cumulative expected value of the objective function in Eq. (5.2) when the decision maker interacts with the environment. The environment has a Markov decision process property. The decision maker runs the Monte Carlo simulation given decision x at time t to maximize the profit. Monte Carlo simulation generates the candidates for the next state of the Markov decision process. The state variable s_t contains all the information related to the state of the system at time t. It also has all information related to uncertain parameters (i.e., ξ) at time t. The Markov decision process consists of (s_t, x_t, g_t, s_{t+1}), the state at time t, decision at time t, the objective function value evaluated by simulation at time t, and next state of the system at time t + 1 which depends on the decision and state at time t.

The Bellman equation is used as a foundational piece to derive the Q-learning algorithm:

$$Q(s_t, x_t) = g_t + \gamma \max_{\mathbf{v}} Q(s_{t+1}, x_t)$$
(5.3)

where γ is a parameter to discount maximum Q at state s_{t+1} . The Q (i.e., quality) in Q-learning represents how useful a given decision is in evaluating the future value of the objective function. The Q-learning algorithm improves its ability to evaluate the quality of a decision at each state (Watkins and Dayan, 1992). The function $Q(s_t, x_t)$ approximates the value of the objective function from the current time t until the end of planning at time T. The goal of Q-Learning algorithm is to maximize total reward (here objective function). It adds the maximum reward attainable from future states which is the a weighted sum of the expected values of the rewards of all future steps starting from the current state.

We can iteratively approximate $Q(s_t, x_t)$ where α is the learning rate between 0 and 1:

$$Q(s_t, x_t) \leftarrow Q(s_t, x_t) + \alpha \left(g_t + \gamma \max_X Q(s_{t+1}, x_{t+1}) - Q(s_t, x_t) \right)$$
(5.4)

Equation (5.4) is the main idea behind the Q-learning algorithm. This algorithm is an iterative process where ,in this study, $Q(s_t, x_t)$ is using simulation to calculate the objective function and randomly samples the next state of the system. In the Q-learning algorithm, the decision maker chooses a decision *x* to evaluate in state *s* based on the epsilon-greedy policy. A policy is ε -greedy with respect to the *Q*, if for every state $s \in S$, the decision maker selects the greedy decision with probability 1- ε and selects a different decision at random from the set of available (both greedy and non-greedy) decisions with probability ε . Each iteration of the algorithm is called episode and ε at episode e can have the following form: $\varepsilon_e = \max{\{\varepsilon_{end}, \varepsilon_{decay}\varepsilon_{e-1}\}}$ where ε_{decay} is the rate of decay for ε (e.g., 0.999) and ε_{e-1} is the value of epsilon at episode e - 1. The parameter ε starts with a number close to one ($\varepsilon_1 = 1$) and it gradually decreases after the algorithms learns the optimal policy. When ε is large, the algorithm picks random decisions to explore and learn the environment, and when ε is small, the algorithm chooses the best decision at each state to maximize the value of Q.

Algorithm 7 shows the Q-learning algorithm (Wang et al., 2013a). After the decision maker repeats this process a sufficient number of times, $Q(s_t, x_t)$ converges to the optimal value ((Melo, 2001)), where:

$$0 \leftarrow \left| g_t + \gamma \max_X Q\left(s_{t+1}, x_{t+1} \right) - Q\left(s_t, x_t \right) \right|$$
(5.5)

Algorithm 7 Q-learning Algorithm.

1: Initialize *Q* values arbitrarily (e.g., Q(s,x) = 0 for all $s \in S$ and $x \in X(s)$)

- 2: for $i \leftarrow 1$ to Total Number of Episodes (E) do
- 3: $\varepsilon \leftarrow \varepsilon_i$
- 4: Reset the simulation environment parameters
- 5: $t \leftarrow 1$

6: Select either random or optimal greedy values for decision variables x_t using epsilon policy algorithm, fulfilling constraints $h(\xi_t, x_t) = b_t(\xi_t)$

- 7: Run simulation model to evaluate x_t given uncertainty at time t (ξ)
- 8: Evaluate objective function at time $t(g_t)$
- 9: $Q(s_t, x_t) \leftarrow Q(s_t, x_t) + \alpha(g_t + \gamma \max_X Q(s_{t+1}, x_{t+1}) Q(s_t, x_t))$
- 10: $t \leftarrow t + 1$
- 11: **until** *t* is end of planning horizon
- 12: end for
- 13: return Q

14: Output: State-decision value function (Q)

A Q-table stores the value of Q for each (s_t, x_t) pairs. During training, the Q value for each pair is updated as the algorithm proceeds. After the algorithm converges, the Q-table shows the optimal decision for each state of the system. The Q-learning algorithm is guaranteed to converge to the optimal solution (see (Melo, 2001)) as long as the step-size parameter α is sufficiently small and every (s_t, x_t) pair, for all $s \in S$ and $x \in X(s)$, is visited infinitely many times, and the policy converges to a policy. The optimal policy can be calculated with Eq. (5.6). The optimal policy is the policy that maximizes Q(s,x) for each (s_t,x_t) pair. The optimal policy shows the optimal decision under any realization of the uncertain parameter.

$$\pi^*(s) = \arg\max_X Q^*(s, x) \quad \forall s \in S$$
(5.6)

Traditional reinforcement learning algorithms such as Q-learning can find the optimal policy for relatively small problems. The decision maker learns via simulation and improves upon the objective function. At each state, the decision maker inputs either a greedy or random decision into the simulation and observes the expected profit from the current time t to t + 1. If many state-decision combinations exist, a traditional Q-learning algorithm may not be able to fully solve a sequential decision problem that depends on a Monte Carlo simulation. The Deep Q-learning algorithm improves upon the Q-learning algorithm and is the actual algorithm used to solve Eq. (5.2).

5.3.2 Deep Q-Learning

The Q-learning algorithm can solve problem for only a limited number of states. If the number of states increases to thousands, the curse of dimensionality may appear as the state-decision values would need to be stored in a huge table. Therefore it is practically impossible to solve the problem if thousands of possible states exist. Deep Q-learning algorithms can estimate $Q(s_t, x_t)$ within an acceptable error (Hester et al., 2017).

Deep Q-Learning combines Q-learning with a flexible deep neural network and has been tested on a varied and large set of Atari games, reaching human-level performance on many games (Van Hasselt et al., 2016). Many problems are too large to learn all decision values in all states separately. Evaluating the true value for the decision-state value function is practically impossible for large problems such as a multi-stage simulation optimization problem. A Deep-Q learning algorithm estimates the decision-state value function with a Deep neural network. Using Deep-Q learning to solve a multi-stage stochastic programming problem where the objective function and constraints are evaluated via simulation represents a novel development in the field of engineering system design.

Algorithm 8 Deep Q-learning Algorithm.

```
1: Initialize neural network weights w^- \leftarrow w
```

- 2: for $i \leftarrow 1$ to E do
- 3: $\varepsilon \leftarrow \varepsilon_i$
- 4: $t \leftarrow 0$
- 5: Repeat
- 6: Find feasible decision variable x_t by fulfilling constraints $h(\xi_t, x_t) \le b_t(\xi_t)$ and using policy $\pi \leftarrow \varepsilon$ greedy $(\hat{Q}(s_t, x_t, w))$
- 7: Run simulation model to evaluate x_t given uncertain parameters value at time t.
- 8: Find objective function at time $t(g_t)$ by simulation
- 9: Generate random sample from uncertain parameters distributions for the next period t + 1 and update state s_{t+1}
- 10: Store experience tuple (s_t, x_t, g_t, s_{t+1})
- 11: Obtain random minibatch of tuples $(s^j, x^j, g_t^j, s^{j+1})$
- 12: Set target $y_t^j = g_t^j + \gamma \max_X \hat{Q}(s_t^{j+1}, x_t, w^-)$
- 13: Update $\Delta w = \alpha (y_t^j \hat{Q}(s_t^j, x_t, w)) \nabla_w \hat{Q}(s_t^j, x_t, w)$
- 14: Reset $w^- \leftarrow w$ every C steps
- 15: **until** *t* is end of planning horizon
- 16: **end for**
- 17: return \hat{Q}

18: Output: State-decision value function approximation (\hat{Q})

In a multi-stage decision making problem, the uncertainty is revealed gradually over time. The decision at time t depends only on the information available at the beginning of t. In other words, if the revealed uncertainty data up to time t in two scenarios is the same, then the decision made at time t should be exactly the same, no matter how different they will be in the future (Cardin et al., 2017). The optimal decision at state s should not depend on the future value of the uncertain parameters. Algorithm 8 shows the Deep Q-learning algorithm to solve the multi-stage stochastic program described in the stochastic program in (5.2). In this algorithm, a decision at each state is selected based on the feasible solutions at that state (i.e., without violating constraints). The goal of this algorithm is to find a decision at each state that can maximize the objective function (e.g., expected profit) when a sequence of decisions should be made to find the optimal policy in the multi-stage stochastic setting for the engineering system design. The proposed framework is generic enough that it can be applied to any type of simulation with any type of constraints when uncertainty exists around the parameters and the decision variables are discrete.

Algorithm 8 shows a step-by-step framework to optimize engineering system design when the objective function is evaluated with the simulation. In the beginning of the algorithm, random numbers are assigned to the weights of the neural network. The algorithm proposed in Algorithm 8 repeats many times where E represents the total number of episodes or iterations. At each episode, the simulation environment including the state variable *s* is reset to start at time t = 1.

Given the state of the system at time *t*, the decision variable is selected with the epsilon greedy algorithm satisfying constraints in (5.2). The state of the system including uncertain parameters ξ and time *t* are inputs into the neural network. The Q-value for each possible decision from the decision variable (*X*) is the output of the neural network. For example, if the decision variable *X* can only be an integer value in [0,10], then the neural network calculates one approximation for the Q-value for each possible decision. The neural network approximates $Q(s_t, x_t)$ for each decision at each state as described in Eq. (5.3). The decision maker interacts with the simulation environment by sampling from the uncertain parameters. The random sample is an input into the deep neural network and the decision is chosen using the ε -greedy policy based on the outputs of the neural network.

The deep neural network acts as a function approximator. The state of the system is passed to the neural network and the neural network produces a vector of decision values with the maximum value indicating the decision to take. In the beginning when the neural network is initialized with random values, the sampled decisions are sparse and random which will likely result in poor decisions. Over time, the Deep Q-learning algorithm finds the appropriate decisions and learns the best decisions at each state of the environment. Unlike the traditional reinforcement learning algorithms such as Q-learning where only one Q-value is produced a time, the Deep Q-Learning algorithm is designed to produce a Q-value for every possible decision in a single forward pass.

After the objective function is calculated via a simulation, the next state of the system s_{t+1} is calculated by sampling from the distribution of the random variable (ξ). A decision can be selected based on the output of the neural network and using epsilon-greedy algorithm satisfying constraints. The weight of neural network will be updated with the gradient descent algorithm.



Figure 5.1: Proposed framework for solving multi-stage stochastic problem

After reaching the end of planning horizon, the algorithm resets the simulation environment and begins a new episode. This process iterates until the decision maker learns the environment and finds the optimal policy that maximizes the objective function. The objective function can be profit or any other output from simulation. At the end of training, the optimal policy π^* is identified. The optimal policy is a trained neural network (\hat{Q}). The optimal policy provides the optimal decision given the input (state of the system including uncertain parameters). The proposed algorithm is also described in Figure 5.1. For example, at t = 3, for any evaluation of the uncertain parameters the output of the neural network is the best decision given any realization of the uncertain parameter. The objective function in (5.2) can be approximated by simulating the optimal policy (trained neural network) M number of times by randomly sampling ξ and using policy π^* :

$$\max f(x,\xi) = \frac{1}{K} \sum_{m=1}^{M} \sum_{t=1}^{T} \hat{Q}_{\pi^*}(x_t^*,\xi_m)$$
(5.7)

5.4 Engineering System Design Illustrative Examples

The proposed framework in this paper can be applied to dynamic stochastic programming problems with a discrete number of decisions available at each stage. The illustrative examples presented in this section provide a proof-of-concept demonstration of the potential of the proposed framework. The illustrative examples are relatively simple, and their purpose is to demonstrate how the algorithm functions. The results show that the Deep Q-learning algorithm can be applied to engineering design problems with a sequential decision-making process under uncertainty and where the objective function is evaluated via simulation. The proposed framework will enable a system design evaluated via simulation to be optimized over a wide range of uncertain parameters.

5.4.1 Capacity Expansion Problem with Price Uncertainty: Problem Formulation

The illustrative example is a capacity expansion problem. In the capacity expansion problem under uncertainty, a decision maker can choose whether or not to expand its operational capacity at different points in time. For example, capacity expansions decisions exist in power plant design (Murphy and Smeers, 2005; Wogrin et al., 2011) and transportation network design (Mathew and Sharma, 2009). In the power plant capacity expansion problem, the designers may make a decision about adding capacity to the existing capacity of the plants (e.g., wind turbines). The designers would like to plan for when they should expand the capacity of their operations, but uncertainty in the future makes the decision of whether to expand their capacity challenging. The designers may choose to expand their capacity under some scenarios and choose not to expand their capacity under other scenarios.

The decision maker's goal is to find the optimal policy to design a system that operates for *T* time periods. The problem is a multi-stage stochastic program. The decision maker determines x_t , the additional units of capacity to add to the system at time *t*. The decision maker's objective is to maximize $f(x, \xi)$, the expected profit of the system. The expected profit is the expected revenue minus the cost of expanding and operating the system over the *T* time periods. The revenue is uncertain and ξ is the future price p_t gained from selling one unit of capacity for one duration of time. We assume there are *u* time units of duration in each time period and the revenue at time *t* is $up_t \sum_{t'=1}^{t} x_{t'}$. The parameter *u* could also represent the number

of units produced for each unit of capacity. When the decision maker determines x_t , the decision maker knows p_t but the future price p_{t+1} is uncertain and depends on the price at time t. The problem is defined as follows:

$$\max f(x,\xi) = (up_1 - c_{om} - c_{inv})x_1 + E\left[\sum_{t=2}^T \frac{(up_t - c_{om})\sum_{t'=1}^t x_{t'} - c_{inv}x_t}{(1+i)^{t-1}}\right]$$

subject to $p_{t+1} = p_t e^{N(\mu_1, \sigma_1)}, \ t = 1, \dots, T-1$
$$\sum_{t=1}^T x_t \le 1$$

 $x_t \in \{0,1\}, \ t = 1, \dots, T$ (5.8)

where c_{om} is the annual operating cost, c_{inv} is the cost of adding capacity to the system, *i* is the interest rate, and μ_1 and σ_1 represent the mean and standard deviation to describe the random evolution of the price.

The optimization problem in (5.8) is formulated as a multi-stage stochastic program similar to (5.2). The optimal solution is solved at each planning period for all possible values of p_t , t = 1, 2, ..., T. Since the sum of capacities is constrained to be less than or equal to 1, this problem assumes that the decision maker can only add capacity in one of the stages. This simplified capacity expansion problem focuses on if and when to build capacity. The system has no initial capacity. At time *t*, the system gains revenue by selling accumulative capacity (i.e., $\sum_{t'=1}^{t} x_{t'}$) at price p_t , where the ratio of consecutive prices follows a lognormal distribution with parameters μ_1 and σ_1 . The operations cost represented by c_{om} is the cost to operate the total capacity existing at time *t*. The investment cost represented by c_{inv} only occurs if capacity is added at time *t* (i.e., x_t).

5.4.2 Capacity Expansion Problem with Price Uncertainty: Solution

We first define the state (*S*), decision variable (*X*) and the objective function in detail. The system state *S* consists of two components: the current price p_t and the remaining capacity at time t, $1 - \sum_{t'=1}^{t} x_{t'}$. The decision is whether or not to add capacity in each stage of the decision-making process. The decision is a discrete variable and the algorithm makes decision at time t given state s. At each step, the decision maker

earns a reward $g(p_t, x_t) = [(up_t - c_{om})\sum_{t'=1}^{t} x_{t'} - c_{inv}x_t] / (1+i)^{t-1}$ after executing decision x_t and evaluating it through simulations. The objective is to find the maximum expected profit while fulfilling the constraints.

Since p_t is a continuous random variable, the algorithm selects 10,000 samples from the distribution of the price at each time period. In this problem, $c_{om} = 300$, $c_{inv} = 20$, u = 2920, $\mu_1 = 0.05$, $\sigma_1 = 0.1$, and $p_1 = 0.1$. The number of episodes (iterations) for the DQN algorithm is 150,000. The parameter $\varepsilon_e = max(\varepsilon_{end}, \varepsilon_{decay} \times \varepsilon_{t-1})$ where $\varepsilon_1 = 1$, $\varepsilon_{end} = 0.001$ and $\varepsilon_{decay} = 0.99995$.

We use this framework to solve two examples from the capacity expansion problem in (5.8). In the first example, the number of stages is T = 2. The decision maker should choose $x_1 = 0$ at time t = 1. The optimal decision at time 2 depends on the price. If $p_2 \ge 0.1096$, the optimal decision is $x_2 = 1$, and if $p_2 < 0.1096$, the optimal decision is $x_2 = 0$. Since this problem is relatively simple, the optimal solution can be solved analytically where $x_2 = 1$ if $x_1 = 0$ and $up_2 - c_{om} - c_{inv} > 0$, which is true if $p_2 \ge 0.1096$. The algorithm's threshold for p_2 when $x_2 = 1$ is with 0.0001 of the analytical solution. The simulated expected profit of this policy is 7.38. The algorithm takes 980 seconds to converge to the optimal solution. Figure 5.2 depicts the optimal decision at t = 2 given p_2 .

The second example increases the number of stages to T = 3. Again, the decision maker should choose $x_1 = 0$ at time t = 1. The algorithm converges to the optimal solution after approximately 80,000 episodes. It takes 1350 seconds to find the optimal solution. As shown in Figure 5.3, the optimal policy depends on p_t in both stages 2 and 3. The algorithm identifies that the decision maker should add one capacity to the system at t = 2 if $p_2 \ge 0.1072$. If $p_2 < 0.1072$ the algorithm determines that $x_2 = 0$ and $x_3 = 1$ if $p_3 > 0.1110$. This policy is found by simulating the system and through generating random samples from the price distribution and finding the optimal decision given each state value with the trained neural network and estimated with Eq. (5.7). The expected profit of this policy is 32.5. According to an analytical solution, the decision maker should add one capacity at stage 3 if $p_3 > 0.1096$ and no capacity is added in stage 2. The decision maker should add capacity in stage 2 if

$$up_{2} - c_{om} - c_{inv} + \frac{u \mathbb{E}[p_{3}|p_{2}] - c_{om}}{1 + i} > P\left(p_{3} > \frac{c_{om} + c_{inv}}{u} \middle| p_{2}\right) \frac{u \mathbb{E}[p_{3}|p_{2}, p_{3} > \frac{c_{om} + c_{inv}}{u}] - c_{om} - c_{inv}}{1 + i}.$$
(5.9)



Figure 5.2: Optimal decision at stage two for two-stages problem with price uncertainty

Using Monte Carlo simulation, we find the decision maker should add capacity at stage if $p_2 > 0.1061$. The Deep-Q learning algorithm's thresholds for p_2 and p_3 are within 0.0011 and 0.0014, respectively, of the true thresholds. The expected profits of the two solutions only differ by approximately 0.08 or 0.2%, however, which is a relatively small difference.

5.4.3 Capacity Expansion Problem with Price and Demand Uncertainty: Problem Formulation

The Deep Q-learning algorithm can handle multiple sources of uncertainty. The uncertain parameters are stored as a tuple of parameters in the state variable and are passed to the Deep neural network as an input. The neural network approximates the relationship between the inputs (state) and the outputs (decision) while new stream of data—produced by simulation—comes to the model. The reinforcement learning algorithm enables the decision maker to explore the simulation environment and learn the optimal policy.



Figure 5.3: Optimal decision at stage 2 and 3 for three-stages problem with price uncertainty

We add demand as another source of uncertainty in this illustrative capacity expansion example. In many engineering problems, demand is an uncertain variable that can have a significant impact on how a system is constructed and how much capacity is required. In this example, the decision maker can decide to add a total of *K* units of capacity to the system. If the demand is high, then multiple units of capacity may be needed. The decision maker will decide when and under what conditions to add a new capacity. The decision maker's objective is to maximize the expected profit but the system will only receive revenue for what is demanded, and the revenue at time *t* is $up_t \times \min\{d_t, c_p \sum_{t'=1}^t x_{t'}\}$ where d_t is the demand at time *t* and c_p is the units of demand that can be satisfied for each unit of capacity. When the decision maker determines x_t , the decision maker knows p_t and d_t , but the future price p_{t+1} and demand d_{t+1} are uncertain and depends on the price and demand at time *t*. The problem is defined as follows:



Figure 5.4: Distribution of uncertain parameters during the planning horizon

$$\max f(x,\xi) = up_{1} \times \min\{d_{1}, c_{p}x_{1}\} - (c_{om} - c_{inv})x_{1} + E\left[\sum_{t=2}^{T} \frac{up_{t} \times \min\{d_{t}, c_{p}\sum_{t'=1}^{t} x_{t'}\} - c_{om}\sum_{t'=1}^{t} x_{t'} - c_{inv}x_{t}}{(1+i)^{t-1}}\right]$$

subject to $p_{t+1} = p_{t}e^{N(\mu_{1},\sigma_{1})}, \ t = 1, \dots, T-1$
 $d_{t+1} = d_{t}e^{N(\mu_{2},\sigma_{2})}, \ t = 1, \dots, T-1$
 $\sum_{t=1}^{T} x_{t} \le K$
 $x_{t} \in \{0, \dots, K\}, \ t = 1, \dots, T$

$$(5.10)$$

5.4.4 Capacity Expansion Problem with Price and Demand Uncertainty: Solution

To evaluate the performance of the proposed framework on the capacity expansion problem with multiple sources of uncertainty, we run the algorithm to find the optimal policy for the problem described in Eq. (5.10). ξ_t is a tuple of p_t and d_t which makes the stochastic problem more complex than the problem with only one source of uncertainty. Since p_t and d_t are continuous random variables, the algorithm selects 100,000 samples from the distribution of the price and demand at each time period. Therefore 10^{10} different scenarios are generated at each time. In this example, $d_1 = 1$, $\mu_2 = 0.2$, $\sigma_2 = 0.1$, and $c_p = 1$.

Figure 5.4a and 5.4b shows price and demand, respectively. These figures show that the demand and price are highly uncertain and combination of these two sources of uncertainty creates many scenarios.

(Expected Profit, Run Time (sec))	Number of Stages				
K	3	4	5		
2	(33.1,1411)	(77.8,1650)	(135.3,2052)		
3	-	(80.1,1753)	(146.5,2109)		

(150.8, 2172)

4

Table 5.1: Expected profit of multi stage stochastic program under demand and price uncertainty

We use the proposed framework to solve the problem for T = 3,4, and 5 stages. Table 5.1 shows the optimal expected profit when the number of stages T varies between 3 and 5 and maximum capacity (K)varies between 2 and 4. Table 5.1 also shows the time it takes to run each of the configurations.

When T = 3 and K = 2, the algorithm converges to a solution after 100,000 episodes as seen in Figure 5.5d. The expected profit is 33.1. As with the previous example, the decision maker should choose $x_1 = 0$.

Since an analytical solution can use backward dynamic programming techniques, the analysis of the solution will begin with the decision in the last stage (t = 3) and proceed to the decision at t = 2. An analytical solution reveals that if $x_2 = 0$, the decision maker should choose $x_3 = 1$ if $up_3 \times \min\{d_3, 1\}$ – $c_{om} - c_{inv} > 0$ and choose $x_3 = 2$ if $up_3 \times \min\{d_3, 2\} - 2(c_{om} - c_{inv}) > up_3 - c_{om} - c_{inv} > 0$. If $x_2 = 1$, the decision maker should choose $x_3 = 1$ if $up_3 \times \min\{d_3 - 1, 1\} - c_{om} - c_{inv} > 0$. Given the numbers in this example, if $x_2 = 0$, then $x_3 = 2$ if $p_3 \times \min\{d_3 - 1, 1\} > 0.1906$ and $x_3 = 1$ if $p_3 \times \min\{d_3, 1\} > 0.1096$ and the condition for $x_3 = 2$ is not met. Figure 5.5b depicts the algorithm's solution for x_3 if $x_2 = 0$. The algorithm finds a threshold for p_3 that separates $x_3 = 0$ and $x_3 = 1$ when $d_3 \ge 1$. This threshold occurs at approximately $p_3 = 0.108$, which is within 0.0016 of the analytical threshold. When $d_3 < 1$, the dividing line between $x_3 = 0$ and $x_3 = 1$ approximately follows $p_3d_3 = 0.1906$. The Deep-Q learning algorithm never finds $x_3 = 2$ as an optimal policy perhaps because only a few instances exist when $x_3 = 2$ should be optimal. If $x_2 = 1$, then $x_3 = 1$ if $p_3 \times \min\{d_3 - 1, 1\} > 0.1906$. Figure 5.5c displays the algorithm's solution for x_3 if $x_2 = 1$. The algorithm finds a dividing line between $x_3 = 0$ and $x_3 = 1$ that approximately follows $p_3 \min\{d_3 - 1, 1\} = 0.1906$ when $x_2 = 1$.

Figure 5.5a shows the algorithm's solution for x_2 . The algorithm finds a threshold that separates $x_2 = 0$ and $x_2 = 1$ if $d_2 > 1.2$ and $p_2 = 0.104$ If $d_3 < 1.2$, the threshold separating $x_2 = 0$ and $x_2 = 1$ appears to follow $p_2 d_2 = 0.077$.





(d) Algorithm convergence to the optimal policy

Figure 5.5: Three-stage problem with price and demand uncertainties and K = 2

If T = 4 and K = 3, the algorithm finds a solution with an expected profit of 80.1. If $x_2 = x_3 = 0$, the final decision $x_4 = 1$ if $d_4 < 1$ and $p_4d_4 > 0.1906$, or if $d_4 \ge 1$ and $p_4 > 0.1906$. If $x_2 = x_3 = 0$, the final decision $x_4 = 2$ if $p_4 \times \min\{d_4 - 1, 1\} > 0.1906$. As shown in Figure 5.6e, the Deep-Q learning algorithm seems to identify $p_4 = 0.1906$ as a dividing line between $x_4 = 0$ and $x_4 = 1$, but the line begins at approximately $d_4 = 1.2$ rather than at $d_4 = 1$. The algorithm does not any scenarios where $x_4 = 2$. If either $x_2 = 1$ or $x_3 = 1$, then $x_4 = 1$ if $p_4 \times \min\{d_4 - 1, 1\} > 0.1906$. Figure 5.6d shows that the Deep-Q learning algorithm's solution approaches the analytical solution although the slope of the dividing line between $x_4 = 0$ and $x_4 = 1$ is less steep than the true solution when $d_4 < 2$.

Figure 5.6b depicts the algorithm's solution for choosing $x_3 = 0$ or $x_3 = 1$ when $x_2 = 0$. The algorithm identifies a pretty clear threshold, and the slope of this dividing line is steep when $d_3 < 1.15$ and much less steep when $d_3 > 1.3$. The algorithm does not identify any situations when $x_3 \ge 2$ or when $x_3 = 2$ given $x_2 = 1$. As seen in Figure 5.6a, a fairly clear threshold exists for the decision at t = 2.



(a) Optimal decision at stage 2



(b) Optimal decision at stage 3 given x2=0



(c) Optimal decision at stage 3 given x2=1



(d) Optimal decision at stage 4 given x2+x3=1



(e) Optimal decision at stage 4 givenx2=0,x3=0





Figure 5.6: Four stages problem with maximum capacity of three

5.5 Conclusion

This paper provides a framework to find the optimal policy for the design of the engineered systems. Designing an engineering system that operates for long time requires the consideration of an uncertain future in the decision-making process. Our proposed framework finds the optimal design of an engineering system when it is evaluated with a Monte Carlo simulation and it faces multiple sources of uncertainties. The proposed methodology is designed to find the optimal design of engineering system through simulation instead of solving many optimization problems. The goal is to find the optimal policy that can maximize the output of a simulation model given a multiple sources of uncertainties. The algorithm is able to solve linear and non-linear multi-stage stochastic program where the decision variables are discrete and the objective function and the constraints are evaluated with Monte Carlo simulation.

The proposed algorithm is applied to two illustrative engineering design problems. In the first one, the optimal policy for a simple problem with one source of uncertainty and linear objective function is calculated. In the second example, optimal policy for a problem with two sources of uncertainties and non-linear objective function is calculated. Multiple configurations of the problem are discussed to show how our proposed methodology is capable to identify the optimal policy under different uncertain conditions with less number of learning episodes compared to the number of scenarios. The objective function and the constraints for both of the problems are evaluated with Monte Carlo simulation where in each run of the simulation the value of the objective function can change based on the valuation of the uncertain parameters.

The findings of this study have to be seen in light of some limitations. Although the algorithm can find the optimal policy, there is an error in the expected profit. For example, in the first illustrative example, the expected profits of the analytical and Deep Q-learning solutions differ by approximately 0.2%. For some configurations, we ran the algorithm multiple times so that it can converge to the optimal solution. There are also some outliers in the results especially for the scenarios that are close to the threshold that the optimal policy changes. Another limitation of the paper is that our proposed framework may not be able to solve multi-stage stochastic problem with a continuous decision variables. Further research could apply new reinforcement learning techniques such as policy gradient and actor critic to solve multi-stage stochastic problem with continuous decision variables. Future works can also consider correlation between uncertain parameters in the simulating the uncertainty scenarios and include the correlation in the decision making process.

Although the examples provide an illustration of how the Deep Q-learning algorithm can be applied to engineering design problems, the examples are relatively simple. Future research can apply the framework in this paper to a real engineering design problem, which will provide more insight into the potential benefits as well as drawbacks of this approach. However, the proposed framework can benefit the decision-making process for the design of engineering systems where the decision makers can find the optimal policy for a multi-stage stochastic problem without solving numerous optimization problems and instead learn the optimal policy by running the simulation and evaluating the objective function. The algorithm is able to solve, for example four stages, with 10,000 possible scenarios for the uncertain parameters with only 150,000 iterations instead of solving $10,000^4$ optimization problems (for each scenario at each stage). The optimal policy generated by the algorithm enables the designers of the engineering systems to make optimal decision under any possible future uncertainty.

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CHAPTER 6. SUMMARY AND DISCUSSION

6.1 Thesis Contributions

This thesis develops simulation optimization frameworks to identify optimal solutions for engineering design problems. Simulation optimization and sequential decision-making frameworks are developed in order to optimize the design of complex engineering systems in four different studies: (i) designing a resilient wind turbine system for risk-averse decision-makers, (ii) improving the reliable design of airfield concrete pavement, (iii) incorporating flexibility into the design of an HRES, and (iv) using reinforcement learning for dynamic engineering design decisions.

Chapter 2 provides a framework to incorporate risk aversion into a firm's design decisions for a resilient engineered system. Applying the Bayesian optimization algorithm alongside the sequential Monte Carlo simulation enables the designers to find the optimal characteristics of the engineered system for both risk-neutral and risk-averse decision makers. This approach can help in the early stages of design by capturing the risk attitude of decision makers as they consider the trade-offs among the initial costs, resilience, and future profits. The results show that the design features for resilience change when we incorporate risk attitude within the design framework. The use of exponential utility and VAR metric for the design of engineered systems when the performance of the systems is evaluated with simulation and the optimal design is found with the Bayesian optimization represents unique contributions to the design of more resilient systems.

Chapter 3 describes the development of a comprehensive reliability-based simulation-optimization framework for finding the optimal design of airfield concrete pavement. The objective of chapter 3 is to develop a new design methodology called SOARP. SOARP is a comprehensive reliability-based simulationoptimization framework. The novelty of this study and its primary difference with FAARFIELD's design methods and other methods in the literature lie in its use of the simulation optimization framework while generating thousands of scenarios for the uncertain parameters to find the optimal design of the airfield rigid pavement. Thousands of scenarios are generated to simulate real-world conditions for long-term usage of the airfield. The design optimization is aimed at minimizing design cost while using a reliability constraint to keep pavement fatigue failure under an allowable amount. The design optimization framework is developed to find the optimal design for multiple design lives and reliability levels.

Chapter 4 makes an important contribution to the literature of flexible design by measuring the value of flexibility in a complex engineered systems which require the use of computationally expensive simulations to evaluate the objective function. The model optimizes the design of an HRES by using a probability distributions to forecast uncertain demand 20 years into the future. A multi-stage flexibility modeling algorithm is developed to evaluate the value of flexibility. A flexible design allows the designers to modify the initial design in the future. The uniqueness of this chapter is that it measures the value of flexibility in complex engineered systems that require using computationally expensive simulations to evaluate the objective function, and the paper develops a model to optimize the design of such systems under highly uncertain parameters.

Chapter 5 provides a framework to find the optimal policy for the design of the engineered systems. The proposed framework identifies the optimal design of an engineered system when it is evaluated with a Monte Carlo simulation that incorporates multiple sources of uncertainties. The proposed framework can benefit the decision-making process for the design of engineered systems for a multi-stage stochastic problem without solving numerous optimization problems. Rather, the framework learns the optimal policy by running the simulation and evaluating the objective function. The optimal policy generated by the algorithm enables designers to make optimal decisions under any possible future uncertainty. The uniqueness of this paper is that our proposed framework uses a Deep Q-learning to find the optimal design of an engineered system when the performance of the system is evaluated with a Monte Carlo simulation and multiple sources of uncertainty influence the performance and desirability of the system.

6.2 Future Research

Engineering systems may operate in an unstable and dynamic environment under high uncertainty. Designers should find the optimal initial design and they should also take appropriate actions in the future to modify the initial design. Owners and operators may need to make decisions at different points in time during a system's lifecycle. Simulation models can evaluate the system's performance during a highly uncertain environment and be used to support and inform decisions about the system. Reinforcement learning algorithms are powerful techniques to help designers to make decisions over time as these algorithms seek to learn the uncertain environments and make the best decisions based on the available information and previous experiences. These algorithms can facilitate decision-making processes for engineering system design. The use of reinforcement learning algorithms to solve dynamic decision making problems represents a fruitful area of study.

Future research could focus on improving the quality of the solution at each iteration of Deep Q-learning. Optimization algorithms such as Bayesian optimization can be combined with the epsilon greedy algorithm to find a better decision at each iteration which could generate the optimal policy in a shorter time than the original Deep Q-learning algorithm.

Hyperparameter optimization methods such as grid search and genetic algorithms can be utilized to find the optimal design for the neural network. These methods can help the decision maker to find the optimal combination of the number of layers and the neurons of the neural network.

Instead of estimating the Q-value for each decision (action) at each state, new algorithms can be developed to estimate Q for any continuous decision variable. Further research could apply new reinforcement learning techniques such as policy gradient and actor-critic to solve a multi-stage stochastic problem with continuous decision variables. These methods could be used to solve complex design problems where the decision space is continuous and many constraints exist.