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Novel Optimization Approaches for Integrated Design and Operation of Smart Manufacturing and Energy Systems

A Dissertation Presented to the Graduate School of Clemson University

In Partial Fulfillment of the Requirements for the Degree Doctor of Philosophy Chemical Engineering

> by Alphonse Hakizimana December 2019

Accepted by: Dr. Joseph K. Scott, Committee Chair Dr. Rachel Getman Dr. Sandra D. Eksioglu Dr.Burak Eksioglu Dr. Sapna Sarupria

Abstract

This dissertation contributes novel theoretical results that enable the use of efficient optimization algorithms for the design of energy and manufacturing systems with high operational flexibility. Operational flexibility is a central theme of the smart grid and smart manufacturing paradigms because it enables systems to optimally adapt to highly dynamic and uncertain operating environments. Such environments are increasingly prevalent in the energy and manufacturing industries due to factors such as the increasing use of variable renewable energy resources (e.g., wind and solar) and the potential benefits of responding quickly to variations in product demands, real-time electricity markets, etc. For systems such as microgrids, combined heat and power plants, multiproduct chemical plants, and biorefineries, such flexibility has the potential to provide huge economic and environmental benefits. However, it also requires systems to make substantial changes in their operating modes of process equipment (e.g., on/off) or the portfolio of products being produced.

Designing systems with such operational flexibility requires consideration of the short-term operational details (e.g., minutes to hours) and future uncertainties that will affect system's performance over its entire lifetime (e.g., decades). This gives rise to a complex optimization problem called integrated design and operation under uncertainty. This problem is complex mainly because the long-term design decisions of interest are tightly coupled with a very large number of short-term operational decisions that must be made over many operational periods and under significant uncertainty. Moreover, these operational decision are mixed-integer decisions, which are particularly challenging for optimization, because they are used to model both discrete and continuous changes in operations. Unfortunately, such problems cannot be solved both accurately and efficiently by standard mathematical programming approaches without major simplifications. At the same time, simplifications that are computationally tractable significantly reduce the level of operational detail that can be captured by the optimization model, which often result in system designs that are sub-optimal or even infeasible for real operations.

An alternative approach, which we refer to as the simulation-based optimization (SO) approach, is to evaluate candidate system designs using a stochastic simulation of the system's operations over all operational periods and in multiple uncertain scenarios. The design problem is then solved by optimizing the output of this simulation with respect to the design decisions. This approach is scalable to models with much more operational detail in terms of the number of operational periods and the number of uncertain scenarios considered, both of which are essential for representing operational flexibility. However, this approach results in highly complex and discontinuous optimization problems due to the discrete decisions that are made within the simulation to represent short-term operations. Hence, solving this formulation usually requires heuristic gradient-free optimization algorithms that are extremely inefficient for high-dimensional problems and offer no theoretical guarantee of finding an optimal design.

To address these challenges, this dissertation presents novel theoretical results that enable the SO formulation to be solved much more efficiently using gradient-based local optimization algorithms. In contrast to the common practice of approximating the cost function as a finite sum of costs associated with discrete uncertain scenarios (i.e., sampleaverage approximation), we instead model the cost as the true expected value over all possible scenarios described by a continuous probability distribution. In this context, our key insight is that averaging over uncertain scenarios is a smoothing operation, and hence this expected cost can be a smooth function of the design decisions despite the fact that sample average approximations are discontinuous. When this is true, the SO formulation can be solved efficiently using gradient-based optimization methods. In Chapter 2, we develop this approach assuming that the operational decisions within the simulation are made with a logical control policy that is specified a priori. Specifically, we consider a type of controller called an energy management policy that is in common use in microgrid simulations. We then derive and rigorously prove two sets of sufficient conditions on the energy management policy under which the expected cost of the simulation is smooth. We demonstrate that these conditions are easily verifiable and often satisfied in practical applications. Finally, we implement different gradient-based algorithms, including a custom-made stochastic gradient descent algorithm, to solve the SO formulation for a representative example problem and show that this approach significantly outperforms derivative-free algorithms in both computational speed and solution quality.

In Chapter 3, we extend this approach to address a much more general mathematical programming formulation of the integrated design and operation problem called multistage stochastic programming (MSP). We argue that this general MSP formulation can be accurately approximated by making all operational decisions using a parameterized mixed-integer decision rule, which reduces the MSP to an SO problem that can be solved efficiently as in Chapter 2. We then extend the smoothness conditions developed in Chapter 2. To develop this approach, we first propose a very general class of mixed-integer decision rules that is flexible enough to approximate near-optimal operational decisions for general MSPs, and then extend the sufficient conditions developed in Chapter 2 to rigorously establish smoothness of the resulting SO approximation. The resulting sufficient conditions are significantly more general than those in Chapter 2, and therefore apply to a much larger class of problems. We then show that these conditions are often satisfied in practice, and that they can always be made to hold by randomizing the decision rule. Finally, we implement different gradient-based algorithms to solve the SO approximation for a representative example problem and show that this approach significantly outperforms derivative-free algorithms in both computational speed and solution quality. Overall, the novel theoretical results developed in this dissertation are shown to enable efficient solution of significantly larger integrated design and operation problems than could be solved by existing approaches.

Dedication

This dissertation is dedicated to my whole family, but especially my loving parents. Their enduring sacrifices and encouragement made it possible for me to escape from a small village in Rwanda to becoming one of the best high school students in the entire country. This led to the opportunity for a scholarship to attend college in the US which, in return, led to yet another opportunity to attend graduate school at Clemson University. Without their initial financial support and their continual encouragement and belief that I was "smart", I would probably never have gotten to receive the honor of becoming the very first family member to earn a PhD.

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Chapter 1

Introduction

This dissertation concerns the development of novel optimization algorithms for solving the problem of integrated process design and operation under uncertainty. Our main motivation for considering this class of problems is to address the optimal design of highly *flexible* manufacturing and energy systems. Flexible systems are defined here as systems with the ability to make substantial changes in their operating mode, including discrete changes in the assignment of equipment to tasks or the portfolio of products being produced, over short time-scales in order to accommodate or exploit variability in the systems operating environment. Variability in the operating environment may arise from the use of variable renewable power sources or feedstocks, participation in real-time markets, contingencies, etc. For such systems, making optimal design decisions requires detailed consideration of how the system will operate under uncertain future conditions therefore, the design decisions are coupled with operational decisions, leading to the class of integrated design and operation problems considered here.

1.1 Motivation for Flexible Manufacturing and Energy Systems

By some estimates, the global energy demand is expected to increase by a staggering 53% from 2008 to 2035 [1]. Meeting this rapidly increasing demand is an outstanding challenge that is aggravated by the environmental and economic concerns surrounding traditional energy generation technologies, which are primarily based on fossil fuels [2]. Tackling this challenge requires a paradigm shift towards more energy efficient operations and the integration of cheap renewable resources in both the power generation and manufacturing industries [3, 4]. Enabling energy and manufacturing processes with much higher *operational flexibility* is essential for making this shift [5, 6]. Systems with this feature can achieve more economical and efficient operations because it endows them with the ability to optimally adapt to highly dynamic and uncertain operating conditions [5, 7, 8] that are increasingly prevalent in the power and manufacturing industries [8–10].

In the power generation industry, renewable energy from wind and solar resources is projected to be the fastest growing contributor to U.S. electricity generation, increasing by nearly 120% from 2015 to 2040 [11]. However, despite their promise of enormous socioeconomic benefits, wind and solar are geographically distributed and highly intermittent (i.e., variable and uncertain), with unpredictable fluctuations occurring over time scales from minutes to hours [12]. This makes their integration at large scales tremendously challenging because the existing power grid is designed for centralized on-demand power generation and has slow dynamic response capabilities [3]. To address this challenge, the power industry is considering major transformations, including the adoption of distributed microgrids and other *smart grid* technologies [13–15], with the potential to enable more flexible and efficient operations. Microgrid systems are autonomous power systems capable of operating in isolation from the grid by pairing local loads and resources. Thus, they are widely regarded as a key technology for enabling efficient integration of distributed renewable energy [3]. However, designing microgrids that can deal with the highly variable and uncertain nature of wind and solar resources is still a challenge. Specifically, dealing with this intermittency requires microgrids to coordinate multiple generation, storage, and back-up units (photovoltaics, wind turbines, diesels, batteries, hydrogen storage, etc.) and to make real-time decisions about which of these units to use based on the current demand and renewable resource availability [16, 17]. These decisions consist of discrete statuses (e.g., on/off) and power set-points that must made on the order of minutes to hours for each generator, storage unit, and controllable load [12]. Moreover, these decisions must be made while also enforcing operational limits on each unit (e.g., minimum uptime/downtime and ramp up/down constraints). Therefore, making these decisions requires solving a complex online control problem (e.g., unit commitment [18]) to coordinate these units so that the demand is met reliably and at the lowest cost despite the fluctuations in wind and solar power generation. However, although these features have the potential to enable microgrids to operate flexibly, the adoption of microgrids is currently hindered by the fact that flexible operations are impractical to achieve unless considered during the design stage of the system [19, 20]. This is true because operational flexibility is a function of the system design. To see this, suppose for example a microgrid system experiences a generator unit failure, a sudden drop in renewable energy generation, or a sudden increase in power demand. To cover such situations, the system needs to capitalize on back-up generators or energy storage units (thermal or battery) [5, 9, 21, 22]. But, these units must already be built in the system design. Thus, design decisions are coupled with operational decisions that have to be made by solving the complex online control problem. Unfortunately, this gives rise to a complex integrated system design and operation problem that cannot be solved both accurately and efficiently by the existing optimization approaches. Efficient approaches often require making major simplifications of operational details, which leads to very expensive, overly conservative designs, hindering advancements in the adoption of microgrids. The novel approaches developed in this dissertation will enable the efficient solution of this problem to achieve more economical designs and therefore, to advance the adoption of microgrid systems.

Operational flexibility is also a critical feature of major transformations, under the umbrella of *smart manufacturing* technologies [23] being considered in the manufacturing industry, which accounts for more than 30% of global energy consumption [24]. By some estimates, smart manufacturing technologies could save a staggering \$10–15 trillion globally by 2035, including \$7–25 billion/year in energy costs alone [25, 26]. However, the realization of this promise will require more flexible operations in systems such as multiproduct chemical manufacturing plants, bio-refineries, and smart utility systems for energy-intensive chemical manufacturing processes. Multiproduct chemical plants and bio-refineries consume low-value raw materials/feedstock to produce multiple high-value products. The ability to enable operational flexibility in these systems, e.g., by increasing their production ramp up/down capabilities, can potentially endow them the ability to adapt to short-term fluctuations in product demands, market prices, raw material/feedstock availability, processing times, and process yields, which can result in significant economic and efficiency gains [27– 32]. Flexible smart utility systems can also offer similar benefits. For example, combined heat and power (CHP) systems produce power while simultaneously recovering heat, a byproduct that usually goes to waste. This heat can then be used to make other useful products, such as steam at different pressures [33]. This heat recovery allows CHPs to boost their energy efficiency by up to 40% relative to separate production of heat and power [34]. The ability to design flexible CHP systems (e.g., CHPs that can quickly ramp up/down their power output) can potentially enable them to be used as highly efficient smart utility systems that endows energy-intensive chemical processes (e.g., pulp and paper mills) the ability to exploit volatile electricity prices in real-time [33, 35]. This can lead to significant economic savings because these processes can use the CHP when prices are high and can use power from the grid when prices are low. However, as in the case of microgrids, the design of flexible multiproduct chemical plants, bio-refineries, and smart utility systems requires coordination of multiple components in order to accommodate multiple resource inputs and product outputs, both of which can be highly variable and uncertain due to external or internal fluctuations [5, 15, 36]. For example, multiproduct chemical plants require multi-

ple multipurpose processing units to accommodate various product demands and achieve optimal operation. However, the adaptability of these plants to short-term fluctuations in, for example product demands, depends heavily on their ability to quickly decide appropriate levels of their production rates and which of the processing units to use in each task involved in the production of each product. This results in a complex operational problem (e.g., adaptive/reactive scheduling) [10, 36]. At the same time, operational adaptability is a function of the system design. To see this, suppose an unpredicted increase in a product demand occurs during the operation of some process in the plant. To accommodate this increase, the process must adapt by ramping up its production. However, it cannot ramp up beyond its capacity, which is fixed by its design. Therefore, system design decisions are coupled with the complex operations, which leads to an unresolved integrated design and operation problem. The inability of existing approaches to accurately solve this problem leads to system designs that are unable to adapt in uncertain and dynamic operating conditions. The efficient approaches developed in this dissertation to solve this problem will lead to the effective design of flexible systems, which will immensely contribute to the realization of the promise of smart manufacturing technologies.

From these discussions, it is clear that smart manufacturing and energy systems have huge potential to address environmental and economic concerns surrounding traditional manufacturing and energy generation technologies. However, the ability to design systems that can operate flexibly in dynamic and uncertain environments is critically important. Unfortunately, designing such systems requires coordination of multiple components which increases the complexity of system operations that must be coupled with design decisions. This leads to a complex integrated design and operation problem that remains unresolved, hindering the advancement in the design and adoption of flexible systems. This dissertation addresses this issue by developing efficient solution approaches for complex integrated design and operation problems.

1.2 Review of Existing Approaches and Challenges

The main objective of this dissertation is to develop novel mathematical modeling and optimization algorithm to advance the design (e.g., process unit sizing and technology selection) of highly flexible manufacturing and energy systems. As discussed in the previous section, this requires making design decisions with the consideration of both the future uncertainties that will affect system operations. Unfortunately, this gives rise to an integrated design and operation problem with the following features that make standard mathematical programming formulations practically intractable and therefore raising the need for novel formulations and optimization strategies for its solution:

- (i) Relevant operational details and uncertainties often occur on time-scales much shorter than the lifetime of a system [15, 36–38]. For example, the value of an energy storage system with a lifetime of 10 years may depend critically on its ability to enhance responsiveness to hourly variations in electricity pricing or renewable power generation [36, 39]. This results in problem formulations with very many operational time periods (e.g., hundreds or thousands) in each of which operational decisions must be made.
- (ii) Many critical operational decisions are discrete (e.g., adaptive scheduling and unit commitment) [10, 18, 36], resulting in problem formulations with mixed-integer decisions.
- (iii) Many important uncertainties are best described by continuous random variables with significant variance, resulting in problem formulations that are not easily approximated using a few discrete uncertainty scenarios (e.g., demands, natural resource availability, process yields, etc.) [40–42].

The integrated design and operation under uncertainty is a minimization problem that aims to find a system design (i.e., component sizes and technology selection) that minimizes the investment cost plus the expected value of the sum of operational costs that the system will incur in each operational time period/stage (e.g., fuel cost associated with the decision to run a diesel generator in each hour) over its entire lifetime (e.g., decades). Notably, the values of these stage costs depend on the realized value of the uncertain inputs. For example, a low power demand realization requires less power from a diesel generator, which gives a lower fuel cost. The opposite happens for a high demand realization which requires more fuel, resulting in a higher fuel cost. The expected value accounts for all possible future scenarios, and hence is an appropriate measure of system performance. Therefore, the problem of integrated design and operation under uncertainty is typically formulated using stochastic models expressed in the framework of either mathematical programming or simulation-optimization.

1.2.1 Stochastic Mathematical Programming Approaches

The integrated design and operation problem can be formulated using two main mathematical programming models, namely multistage stochastic programs (MSPs) and stochastic multilevel programs (SMLPs), both with mixed-integer operational decisions in all periods. Note that, in the settings of the integrated problems we consider in this dissertation, a stage in the term multistage and a level in the term multilevel pertains to an operational period. In both formulations the operational decisions are *recourse* decisions, meaning that they are made after an uncertainty realization has occurred, as opposed to the design decisions which are made without knowledge of the uncertainty. The objective function in both of these models consists of the investment cost and the expected value of the sum of the operational costs in all operational periods. The minimization of this objective with respect to the design decisions is subject to operational constraints that include a dynamic model that represents how the system state (e.g., product inventory level, battery state of charge) evolves over each period, and flexibility constraints such as minimum uptime/downtime and ramp up/down constraints for units in the system. Both models allow some of the operational constraints to be enforced in a probabilistic sense as chance constraints. In general, however, MSPs are distinct from SMLPs in that SMLPs include at least one optimization sub-problem in their constraints while MSPs do not. For the integrated problems of interest here, MSPs will have as many stages as the number of operational periods and SMLPs will include an auxiliary optimization sub-problem for each operational period, while MSPs do not. Furthermore, in MSP models, the recourse decisions are *free*, meaning that they are not enforced by some control law. In contrast, SMLPs enforce a control law which is often represented by the auxiliary sub-problem. In fact, the auxiliary sub-problem is often introduced in order to represent an advanced control strategy that will be used to make operational decisions once the system is built. For example, model predictive control (MPC) is an advanced control strategy that is widely used for the operation of energy systems such as microgrids and CHPs [43–45] and for the dynamic control of multi-product chemical manufacturing processes [36, 46, 47].

However, despite this difference, MSP and SMLP models have two more important features in common. Specifically, in both models, all of the operational decisions in all of the operational periods are taken as optimization variables in the overall problem. Moreover, to model system adaptability in uncertain conditions, these operational variables naturally take different values for different uncertainty scenarios, making them functions of the uncertainty. An obvious unfavorable consequence of this is that the optimization problems resulting from both these formulations scale in the number of operational periods and uncertainty scenarios considered, both of which can be extremely large due to features (i) and (iii). Combined with nonlinearities in system models and the presence of integer operational decisions (feature (ii)), the standard scenario-based solution paradigm (i.e., sample average approximation), which consists of sampling discrete scenarios and co-optimizing design decisions with operational decisions for every stage and every scenario, easily results in huge mixed-integer nonlinear programs (MINLPs) (e.g., hundreds of thousands of optimization variables) that are far beyond the capabilities of existing optimization solvers.

In some special cases (e.g., linear models and no integer decisions), decomposition and reformulation techniques exist that can help alleviate the computational burden of these models. Moreover, a few rigorous decomposition methods have recently been developed for general models with mixed-integer decisions and non-convexities [48–50]. Unfortunately, these are still nascent and have significant limitations that prohibit their use for problems with features (i)–(iii) (e.g., their computational cost is relatively high; they only apply to MSPs with two-stages; they impose restrictions on which stage/level can have continuous or integer decisions [48, 51–53]). Furthermore, SMPLs can be transformed into single-level optimization problems using reformulations that replace the lower-level sub-problems by their KKT conditions [54–57] or their explicit multiparametric solutions [58–62]. However, the KKT reformulation does not work when the sub-problems are non-convex because KKT conditions are necessary but not sufficient for optimality in these cases. The sub-problems are non-convex in the integrated problems of interest here because of feature (ii), which dictates the presence of discrete operational decisions in the sub-problem (e.g., hourly decisions to turn generators on/off by solving a unit commitment optimization sub-problem [43]). Moreover, the multiparametric programming approach does not scale well to problems with a large number of parameters. This is true because the number of equations and inequalities characterizing the multiparametric solution can potentially grow exponentially in the number of problem parameters [10, 63], leading to prohibitively large reformulations. In our case, a large number of variables parameterizing each sub-problem (e.g., system design variables, system state variables, and uncertain variables) is likely to occur due to the complexity of flexible manufacturing and energy systems as described above (e.g., multiple source of uncertainties and multiple process units).

In the light of these issues, tractable approximations are often achieved through aggressive simplifications of features (i)–(iii). For MSPs, such simplifications include lumping operational periods into a few [40, 64]; relaxing integrality of the operational decisions [65, 66]; using deterministic approximations [37, 65] that make operational decisions with perfect foresight rather than under uncertainty; using linearized rather than realistic nonlinear models [15, 37]; aggregating uncertainty scenarios in each operational period into a few [67, 68]; decoupling consecutive operational periods using static process models [64, 69]; etc. Notably, similar simplifications are often adopted for SMLPs [54–57]. Critically, although these simplifications may significantly reduce the size of the problem and are appropriate in some applications, they are not appropriate for the problems of interest here because they degrade the optimization model in exactly the aspects that are most essential for assessing operational flexibility and system responsiveness in dynamic and uncertain environments. Thus, these simplifications may lead to system designs that are highly sub-optimal or even infeasible in real operating conditions. Consequently, simulation-optimization approaches have been considered in the literature as an alternative to formulate integrated problems in an efficient way that retains the critical operational flexibility details in these problems.

1.2.2 Decision Rule-Embedded Simulation-Optimization (DR-SO) Approaches

Simulation-optimization (SO) approaches are widely regarded as the most general and natural approaches to formulate complex problems of integrated design and operation [70–73]. A typical SO formulation consists of an outer optimization problem over the design decisions and an *inner* stochastic time series simulation that is used to evaluate the expected operational cost and constraints of the outer problem. For any fixed system design, the simulation mimics how the system will be operated once it is designed and implemented. In practice, the systems we consider are operated using a decision rule (DR). Loosely speaking, a DR can be thought of as an explicit expression with a fixed functional form that is executed using as input the available data in the current operational period (e.g., the uncertainty realization and system state) to produce values of the operational decisions in that period. For example, an energy management policy (EMP) is a set of logical rules that are typically used to determine when and how each component in a microgrid system is used [16]. A typical EMP rule involves setting thresholds on the system state (i.e., battery state of charge) and the available net power (i.e., difference between power demand and power from renewable resources such as wind and solar) and deciding on/off statuses of other components (e.g., generators) based on whether those thresholds are exceeded or not. Besides microgrid systems, DRs are used in other practical applications. For example, hedging rules are used in water resource management [74] and dispatching rules are used in flexible manufacturing systems [75, 76]. To mimic this practical DR-based operation for a fixed system design and uncertainty scenario (i.e., a time series of sampled uncertainty in each period), systems of interest are typically simulated using a time-stepping process that sequentially executes the DR in every operational period to determine mixed-integer operational decisions. The latter are then used to compute the operational costs (e.g., fuel cost for running a generator). Such a process constitutes one stochastic simulation that can be performed multiple times to approximate the expected operational cost using the standard sample average.

Compared to the MSP and SMLP formulations, the critical advantage of the decision-rule embedded simulation-optimization (DR-SO) formulation is its high scalability to problems with very many operational periods and uncertainty scenarios. In particular, specifying a DR can be regarded as an offline specification of the operational decisions for each period and scenario, which are all optimization variables in the MSP and SMLP formulations. Therefore, the size of the outer optimization problem in the DR-SO formulation is completely independent of the number of operational periods and uncertainty scenarios. Thus, in contrast to the MSP and SMLP models that would have hundreds of thousands of decision variables due to features (i)-(iii), the DR-SO formulation will have very few optimization variables, including only the design decisions and a few more variables that might be desirably added to parametrize the DR in attempt to enhance the quality of operational decisions that it provides. Thus, the DR-SO formulation can accommodate relatively many scenarios an operational periods as required by features (i) and (iii). This claim is further justified by the fact that the computational cost of each stochastic simulation scales only linearly in the number of operational periods and the computational cost of a sample average approximation of the expected cost increases linear in the number of scenarios considered. Furthermore, the DR-SO formulation offers tremendous modeling flexibility because it can readily accommodate realistic nonlinear and nonconvex models, all of which would further complicate the MSP and SMLP formulations. Hence, the DR-SO formulation is seemingly more likely to provide higher-quality designs since many of the aggressive simplifications required to make MSP and SMLP formulations tractable are no longer necessary. In fact, on the basis of these advantages, the DR-SO formulation is the backbone of many popular energy systems sizing softwares such as HOMER [73].

However, although decision-rule embedded simulations are undeniably well-suited for effective modeling of features (i)–(iii), the solution of DR-SO problems is not well addressed by existing solution approaches. This is due to the fact that the outer optimization problem in the DR-SO formulation is often extremely complex despite being lowdimensional. Specifically, the critical drawback of the DR-SO approach is that the integer operational decisions made by the embedded DR make the simulated cost and constraint functions discontinuous with respect to the outer optimization variables (i.e., design decisions and DR parameters) for any fixed uncertainty scenario. This is true because the DR is a function of these decision variables and so, a perturbation of any of these variables may cause the DR output to jump from one discrete operational decision value to a different discrete value. Clearly, this jump will cause a discontinuity in the operational cost. Since this may occur for every operational period and every simulated scenario, the number of such discontinuities can be huge because of features (i)–(iii). Consequently, a sample average approximation (SAA) makes the DR-SO problem extremely irregular and difficult to solve. As a result, in practice, DR-SO are commonly solved using human-guided trial-and-error approaches, or by exhaustively evaluating a set of candidate designs, as is done in HOMER [73]. Furthermore, population-based heuristic algorithms (e.g., particle swarm optimization, genetic algorithms, tabu search, etc.) are used extensively in practice [72, 77, 78]. This is due to the fact that these approaches are *black-box* approaches, meaning that the optimizer simulates candidate system designs, but without exploiting any mathematical structure of the simulation model. Consequently, these approaches are extremely easy to implement and are broadly applicable, even for complex simulations with highly discontinuous outputs. Unfortunately, however, these approaches are not guaranteed to find an optimal solution finitely. Moreover, since these approaches do not use derivative information which, whenever available, is critical in guiding the solution search, they often suffer from slow convergence compared to gradient-based algorithms [79, 80]. Thus, in practice, derivative-free methods often require prohibitive computational effort and may locate sub-optimal solutions, particularly for high dimensional problems [72, 78].

To summarize the discussion above, the DR-SO approach addresses many challenges associated with mathematical programing formulations highlighted above. However, the outstanding issue we aim to address in this dissertation is that the presence of discrete operational decisions makes DR-SO formulations highly discontinuous, making them unsuited for gradient-based algorithms which are much more reliable and computationally efficient relative to gradient-free approaches.

1.3 Thesis Contributions

The central insight we aim to lay out rigorously in this dissertation is that, despite the fact that integer operational decisions unavoidably introduce many discontinuities in the DR-SO problem through the actions of the DR in each time period and for any fixed finite number uncertainty scenarios (i.e., SAA), the *true* expected-value over all possible scenarios described by a continuous probability distribution might be nonetheless smooth. When the smoothing happens, the overwhelming discontinuous character of the finite-sample SAA is entirely eliminated. In this case, simulations will return stochastic estimates of the smooth function rather than the discontinuous one. Therefore, the DR-SO problem is amenable to stochastic gradient-based solution algorithms, which are expected to significantly outperform heuristic gradient-free approaches. However, despite that some smoothing may occur due to the inherent smoothing property of expectation, this is not generally guaranteed. Overall, this dissertation is dedicated to the discovery of novel, easily verifiable, non-restrictive, and sufficient conditions that will always guarantee smoothness of DR-SO problems and the development of a general framework that capitalizes on the combination of these conditions and the DR-SO formulation for a more effective solution of the otherwise intractable MSP models. Our first contribution is given in Chapter 2 and consists of a set of sufficient conditions that always guarantee smoothness of DR-SO problems for a special class of mixed-integer DRs commonly used for microgrid systems operations. The second contribution of this dissertation is given in Chapter 3. In this chapter, we extend the conditions developed in Chapter 2 to a much more general class of mixed-integer DRs. The main objective of this chapter is to demonstrate that the application of DRs belonging to the proposed class and satisfying the extended conditions endows the DR-SO approach the ability to be used as a highly efficient solution approach for MSPs that are intractable by any other means. These contributions are detailed in their respective chapters, but we give a brief summary for each in the following subsections.

1.3.1 Smoothness of DR-SO Problems for Microgrids Application (Chapter 2)

In Chapter 2, we consider the problem of integrated design and operation of microgrid energy systems under uncertain time-series of power demand and solar energy generation. This problem is formulated as a DR-SO and we adopt a typical microgrid simulation paradigm in which mixed-integer operational decisions (e.g., on/off statuses and power set points of each microgrid component) are made on a hourly basis over a year using a class of threshold-type DRs called *energy management policies* (EMPs) [16]. The objective function of this problem consists of the capital cost for buying system components (e.g., PVs, battery banks, and diesel generators) and the expected operational cost (e.g., fuel cost and penalties for unmet demand) computed using the yearly randomized time series simulations. We first introduce the typical microgrid simulation as a discrete-time stochastic hybrid system (DTSHS). This model is based on an EMP-type class of DRs consisting of checking the signs of a set of smooth threshold functions that may depend arbitrarily on the system state, the current uncertainty, and the design decision variables. Each of these signs corresponds to a binary outcome which is directly related to the operation of the system. In fact, one subset of these binary outcomes will represent the actual discrete operational decisions (e.g., on/off statuses of generators) and the other subset will indicate operational events (e.g., battery overcharge, power surplus/power deficit) that are used in determining other useful operational information (e.g., penalty cost for unmet demand or overcharging a battery). DTSHSs emerge as a result of using these binary outcomes as inputs to the system's dynamic model responsible for updating system state in every hour of the year.

Consequently, the DR-SO formulation we consider involves an expected-value minimization subject to DTSHSs. It is important to note that the class of EMP-type DRs we consider are discontinuous since their outcomes are binary sequences. Therefore, these DRs cause many discontinuities in the SAA of the DR-SO problem, which then has to be solved using heuristic gradient-free algorithms with well-known limitations. In the interest of enabling more efficient optimization approaches, we consider the important question of whether or not the expected-cost is a continuously differentiable function of the design decision and the EMP rule parameters. Our findings in answering this question show that the expected-value of the cost function is continuously differentiable under very general conditions requiring that (1) the uncertain variables are continuously distributed, and (2)the smooth threshold functions defining the EMP satisfy a set of non-degeneracy conditions that we characterize theoretically. We demonstrate the verification of these conditions for some representative microgrid models and we also highlight particular model features and EMP rules that may lead to violations of these conditions. Finally, we present optimization results for illustrative microgrid design and capacity expansion examples in which we show that even an immature stochastic gradient-descent algorithm outperforms state-of-the-art gradient-free approaches in both computational efficiency and solution quality.

1.3.2 The DR-SO Approach to Multistage Stochastic Programs (Chapter 3)

Chapter 3 extends the approach developed in Chapter 2 to address general MSP formulations of the integrated design and operation problem in which a specific decision rule is no longer specified as part of the problem statement. The key idea is to use a more flexible general class of parameterized mixed-integer decision rules to obtain an accurate

approximation of the original MSP in the form of a DR-SO problem. As discussed in the previous sub-section, this approximation will be tractable provided that this class of DRs results in a smooth DR-SO problem. The extensions of the results from Chapter 2 are necessary because the class of DRs proposed there and the sufficient conditions developed there impose many restrictions that limit their application to the general MSPs we consider. For example, the conditions are violated by DRs defined by threshold functions that enforce minimum uptime/downtime constraints. In practice, enforcing these constraints is often required for some system units, but also enforcing them in the problem is essential for representing operational flexibility. As our first contribution, we propose a general class of mixed-integer DRs that is flexible in that it provides a general framework for modeling many decision rules found in the literature. These include linear and nonlinear decision rules found in the robust optimization literature [81–86], and logic controllers such as the EMPtype rules considered in Chapter 2 for microgrid systems operations, hedging rules in water resource management, and dispatching rules in flexible manufacturing [16, 74, 75]. The basic structure of the proposed class of DRs uses the idea that mixed-integer operational decisions (i.e., the recourse decisions) can be determined through a process that involves a step consisting of checking the signs of a set of smooth threshold functions. Thus, this class has some relation to the class proposed in Chapter 2. As our second contribution, we develop a new set of sufficient conditions on the proposed class of DRs that guarantee continuous differentiability of the DR-SO problem. The new set of conditions are a relaxation of the conditions developed in Chapter 2. Notably these new conditions are still only imposed on the threshold functions defining the DR. More importantly, the added relaxations enable use of DRs with threshold functions that depend on discrete system states. Discrete states are allowed by the general MSP model we consider and are typically required to enforce operational flexibility constraints such as the minimum uptime/downtime constraints which are usually enforced by a suitably constructed DR. Consideration of DRs involving discrete states is not possible with the conditions developed in Chapter 2. Moreover, note that smoothness of the DR-SO problem requires smoothness of both the expected value and chance constraints functions, all of which are part of the general MSP model we consider. As our third contribution, we apply the new sufficient conditions to address smoothness of chance constraints, which were not treated in Chapter 2. For our final contribution, we provide a trivial, but systematic way to modify any DR of the proposed class such that the resulting DR is free of any violations of the conditions developed in both Chapter 2 and 3. Notably, although this modification guarantees that the conditions in Chapter 2 will always hold, it relies on randomizing the DR with violations. Unfortunately, this randomization might not be desirable in some important practical cases. For example, randomizing DRs that enforce minimum uptime/downtime constraints will lead to the violation of these constraint with a non-trivial probability. However, the new conditions developed in Chapter 3 are able to prevent many of such undesirable randomizations. Using an illustrative twoproduct manufacturing inventory system design example, we demonstrate the application of these contributions. In particular, we show that significant improvements in the optimization results are obtained with an algorithm that relies on differentiability of the DR-SO problem as compared to state-of-the-art gradient-free algorithms.

Chapter 2

Differentiability Conditions for Stochastic Hybrid Systems with Application to the Optimal Design of Microgrids

2.1 Abstract

This chapter considers the regularity of expected value minimization problems subject to discrete-time stochastic hybrid systems. A primary motivation is the optimal design of microgrids subject to detailed operational simulations with renewable resources and discrete dispatching. For such problems, hybrid behavior can make the cost function discontinuous for any fixed realization of uncertainty, which has led to the widespread use of derivative-free optimizers with well known limitations. In contrast, we provide sufficient conditions under which the expected value of the cost is continuously differentiable. We verify these conditions for a simple example and show promising preliminary optimization results using a stochastic gradient-descent method.

2.2 Introduction

This chapter considers expected value minimization problems subject to discretetime nonlinear dynamic systems with stochastic inputs and hybrid discrete-continuous behavior. The optimization of hybrid systems arises in chemical processing, systems biology, and robotics to name only a few [87]. However, the formulation here is largely motivated by the problem of integrated planning and scheduling under uncertainty, which arises broadly in power systems, multiproduct chemical plants, flexible manufacturing, etc. [37, 88]. Such problems aim to co-optimize long-term investment decisions with mixed-integer operational decisions that occur on much shorter time-scales. In full generality, these are multistage stochastic programs with mixed-integer recourse, and are intractable without major simplifications when many stages are considered [40]. Unfortunately, this makes it difficult to model process operations in sufficient detail when optimizing important investment decisions [88]. However, in many applications it is sensible to formulate an explicit decision rule that determines (suboptimal) operational decisions in each stage and scenario, e.g. by checking a set of logical conditions or thresholds. In many cases, such rules describe how the system will be operated in practice, which is rarely optimal (e.g., energy management policies in microgrids, dispatching rules in flexible manufacturing, and hedging rules in water management [16, 74, 75]). In other cases, such rules approximate optimal operations (truly optimal rules are sometimes computable via multi-parametric programming) [10, 89]. In principle, decision rules greatly simplify integrated planning and scheduling problems by eliminating a potentially huge number of recourse decisions and producing a single stage approximation. Indeed, for multistage linear programs with continuous recourse, decision rules often lead to simple linear or second-order cone programs [82]. However, problems with integer recourse require discrete decision rules, for which existing approaches lead to much more demanding reformulations (e.g., semi-infinite mixed-integer programs in [90]). In general, substituting a discrete decision rule into the operational dynamics of a system results in a stochastic hybrid system. Accordingly, there is significant interest in efficient algorithms for optimizing such systems.

Given a stochastic hybrid system and an associated cost, the goal of this work is to determine when the expected value of the cost is differentiable, and hence amenable to efficient optimization by gradient-based methods. To see the significance of this question, note that the hybrid behavior can make the cost discontinuous when evaluated at a *fixed* realization of uncertainty (i.e., scenario). For example, in integrated planning and scheduling, a perturbation of a planning decision may induce a change in a discrete operational decision through the action of an embedded decision rule. Moreover, such discontinuities can arise in every operational stage, and every scenario. Thus, the common approach of optimizing a sample-averaged cost easily results in a problem with thousands of discontinuities (see $\S2.6$). Clearly, eliminating these through the introduction of binary variables is intractable. Thus, these problems are commonly addressed using derivative-free algorithms [77, 91, 92]. However, while these methods are easy to implement and avoid local minima, they are not guaranteed to find optimal solutions finitely, and do not enjoy the fast convergence of gradient-based algorithms [79, 80]. Thus, in practice, derivative-free methods often require prohibitive computational effort and may locate suboptimal solutions, especially for high dimensional problems.

In contrast, this chapter takes an important step towards gradient-based optimization of stochastic hybrid systems based on the following insight: Although hybrid behavior can introduce discontinuities in the cost for any fixed scenario, the expected value of the cost over a continuous probability distribution may nonetheless be smooth. In other words, while existing optimization formulations using sample-averaged costs with fixed samples are highly discontinuous, minimizing the true expected cost may be a smooth NLP, albeit with a complex objective. This is demonstrated by example in §2.6. To formalize this, we introduce a general class of discrete-time stochastic hybrid systems (DTSHS) and prove two sets of sufficient conditions under which the expected cost is continuously differentiable. We then demonstrate using an illustrative microgrid optimization problem that these conditions are verifiable and broadly applicable. Finally, we show that exploiting noisy gradient estimates in a rudimentary stochastic gradient descent algorithm can lead to significant efficiency gains relative to two standard derivative-free approaches.

The smoothing of discontinuities under the expectation forms the basis for several existing optimization algorithms used in communications, manufacturing, and finance [93, 94]. Unfortunately, existing smoothness results do not address the general form of hybrid system analyzed here. Many results apply to discrete-event systems, which are distinct from the time-driven simulation paradigm used here [95]. Moreover, our systems violate central assumptions in existing results. Infinitesimal perturbation analysis (IPA) fails for discontinuous costs, and the likelihood ratio method only permits decision dependence in the probability density, not in the cost [93]. Smoothed IPA and the 'push-out' method overcome these problems, but require problem specific methods. Weak derivative approaches require abstract assumptions that have only been reduced to verifiable conditions for several academic examples [96]. The article [97] gives differentiability conditions for Markov processes with optimal discrete actions taken in each time-step, but does not address more general discrete events that can occur in hybrid systems. Thus, this chapter develops a new approach to differentiability analysis for general DTSHSs.

2.2.1 Application to the Optimal Design of Microgrids

Microgrids are autonomous power systems capable of operating in isolation from the grid by pairing local loads and resources, and are widely regarded as an enabling technology for the integration of distributed renewable energy [3]. However, the highly variable and uncertain nature of wind and solar resources poses serious complications, often requiring microgrids to coordinate multiple generation and storage technologies (photovoltaics, wind turbines, diesels, batteries, hydrogen storage, etc.) [16, 17]. This gives rise to a complex operational problem in which the discrete status (e.g., on/off) and power set-point for each generator, storage unit, and controllable load must be determined to balance supply and demand on the order of minutes to hours, while also hedging against future uncertainties. This *energy management* problem combines the tasks commonly referred to as unit commitment

and economic dispatch in larger power systems, and is distinct from power management, which concerns power quality control on subsecond time-scales [98]. Energy management decisions strongly impact the economics and reliability of systems with large shares of wind and solar power. At the same time, these decisions are constrained by capital investments, such as storage capacity. Thus, microgrid investment decisions, which typically consider horizons of 20 years or more, are tightly coupled with operational decisions on time-scales of hours to minutes [17].

Microgrid design fits within the broader context of power system expansion planning [69, 99], and is most closely related to formulations with detailed unit commitment constraints [37, 65, 100]. Such problems can generally be cast as multistage stochastic programs [101] in which the load and renewable generation are random variables and unit commitment is modeled by mixed-integer recourse decisions in each stage (e.g., hour). However, solving such problems often requires approximations that can significantly degrade operational detail. For example, long planning horizons are commonly addressed using aggregated, non-chronological representations of the load and resource data (and hence of system operations), such as load-duration or screening curves [64, 69, 102]. In contrast, models with hourly resolution often use simplified unit commitment models that relax binary decisions [65, 66, 103], or consider only a small number of representative days in the planning horizon [37, 104]. In some cases, decomposition methods are also used [66, 105]. Another common but potentially drastic simplification is to consider fixed rather than stochastic load and resource data, which allows operational decisions to be made with perfect foresight [37, 66, 100]. In contrast, many models have considered uncertainty using scenario-based, chanceconstrained, and robust formulations [67, 106–108]. However, very few works have yet incorporated detailed unit commitment models into stochastic formulations [105]. Finally, linearized models are predominantly used to maintain computational tractability [103, 104]. The reader is referred to [109] for further details on expansion planning formulations.

In contrast to larger power systems, detailed operational decisions in microgrids are typically made in practice using a logical controller called the *energy management policy* (EMP) [16]. Moreover, such policies have been widely adopted in microgrid simulation codes that are naturally described as discrete-time stochastic hybrid systems (DTSHSs) [73, 110]. Such simulations typically consider hourly time-steps over a year or more, and are increasingly used to evaluate detailed operational considerations in the context of longterm investment decisions [110]. However, as described above, discrete actions of the EMP can make the system cost highly discontinuous for fixed load and resource data. Likely for this reason, existing approaches for optimizing microgrid simulations have exclusively used derivative-free methods [17, 77, 91, 92]. In contrast, we show in §2.6 that the differentiability conditions for DTSHS proven here hold for a simple but representative microgrid model, and enable significantly faster optimization via gradient-based methods.

2.3 Problem Statement

To avoid cumbersome indexing, we denote scalars and vectors without emphasis and use bold font for sequences $\mathbf{x} = (x_0, \ldots, x_N)$ associated with the discrete-time system below. $B_{\eta}(v)$ is the open ball of radius $\eta > 0$ around v. $C^k(D, \mathbb{R}^m)$ is the set of k-times continuously differentiable maps from D into \mathbb{R}^m . Let $S \subset \mathbb{R}^{n_s}$, $R \subset \mathbb{R}^{n_r}$, and $\ell \in C^k(S \times R, \mathbb{R}^m)$ with $k \ge 1$. For any $(\hat{s}, \hat{r}) \in S \times R$, the Jacobian matrix of $\ell(\hat{s}, \cdot)$ at \hat{r} is $\frac{\partial \ell}{\partial r}(\hat{s}, \hat{r})$ or $\nabla_r^{\mathrm{T}} \ell(\hat{s}, \hat{r})$.

Consider the discrete-time stochastic hybrid system (DTSHS)

$$\sigma_{k,i} = \begin{cases} 1, & \text{if } h_i(k, \sigma_{k,1:i-1}, x_k, w_k, \theta) \le 0, \\ -1, & \text{otherwise} \end{cases}, \quad \forall i \in \{1, \dots, n_\sigma\}, \qquad (2.1)$$

$$x_{k+1} = f(k, \sigma_k, x_k, w_k, \theta), \tag{2.2}$$

with state $x_k \in \tilde{X} \subset \mathbb{R}^{n_x}$, input $w_k \in \tilde{W} \subset \mathbb{R}^{n_w}$, parameters $\theta \in \tilde{\Theta} \subset \mathbb{R}^{n_\theta}$, and discrete mode $\sigma_k \in \{-1, 1\}^{n_\sigma}$. The sets \tilde{X} , \tilde{W} , and $\tilde{\Theta}$ are open, as indicated by the tilde, and we denote $S = \{-1, 1\}$ and $\mathcal{K} = \{0, \dots, N-1\}$ with N > 0. Then, $f : \mathcal{K} \times S^{n_\sigma} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \tilde{X}$ and $h_i : \mathcal{K} \times S^{i-1} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \mathbb{R}$. The functions $h = (h_1, \dots, h_{n_\sigma})$ are called *event* functions. Note that h_i can depend on the discrete outcome of all previous event functions in the same step k, $\sigma_{k,1:i-1} = (\sigma_{k,1}, \ldots, \sigma_{k,i-1})$, and h_1 has no dependence on σ_k . This is necessary for representing, e.g., microgrid EMPs, which often make dispatching decisions sequentially in a single time-step. The reader is referred to §2.6.1 for an example of using (2.1)-(2.2) to model a simple microgrid.

The initial condition x_0 and inputs w_0, \ldots, w_{N-1} are random variables. The case where x_0 has deterministic elements is not considered here, but the necessary modifications are discussed in Remark 2.5.2 in §2.5. Define the shorthand $\boldsymbol{\omega} := (x_0, w_0, \ldots, w_{N-1})$ and $\tilde{\Omega} := \tilde{X} \times \tilde{W} \times \cdots \times \tilde{W}$. Furthermore, let $X_0 := [x_0^L, x_0^U] \subset \tilde{X}$ and $W := [w^L, w^U] \subset \tilde{W}$ be compact n_x - and n_w -dimensional intervals with nonempty interiors, and let $\Omega := X_0 \times W \times \cdots \times W$.

Assumption 2.3.1. $\boldsymbol{\omega}$ has a probability density $p: \tilde{\Omega} \subset \mathbb{R}^{n_x + Nn_w} \to \mathbb{R}$ that is zero outside Ω and continuous on the interior of Ω .

Define the solution map $\phi_k : \tilde{\Omega} \times \tilde{\Theta} \to \mathbb{R}^{n_x}$ by $\phi_k(\boldsymbol{\omega}, \theta) = x_k$, where x_k is the state of (2.1)–(2.2) at k given $(\boldsymbol{\omega}, \theta)$. It will be understood without complicating the notation that ϕ_k depends only on $(x_0, w_0, \dots, w_{k-1})$. Let $\ell_S : \mathcal{K} \times \mathcal{S}^{n_\sigma} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \mathbb{R}$ and $\ell_T : \tilde{X} \times \tilde{\Theta} \to \mathbb{R}$ denote stage and terminal costs associated with (2.1)–(2.2), respectively. Thus, the total cost of a trajectory of (2.1)–(2.2) given $(\boldsymbol{\omega}, \theta)$ is

$$\ell(\theta, \boldsymbol{\omega}) := \sum_{k=0}^{N-1} \ell_S(k, \sigma_k, \phi_k(\boldsymbol{\omega}, \theta), w_k, \theta) + \ell_T(\phi_N(\boldsymbol{\omega}, \theta), \theta).$$
(2.3)

We are interested in the dynamic optimization problem

$$\min_{\theta \in \Theta} \mathcal{L}(\theta), \quad \mathcal{L}(\theta) := \mathbb{E}[\ell(\theta, \omega)] = \int_{\Omega} \ell(\theta, \omega) p(\omega) \mu(d\omega), \quad (2.4)$$

where $\Theta \subset \tilde{\Theta}$ is compact, \mathbb{E} denotes the expected value, and μ is the Lebesgue measure on $\tilde{\Omega}$. Existence of the integral is proven in Lemma 2.4.4.

Assumption 2.3.2. For each $k \in \mathcal{K}$ and $\sigma \in \mathcal{S}^{n_{\sigma}}$, the functions $f(k, \sigma, \cdot, \cdot, \cdot)$, $\ell_{S}(k, \sigma, \cdot, \cdot, \cdot)$, and $h_{i}(k, \sigma_{1:i-1}, \cdot, \cdot, \cdot)$, $\forall i \in \{1, \ldots, n_{\sigma}\}$, are continuously differentiable on $\tilde{X} \times \tilde{W} \times \tilde{\Theta}$ and
$\ell_T \in C^1(\tilde{X} \times \tilde{\Theta}, \mathbb{R}).$

Despite Assumption 2.3.2, the solution ϕ_k and cost ℓ are discontinuous in general due to the discrete events in (2.1). However, it may still happen that $\mathcal{L} \in C^1(\tilde{\Theta}, \mathbb{R})$, enabling the use of gradient-based algorithms to solve (2.4). Our objective is to derive verifiable sufficient conditions on f, h, ℓ_S and ℓ_T such that this holds. See §2.6 for an example where ℓ is discontinuous and \mathcal{L} is smooth.

2.4 General Sufficient Conditions for Differentiability

This section formulates sufficient conditions for continuous differentiability of \mathcal{L} as defined in (2.4). These are motivated by existing results on the regularity of integrals over parametric regions [111–113], which we relate to (2.4) through *discontinuity-locked models*, or in short, σ -locked models.

For each mode sequence $\boldsymbol{\sigma} \in \mathcal{S}^{Nn_{\sigma}}$, the $\boldsymbol{\sigma}$ -locked model is defined by applying (2.2) with $\boldsymbol{\sigma}$ fixed; i.e., (2.1) is not used. Let $\phi_k^{dl} : \mathcal{S}^{Nn_h} \times \tilde{\Omega} \times \tilde{\Theta} \to \mathbb{R}^{n_x}$ be defined by $\phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta) = x_k$, where x_k is the solution of the $\boldsymbol{\sigma}$ -locked model given $(\boldsymbol{\omega}, \theta)$. Furthermore, define

$$\ell^{dl}(\boldsymbol{\sigma},\boldsymbol{\omega},\boldsymbol{\theta}) := \sum_{k=0}^{N-1} \ell_S(k,\sigma_k,\phi_k^{dl}(\boldsymbol{\sigma},\boldsymbol{\omega},\boldsymbol{\theta}),w_k,\boldsymbol{\theta}) + \ell_N(\phi_N^{dl}(\boldsymbol{\sigma},\boldsymbol{\omega},\boldsymbol{\theta}),\boldsymbol{\theta}).$$
(2.5)

In the arguments below, we first show that Ω can be partitioned into sets $\Omega(\boldsymbol{\sigma}, \theta)$ (Definition 2.4.1) on which ϕ_k and ℓ agree with the $\boldsymbol{\sigma}$ -locked models just defined (Lemma 2.4.1). Furthermore, the $\boldsymbol{\sigma}$ -locked models are C^1 (Lemma 2.4.2). We then impose two assumptions on the regularity of the boundaries of the sets $\Omega(\boldsymbol{\sigma}, \theta)$. These permit \mathcal{L} to be written as a sum of integrals over the sets $\Omega(\boldsymbol{\sigma}, \theta)$ (Lemma 2.4.4), each with C^1 integrands. Moreover, they imply that each of these integrals, and hence \mathcal{L} , is in $C^1(\tilde{\Theta}, \mathbb{R})$ (Theorem 2.4.1). **Definition 2.4.1.** For every $k \in \mathcal{K}$, $i \in \{1, \ldots, n_{\sigma}\}$, and $\sigma \in \mathcal{S}^{Nn_{\sigma}}$, define

$$\tilde{\psi}_{ki}(\boldsymbol{\sigma},\boldsymbol{\omega},\boldsymbol{\theta}) := \sigma_{k,i}h_i(k,\sigma_{k,1:i-1},\phi_k^{dl}(\boldsymbol{\sigma},\boldsymbol{\omega},\boldsymbol{\theta}),w_k,\boldsymbol{\theta}), \quad \forall (\boldsymbol{\omega},\boldsymbol{\theta}) \in \tilde{\Omega} \times \tilde{\Theta}.$$
(2.6)

We regard $\tilde{\psi}$ as a map into $\mathbb{R}^{Nn_{\sigma}}$, but use the index ki for clarity. Denote the interval Ω by $[\boldsymbol{\omega}^{L}, \boldsymbol{\omega}^{U}]$ and define $\psi^{L}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta) := \boldsymbol{\omega}^{L} - \boldsymbol{\omega}, \ \psi^{U}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta) := \boldsymbol{\omega} - \boldsymbol{\omega}^{U}, \ \psi := (\tilde{\psi}, \psi^{L}, \psi^{U}),$ and $n_{\psi} := Nn_{\sigma} + 2(n_{x} + Nn_{w})$. Finally, define the sets

 $\Omega(\boldsymbol{\sigma}, \theta) := \{ \boldsymbol{\omega} \in \tilde{\Omega} : \psi(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta) \le 0 \},$ (2.7)

$$\hat{\Omega}(\boldsymbol{\sigma}, \theta) := \{ \boldsymbol{\omega} \in \tilde{\Omega} : \psi(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta) < 0 \}.$$
(2.8)

Lemma 2.4.1. For every $k \in \mathcal{K}$, $\boldsymbol{\sigma} \in \mathcal{S}^{Nn_{\sigma}}$, and $\theta \in \tilde{\Theta}$,

- 1. $\phi_k(\boldsymbol{\omega}, \theta) = \phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), \ \forall \boldsymbol{\omega} \in \hat{\Omega}(\boldsymbol{\sigma}, \theta).$
- 2. $\ell(\boldsymbol{\omega}, \boldsymbol{\theta}) = \ell^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \boldsymbol{\theta}), \, \forall \boldsymbol{\omega} \in \hat{\Omega}(\boldsymbol{\sigma}, \boldsymbol{\theta}).$

Proof Choose $\boldsymbol{\sigma} \in \mathcal{S}^{Nn_{\sigma}}$, $\theta \in \tilde{\Theta}$, and $\boldsymbol{\omega} \in \hat{\Omega}(\boldsymbol{\sigma}, \theta)$. Assume Conclusion 1 holds with some $k \in \mathcal{K}$, which is true with k = 0 since $\phi_k(\boldsymbol{\omega}, \theta) = \phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta) = x_0$. Let $\hat{\sigma}_k$ be the vector obtained by applying (2.1) with w_k and $x_k = \phi_k(\boldsymbol{\omega}, \theta)$. We show that $\hat{\sigma}_k = \sigma_k$. Choose $i \geq 1$ and assume $\hat{\sigma}_{k,1:i-1} = \sigma_{k,1:i-1}$, which holds for i = 1. By definition, $\boldsymbol{\omega} \in \hat{\Omega}(\boldsymbol{\sigma}, \theta)$ implies $\sigma_{k,i}h_i(k, \sigma_{k,1:i-1}, \phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_k, \theta) < 0$. But since $\phi_k(\boldsymbol{\omega}, \theta) = \phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta)$ and $\sigma_{k,1:i-1} = \hat{\sigma}_{k,1:i-1}$, this gives $\sigma_{k,i}h_i(k, \hat{\sigma}_{k,1:i-1}, \phi_k(\boldsymbol{\omega}, \theta), w_k, \theta) < 0$. By (2.1), it follows that $\hat{\sigma}_{k,i} = \sigma_{k,i}$. Induction on i shows $\hat{\sigma}_k = \sigma_k$, and (2.2) then gives $\phi_{k+1}(\boldsymbol{\omega}, \theta) = \phi_{k+1}^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta)$. By induction on k, Conclusion 1 holds $\forall k \in \mathcal{K}$, and Conclusion 2 follows immediately. \Box

Lemma 2.4.2. For every $k \in \mathcal{K}$ and $\boldsymbol{\sigma} \in \mathcal{S}^{Nn_{\sigma}}$, $\phi_{k}^{dl}(\boldsymbol{\sigma},\cdot,\cdot) \in C^{1}(\tilde{\Omega} \times \tilde{\Theta}, \mathbb{R}^{n_{x}})$, $\ell^{dl}(\boldsymbol{\sigma},\cdot,\cdot) \in C^{1}(\tilde{\Omega} \times \tilde{\Theta}, \mathbb{R})$, and $\psi(\boldsymbol{\sigma},\cdot,\cdot) \in C^{1}(\tilde{\Omega} \times \tilde{\Theta}, \mathbb{R}^{n_{\psi}})$.

Proof Since $\boldsymbol{\sigma}$ is fixed in the definition of $\phi_k^{dl}(\boldsymbol{\sigma},\cdot,\cdot)$, continuous differentiability follows by a standard inductive argument using Assumption 2.3.2. The remaining claims follow immediately by composition.

We now make two assumptions on the sets $\Omega(\boldsymbol{\sigma}, \theta)$ that imply $\mathcal{L} \in C^1(\tilde{\Theta}, \mathbb{R})$. These are reduced to verifiable conditions on (2.1)–(2.2) in §2.5.

Definition 2.4.2. For every $\boldsymbol{\sigma} \in \mathcal{S}^{Nn_w}$ and $\boldsymbol{\theta} \in \tilde{\Theta}$, define

$$\partial_i \Omega(\boldsymbol{\sigma}, \theta) := \{ \boldsymbol{\omega} \in \Omega(\boldsymbol{\sigma}, \theta) : \psi_i(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta) = 0 \}, \quad \forall i \in \{1, \dots, n_{\psi}\}.$$
 (2.9)

Assumption 2.4.1. For every $\boldsymbol{\sigma} \in \mathcal{S}^{Nn_w}$, $\boldsymbol{\theta} \in \tilde{\Theta}$, and $i \in \{1, \dots, n_{\psi}\}$, we have $\|\frac{\partial \psi_i}{\partial \boldsymbol{\omega}}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \boldsymbol{\theta})\| > 0, \forall \boldsymbol{\omega} \in \partial_i \Omega(\boldsymbol{\sigma}, \boldsymbol{\theta}).$

Assumption 2.4.2. For every $\boldsymbol{\sigma} \in \mathcal{S}^{Nn_w}$, $\boldsymbol{\theta} \in \tilde{\Theta}$, and $i, j \in \{1, \dots, n_{\psi}\}$ with $i \neq j$, $\frac{\partial \psi_i}{\partial \boldsymbol{\omega}}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \boldsymbol{\theta})$ and $\frac{\partial \psi_j}{\partial \boldsymbol{\omega}}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \boldsymbol{\theta})$ are linearly independent for all $\boldsymbol{\omega} \in (\partial_i \Omega(\boldsymbol{\sigma}, \boldsymbol{\theta}) \cap \partial_j \Omega(\boldsymbol{\sigma}, \boldsymbol{\theta}))$.

Conceptually, Assumptions 2.4.1–2.4.2 imply that θ must change the measure of each $\Omega(\boldsymbol{\sigma}, \theta)$, and hence the probability that $\boldsymbol{\omega} \in \Omega(\boldsymbol{\sigma}, \theta)$, smoothly. To see this, consider the simple examples $\Omega(\boldsymbol{\sigma}, \theta) = \{\boldsymbol{\omega} : 0 \leq \boldsymbol{\omega} \leq 1, \ 0 \leq \theta\}$ and $\Omega(\boldsymbol{\sigma}, \theta) = \{\boldsymbol{\omega} : 0 \leq \boldsymbol{\omega} \leq 1, \ \boldsymbol{\omega} \leq \theta\}$. For the first, $\boldsymbol{\psi} = (\boldsymbol{\omega}, \boldsymbol{\omega} - 1, -\theta)$, and for the second, $\boldsymbol{\psi} = (\boldsymbol{\omega}, \boldsymbol{\omega} - 1, \boldsymbol{\omega} - \theta)$. The first set violates Assumption 2.4.1 at $\theta = 0$ because $\psi_3 = 0$ and $\frac{\partial \psi_3}{\partial \boldsymbol{\omega}} = 0$, and indeed its measure jumps from 0 to 1 there. The second violates Assumption 2.4.2 for $\theta \in \{0, 1\}$, and its measure is nonsmooth at both points. For example, with $\theta = 0$ we have $\psi_1 = \psi_3 = \boldsymbol{\omega}$, which are linearly dependent for all $\boldsymbol{\omega}$. Next, we use Assumption 2.4.1 to express \mathcal{L} as a sum of integrals over the sets $\Omega(\boldsymbol{\sigma}, \theta)$.

Lemma 2.4.3. Under Assumption 2.4.1, $\mu(\partial_i \Omega(\boldsymbol{\sigma}, \theta)) = 0$ for all $\boldsymbol{\sigma} \in S^{Nn_w}$, $\theta \in \tilde{\Theta}$, and $i \in \{1, \ldots, n_{\psi}\}$.

Proof By Assumption 2.4.1, $\exists \delta > 0$ such that $\|\frac{\partial \psi_i}{\partial \omega}(\boldsymbol{\sigma}, \cdot, \theta)\| > 0$ on the superset of $\partial_i \Omega(\boldsymbol{\sigma}, \theta)$ defined by $\{\boldsymbol{\omega} \in \Omega(\boldsymbol{\sigma}, \theta) + B_{\delta}(0) : \psi_i(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta) = 0\}$. By Theorem 2.1.2 and §3.3.17.2 of [114], this set is a C^1 submanifold of $\mathbb{R}^{n_{\boldsymbol{\omega}}}$ of dimension $(n_{\boldsymbol{\omega}} - 1)$, and hence has Lebesgue measure zero in $\mathbb{R}^{n_{\boldsymbol{\omega}}}$. **Lemma 2.4.4.** Under Assumption 2.4.1, $\mathcal{L}(\theta)$ exists and satisfies

$$\mathcal{L}(\theta) = \sum_{\boldsymbol{\sigma}} \int_{\Omega(\boldsymbol{\sigma},\theta)} \ell^{dl}(\boldsymbol{\sigma},\boldsymbol{\omega},\theta) p(\boldsymbol{\omega}) \mu(d\boldsymbol{\omega}), \quad \forall \theta \in \tilde{\Theta}.$$
(2.10)

Proof Choose $\theta \in \tilde{\Theta}$ and let $L(\theta)$ be the right-hand side of (2.10). By Lemma 2.4.2, $L(\theta)$ exists because each $\Omega(\boldsymbol{\sigma}, \theta)$ is closed and hence measurable. By Lemma 2.4.3, $\mu(\Omega(\boldsymbol{\sigma}, \theta)) = \mu(\hat{\Omega}(\boldsymbol{\sigma}, \theta))$. Thus, $L(\theta) = \sum_{\boldsymbol{\sigma}} \int_{\hat{\Omega}(\boldsymbol{\sigma}, \theta)} \ell(\boldsymbol{\omega}, \theta) p(\boldsymbol{\omega}) \mu(d\boldsymbol{\omega})$, where Lemma 2.4.1 has been used to replace ℓ^{dl} with ℓ . But $\cup_{\boldsymbol{\sigma}} \Omega(\boldsymbol{\sigma}, \theta) = \Omega$, so the disjoint sets $\hat{\Omega}(\boldsymbol{\sigma}, \theta)$ cover all of Ω except for a set of measure zero. Thus, $L(\theta) = \int_{\Omega} \ell(\boldsymbol{\omega}, \theta) p(\boldsymbol{\omega}) \mu(d\boldsymbol{\omega}) = \mathcal{L}(\theta)$. \Box

Theorem 2.4.1. Under Assumption 2.4.1, \mathcal{L} is continuous on $\tilde{\Theta}$. If Assumption 2.4.2 also holds, then $\mathcal{L} \in C^1(\tilde{\Theta}, \mathbb{R})$.

Due to excessive length, the proof of Theorem 2.4.1 is provided in the appendix of this chapter. In brief, the proof first verifies continuity and continuous differentiability of the integrals over θ -dependent domains in (2.10). Continuity of such integrals under Assumption 2.4.1 is typically attributed to Raik [111], which is only available in Russian, so the result is proven here. Differentiability under Assumptions 2.4.1–2.4.2 is due to Kibzun and Uryasev [112, 113]. The extension to continuous differentiability, which is essential for gradient-based optimization, is new. Since many intermediate results are required using mostly standard constructions (e.g., the surface integral over a C^1 manifold), this development has been relegated to the appendix for brevity.

2.5 Verifiable Differentiability Conditions for DTSHS

The differentiability conditions established in §2.4 require assumptions on the vector function ψ defined in Definition 2.4.1. These conditions are difficult to verify in practice, first because ψ is very high-dimensional when the horizon N is large, and second because the elements of ψ are defined recursively through the DTSHS (2.1)–(2.2), and thus are not known in a convenient form for analysis. The objective of this section is to reduce Assumptions 2.4.1–2.4.2 to two sets of easily verifiable conditions on the event functions h and right-hand side functions f in (2.1)–(2.2). The distinct advantage is that the developed conditions are verifiable at each k independently. The implications linking these verifiable conditions to the general assumptions of §2.4 are summarized in Figure 2.1.



Figure 2.1: Summary of implications (arrows) linking the 1^{st} (grey) and 2^{nd} (cyan) sets of verifiable conditions in §2.5 to the general assumptions in §2.4.

2.5.1 A First Set of Sufficient Conditions: No Pure-State Events

This section provides sufficient conditions that impose strong requirements on h, but require nothing of f beyond Assumption 2.3.2. These conditions are easier to verify than those in §2.5.2, and should serve as a first check. The key requirement is that hhas nontrivial dependence on w. Thus, we exclude events that depend only on the state x_k , which we call *pure-state events*. We require the sets $\mathcal{M}(k,\sigma,\theta)$ defined below, which partition the joint state and uncertainty set $\tilde{X} \times W$ at each k just as the sets $\Omega(\sigma, \theta)$ partition the cumulative uncertainty set $\tilde{\Omega}$ in §2.4. To ease notation, we will write $h_i(k,\sigma,z,w,\theta)$ with the understanding that h_i depends only on $\sigma_{1:i-1}$.

Definition 2.5.1. For every $k \in \mathcal{K}$, $\sigma \in \mathcal{S}^{n_{\sigma}}$, and $\theta \in \tilde{\Theta}$, define the sets

$$\mathcal{M}(0,\sigma,\theta) := \{ (z,w) \in X_0 \times W : \sigma_i h_i(k,\sigma,z,w,\theta) \le 0, \ \forall i \},$$
(2.11)

$$\mathcal{M}(k,\sigma,\theta) := \{ (z,w) \in \tilde{X} \times W : \sigma_i h_i(k,\sigma,z,w,\theta) \le 0, \ \forall i \}, \ \forall k > 0,$$
(2.12)

$$\partial_i \mathcal{M}(k,\sigma,\theta) := \{ (z,w) \in \mathcal{M}(k,\sigma,\theta) : h_i(k,\sigma,z,w,\theta) = 0 \}, \quad \forall k \ge 0.$$
(2.13)

Remark 2.5.1. It follows immediately from Definition 3.4.3 that

$$\Omega(\boldsymbol{\sigma}, \theta) = \{ \boldsymbol{\omega} \in \tilde{\Omega} : (\phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_k) \in \mathcal{M}(k, \sigma_k, \theta), \ \forall k \in \mathcal{K} \}.$$
(2.14)

Condition 2.5.1. For any $k \in \mathcal{K}$, $\sigma \in \mathcal{S}^{n_{\sigma}}$, $\theta \in \tilde{\Theta}$, and $i \in \{1, \ldots, n_{\sigma}\}$,

$$\frac{\partial h_i}{\partial w}(k,\sigma,z,w,\theta) \neq 0, \quad \forall (z,w) \in \partial_i \mathcal{M}(k,\sigma,\theta).$$
(2.15)

Condition 2.5.2. Choose any $k \in \mathcal{K}$, $\sigma \in \mathcal{S}^{n_{\sigma}}$, $\theta \in \tilde{\Theta}$, $i, j \in \{1, \ldots, n_{\sigma}\}$ with $i \neq j$, and $p \in \{1, \ldots, n_w\}$. With all derivatives evaluated at $(k, \sigma, z, w, \theta)$,

1. rank $\begin{bmatrix} \frac{\partial h_i}{\partial w}\\ \frac{\partial h_j}{\partial w} \end{bmatrix} = 2, \ \forall (z,w) \in \partial_i \mathcal{M}(k,\sigma,\theta) \cap \partial_j \mathcal{M}(k,\sigma,\theta).$ 2. rank $\begin{bmatrix} \frac{\partial h_i}{\partial w}\\ e_p^T \end{bmatrix} = 2, \ \forall (z,w) \in \partial_i \mathcal{M}(k,\sigma,\theta) \ \text{with} \ w_p = w_p^L \ \text{or} \ w_p = w_p^U.$

Condition 3.4.1 states that an event function h_i must have $\frac{\partial h_i}{\partial w} = 0$ whenever it is active (i.e., $h_i = 0$). By Condition 2.5.2, any two event functions that are active at the same time must have linearly independent w-derivatives. We show below that these conditions imply Assumptions 2.4.1–2.4.2, and hence $\mathcal{L} \in C^1(\tilde{\Theta}, \mathbb{R})$, as shown in Fig. 2.1. Recall that each h_i is related to the function ψ in Assumptions 2.4.1–2.4.2 through (2.6). Thus, we simply apply Conditions 3.4.1–2.5.2 to verify Assumptions 2.4.1–2.4.2 for every ψ_r and ψ_s with $r \neq s$.

Lemma 2.5.1. Condition 3.4.1 implies Assumption 2.4.1.

Proof Choose $\boldsymbol{\sigma} \in \mathcal{S}^{Nn_{\sigma}}, \ \theta \in \tilde{\Theta}, \ r \in \{1, \dots, n_{\psi}\}, \ \text{and } \boldsymbol{\omega} \in \partial_{r}\Omega(\boldsymbol{\sigma}, \theta).$ To verify Assumption 2.4.1, we show $\frac{\partial \psi_{r}}{\partial \boldsymbol{\omega}}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta) \neq 0.$ Since $\psi = (\tilde{\psi}, \psi^{L}, \psi^{U})$, there are two cases: $r \in \{1, \dots, Nn_{\sigma}\}$ and $r \in \{Nn_{\sigma} + 1, \dots, n_{\psi}\}.$ In the latter, either $\psi_{r} = \psi_{p}^{L}$ or $\psi_{r} = \psi_{p}^{U}$ with $p \in \{1, \dots, n_{x} + Nn_{w}\}.$ Thus, $\frac{\partial \psi_{r}}{\partial \boldsymbol{\omega}} \neq 0$ since

$$\frac{\partial \psi^L}{\partial \boldsymbol{\omega}}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \boldsymbol{\theta}) = -\mathbf{I}, \quad \frac{\partial \psi^U}{\partial \boldsymbol{\omega}}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \boldsymbol{\theta}) = \mathbf{I}.$$
(2.16)

In the former, $\tilde{\psi}_r(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta) = \sigma_{k,i}h_i(k, \sigma_k, \phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_k, \theta)$ for some $k \in \mathcal{K}$ and $i \in \{1, \dots, n_{\sigma}\}$. Then $\frac{\partial \psi_r}{\partial \boldsymbol{\omega}} = \begin{bmatrix} \frac{\partial \psi_r}{\partial x_0} & \frac{\partial \psi_r}{\partial w_{0:k-1}} & \frac{\partial h_i}{\partial w} & 0_{n_w}^{\mathrm{T}} & \cdots & 0_{n_w}^{\mathrm{T}} \end{bmatrix}$, with $\frac{\partial h_i}{\partial w}$ evaluated at $(k, \sigma, \phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_k, \theta)$ and the derivatives of ψ_r at $(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta)$. But $\boldsymbol{\omega} \in \partial_r \Omega(\boldsymbol{\sigma}, \theta)$ implies $(\phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_k) \in \partial_i \mathcal{M}(k, \sigma_k, \theta)$, so $\frac{\partial \psi_r}{\partial \boldsymbol{\omega}}$ is nonzero by Condition 3.4.1. Thus, Assumption 2.4.1 holds.

Lemma 2.5.2. Conditions 3.4.1 and 2.5.2 imply Assumption 2.4.2.

Proof Choose any $\boldsymbol{\sigma} \in \mathcal{S}^{Nn_{\boldsymbol{\sigma}}}, \ \theta \in \tilde{\Theta}, \ r,s \in \{1,\cdots,n_{\psi}\}$ with $s \neq r$ and let $\boldsymbol{\omega} \in (\partial_r \Omega(\boldsymbol{\sigma},\theta) \cap \partial_s \Omega(\boldsymbol{\sigma},\theta))$. To verify Assumption 2.4.2, we show that $\frac{\partial \psi_r}{\partial \boldsymbol{\omega}}(\boldsymbol{\sigma},\boldsymbol{\omega},\theta)$ and $\frac{\partial \psi_s}{\partial \boldsymbol{\omega}}(\boldsymbol{\sigma},\boldsymbol{\omega},\theta)$ are linearly independent in three cases.

Case 1: $r, s \in \{Nn_{\sigma} + 1, ..., n_{\psi}\}$. In this case, $\exists p, q \in \{1, ..., n_x + Nn_w\}$ such that $\psi_r = \psi_p^L$ or $\psi_r = \psi_p^U$, and $\psi_s = \psi_q^L$ or $\psi_s = \psi_q^U$. Since $\psi_r = \psi_s = 0$ and $\omega^L < \omega^U$, we must have $p \neq q$. Thus, the gradients of ψ_r and ψ_s at $(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta)$ are linearly independent by (2.16).

Case 2: $r, s \in \{1, \ldots, Nn_{\sigma}\}$. In this case, $\exists k, m \in \mathcal{K}$ and $i, j \in \{1, \ldots, n_{\sigma}\}$ such that $\psi_r = \tilde{\psi}_{ki}$ and $\psi_s = \tilde{\psi}_{mj}$. If k = m, then $i \neq j$ and

$$\begin{bmatrix} \frac{\partial \psi_r}{\partial \boldsymbol{\omega}} \\ \frac{\partial \psi_s}{\partial \boldsymbol{\omega}} \end{bmatrix} = \begin{bmatrix} \frac{\partial \psi_r}{\partial x_0} & \frac{\partial \psi_r}{\partial w_{0:k-1}} & \frac{\partial h_i}{\partial w} & \mathbf{0}_{n_w}^{\mathrm{T}} & \cdots & \mathbf{0}_{n_w}^{\mathrm{T}} \\ \frac{\partial \psi_s}{\partial x_0} & \frac{\partial \psi_s}{\partial w_{0:k-1}} & \frac{\partial h_j}{\partial w} & \mathbf{0}_{n_w}^{\mathrm{T}} & \cdots & \mathbf{0}_{n_w}^{\mathrm{T}} \end{bmatrix},$$
(2.17)

where the derivatives of ψ_r and ψ_s are evaluated at $(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta)$ and those of h_i and h_j at $(k, \sigma, \phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_k, \theta)$. But $\boldsymbol{\omega} \in (\partial_r \Omega(\boldsymbol{\sigma}, \theta) \cap \partial_s \Omega(\boldsymbol{\sigma}, \theta))$ implies that $(\phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_k) \in \partial_i \mathcal{M}(k, \sigma_k, \theta) \cap \partial_j \mathcal{M}(k, \sigma_k, \theta)$. Thus, Condition 2.5.2.1 implies that $\frac{\partial h_i}{\partial w}$ and $\frac{\partial h_j}{\partial w}$ are linearly independent, and hence so are $\frac{\partial \psi_r}{\partial \boldsymbol{\omega}}$ and $\frac{\partial \psi_s}{\partial \boldsymbol{\omega}}$. Alternatively, if $k \neq m$ (assume k > m w.l.o.g.), then

$$\begin{bmatrix} \frac{\partial \psi_r}{\partial \boldsymbol{\omega}} \\ \frac{\partial \psi_s}{\partial \boldsymbol{\omega}} \end{bmatrix} = \begin{bmatrix} \frac{\partial \psi_r}{\partial x_0} & \frac{\partial \psi_r}{\partial w_{0:m-1}} & \frac{\partial \psi_r}{\partial w_m} & \cdots & \frac{\partial \psi_r}{\partial w_{k-1}} & \frac{\partial h_i}{\partial w} & \mathbf{0}_{n_w}^{\mathrm{T}} & \cdots & \mathbf{0}_{n_w}^{\mathrm{T}} \\ \frac{\partial \psi_s}{\partial x_0} & \frac{\partial \psi_s}{\partial w_{0:m-1}} & \frac{\partial h_j}{\partial w} & \cdots & \mathbf{0}_{n_w}^{\mathrm{T}} & \mathbf{0}_{n_w}^{\mathrm{T}} & \mathbf{0}_{n_w}^{\mathrm{T}} & \cdots & \mathbf{0}_{n_w}^{\mathrm{T}} \end{bmatrix},$$
(2.18)

where $\frac{\partial h_j}{\partial w}$ is now evaluated at $(m, \sigma_m, \phi_m^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_m, \theta)$. But $\boldsymbol{\omega} \in \partial_r \Omega(\boldsymbol{\sigma}, \theta)$

implies $(\phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_k) \in \partial_i \mathcal{M}(k, \sigma_k, \theta)$ and $\boldsymbol{\omega} \in \partial_s \Omega(\boldsymbol{\sigma}, \theta)$ implies that $(\phi_m^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_m) \in \partial_j \mathcal{M}(m, \sigma_m, \theta)$. Thus, by Condition 3.4.1, both $\frac{\partial h_i}{\partial w}$ and $\frac{\partial h_j}{\partial w}$ are nonzero, and hence $\frac{\partial \psi_r}{\partial \boldsymbol{\omega}}$ and $\frac{\partial \psi_s}{\partial \boldsymbol{\omega}}$ are linearly independent by (2.18).

Case 3: $r \in \{1, ..., Nn_{\sigma}\}, s \in \{Nn_{\sigma} + 1, ..., n_{\psi}\}$. In this case, there exist $k \in \mathcal{K}$ and $i \in \{1, ..., n_{\sigma}\}$ such that $\psi_r = \tilde{\psi}_{ki}$ and either $\psi_s = \psi_p^U$ or $\psi_s = \psi_p^L$ for some $p \in \{1, ..., n_x + Nn_w\}$. Thus,

$$\begin{bmatrix} \frac{\partial \psi_r}{\partial \boldsymbol{\omega}} \\ \frac{\partial \psi_s}{\partial \boldsymbol{\omega}} \end{bmatrix} = \begin{bmatrix} \frac{\partial \psi_r}{\partial x_0} & \frac{\partial \psi_r}{\partial w_{0:k-1}} & \frac{\partial h_i}{\partial w} & 0_{n_w}^{\mathrm{T}} & \cdots & 0_{n_w}^{\mathrm{T}} \\ & & e_p^{\mathrm{T}} & & \end{bmatrix}, \qquad (2.19)$$

where the derivative of h_i is evaluated at $(k, \sigma_k, \phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_k, \theta)$. But $\boldsymbol{\omega} \in (\partial_r \Omega(\boldsymbol{\sigma}, \theta) \cap \partial_s \Omega(\boldsymbol{\sigma}, \theta))$ implies that $(\phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_k) \in \partial_i \mathcal{M}(k, \sigma_k, \theta)$ and either $\omega_p = \omega_p^L$ or $\omega_p = \omega_p^U$. Thus, by Condition 2.5.2.2, $\frac{\partial \psi_r}{\partial \boldsymbol{\omega}}$ and $\frac{\partial \psi_s}{\partial \boldsymbol{\omega}}$ must be linearly independent if the 1 in e_p^T appears in the third block column of (2.19). Yet, if the 1 appears elsewhere, then linear independence follows from $\frac{\partial h_i}{\partial w} \neq 0$ by Condition 3.4.1. Thus, Assumption 2.4.2 is verified.

Theorem 2.5.1. Under Condition 3.4.1, \mathcal{L} is continuous on $\tilde{\Theta}$. If Condition 2.5.2 also holds, then $\mathcal{L} \in C^1(\tilde{\Theta}, \mathbb{R})$.

Proof The result follows from Theorem 2.4.1 with Lemmas 2.5.1 and 2.5.2. \Box

2.5.2 A Second Set of Sufficient Conditions: Allowing Pure-State Events

The conditions in §2.5.1 fail whenever $\frac{\partial h_i}{\partial w} = 0$, while in applications it is common to have events that depend only on the state x_k (i.e., *pure-state events*). Here, we develop a second set of conditions that permits $\frac{\partial h_i}{\partial w} = 0$. The central idea is that, if h_i has trivial dependence on w_k , then it must have nontrivial dependence on w_{k-1} via x_k . These conditions involve both h and f, which makes them less restrictive but also harder to verify than those in §2.5.1. They require the following extension of the sets $\mathcal{M}(k, \sigma, \theta)$ in §2.5.1: **Definition 2.5.2.** For every $k > 0, \sigma_{-}, \sigma \in \mathcal{S}^{n_{\sigma}}$, and $\theta \in \tilde{\Theta}$, define

$$\mathcal{M}_f^2(k,\sigma_-,\sigma,\theta) := \{ (z_-, w_-, z, w) \in \mathcal{M}(k-1, \sigma_-, \theta) \times \mathcal{M}(k, \sigma, \theta) : \qquad (2.20)$$
$$z = f(k-1, \sigma_-, z_-, w_-, \theta) \}.$$

Furthermore, let $\partial_i \mathcal{M}_f^2(k, \sigma_-, \sigma, \theta)$ and $\partial_i^- \mathcal{M}_f^2(k, \sigma_-, \sigma, \theta)$ be the restrictions of $\mathcal{M}_f^2(k, \sigma_-, \sigma, \theta)$ to points such that $(z, w) \in \partial_i \mathcal{M}(k, \sigma, \theta)$ and $(z_-, w_-) \in \partial_i \mathcal{M}(k - 1, \sigma_-, \theta)$, respectively.

In words, $\mathcal{M}_{f}^{2}(k, \sigma_{-}, \sigma, \theta)$ is the set of states and uncertainties in two consecutive time steps that satisfy the system dynamics and are consistent with the mode sequence (σ_{-}, σ) . The sets $\partial_{i}^{-}\mathcal{M}_{f}^{2}(k, \sigma_{-}, \sigma, \theta)$ and $\partial_{i}\mathcal{M}_{f}^{2}(k, \sigma_{-}, \sigma, \theta)$ additionally require that $h_{i} = 0$ in the first or second time step, respectively. For readability in the conditions below, derivatives evaluated at $(k, \sigma, z, w, \theta)$ are written without arguments, while those evaluated at $(k - 1, \sigma_{-}, z_{-}, w_{-}, \theta)$ are written with the argument (*).

Condition 2.5.3. For any $k > 0, \sigma_{-}, \sigma \in \mathcal{S}^{n_{\sigma}}, \theta \in \tilde{\Theta}$, and $i \in \{1, \ldots, n_{\sigma}\}$,

$$\left[\frac{\partial h_i}{\partial x}\frac{\partial f}{\partial w}(*) \; \frac{\partial h_i}{\partial w}\right] \neq 0, \quad \forall (z_-, z, w_-, w) \in \partial_i \mathcal{M}_f^2(k, \sigma_-, \sigma, \theta).$$
(2.21)

Condition 2.5.4. Choose any k > 0, $\sigma_{-}, \sigma \in S^{n_{\sigma}}, \theta \in \tilde{\Theta}, i, j \in \{1, \dots, n_{\sigma}\}$ with $i \neq j$, and $p \in \{1, \dots, 2n_w\}$. Abbreviating $\mathcal{M}_f^2 := \mathcal{M}_f^2(k, \sigma_{-}, \sigma, \theta)$,

$$1. \operatorname{rank} \begin{bmatrix} \frac{\partial h_i}{\partial x} \frac{\partial f}{\partial w}(*) & \frac{\partial h_i}{\partial w} \\ \frac{\partial h_j}{\partial x} \frac{\partial f}{\partial w}(*) & \frac{\partial h_j}{\partial w} \end{bmatrix} = 2, \forall (z_-, z, w_-, w) \in \partial_i \mathcal{M}_f^2 \cap \partial_j \mathcal{M}_f^2.$$

$$2. \operatorname{rank} \begin{bmatrix} \frac{\partial h_i}{\partial x} \frac{\partial f}{\partial w}(*) \\ \frac{\partial h_j}{\partial w}(*) \end{bmatrix} = 2, \forall (z_-, z, w_-, w) \in \partial_i \mathcal{M}_f^2 \cap \partial_j^- \mathcal{M}_f^2 \text{ with } \frac{\partial h_i}{\partial w} = 0 \text{ and } \frac{\partial h_j}{\partial w}(*) \neq 0.$$

$$3. \operatorname{rank} \begin{bmatrix} \frac{\partial h_i}{\partial x} \frac{\partial f}{\partial w}(*) \\ e_p^T \end{bmatrix} = 2, \forall (z_-, z, w_-, w) \in \partial_i \mathcal{M}_f^2 \text{ with } [\frac{w_-}{w}]_p = \begin{bmatrix} w_L^L \\ w^L \end{bmatrix}_p \text{ or } [\frac{w_-}{w}]_p = \begin{bmatrix} w_U^U \\ w^U \end{bmatrix}_p.$$

Condition 2.5.3 ensures that, at any k, each event function h_i has nontrivial dependence on either w_k or w_{k-1} (via x_k) if it is active (i.e., $h_i = 0$). Condition 2.5.4 ensures that any two active event functions, chosen in any combination from either time k or k - 1, are linearly independent as functions of (w_{k-1}, w_k) . The next two conditions are special cases of Conditions 2.5.3–2.5.4 for k = 0.

Condition 2.5.5. For k = 0 and any $\sigma \in S^{n_{\sigma}}$, $\theta \in \tilde{\Theta}$, and $i \in \{1, \ldots, n_{\sigma}\}$,

$$\left[\frac{\partial h_i}{\partial x} \ \frac{\partial h_i}{\partial w}\right](k,\sigma,z,w,\theta) \neq 0, \quad \forall (z,w) \in \partial_i \mathcal{M}(k,\sigma,\theta).$$
(2.22)

Condition 2.5.6. Let k = 0 and choose any $\sigma \in S^{n_{\sigma}}$, $\theta \in \tilde{\Theta}$, $i, j \in \{1, ..., n_{\sigma}\}$ with $i \neq j$, and $p \in \{1, ..., n_x + n_w\}$. With the abbreviation $\mathcal{M} := \mathcal{M}(0, \sigma, \theta)$ and all the derivatives evaluated at $(0, \sigma, z, w, \theta)$:

1. rank $\begin{bmatrix} \frac{\partial h_i}{\partial x} & \frac{\partial h_i}{\partial w} \\ \frac{\partial h_j}{\partial x} & \frac{\partial h_j}{\partial w} \end{bmatrix} = 2, \ \forall (z, w) \in \partial_i \mathcal{M} \cap \partial_j \mathcal{M}.$ 2. rank $\begin{bmatrix} \frac{\partial h_i}{\partial x} & \frac{\partial h_i}{\partial w} \\ e_p^T \end{bmatrix} = 2, \ \forall (z, w) \in \partial_i \mathcal{M} \text{ with } \begin{bmatrix} z \\ w \end{bmatrix}_p = \begin{bmatrix} x_0^L \\ w^L \end{bmatrix}_p \text{ or } \begin{bmatrix} z \\ w \end{bmatrix}_p = \begin{bmatrix} x_0^U \\ w^U \end{bmatrix}_p.$

We show below that Conditions 2.5.3–2.5.6 imply Assumptions 2.4.1–2.4.2, and hence $\mathcal{L} \in C^1(\tilde{\Theta}, \mathbb{R})$, as shown in Fig. 2.1. Again, we simply apply Conditions 2.5.3–2.5.6 to verify Assumptions 2.4.1–2.4.2 using the relation (2.6).

Lemma 2.5.3. Conditions 2.5.3 and 2.5.5 imply Assumption 2.4.1.

Proof Choose $\boldsymbol{\sigma} \in \mathcal{S}^{Nn_{\sigma}}, \ \theta \in \tilde{\Theta}, \ r \in \{1, \cdots, n_{\psi}\}, \ \text{and} \ \boldsymbol{\omega} \in \partial_{r}\Omega(\boldsymbol{\sigma}, \theta).$ If $r \in \{Nn_{\sigma} + 1, \ldots, n_{\psi}\}, \ \text{then} \ \frac{\partial \psi_{r}}{\partial \boldsymbol{\omega}}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta) \neq 0 \ \text{by} \ (2.16).$ Otherwise, $\psi_{r}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta) = \sigma_{k,i}h_{i}(k, \sigma_{k}, \phi_{k}^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_{k}, \theta) \ \text{for some} \ k \ \text{and} \ i.$ If $k = 0, \ \text{then} \ \frac{\partial \psi_{r}}{\partial \boldsymbol{\omega}} = \left[\frac{\partial h_{i}}{\partial x} \ \frac{\partial h_{i}}{\partial w} \ 0^{\mathrm{T}}_{(N-1)n_{w}}\right] \ \text{with} \ \frac{\partial h_{i}}{\partial w} \ \text{and} \ \frac{\partial h_{i}}{\partial x} \ \text{evaluated} \ \text{at} \ (0, \sigma_{0}, x_{0}, w_{0}, \theta).$ But $(x_{0}, w_{0}) \in \partial_{i}\mathcal{M}(0, \sigma_{0}, \theta) \ \text{because} \ \boldsymbol{\omega} \in \partial_{r}\Omega(\boldsymbol{\sigma}, \theta).$ Thus, Condition 2.5.5 implies $\frac{\partial \psi_{r}}{\partial \boldsymbol{\omega}}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta) \neq 0.$ If k > 0, then

$$\frac{\partial \psi_r}{\partial \boldsymbol{\omega}} = \begin{bmatrix} \frac{\partial \psi_r}{\partial x_0} & \frac{\partial \psi_r}{\partial w_{0:k-2}} & \frac{\partial h_i}{\partial x} \frac{\partial f}{\partial w} & \frac{\partial h_i}{\partial w} & \mathbf{0}_{n_w}^{\mathrm{T}} & \cdots & \mathbf{0}_{n_w}^{\mathrm{T}} \end{bmatrix}, \qquad (2.23)$$

where the derivatives of ψ_r are evaluated at $(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta)$ and the derivatives of h_i and f at $(k, \sigma_k, \phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_k, \theta)$ and $(k - 1, \sigma_{k-1}, \phi_{k-1}^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_{k-1}, \theta)$, respectively. But

 $(\phi_{k-1}^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_{k-1}, \phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_k) \in \partial_i \mathcal{M}_f^2(k, \sigma_{k-1}, \sigma_k, \theta)$ because $\boldsymbol{\omega} \in \partial_r \Omega(\boldsymbol{\sigma}, \theta)$. Thus, Condition 2.5.3 implies $\frac{\partial \psi_r}{\partial \boldsymbol{\omega}} \neq 0$.

Lemma 2.5.4. Conditions 2.5.3–2.5.6 imply Assumption 2.4.2.

Proof Choose $\boldsymbol{\sigma} \in \mathcal{S}^{Nn_{\sigma}}$, $\boldsymbol{\theta} \in \tilde{\Theta}$, $r, s \in \{1, \dots, n_{\psi}\}$ with $s \neq r$ and let $\boldsymbol{\omega} \in (\partial_r \Omega(\boldsymbol{\sigma}, \boldsymbol{\theta}) \cap \partial_s \Omega(\boldsymbol{\sigma}, \boldsymbol{\theta}))$. We show that $\frac{\partial \psi_r}{\partial \boldsymbol{\omega}}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \boldsymbol{\theta})$ and $\frac{\partial \psi_s}{\partial \boldsymbol{\omega}}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \boldsymbol{\theta})$ are linearly independent. Three cases are considered.

Case 1: $r, s \in \{1, ..., Nn_{\sigma}\}$. For this case, $\exists k, m \in \mathcal{K}$ and $i, j \in \{1, ..., n_{\sigma}\}$ such that $\psi_r = \tilde{\psi}_{ki}$ and $\psi_s = \tilde{\psi}_{mj}$. If k, m = 0, then $i \neq j$ because $r \neq s$, and

$$\begin{bmatrix} \frac{\partial \psi_r}{\partial \boldsymbol{\omega}} \\ \frac{\partial \psi_s}{\partial \boldsymbol{\omega}} \end{bmatrix} = \begin{bmatrix} \frac{\partial h_i}{\partial x} & \frac{\partial h_i}{\partial w} & \mathbf{0}_{n_w}^{\mathrm{T}} & \cdots & \mathbf{0}_{n_w}^{\mathrm{T}} \\ \frac{\partial h_j}{\partial x} & \frac{\partial h_j}{\partial w} & \mathbf{0}_{n_w}^{\mathrm{T}} & \cdots & \mathbf{0}_{n_w}^{\mathrm{T}} \end{bmatrix},$$
(2.24)

where the derivatives of h_i and h_j are evaluated at $(0, \sigma_0, x_0, w_0, \theta)$. But $(x_0, w_0) \in (\partial_i \mathcal{M}(0, \sigma_0, \theta) \cap \partial_j \mathcal{M}(0, \sigma_0, \theta)$ because $\boldsymbol{\omega} \in (\partial_r \Omega(\boldsymbol{\sigma}, \theta) \cap \partial_s \Omega(\boldsymbol{\sigma}, \theta))$. Thus, $\left[\frac{\partial h_i}{\partial x} \frac{\partial h_i}{\partial w}\right]$ and $\left[\frac{\partial h_j}{\partial x} \frac{\partial h_j}{\partial w}\right]$ are linearly independent by Condition 2.5.6.1, and hence so are $\frac{\partial \psi_r}{\partial \boldsymbol{\omega}}$ and $\frac{\partial \psi_s}{\partial \boldsymbol{\omega}}$.

If k = m > 0, then again $i \neq j$, and

$$\begin{bmatrix} \frac{\partial \psi_r}{\partial \boldsymbol{\omega}} \\ \frac{\partial \psi_s}{\partial \boldsymbol{\omega}} \end{bmatrix} = \begin{bmatrix} \frac{\partial \psi_r}{\partial x_0} & \frac{\partial \psi_r}{\partial w_{0:k-2}} & \frac{\partial h_i}{\partial x} \frac{\partial f}{\partial w} & \frac{\partial h_i}{\partial w} & \mathbf{0}_{n_w}^{\mathrm{T}} & \cdots & \mathbf{0}_{n_w}^{\mathrm{T}} \\ \frac{\partial \psi_s}{\partial x_0} & \frac{\partial \psi_s}{\partial w_{0:k-2}} & \frac{\partial h_j}{\partial x} \frac{\partial f}{\partial w} & \frac{\partial h_j}{\partial w} & \mathbf{0}_{n_w}^{\mathrm{T}} & \cdots & \mathbf{0}_{n_w}^{\mathrm{T}} \end{bmatrix},$$
(2.25)

with derivatives of h_i and h_j evaluated at $(k, \sigma_k, \phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_k, \theta)$ and those of f at $(k - 1, \sigma_{k-1}, \phi_{k-1}^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_{k-1}, \theta)$. But $\boldsymbol{\omega} \in \partial_r \Omega(\boldsymbol{\sigma}, \theta) \cap \partial_s \Omega(\boldsymbol{\sigma}, \theta)$, so $(\phi_{k-1}^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_{k-1}, \phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_k)$ is in both $\partial_i \mathcal{M}_f^2(k, \sigma_{k-1}, \sigma_k, \theta)$ and $\partial_j \mathcal{M}_f^2(k, \sigma_{k-1}, \sigma_k, \theta)$. Thus, by Condition 2.5.4.1, $\left[\frac{\partial h_i}{\partial x} \frac{\partial f}{\partial w} \frac{\partial h_i}{\partial w}\right]$ and $\left[\frac{\partial h_j}{\partial x} \frac{\partial f}{\partial w} \frac{\partial h_j}{\partial w}\right]$ are linearly independent, and by (2.25), so are $\frac{\partial \psi_r}{\partial \boldsymbol{\omega}}$ and $\frac{\partial \psi_s}{\partial \boldsymbol{\omega}}$. If $k \neq m$, assume w.l.o.g. that k > m. If m = k - 1, then

$$\begin{bmatrix} \frac{\partial \psi_r}{\partial \boldsymbol{\omega}} \\ \frac{\partial \psi_s}{\partial \boldsymbol{\omega}} \end{bmatrix} = \begin{bmatrix} \frac{\partial \psi_r}{\partial x_0} & \frac{\partial \psi_r}{\partial w_{0:k-2}} & \frac{\partial h_i}{\partial x} \frac{\partial f}{\partial w} & \frac{\partial h_i}{\partial w} & \mathbf{0}_{n_w}^{\mathrm{T}} & \cdots & \mathbf{0}_{n_w}^{\mathrm{T}} \\ \frac{\partial \psi_s}{\partial x_0} & \frac{\partial \psi_s}{\partial w_{0:k-2}} & \frac{\partial h_j}{\partial w} & \mathbf{0}_{n_w}^{\mathrm{T}} & \mathbf{0}_{n_w}^{\mathrm{T}} & \cdots & \mathbf{0}_{n_w}^{\mathrm{T}} \end{bmatrix},$$
(2.26)

where the derivatives of h_i and f are evaluated as in (2.25) and the derivative of h_j is evaluated at $(k - 1, \sigma_{k-1}, \phi_{k-1}^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_{k-1}, \theta)$. In this case, $\boldsymbol{\omega} \in \partial_r \Omega(\boldsymbol{\sigma}, \theta) \cap \partial_s \Omega(\boldsymbol{\sigma}, \theta)$ implies that $(\phi_{k-1}^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_{k-1}, \phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_k)$ is in both $\partial_i \mathcal{M}_f^2(k, \sigma_{k-1}, \sigma_k, \theta)$ and $\partial_j^- \mathcal{M}_f^2(k, \sigma_{k-1}, \sigma_k, \theta)$. Thus, if $\frac{\partial h_i}{\partial w} = 0$ and $\frac{\partial h_j}{\partial w} \neq 0$, then Condition 2.5.4.2 implies $\left[\frac{\partial h_i}{\partial x} \frac{\partial f}{\partial w}\right]$ and $\left[\frac{\partial h_j}{\partial w}\right]$ are linearly independent. Hence, $\frac{\partial \psi_r}{\partial \omega}$ and $\frac{\partial \psi_s}{\partial \omega}$ are linearly independent. Alternatively, if $\frac{\partial h_i}{\partial w} \neq 0$ or $\frac{\partial h_j}{\partial w} = 0$, the only way $\frac{\partial \psi_r}{\partial \omega}$ and $\frac{\partial \psi_s}{\partial \omega}$ are linearly dependent is if the second row of (2.26) is zero. But this is prohibited by Assumption 2.4.1, which is implied by Conditions 2.5.3 and 2.5.5, because $\boldsymbol{\omega} \in \partial_s \Omega(\boldsymbol{\sigma}, \theta)$.

Finally, if m < k - 1, then

$$\begin{bmatrix} \frac{\partial \psi_r}{\partial \boldsymbol{\omega}} \\ \frac{\partial \psi_s}{\partial \boldsymbol{\omega}} \end{bmatrix} = \begin{bmatrix} \frac{\partial \psi_r}{\partial x_0} & \frac{\partial \psi_r}{\partial w_{0:m-1}} & \frac{\partial \psi_r}{\partial w_m} & \cdots & \frac{\partial h_i}{\partial x} \frac{\partial f}{\partial w} & \frac{\partial h_i}{\partial w} & \mathbf{0}_{n_w}^{\mathrm{T}} & \cdots & \mathbf{0}_{n_w}^{\mathrm{T}} \\ \frac{\partial \psi_s}{\partial x_0} & \frac{\partial \psi_s}{\partial w_{0:m-1}} & \frac{\partial h_j}{\partial w} & \cdots & \mathbf{0}_{n_w}^{\mathrm{T}} & \mathbf{0}_{n_w}^{\mathrm{T}} & \mathbf{0}_{n_w}^{\mathrm{T}} & \cdots & \mathbf{0}_{n_w}^{\mathrm{T}} \end{bmatrix}, \quad (2.27)$$

where the derivatives of h_i and f are evaluated as in (2.25) and the derivative of h_j is evaluated at $(m, \sigma_m, \phi_m^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_m, \theta)$. In this case, $\boldsymbol{\omega} \in \partial_s \Omega(\boldsymbol{\sigma}, \theta)$ implies that the bottom row of (2.27) is nonzero by Assumption 2.4.1, which is implied by Conditions 2.5.3 and 2.5.5. Thus, $\frac{\partial \psi_r}{\partial \boldsymbol{\omega}}$ and $\frac{\partial \psi_s}{\partial \boldsymbol{\omega}}$ are linearly independent if $\left[\frac{\partial h_i}{\partial x}\frac{\partial f}{\partial \boldsymbol{w}}\frac{\partial h_i}{\partial \boldsymbol{w}}\right] \neq 0$. But this holds by Condition 2.5.3 because $\boldsymbol{\omega} \in \partial_r \Omega(\boldsymbol{\sigma}, \theta)$ implies that $(\phi_{k-1}^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_{k-1}, \phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_k)$ is in $\partial_i \mathcal{M}_f^2(k, \sigma_{k-1}, \sigma_k, \theta)$.

Case 2: $r \in \{1, ..., Nn_{\sigma}\}$ and $s \in \{Nn_{\sigma}+1, ..., n_{\psi}\}$. In this case, $\psi_r = \tilde{\psi}_{ki}$ for some $k \in \mathcal{K}$ and $i, j \in \{1, ..., n_{\sigma}\}$ and either $\psi_s = \psi_p^U$ or $\psi_s = \psi_p^L$ for some $p \in \{1, ..., n_x + Nn_w\}$. If k = 0, then

$$\begin{bmatrix} \frac{\partial \psi_r}{\partial \boldsymbol{\omega}} \\ \frac{\partial \psi_s}{\partial \boldsymbol{\omega}} \end{bmatrix} = \begin{bmatrix} \frac{\partial h_i}{\partial x} & \frac{\partial h_i}{\partial w} & 0_{n_w}^{\mathrm{T}} & \dots & 0_{n_w}^{\mathrm{T}} \\ & & e_p^{\mathrm{T}} \end{bmatrix}, \qquad (2.28)$$

where $\frac{\partial h_i}{\partial w}$ and $\frac{\partial h_i}{\partial x}$ are evaluated as in (2.24). But $\boldsymbol{\omega} \in (\partial_r \Omega(\boldsymbol{\sigma}, \theta) \cap \partial_s \Omega(\boldsymbol{\sigma}, \theta))$ implies $(x_0, w_0) \in \partial_i \mathcal{M}(0, \sigma_k, \theta)$ and $\omega_p \in \{\omega_p^L, \omega_p^U\}$. If the 1 in e_p^T does not appear in the first two block columns of the right-hand side of (2.28), then $\frac{\partial \psi_r}{\partial \boldsymbol{\omega}}$ and $\frac{\partial \psi_s}{\partial \boldsymbol{\omega}}$ are independent by Condition 2.5.5. Otherwise, either $\begin{bmatrix} x_0 \\ w_0 \end{bmatrix}_p = \begin{bmatrix} x_0^L \\ w^L \end{bmatrix}_p$ or $\begin{bmatrix} x_0 \\ w_0 \end{bmatrix}_p = \begin{bmatrix} x_0^U \\ w^U \end{bmatrix}_p$, and independence follows from Condition 2.5.6.2.

If k > 0, then (with derivatives evaluated as in (2.25))

$$\begin{bmatrix} \frac{\partial \psi_r}{\partial \boldsymbol{\omega}} \\ \frac{\partial \psi_s}{\partial \boldsymbol{\omega}} \end{bmatrix} = \begin{bmatrix} \frac{\partial \psi_r}{\partial x_0} & \frac{\partial \psi_r}{\partial w_{0:k-2}} & \frac{\partial h_i}{\partial x} \frac{\partial f}{\partial w} & \frac{\partial h_i}{\partial w} & 0_{n_w}^{\mathrm{T}} & \cdots & 0_{n_w}^{\mathrm{T}} \\ & & e_p^{\mathrm{T}} & & \end{bmatrix}, \qquad (2.29)$$

But $\boldsymbol{\omega} \in \partial_s \Omega(\boldsymbol{\sigma}, \theta)$ implies that $\omega_p \in \{\omega_p^L, \omega_p^U\}$, and $\boldsymbol{\omega} \in \partial_r \Omega(\boldsymbol{\sigma}, \theta)$ implies that $(\phi_{k-1}^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_{k-1}, \phi_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_k) \in \partial_i \mathcal{M}_f^2(k, \sigma_{k-1}, \sigma_k, \theta)$. Thus, if the 1 in e_p^{T} appears in the third or fourth block column of (2.29), then Condition 2.5.4.3 implies that $\frac{\partial \psi_r}{\partial \boldsymbol{\omega}}$ and $\frac{\partial \psi_s}{\partial \boldsymbol{\omega}}$ are linearly independent. Otherwise, linear independence follows by Condition 2.5.3.

Case 3: $r, s \in \{Nn_{\sigma} + 1, ..., n_{\psi}\}$. In this case, $\exists p, q$ such that $\psi_r = \psi_p^L$ or $\psi_r = \psi_p^U$ and $\psi_s = \psi_q^L$ or $\psi_s = \psi_q^U$. Since $\psi_r = \psi_s = 0$ and $\omega^L < \omega^U$, we must have $p \neq q$, and hence $\frac{\partial \psi_r}{\partial \omega}$ and $\frac{\partial \psi_s}{\partial \omega}$ are linearly independent by (2.16).

Theorem 2.5.2. Under Conditions 2.5.3 and 2.5.5, \mathcal{L} is continuous on $\tilde{\Theta}$. If Conditions 2.5.4 and 2.5.6 also hold, then $\mathcal{L} \in C^1(\tilde{\Theta}, \mathbb{R})$.

Proof The result follows from Theorem 2.4.1 with Lemmas 2.5.3 and 2.5.4. \Box

Remark 2.5.2. The proofs of Lemmas 2.5.3–2.5.4 require that x_0 is a random variable; i.e., every element of x_0 appears in $\boldsymbol{\omega}$. If $x_0 = (x_0^r, x_0^d)$ with x_0^r random and x_0^d deterministic, then we must redefine $\boldsymbol{\omega} := (x_0^r, w_0, \dots, w_{N-1})$ so that $\boldsymbol{\omega}$ has a continuous density as per Assumption 2.3.1. The results in this section hold provided that Conditions 2.5.5–2.5.6 hold when $\frac{\partial h_i}{\partial x}$ is replaced by $\frac{\partial h_i}{\partial x^r}$.

2.6 Application to an Illustrative Microgrid Optimization Problem

In this section, the sufficient conditions of §2.5 are used to establish continuous differentiability of a small microgrid system consisting of a 40 kW diesel generator, a photovoltaic (PV) array with capacity C_{PV} kW, and a battery bank with capacity C_B kWh serving 10 homes over 25 years. We first consider a simple design problem with no annual load increase and no capacity expansions after year 1. This model is used to verify differentiability, which is then easily extended to more general cases. Next, we consider expansion planning with an annual load growth of 8% and investments every 5 years.

2.6.1 System Modeling and EMP Description

The system described above can be modeled as a DTSHS (2.1)-(2.2) with an hourly time-step [73]. In the case with no annual load increase, a horizon of 1 year (N = 8760)is sufficient. The design decisions are $\theta = (C_B, C_{PV}, \tilde{s})$, where \tilde{s} is a threshold used in the energy management policy (EMP) below. The state of the DTSHS is the state-of-charge (SOC) of the battery, s_k , and the random input is $w_k = (r_k, \kappa_k)$, where r_k is a random perturbation on the load and κ_k is the *clearness index* (a measure of cloudiness defined as the fraction of extraterrestrial irradiation that falls on a horizontal surface at ground level [115]). The quantities (r_k, κ_k) are used to compute the load in hour k, $P_L(k, r_k)$ kW, and the power generated by the PV in hour k, $P_{PV}(k, \kappa_k, C_{PV})$ kW, as described below. P_{PV} and P_L are used to define the net power $P_N(k, w_k, \theta) := P_{PV}(k, \kappa_k, C_{PV}) - P_L(k, r_k)$. Based on s_k and P_N , dispatching decisions are made to determine the status of the diesel generator and the amount of energy stored in or removed from the battery in hour k. These decisions (i.e., the EMP) are described below and will define the functions h_i , the discrete mode σ_k , and the update of s_k as in (2.1)–(2.2). The diesel is either operated at $P_D = 40$ kW or not at all in hour k. This captures the important fact that generators, like other dispatchable components (e.g. fuel cells, electrolyzers, wind turbines, etc.) cannot operate below a minimum power. Thus, the EMP must make a discrete decision in each hour.

One year of hourly irradiation [116] and residential electric load data ([117], highload case) was obtained for a region in Texas at 32.00°N/102.10°W. The latter was used as $P_{L,k}^d$ to compute $P_L(k, r_k) = P_{L,k}^d + r_k$, where $r_k \in [r^L, r^U]$ is a truncated normal random variable with mean zero and 100 W standard deviation. Truncation is required to satisfy Assumption 2.3.1, but $[r^L, r^U]$ can be chosen arbitrarily large so that little error is introduced. Interestingly, the differentiability analysis below requires $[r^L, r^U]$ to be sufficiently large ($[-10^3, 10^3]$ proves to be adequate). Irradiation data are used to compute daily clearness indices, from which stochastic hourly indices $\kappa_k \in [0, 1]$ are generated by an ARMA(1,0) process $\kappa_k = \rho \kappa_{k-1} + \epsilon_k$ with Gaussian white noise ϵ_k as in [118]. Each κ_k is used to compute irradiation on a tilted PV panel at time k as in [115] with tilt and azimuth angles of 32° and -1° , and ground reflectance 0.6. P_{PV} is correlated to the resulting irradiation as in [73] with de-rating factor 0.95. These models define a smooth nonlinear relation $P_N(k, w_k, \theta)$. Assumption 2.3.1 holds for $\omega := (s_0, w_0, \ldots, w_{N-1})$ with s_0 sampled uniformly in [0, 1] because r_k and κ_k are bounded and have continuous probability densities. For simplicity, we do not consider correlations between r_k and κ_k .

Fig. 2.2 shows the logic for two EMPs based on common heuristics [16]. At the beginning of hour k, both EMPs first determine the diesel generator status d_k using the threshold \tilde{s} (which is a decision variable). In EMP2, \tilde{s} is compared to $s' := s_k$, with the result that $d_k = 1$ (on) if $s' \leq \tilde{s}$ and $d_k = 0$ (off) otherwise. These cases correspond to the discrete modes $\sigma_{k,1} = 1$ and $\sigma_{k,1} = -1$ in (2.1)–(2.2), as shown in Fig. 2.2. In contrast, EMP1 assumes that $P_N(k, w_k, \theta)$ is known immediately at time k, and hence compares \tilde{s} to $s' := s_k + P_N(k, w_k, \theta)/C_B$, which is the value s_{k+1} will take if $d_k = 0$. After d_k is decided, both EMPs check another set of conditions to ensure that the battery SOC remains within its operating limits $[s, \bar{s}] := [0.4, 1]$. In Fig. 2.2, s'' is the value that s_{k+1} will take if the battery is able to supply or store the power $d_k P_D + P_N(k, w_k, \theta)$. If $s'' \in [s, \bar{s}]$ ($\sigma_{k,2} = -1$ and $\sigma_{k,3} = 1$), then the SOC is updated to $s_{k+1} = s''$. Otherwise, there is an excess ($\sigma_{k,2} = \sigma_{k,3} = -1$) or deficit ($\sigma_{k,2} = \sigma_{k,3} = 1$) of power that must be curtailed or dumped,

and s_{k+1} takes one of the values \underline{s} or \overline{s} . Any deficit is recorded as the unmet demand, u_k kW. After execution of the EMP, the stage cost is computed as $\ell_S = \beta_D d_k + \beta_U u_k$, where $\beta_D = \$7.52/h$ is the diesel fuel and operating cost and $\beta_U = \$0.60/kWh$ is a penalty for unmet demand to enforce reliability. The event functions h_i in (2.1) are explicitly given in Table 2.1, while f and ℓ_s in (2.2)–(2.3) are given in Table 2.2. Note that h_i and f satisfy Assumption 2.3.2. The total cost ℓ for 25 years of operation is

$$\ell(\theta, \omega) = 25 \sum_{k=0}^{8759} \ell_S(k, \sigma_k, s_k, w_k, \theta) + \ell_T(s_N, \theta),$$
(2.30)

with $\ell_T(s_N, \theta) = \alpha_{PV}C_{PV} + \alpha_D + \alpha_B C_B$, where $\alpha_{PV} = \$2.941 \times 10^3$ /kW, $\alpha_D = \$2.63 \times 10^4$, and $\alpha_B = \$1.185 \times 10^3$ /kWh are, respectively, the capital costs of the PV, diesel generator, and battery, including expected replacements.



Figure 2.2: Energy Management Policies EMP1 and EMP2. Decisions in \diamond blocks and $\sigma_{k,i}$ values correspond to the event functions $h_i \leq 0$ and $\sigma_{k,i}$ values in (2.1).

Table 2.1: Explicit expressions for the event functions h_i in (2.1) corresponding to Fig. 2.2

h_1	$s_k + P_N(k, w_k, \theta) / C_B - \tilde{s}$ for EMP1 and $s_k - \tilde{s}$ for EMP2							
	If $\sigma_{k,1} = -1$	If $\sigma_{k,1} = 1$						
h_2	$s_k + P_N(k, w_k, \theta) / C_B - \underline{s}$	$s_k + (P_D + P_N(k, w_k, \theta))/C_B - \underline{s}$						
h_3	$s_k + P_N(k, w_k, \theta) / C_B - \overline{s}$	$s_k + (P_D + P_N(k, w_k, \theta))/C_B - \overline{s}$						

Figure 2.3 illustrates the key difference in regularity between $\ell(\boldsymbol{\omega}, \cdot)$ and $\mathcal{L} = \mathbb{E}[\ell(\boldsymbol{\omega}, \cdot)]$ that motivates the analysis in §2.5. With $C_{PV} = 20$ kW and $C_B = 350$

Table 2.2: Explicit expressions for the state update function f in (2.2) and the stage cost ℓ_S in (2.3) for every permissible value of $\sigma_k = (\sigma_{k,1}, \sigma_{k,2}, \sigma_{k,3})$. We abbreviate $P_N := P_N(k, w_k, \theta)$.

σ_k	$f(k, \sigma_k, x_k, w_k, \theta)$	$\ell_s(k,\sigma_k,x_k,w_k, heta)$
(1,-1,1)	$s_k + (P_D + P_N)/C_B$	β_D
(1,-1,-1)	\overline{s}	β_D
(1,1,1)	<u>s</u>	$\beta_D + \beta_u C_B(\underline{s} - s_k - (P_D + P_N)/C_B)$
(-1,-1,1)	$s_k + P_N/C_B$	0
(-1,-1,-1)	\overline{s}	0
(-1,1,1)	<u></u>	$\beta_u C_B(\underline{s} - s_k - P_N/C_B)$



Figure 2.3: Fractional diesel run-time (\circ), normalized unmet demand (\triangle), and normalized operational cost (\Box) versus \tilde{s} with a fixed ω (left) and averaged over 10⁴ random ω 's (right).

kWh fixed, the left panel shows $\ell(\hat{\omega}, \cdot)$ versus \tilde{s} for a single scenario $\hat{\omega}$, while the right shows \mathcal{L} approximated using 10⁴ random samples of ω (for clarity, only operating costs for 1 week in summer are shown). Discontinuities in ℓ arise from the choice of d_k in Fig. 2.2, which leads to discrete changes in the cumulative diesel generator hours and the unmet demand as \tilde{s} is varied. In general, each decision in the EMP can introduce one surface of discontinuity in $\ell(\hat{\omega}, \cdot)$ in every hour of the year. Clearly, this precludes the use of gradient-based optimization. In contrast, \mathcal{L} appears to be smooth (although it is notably nonconvex). In §2.6.2–2.6.3, we apply the results of §2.5 to prove that \mathcal{L} is in fact smooth with one minor exception for EMP1. We assume throughout that

$$0 \le \underline{s} < \tilde{s} \le \overline{s} \le 1. \tag{2.31}$$

2.6.2 Verification of Sufficient Differentiability Conditions for EMP1

Choose any $k \in \mathcal{K}$, $\sigma \in \mathcal{S}^{n_{\sigma}}$, $\theta \in \tilde{\Theta}$, and $(z, w) \in \mathcal{M}(k, \sigma, \theta)$. We show that Condition 3.4.1 holds, and that Condition 2.5.2 holds provided that θ satisfies

$$\overline{s} - \widetilde{s} \neq P_D/C_B. \tag{2.32}$$

Thus, by Theorem 2.5.1, \mathcal{L} is continuous at θ and, under (2.32), is C^1 there.

Recall that $w = (r, \kappa)$ and $P_N(k, w, \theta) = P_{PV}(k, \kappa, C_{PV}) - P_L(k, r)$. Thus, every h_i in Table 2.1 satisfies

$$\frac{\partial h_i}{\partial w} = \frac{1}{C_B} \frac{\partial P_N}{\partial w} = \frac{1}{C_B} \begin{bmatrix} -1 & \frac{\partial P_{PV}}{\partial \kappa} \end{bmatrix} \neq \begin{bmatrix} 0 & 0 \end{bmatrix}.$$
(2.33)

This verifies Condition 3.4.1. However, it also shows that $\frac{\partial h_i}{\partial w}$ and $\frac{\partial h_j}{\partial w}$ are linearly dependent for every *i* and *j*. Thus, to verify Condition 2.5.2.1, it must be shown that the event $h_i = h_j = 0$ is impossible.

Case 1: $h_1 = h_2 = 0$. From Table 2.1, $h_1 = h_2$ implies $\tilde{s} = \underline{s} - P_D/C_B$ if $\sigma_{k,1} = 1$. But $P_D/C_B > 0$, and so $\tilde{s} < \underline{s}$, which violates (2.31). Alternately, $h_1 = h_2$ implies $\tilde{s} = \underline{s}$ if $\sigma_{k,1} = -1$, which also violates (2.31).

Case 2: $h_2 = h_3 = 0$. For any σ_k , this implies $\underline{s} = \overline{s}$ which violates (2.31).

$$z + C_B^{-1}(d_k P_D + P_{PV}(k, \kappa, C_{PV}) - (P_{L,k}^d + r)) \in \{\tilde{s}, \underline{s}, \overline{s}\},$$
(2.34)

for any $d_k \in \{0,1\}$. Thus, we pick $[r^L, r^U]$ large enough that (2.34) is impossible at its endpoints. Noting that $z, \tilde{s}, \underline{s}, \overline{s} \in [0, 1]$, it suffices that, $\forall (\kappa, \theta) \in [0, 1] \times \tilde{\Theta}$,

$$\min(|r^{L}|, |r^{U}|) \ge |C_{B} + P_{PV}(k, \kappa, C_{PV}) - P_{L,k}^{d} + P_{D}|.$$
(2.35)

By Theorem 2.5.1, \mathcal{L} is continuous on $\tilde{\Theta}$ and C^1 at every $\theta \in \tilde{\Theta}$ with the possible exception of one surface of discontinuity at (2.32). Thus, \mathcal{L} is much more regular than $\ell(\hat{\omega}, \cdot)$, which exhibits 8760 discontinuities with fixed $\hat{\omega}$.

2.6.3 Verification of Sufficient Differentiability Conditions for EMP2

The event functions in EMP2 are the same as those in EMP1 except for h_1 . Thus, (2.33) holds for all $i \neq 1$. However, $\frac{\partial h_1}{\partial w} = [0 \ 0]$ and so Conditions 3.4.1–2.5.2 fail. Therefore, we must use Conditions 2.5.3–2.5.6 instead.

To verify Conditions 2.5.5–2.5.6, let k = 0 and choose any $\sigma \in S^{n_{\sigma}}$, $\theta \in \tilde{\Theta}$, and $(z,w) \in \mathcal{M}(0,\sigma,\theta)$. For any $i \in \{1,2,3\}$, $\frac{\partial h_i}{\partial x}(k,\sigma,z,w,\theta) = 1$, so Condition 2.5.5 holds. Condition 2.5.6.1 must be verified for the case $h_2 = h_3 = 0$ and the cases $h_1 = h_i = 0$, $i \in \{2,3\}$. By Table 2.1, the first case implies $\underline{s} = \overline{s}$ which violates (2.31). For the latter cases, Table 2.1 and (2.33) give $\begin{bmatrix} \frac{\partial h_1}{\partial x} & \frac{\partial h_1}{\partial w} \\ \frac{\partial h_1}{\partial x} & \frac{\partial h_1}{\partial w} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & -\frac{1}{C_B} & \frac{1}{C_B} & \frac{\partial P_N}{\partial \kappa} \end{bmatrix}$, which has rank 2 as required. For Condition 2.5.6.2, suppose $h_i = 0$ for some $i \in \{1, 2, 3\}$ and note that $\begin{bmatrix} \frac{\partial h_i}{\partial x} & \frac{\partial h_i}{\partial w} \\ e_p^T \end{bmatrix} = \begin{bmatrix} 1 & \frac{\partial h_i}{\partial w} & \frac{\partial h_i}{\partial w} \\ e_p^T \end{bmatrix}$. If $p \in \{2, 3\}$, then this matrix has rank 2 as required. If p = 1 and $i \in \{2, 3\}$, then (2.33) again implies that this matrix has rank 2. Finally, if p = 1 and i = 1, then $s_0 = \tilde{s}$ and $s_0 \in \{s_0^L, s_0^U\} = \{\underline{s}, \overline{s}\}$, which violates (2.31).

To verify Conditions 2.5.3–2.5.4, choose any $k > 0, \sigma_{-}, \sigma \in S^{n_{\sigma}}, \theta \in \tilde{\Theta}$, and $(z_{-}, z, w_{-}, w) \in \mathcal{M}_{f}^{2}(k, \sigma_{-}, \sigma, \theta)$. We first show the following implications:

$$h_1 = 0 \implies z \notin \{\underline{s}, \overline{s}\} \text{ and } \frac{\partial f}{\partial w}(*) = \begin{bmatrix} -\frac{1}{C_B} & \frac{1}{C_B} \frac{\partial P_N}{\partial \kappa} \end{bmatrix},$$
 (2.36)

$$h_i(*) = 0, \ i \in \{2, 3\}, \qquad \Longrightarrow \qquad z \in \{\underline{s}, \overline{s}\}, \tag{2.37}$$

where all functions are evaluated at $(k, \sigma, z, w, \theta)$ unless marked with $(*) := (k - 1, \sigma_{-}, z_{-}, w_{-}, \theta)$. By Definition 2.5.2, z = f(*). If $h_1 = 0$, then $\tilde{s} = z = f(*)$. Then, by (2.31) $z = f(*) \notin \{\underline{s}, \overline{s}\}$, and it follows from Table 2.2 and the definition of P_N that f must satisfy (2.36). To see (2.37), consider Fig. 2.2 at k - 1. If, e.g., $h_2(*) = 0$, then $s'' = \underline{s}$ and, regardless of $\sigma_{-,2}$, the outcome is $z = f(*) = s'' = \underline{s}$. An analogous argument shows that $z = \overline{s}$ if $h_3(*) = 0$.

For $i \in \{2,3\}$, Condition 2.5.3 holds because $\frac{\partial h_i}{\partial w} \neq 0$ by (2.33). For i = 1, $\frac{\partial h_i}{\partial x} = 1$ and $\frac{\partial f}{\partial w}(*) \neq 0$ by (2.36), so Condition 2.5.3 again holds. (2.31).

Condition 2.5.4.1 must be verified for $h_2 = h_3 = 0$ and the cases $h_1 = h_i = 0$, $i \in \{2,3\}$. The first case implies $\underline{s} = \overline{s}$, which contradicts (2.31). For the latter cases (2.33) gives $\begin{bmatrix} \frac{\partial h_1}{\partial x} \frac{\partial f}{\partial w}(*) & \frac{\partial h_1}{\partial w} \\ \frac{\partial h_i}{\partial x} \frac{\partial f}{\partial w}(*) & \frac{\partial h_i}{\partial w} \end{bmatrix} = \begin{bmatrix} \frac{\partial f}{\partial w}(*) & 0 & 0 \\ \frac{\partial f}{\partial w}(*) - \frac{1}{C_B} & \frac{1}{C_B} \frac{\partial P_N}{\partial \kappa} \end{bmatrix}$. But $\frac{\partial f}{\partial w}(*) \neq 0$ by (2.36), so this matrix has rank 2 as required.

For Condition 2.5.4.2, choose $i, j \in \{1, 2, 3\}$ and suppose that $h_i = 0, h_j(*) = 0$, $\frac{\partial h_i}{\partial w} = 0$, and $\frac{\partial h_j}{\partial w}(*) \neq 0$. From Table 2.1, the only *i* and *j* consistent with these requirements are i = 1 and $j \in \{2, 3\}$. But these cases are impossible because the conclusions of (2.36) and (2.37) are mutually exclusive.

For Condition 2.5.4.3, suppose that $h_i = 0$ for some $i \in \{1, 2, 3\}$ and note that $\begin{bmatrix} \frac{\partial h_i}{\partial x} \frac{\partial f}{\partial w} \frac{\partial h_i}{\partial w} \\ e_p^T \end{bmatrix} = \begin{bmatrix} \frac{\partial f}{\partial w_1} \frac{\partial f}{\partial w_2} \frac{\partial h_i}{\partial w_2} \frac{\partial h_i}{\partial w_2} \\ e_p^T \end{bmatrix}$. From (2.36) and (2.33) it is simple to show that this matrix has rank 2 for the following cases: i = 1 and $p \in \{2, 3, 4\}$, $i \in \{2, 3\}$ and $p = \{1, 2, 4\}$. We show that the remaining cases cannot occur. If i = 1 and p = 1, then $\tilde{s} = z, r_- \in \{r^L, r^U\}$, and by (2.36) and Table 2.2,

$$\tilde{s} = z = f(*) = z_{-} + C_B^{-1} \left(d_{k-1} P_D + P_N(k-1, w_{-}, \theta) \right), \qquad (2.38)$$

where $d_{k-1} = 1$ if $\sigma_{-,1} = 1$ and $d_{k-1} = 0$ otherwise. But, using the definition of P_N and $\tilde{s} - z_- \in [-1, 1]$, it is simple to show that this contradicts (2.35). Finally, if p = 3 and

 $i \in \{2, 3\}$, then $r \in \{r^L, r^U\}$ and $h_i = 0$ implies

$$z + C_B^{-1} \left(d_k P_D + P_N(k, w, \theta) \right) \in \{ \underline{s}, \overline{s} \},$$

$$(2.39)$$

where $d_k = 1$ if $\sigma_1 = 1$ and $d_k = 0$ otherwise. But again, noting that $\underline{s} - z, \overline{s} - z \in [-1, 1]$, it is straightforward to show that this contradicts (2.35). Thus, Conditions 2.5.3–2.5.6 hold and $\mathcal{L} \in C^1(\tilde{\Theta}, \mathbb{R})$ by Theorem 2.5.1.

2.6.4 Optimization Results

This section illustrates the advantages of exploiting differentiability to minimize $\mathcal{L}(\theta) = \mathbb{E}[\ell(\omega, \theta)]$. First, consider the case with no annual load increase and only 3 decisions $\theta = (C_B, C_{PV}, \tilde{s})$ with feasible set $\Theta = [\theta^L, \theta^U]$, where $\theta^L = (10, 10, 0.41)$ and $\theta^U = (1.5 \times 10^3, 1.5 \times 10^3, 0.99)$. We use a year-long stochastic simulation with EMP2 to evaluate $\ell(\omega, \theta)$. Although this problem seems very simple, a typical MILP formulation requires integer variables to describe the diesel status in each hour of the year and each scenario ω . In fact, CPLEX 12.6 required more than 12 hours to solve this problem as an expected value minimization subject to a DTSHS using stochastic gradient-descent (SGD). We implement SGD as $\theta_{j+1} = \Psi[\theta_j + \alpha_j d_j]$, where $\Psi[y]$ is the projection of y onto Θ, α_j is the step-size, and the search direction is $d_j = -\frac{D\mathcal{G}(\omega, \theta_j)}{\|D\mathcal{G}(\omega, \theta_j)\|}$, where $D = \text{diag}(10^5, 10^6, 0.1)$ is a scaling matrix and $\mathcal{G}(\omega, \theta_j)$ is a finite-difference (FD) approximation of $\nabla \mathcal{L}(\theta_j)$. Specifically, in each iteration j, we generate a random $\hat{\omega}_j$ and compute

$$\mathcal{G}_i(\hat{\boldsymbol{\omega}}_j, \theta_j) = (2\delta_i)^{-1} [\ell(\hat{\boldsymbol{\omega}}_j, \theta_j + e_i\delta_i) - \ell(\hat{\boldsymbol{\omega}}_j, \theta_j - e_i\delta_i)], \qquad (2.40)$$

with $\delta = (12.5, 5.3, 0.1)$. Although this looks like an FD approximation of $\ell(\hat{\omega}_j, \cdot)$, which may not be differentiable at θ_j , it is an unbiased estimator of the divided difference $(2\delta_i)^{-1}[\mathcal{L}(\theta_j + e_i\delta_i) - \mathcal{L}(\theta_j - e_i\delta_i)]$, which can be made arbitrarily close to the true derivative of \mathcal{L} since $\mathcal{L} \in C^1(\tilde{\Theta}, \mathbb{R})$. The step size α_k is determined using bisection to satisfy the Armijo inequality

$$\ell(\hat{\boldsymbol{\omega}}_k, \theta_k) - \ell(\hat{\boldsymbol{\omega}}_k, \theta_k + \alpha_k d_k) \ge -\rho \alpha_k \mathcal{G}(\hat{\boldsymbol{\omega}}_k, \theta_k)^{\mathrm{T}} d_k, \quad \rho = 0.02.$$
(2.41)

Since $\mathcal{G}_i(\hat{\omega}_j, \theta_j)$ may not be a descent direction for every $\hat{\omega}_j$, the line search may fail (i.e., $\alpha_k < 10^{-6}$) away from a local minimum, in which case $\hat{\omega}_j$ is re-sampled. The algorithm terminates if either (a) the line search fails more than 6 times, (b) for any $j > 6, \frac{1}{6} \sum_{n=j-6}^{j} |\theta_{n+1,i} - \theta_{n,i}| \le T_i, \forall i \in \{1,2,3\}, \text{ where } T = (0.5, 0.5, 0.006), \text{ or (c)}$ $\frac{1}{6} \sum_{n=j-6}^{j} |\ell(\hat{\omega}_{n+1}, \theta_{n+1}) - \ell(\hat{\omega}_n, \theta_n)| \le 500.$

Figure 2.4 compares our SGD results with the particle swarm optimization (PSO) code particleswarm and the genetic algorithm (GA) code ga in MATLAB R2015a. The initial population size was 20 and 50 for particleswarm and ga, respectively. With default settings for other parameters, the solvers terminated when the relative change in the best objective value was less than 10^{-6} in the last 20 iterations for PSO and 50 generations for GA. Because these algorithms are stochastic and \mathcal{L} may have several local minima. all algorithms were initiated at 100 random initial guesses and $\mathcal{L}(\theta_{\min})$ was estimated at each solution using 1000 random $\boldsymbol{\omega}$'s. PSO terminated with $\mathcal{L}(\theta_{\min}) = \2.16×10^6 for all initial guesses. This was the best point found by any solver. SGD terminated at this point often, but also frequently found two other points with $\mathcal{L}(\theta_{\min}) = \2.17×10^6 and $\mathcal{L}(\theta_{\min}) =$ \$2.3 × 10⁶. All three were visually confirmed to be local minima, indicating that SGD performs as expected. In contrast, GA terminated at arbitrary non-stationary points in about 20% of cases. Most importantly, the average number of function evaluations required by the solvers varied greatly: 1860 for PSO, 6560 for GA, and only 500 for SGD, including the evaluations for computing \mathcal{G} and executing line search. Since the optimization time is dominated by function evaluations, which take approximately $0.36s^1$, our rudimentary gradient-based algorithm provides speed-ups of $13 \times$ over a mature GA code and $3.7 \times$ over PSO. Moreover, at 180 CPUs, the SGD solution time using year-long simulations is $240 \times$

¹Dell Precision T3600, 3.0 GHz Intel Xeon, 4GB RAM, Windows 7, MATLAB R2015a



Figure 2.4: Frequency of solutions found by PSO, GA, and SGD out of 100 initial guesses versus the corresponding expected costs (million dollars).



Figure 2.5: Detailed operation of the optimal system over 7 days in September. Squares indicate the diesel on (1) and off (0) statuses.

faster than solving the MILP formulation discussed above over only 5 days. The operation of the optimal system is demonstrated in Fig. 2.5.

To test SGD on larger problems, we considered two extensions. First, we split the year into 40 periods of 219 h and allowed a distinct threshold \tilde{s} in each, resulting in 42 decisions in total. PSO and SGD found similar ranges of solutions, with the best having $\mathcal{L}(\theta_{\min}) = \1.81×10^6 at $(C_{PV}, C_B) = (149,506)$ for SGD and (144,511) for PSO. Fig. 2.6 shows the optimal thresholds, which are high in summer (indicating more diesel use) due to high cooling demands in Texas. Computationally, SGD again outperformed PSO, but by a smaller margin, requiring 1123 function evaluations versus 3800 for PSO.

Next, we considered an expansion planning problem with five investment periods over a 25 years. Capacities C_{PV} and C_B are purchased at the start of period 1 and allowed to increase in each successive period. We used a distinct threshold \tilde{s} in each period, making 15 decisions in total. We used data for 32.45°N and 112.10°W (Arizona) with a constant interest rate of 6%/yr (for investment discounting) and a load growth rate of 8%/yr.



Figure 2.6: Optimal EMP thresholds found by PSO (\circ) and SGD (\star) versus time (months).



Figure 2.7: Frequency of solutions found by PSO and SGD out of 100 initial guesses versus the corresponding expected costs (million dollars) for the expansion planning problem.

Note that planning models based on load duration curves are not applicable here because they ignore the chronology of the load and resource profiles [64]. Here, dispatching decisions are coupled through the battery SOC, and their costs must be evaluated by hourly simulations, as in Fig. 2.5. Nonetheless, we opted to consider only two weeks from each season of each year, or 3.36×10^4 h in total, which is common in expansion planning models with discrete decisions at the hourly level [37, 104, 105] and reduces our simulation times by about $6.5 \times$.

Fig. 2.7 shows that both PSO and SGD find several local minima, with the best found most frequently. SGD is again much faster, with 2918 function evaluations on average versus 17152 for PSO. Table 2.3 shows the best expansion plans for both solvers. Capacity grows considerably until the fourth period, where investments drop off. Moreover, the EMP thresholds increase after the first stage, meaning that the system is favoring more frequent use of the diesel.

	PSO					SGD				
Period	1	2	3	4	5	1	2	3	4	5
C_{PV}	67.8	89.8	127.8	13.90	0	65.0	92.9	124.0	13.4	0
C_B	70.7	243	0	0	0	71.3	211.0	0	0	0
\tilde{s}	0.70	0.94	0.95	0.94	0.94	0.64	0.94	0.95	0.94	0.89

Table 2.3: Optimal expansion plans found by PSO and SGD over 5 investment periods

2.7 Conclusions

This chapter analyzed the regularity of expected costs associated with stochastic hybrid systems. The main results are two sets of sufficient conditions for continuous differentiability of such functions. The first is a special case of the second that is simpler to verify in practice. These conditions were successfully applied to a representative microgrid optimization problem, suggesting that many problems of interest are smooth in expectation, even while sample-average approximations are discontinuous. This is important because it enables the use of gradient-based algorithms that can potentially achieve higher solution quality and efficiency than the derivative-free algorithms that currently dominate the microgrid literature. Significant gains were achieved here using a simple stochastic gradient descent algorithm. General purpose algorithms and more comprehensive comparisons will be considered in future work.

2.8 Appendix

2.8.1 Introduction

The purpose of this appendix is to provide a self-contained proof of Theorem 2.4.1. To simplify notation, we redefine some nomenclature with obvious correlations. Let $\tilde{\Omega} \subset \mathbb{R}^{n_{\omega}}$ and $\tilde{\Theta} \subset \mathbb{R}^{n_{\theta}}$ be open sets, let $\psi \in C^1(\tilde{\Omega} \times \tilde{\Theta}, \mathbb{R}^{n_{\psi}})$, and let $g : \tilde{\Omega} \times \tilde{\Theta} \to \mathbb{R}$ be continuous and satisfy $g(\cdot, \omega) \in C^1(\tilde{\Theta}, \mathbb{R}), \forall \omega \in \tilde{\Omega}$. Furthermore, define

$$\mathcal{G}(\theta) := \int_{\Omega(\theta)} g(\omega, \theta) \mu(d\omega), \qquad (2.42)$$

$$\Omega(\theta) := \{ \omega \in \tilde{\Omega} : \psi(\omega, \theta) \le 0 \},$$
(2.43)

$$\partial_i \Omega(\theta) := \{ \omega \in \Omega(\theta) : \psi_i(\omega, \theta) = 0 \}, \quad \forall i \in \{1, \dots, n_{\psi}\},$$
(2.44)

$$\partial_i \tilde{\Omega}(\theta) := \{ w \in \tilde{\Omega} : \psi_i(\omega, \theta) = 0 \}, \quad \forall i \in \{1, \dots, n_\psi\}.$$
(2.45)

Assumption 2.8.1. $\exists \Omega_C \subset \tilde{\Omega}$ compact and such that $\Omega(\theta) \subset \Omega_C, \forall \theta \in \tilde{\Theta}$.

Assumption 2.8.2. For every $\theta \in \tilde{\Theta}$ and each i, $\|\frac{\partial \psi_i}{\partial \omega}(\omega, \theta)\| > 0$, $\forall \omega \in \partial_i \Omega(\theta)$.

Assumption 2.8.3. For every $\theta \in \tilde{\Theta}$ and every *i* and *j* with $i \neq j$, $\frac{\partial \psi_i}{\partial \omega}(\omega, \theta)$ and $\frac{\partial \psi_j}{\partial \omega}(\omega, \theta)$ are linearly independent for all $\omega \in (\partial_i \Omega(\theta) \cap \partial_j \Omega(\theta))$.

In the following sections, it will be proven that \mathcal{G} is continuous on $\tilde{\Theta}$ under Assumptions 2.8.1–2.4.1, and $\mathcal{G} \in C^1(\tilde{\Theta}, \mathbb{R})$ under Assumptions 2.8.1–2.4.2. These results establish Theorem 3.1 because \mathcal{L} is a finite sum of integrals of the form (2.42) by Lemmas 2.3.2 and 2.3.4. Moreover, Assumptions 2.8.2–2.8.3 are exactly Assumptions 2.3.1–2.3.2 with minor changes in notation, and Assumption 2.8.1 holds with $\Omega_C := \Omega$.

2.8.2 Continuity of the Volume Integral \mathcal{G} on $\tilde{\Theta}$

In the following developments, we use the notations $A + B := \{a + b : a \in A, b \in B\}$ and $A \setminus B := \{a \in A : a \notin B\}$. Recall also that $B_{\delta}(y)$ denotes the open ball of radius δ about y. Finally, we denote the closure of $A \subset \mathbb{R}^n$ by clA. **Lemma 2.8.1.** Choose any $\theta^* \in \Theta$ and $\delta > 0$, and define

$$N_{\delta}^{*} = \bigcup_{i=1}^{n_{\psi}} \partial_{i} \Omega(\theta^{*}) + B_{\delta}(0), \quad M_{\delta}^{*} = \Omega_{C} \setminus N_{\delta}^{*}, \quad K_{\delta}^{*} = M_{\delta}^{*} \cap \Omega(\theta^{*}).$$
(2.46)

Under Assumption 2.8.1, $\exists \eta > 0: K^*_{\delta} \subset \Omega(\theta) \subset (K^*_{\delta} \cup N^*_{\delta}), \forall \theta \in B_{\eta}(\theta^*).$

Proof Since N_{δ}^* is open, its complement is closed, and hence M_{δ}^* is compact. Define $r(\omega, \theta) := \max_i(\psi_i(\omega, \theta))$. If $\omega \in M_{\delta}^*$, then either $\omega \in K_{\delta}^*$, in which case $r(\omega, \theta^*) < 0$, or $\omega \notin \Omega(\theta^*)$, in which case $r(\omega, \theta^*) > 0$. Thus, for each $\omega \in M_{\delta}^*$, $|r(\omega, \theta^*)| > 0$ and continuity implies that $\exists \gamma_{\omega}, \eta_{\omega} > 0$ such that |r| > 0 on $B_{\gamma_{\omega}}(\omega) \times B_{\eta_{\omega}}(\theta^*)$. Note that r < 0 on $B_{\gamma_{\omega}}(\omega) \times B_{\eta_{\omega}}(\theta^*)$ if $\omega \in K_{\delta}^*$, and r > 0 otherwise. Since M_{δ}^* is compact and covered by the sets $B_{\gamma_{\omega}}(\omega)$, there exists a finite subcover indexed by ω_i , $i = 1, \ldots, N$. Let $\gamma_i := \gamma_{\omega_i}$ and $\eta_i := \eta_{\omega_i}$.

We show by contradiction that the result holds with $\eta = \min_i \eta_i > 0$. Choose any $\theta \in B_{\eta}(\theta^*)$ and suppose $K^*_{\delta} \not\subset \Omega(\theta)$. Then $\exists \omega \in K^*_{\delta}$ with $r(\omega, \theta) > 0$. But $\omega \in K^*_{\delta}$ and $\theta \in B_{\eta}(\theta^*)$ imply that (ω, θ) belongs to some $B_{\gamma_i}(\omega_i) \times B_{\eta_i}(\theta^*)$ on which r < 0, which is a contradiction. Next, suppose that $\Omega(\theta) \not\subset (K^*_{\delta} \cup N^*_{\delta})$. Then, $\exists \omega \in \Omega(\theta)$ such that $\omega \notin N^*_{\delta}$ and $\omega \notin K^*_{\delta}$. The first of these inclusions implies that $r(\omega, \theta) \leq 0$, while the second implies that $\omega \in M^*_{\delta}$. But $\omega \in M^*_{\delta} \setminus K^*_{\delta}$ and $\theta \in B_{\eta}(\theta^*)$ imply that (ω, θ) belongs to some $B_{\gamma_i}(\omega_i) \times B_{\eta_i}(\theta^*)$ on which r > 0, which is again a contradiction. \Box

Corollary 2.8.1. For any $i \in \{1, ..., n_{\psi}\}$, $\theta^* \in \tilde{\Theta}$, and $\delta > 0$, under Assumption 2.8.1, $\exists \eta > 0$ such that $\partial_i \Omega(\theta) \subset \partial_i \Omega(\theta^*) + B_{\delta}(0)$, $\forall \theta \in B_{\eta}(\theta^*)$.

Proof From the proof of Lemma 2.8.1, r < 0 on $K_{\delta}^* \times B_{\eta}(\theta^*)$, and hence $\partial_i \Omega(\theta)$ does not intersect K_{δ}^* . Then, since $\partial_i \Omega(\theta) \subset \Omega(\theta)$, it follows from the conclusion of Lemma 2.8.1 that $\partial_i \Omega(\theta) \subset N_{\delta}^*$.

Theorem 2.8.1. Under Assumptions 2.8.1–2.4.1, \mathcal{G} is continuous on Θ .

Proof Choose any $\theta^* \in \tilde{\Theta}$ and any $\epsilon > 0$. Choose $\eta_C > 0$ such that $B_{\eta_C}(\theta^*) \subset \tilde{\Omega}$ and let g_C be an upper bound for |g| on $\Omega_C \times clB_{\eta_C}(\theta^*)$. By Lemma 2.3.3, $N^* := \bigcup_i \partial_i \Omega(\theta^*)$ has measure zero, and so is contained in an open set O with $\mu(O) \leq \frac{\epsilon}{2g_C}$. Since N^* is compact, we may choose $\delta > 0$ small enough that $N^*_{\delta} := N^* + B_{\delta}(0) \subset O$, and hence $\mu(N^*_{\delta}) \leq \frac{\epsilon}{2g_C}$. Choose $\eta \leq \eta_C$ satisfying Lemma 2.8.1 with this δ , and note that

$$\mathcal{G}(\theta) = \int_{K_{\delta}^{*}} g(\omega, \theta) \mu(d\omega) + \int_{\Omega(\theta) \setminus K_{\delta}^{*}} g(\omega, \theta) \mu(d\omega), \quad \forall \theta \in B_{\eta}(\theta^{*}).$$
(2.47)

The first term on the right is continuous at θ^* by Theorem 3.103 in [119]. It remains to show continuity of the second term. But, by Lemma 2.8.1,

$$\left| \int_{\Omega(\theta^*) \setminus K^*_{\delta}} g(\omega, \theta^*) \mu(d\omega) - \int_{\Omega(\theta) \setminus K^*_{\delta}} g(\omega, \theta) \mu(d\omega) \right| \le 2 \int_{N^*_{\delta}} g_C \mu(d\omega), \quad (2.48)$$

with $2\int_{N^*_{\delta}}g_C\mu(d\omega) = 2g_C\mu(N^*_{\delta}) \le \epsilon$ for all $\theta \in B_{\eta}(\theta^*)$ by construction. \Box

2.8.3 Surface Measure and Integrals

In §2.8.4, we present an essential result of Kibzun and Uryasev [112] showing that \mathcal{G} is differentiable under Assumptions 2.8.1–2.4.2, and that the derivative can be expressed in terms of surface integrals over the sets $\partial_i \Omega(\theta)$. In this section, these surface integrals are formalized and some properties are established. In general, we follows the standard procedure for defining surface integrals over differentiable manifolds using local coordinate patches and a partition of unity [120]. However, under the standard development, one obtains distinct coordinate patches and partitions of unity corresponding to each $\partial_i \Omega(\theta)$ with $\theta \in \tilde{\Theta}$, making it impossible to analyze how the surface integral itself varies with θ . Here, we modify the standard development to show that one can construct a single, finite partition of unity, dominating a finite set of θ -dependent coordinate patches, which can be used to express the surface integral over all $\partial_i \Omega(\theta)$ with θ in a sufficiently small ball around some $\theta^* \in \tilde{\Theta}$. As a result, we are able to extend the result of Kibzun and Uryasev by establishing continuous differentiability of \mathcal{G} (Theorem 2.8.3). This construction is the content of the following lemma. **Lemma 2.8.2.** Choose any $\theta^* \in \tilde{\Theta}$ and $i \in \{1, \ldots, n_{\psi}\}$. For any $\delta > 0$, denote $N_{\delta,i}^* := \partial_i \Omega(\theta^*) + B_{\delta}(0)$. Under Assumptions 2.8.1–2.4.1, there exists $\eta, \delta > 0$ and functions $\alpha_j \in C^1(E_j \times B_{\eta}(\theta^*), \mathbb{R}^{n_{\omega}})$ and $\phi_j \in C^1(\mathbb{R}^{n_{\omega}}, \mathbb{R}_+), \forall j \in \{1, \ldots, l\}$, such that the following conditions hold $\forall \theta \in B_{\eta}(\theta^*)$ and every j:

- 1. $\sum_{j=1}^{l} \phi_j(\omega) = 1, \ \forall \omega \in N^*_{\delta,i}.$
- 2. $\phi_j(\omega) \ge 0, \forall \omega \in \mathbb{R}^{n_\omega}, and \phi_j(\omega) = 0$ outside of a compact rectangle S_j .
- 3. $\partial_i \Omega(\theta) \subset N^*_{\delta,i}$.
- 4. $E_j \subset \mathbb{R}^{n_\omega 1}$ is open, $\alpha_j(\cdot, \theta)$ is 1-to-1 on E_j , $\alpha_j^{-1}(\cdot, \theta)$ is continuous on $V_j(\theta) := \alpha_j(E_j, \theta)$, and $V_j(\theta)$ is an open subset of $\partial_i \tilde{\Omega}(\theta)$.
- 5. $\frac{\partial \alpha_j}{\partial \xi}(\xi, \theta)$ has full rank $\forall \xi \in E_j$.
- 6. $\alpha_j^{-1}(S_j \cap V_j(\theta), \theta)$ is a compact rectangle in E_j and $S_j \cap \partial_i \tilde{\Omega}(\theta) \subset V_j(\theta)$.

Proof Choose $\omega \in \partial_i \Omega(\theta^*)$. By Assumption 2.4.1, $\frac{\partial \psi_i}{\partial \omega}(\omega, \theta^*)$ has at least one nonzero component. Assume w.l.o.g. that $\omega = (\gamma, \xi), \ \gamma \in \mathbb{R}$, and $\frac{\partial \psi_i}{\partial \gamma}(\omega, \theta^*) \neq 0$. Then, by the Implicit Function Theorem (Theorem 9.2 in [120]), there exist open balls E_{ω}, T_{ω} , and G_{ω} about ξ, θ^* , and γ , respectively, and $h_{\omega} \in C^1(E_{\omega} \times T_{\omega}, G_{\omega})$ such that, $\forall (\xi', \theta') \in E_{\omega} \times T_{\omega},$ $\gamma' := h_{\omega}(\xi', \theta')$ is the unique element of G_{ω} satisfying $\psi_i((\gamma', \xi'), \theta') = 0$.

Let A be the union of the sets $G_{\omega} \times E_{\omega}$, $\forall \omega \in \partial_i \Omega(\theta^*)$. By Theorem 16.3 in [120], there exists a countable partition of unity, $\phi_j \in C^{\infty}(\mathbb{R}^{\omega}, \mathbb{R}_+)$, $\forall j \in \mathbb{N}$, such that $\sum_{j=1}^{\infty} \phi_j = 1$ on A, each ϕ_j is positive and is zero outside of a compact rectangle S_j contained entirely in some $G_{\omega} \times E_{\omega}$, and each $\omega \in A$ has a neighborhood that intersects only finitely many S_j 's. We make this partition finite on a compact subset of A as follows. Since A is open and $\partial_i \Omega(\theta^*)$ compact, we may choose $\delta > 0$ small enough that $N^*_{\delta,i} \subset A$. Now, the closure $clN^*_{\delta,i}$ is compact, and every $\omega \in clN^*_{\delta,i}$ has a neighborhood intersecting only finitely many S_j 's. This forms a cover of $clN^*_{\delta,i}$, and the existence of a finite subcover implies that $clN^*_{\delta,i}$ itself intersects only finitely many S_j 's. Indexing these from 1 to l, Conditions 1 and 2 are proven. For each $j \in \{1, \ldots, l\}$, we have established that there exists some $G_{\omega} \times E_{\omega}$ containing S_j . Denote this neighborhood by $G_j \times E_j$, and let $h_j \in C^1(E_j \times T_j, G_j)$ be the corresponding implicit function. Define $T = \bigcap_{j=1}^l T_j$, which is an open neighborhood of θ^* . By Corollary 2.8.1, $\exists \eta > 0$ such that $B_{\eta}(\theta^*) \subset T$ and Condition 3 holds for all $\theta \in B_{\eta}(\theta^*)$. For each $j \in \{1, \ldots, l\}$, define $\alpha_j \in C^1(E_j \times B_{\eta}(\theta^*), \mathbb{R}^{n_{\omega}})$ by $\alpha_j(\xi, \theta) := (h_j(\xi, \theta), \xi)$. Evidently, $\alpha_j(\cdot, \theta)$ is 1-to-1 and $\alpha_j^{-1}(\cdot, \theta)$ is continuous on $V_j(\theta) := \alpha_j(E_j, \theta)$, for all $\theta \in B_{\eta}(\theta^*)$. Moreover, since $\alpha(\cdot, \theta)$ maps into $\partial_i \tilde{\Omega}(\theta)$, continuity of the inverse proves that $V_j(\theta)$ is open there, so Condition 4 holds. From the definition of α , it is also clear that $\frac{\partial \alpha_j}{\partial \xi}(\cdot, \theta)$ is full rank (i.e., $n_{\omega} - 1$) on E_j , so Condition 5 holds.

To arrange for Condition 6, denote $S_j := G_j^S \times E_j^S \subset E_j \times G_j$ and note that $h_j(E_j^S, T')$ is a compact interval in $G_j \subset \mathbb{R}$ for any compact neighborhood T' of θ^* contained in $B_\eta(\theta^*)$. Thus, we may redefine (if necessary) G_j^S , and hence S_j , so that G_j^S is a compact interval in G_j containing $h_j(E_j^S, T')$ in its interior, and restrict η so that $B_\eta(\theta^*) \subset T'$. Note that this modification does not invalidate Condition 2, and it now holds that

$$\alpha_j^{-1}(S_j \cap V_j(\theta)) = \{\xi \in E_j : (h_j(\xi, \theta), \xi) \in G_j^S \times E_j^S\} = E_j^S,$$
(2.49)

for all $\theta \in B_{\eta}(\theta^*)$. Finally, to show that $S_j \cap \partial_i \tilde{\Omega}(\theta) \subset V_i(\theta)$, choose any $\theta \in B_{\eta}(\theta^*)$ and $\omega = (\gamma, \xi) \in S_j \cap \partial_i \tilde{\Omega}(\theta)$. By construction, $\theta \in T_j$ and $(\gamma, \xi) \in G_j \times E_j$. Thus, by the Implicit Function Theorem, $\gamma' := h_j(\xi, \theta)$ is the unique element of G_j satisfying $\psi_i(\gamma', \xi, \theta) = 0$, and hence $\gamma' = \gamma$. It follows that $\alpha_j(\xi, \theta) = (\gamma, \xi) \in V_j(\theta)$.

Definition 2.8.1. Choose $\theta^* \in \tilde{\Theta}$, $i \in \{1, \ldots, n_{\psi}\}$, and let η , δ , α_j , E_j , $V_j(\theta)$, and l be as in Lemma 2.8.2. For any $\theta \in B_{\eta}(\theta^*)$, a set $Q \subset \partial_i \Omega(\theta)$ is $\mu_i^s(\cdot, \theta)$ -measurable if $\alpha_j^{-1}(Q \cap V_j(\theta), \theta)$ is Lebesgue measurable in $\mathbb{R}^{n_{\omega}-1}$, $\forall j \in \{1, \ldots, l\}$. For any $\mu_i^s(\cdot, \theta)$ -measurable Q, define the surface integral of g over Q as

$$\int_{Q} g(\omega,\theta)\mu_{i}^{s}(d\omega,\theta) := \sum_{j=1}^{l} \int_{\alpha_{j}^{-1}(Q \cap V_{j}(\theta),\theta)} [(\phi_{j}g) \circ \alpha_{j}(\xi,\theta)] V(D\alpha_{j})\mu(d\xi),$$
(2.50)

where $V(D\alpha_j) := \left(\det \left(\frac{\partial \alpha_j}{\partial \xi} \right)^T \left(\frac{\partial \alpha_j}{\partial \xi} \right) \right)^{1/2}$ is a differential volume element.

Remark 2.8.1. Concerning the integrals on the right-hand side of (2.50), note that Q is in $N_{i,\delta}^*$ by Condition 3 of Lemma 2.8.2. Then, using Condition 1 as well, $g(\omega) = \sum_{j=1}^l (\phi_j g)(\omega)$, $\forall \omega \in Q$. Since each term in this sum is zero outside of the corresponding S_j , the domain of integration for each term can be restricted to any superset of $Q \cap S_j$. To perform the integration, this domain must be 'pulled back' into $\mathbb{R}^{n_\omega - 1}$ using the local coordinate patch α_j . This requires that the image $V_j(\theta)$ covers $Q \cap S_j$, which holds by Condition 6 of Lemma 2.8.2.

Remark 2.8.2. The surface measure of $Q \subset \partial_i \Omega(\theta)$ is naturally defined as $\mu_i^s(Q,\theta) := \int_Q \mu_i^s(d\omega,\theta)$, and is zero if an only if $\alpha_j^{-1}(Q \cap V_j(\theta),\theta)$ has Lebesgue measure zero in $\mathbb{R}^{n_\omega - 1}, \forall j \in \{1, \ldots, l\}$.

Remark 2.8.3. For any $\theta \in \tilde{\Theta}$, there may be multiple choices of θ^* with $\theta \in B_{\eta}(\theta^*)$, and hence multiple definitions of the surface measure and integral on $\partial_i \Omega(\theta)$. Nevertheless, since choosing an alternative θ^* simply amounts to covering $\partial \Omega_i(\theta)$ by an alternative partition of unity and collection of coordinate patches, Definition 2.8.1 is unambiguous and independent of θ^* (see §25 in [120]).

In order to define the surface integral of g over $\partial_i \Omega(\theta)$ itself, it remains to ensure that this set is $\mu_i^s(\cdot, \theta)$ -measurable.

Lemma 2.8.3. Let Assumptions 2.8.1–2.4.2 hold, choose $\theta^* \in \tilde{\Theta}$ and $i \in \{1, \ldots, n_{\psi}\}$, and let η , δ , α_j , E_j , $V_j(\theta)$, and l be as in Lemma 2.8.2. Choose any $j \in \{1, \ldots, l\}$, $(\xi, \theta) \in E_j \times B_\eta(\theta^*)$, and $k \neq i$. If $\alpha_j(\xi, \theta) \in \partial_i \Omega(\theta) \cap \partial_k \Omega(\theta)$, then $\frac{\partial}{\partial \xi} \psi_k(\alpha_j(\xi, \theta), \theta) \neq 0$.

Proof If the implication fails, $\exists (\xi, \theta) \in E_j \times B_\eta(\theta^*)$ such that $\psi(\alpha_j(\xi, \theta)) \leq 0$,

$$\begin{bmatrix} \psi_k(\alpha_j(\xi,\theta),\theta)\\ \psi_i(\alpha_j(\xi,\theta),\theta) \end{bmatrix} = 0, \quad \text{and} \quad \begin{bmatrix} \frac{\partial \psi_k}{\partial \omega}(\alpha_j(\xi,\theta),\theta)\\ \frac{\partial \psi_i}{\partial \omega}(\alpha_j(\xi,\theta),\theta) \end{bmatrix} \frac{\partial \alpha_j}{\partial \xi}(\xi,\theta) = 0.$$
(2.51)

The second row follows from Condition 4 of Lemma 2.8.2; i.e., $\psi_i(\alpha_j(\xi', \theta'), \theta') = 0$, $\forall (\xi', \theta') \in E_j \times B_\eta(\theta^*)$. But, by Condition 5 of Lemma 2.8.2, $\frac{\partial \alpha_j}{\partial \xi}(\xi, \theta)$ has rank $n_\omega - 1$, which implies that the rank of the left-hand matrix in (2.51) is at most 1 (it's range lies in the one-dimensional left null space of $\frac{\partial \alpha_j}{\partial \xi}(\xi, \theta)$). But this contradicts Assumption 2.4.2 because $\alpha_j(\xi, \theta) \in \partial_i \Omega(\theta) \cap \partial_k \Omega(\theta)$.

Theorem 2.8.2. Let Assumptions 2.8.1–2.4.2 hold. For every $\theta \in \tilde{\Theta}$ and $i, k \in \{1, ..., n_{\psi}\}$ with $i \neq k$, $\partial_i \Omega(\theta)$ is $\mu_i^s(\cdot, \theta)$ -measurable, $\mu_i^s(\partial_i \Omega(\theta) \cap \partial_k \Omega(\theta), \theta) = 0$, and the surface integral $\int_{\partial_i \Omega(\theta)} g(\omega, \theta) \mu_i^s(d\omega, \theta)$ is continuous at θ .

Proof Choose $\theta \in \tilde{\Theta}$, $i \in \{1, \ldots, n_{\psi}\}$, and let and let η , δ , α_j , E_j , $V_j(\theta)$, and l be as in Lemma 2.8.2. For any $\theta \in B_{\eta}(\theta^*)$, $\partial_i \Omega(\theta)$ is $\mu_i^s(\cdot, \theta)$ -measurable if $\alpha_j^{-1}(\partial_i \Omega(\theta) \cap V_j(\theta), \theta)$ is μ -measurable for all j. But for each j, $\psi_i(\alpha_j(\xi, \theta), \theta) = 0$, $\forall \xi \in E_j$, by definition, and hence

$$\alpha_j^{-1}(\partial_i \Omega(\theta) \cap V_j(\theta), \theta) = \{\xi \in E_j : \psi_m(\alpha_j(\xi, \theta), \theta) \le 0, \ \forall m \neq i\}.$$
(2.52)

Moreover, for any $k \neq i$, $\alpha_j^{-1}(\partial_i \Omega(\theta) \cap \partial_k \Omega(\theta) \cap V_j(\theta))$ is exactly (2.52) with the additional constraint $\psi_k(\alpha_j(\xi,\theta),\theta) = 0$. Thus, the right-hand side of (2.52) is a system of inequalities that satisfies Assumption 2.4.1 by Lemma 2.8.3. It follows that $\alpha_j^{-1}(\partial_i \Omega(\theta) \cap \partial_k \Omega(\theta) \cap V_j(\theta))$ has μ -measure zero in $\mathbb{R}^{n_\omega - 1}$ by Lemma 2.3.3. Then, by definition, $\partial_i \Omega(\theta) \cap \partial_k \Omega(\theta)$ has $\mu_i^s(\cdot, \theta)$ -measure zero. Furthermore, observe that (2.52) can be written as the union of the sets $\alpha_j^{-1}(\partial_i \Omega(\theta) \cap \partial_k \Omega(\theta) \cap V_j(\theta), \theta)$, for all $k \neq i$, with the set $\{\xi \in E_j : \psi_m(\alpha_j(\xi, \theta), \theta) < 0, \forall m \neq i\}$. Since this last set is open, it is μ -measurable in $\mathbb{R}^{n_\omega - 1}$. Thus, (2.52) is μ -measurable because it is a union of μ -measurable sets, and it follows that $\partial_i \Omega(\theta)$ is $\mu_i^s(\cdot, \theta)$ -measurable.

Finally, continuity of the surface integral holds if each volume integral on the righthand side of (2.50) is continuous with $Q = \partial_i \Omega(\theta)$. Note that each of these integrals has continuous integrand, and by Condition 2 of Lemma 2.8.2, its domain of integration can be restricted to $\alpha_j^{-1}(Q \cap S_j \cap V_j(\theta), \theta)$ without affecting its value. Using Condition 6 of Lemma 2.8.2, this restricted set is

$$\{\xi \in E_j^S : \psi_m(\alpha_j(\xi, \theta), \theta) \le 0, \ \forall m \neq i\},\tag{2.53}$$

where E_j^S is a compact rectangle. But (2.53) is a system of inequalities satisfying Assumption 2.8.1 with $\Omega_C := E_j^S$ and satisfying Assumption 2.4.1 by Lemma 2.8.3. Thus, continuity follows from Theorem 2.8.1.

2.8.4 Continuous Differentiability of the Volume Integral

In the following theorem, differentiability follows from the results of Kibzun and Uryasev [112, 113], while continuity of the derivative follows from Theorem 2.8.2.

Theorem 2.8.3. Under Assumptions 2.8.1–2.4.2, $\mathcal{G} \in C^1(\tilde{\Theta}, \mathbb{R})$ and, $\forall \theta \in \tilde{\Theta}$,

$$\frac{\partial \mathcal{G}}{\partial \theta}(\theta) = \int_{\Omega(\theta)} \frac{\partial g}{\partial \theta}(\omega, \theta) \mu(d\omega) - \sum_{i=1}^{n_{\psi}} \int_{\partial_i \Omega(\theta)} \frac{g(\omega, \theta) \nabla_{\theta} \psi_i(\omega, \theta)}{\|\nabla_{\omega} \psi_i(\omega, \theta)\|} \mu_i^s(d\omega, \theta).$$
(2.54)

Proof Define $G(\theta, \eta) := \int_{\Omega(\theta)} g(\omega, \eta) \mu(d\omega), \, \forall (\theta, \eta) \in \tilde{\Theta} \times \tilde{\Theta}$. For any k, Theorem 3.104 in [119] shows that

$$\frac{\partial G}{\partial \eta_k}(\theta,\eta) = \int_{\Omega(\theta)} \frac{\partial g}{\partial \theta_k}(\omega,\eta) \mu(d\omega), \quad \forall (\theta,\eta) \in \tilde{\Theta} \times \tilde{\Theta}.$$
(2.55)

Furthermore, this derivative is continuous in $\tilde{\Theta} \times \tilde{\Theta}$ by Theorem 2.8.1. Thus, by Theorem 6.2 in [120], $G(\theta, \cdot) \in C^1(\tilde{\Theta}, \mathbb{R}), \forall \theta \in \tilde{\Theta}$.

Now, by Theorem 2.4 in [112], $G(\cdot, \eta)$ is also differentiable and

$$\frac{\partial G}{\partial \theta}(\theta,\eta) = -\sum_{i=1}^{n_{\psi}} \int_{\partial_i \Omega(\theta)} \frac{g(\omega,\eta) \nabla_{\theta} \psi_i(\omega,\theta)}{\|\nabla_{\omega} \psi_i(\omega,\theta)\|} \mu_i^s(d\omega,\theta),$$
(2.56)

for all $\forall (\theta, \eta) \in \tilde{\Theta} \times \tilde{\Theta}$, and this derivative is continuous by Theorem 2.8.2. By a final application of Theorem 6.2 in [120], $G \in C^1(\tilde{\Theta} \times \tilde{\Theta}, \mathbb{R})$. Finally, by Theorem 5.1 in [120], \mathcal{G} is continuously differentiable and (2.54) holds.

Chapter 3

Smooth-in-Expectation Decision Rules: A New Approach for Multistage Stochastic Programs with Mixed-Integer Recourse Decisions

3.1 Abstract

A new class of decision rules is presented for formulating tractable approximations of nonlinear multistage stochastic programs (MSPs) with mixed-integer recourse decisions and very many stages (i.e., hundreds). Such MSPs arise in smart manufacturing, renewable energy systems, etc., and are notoriously difficult to solve with scenario-based approaches. A promising alternative is to solve a decision-rule approximation (DRA) wherein recourse decisions are replaced by functions of the random variables parameterized by additional first-stage decisions. For MSPs with continuous recourse, such approximations can often be solved very efficiently. In stark contrast, MSPs with mixed-integer recourse require discontinuous decision rules, resulting in generally intractable DRAs. To address this, we introduce a general class of mixed-integer decision rules that, despite being discontinuous, guarantee continuous differentiability of the DRA. Specifically, for nonlinear MSPs with expected-value objectives and chance constraints over continuous random variables, we establish conditions under which the integrals defining these functions are guaranteed to smooth all discontinuities introduced by the decision rules. These conditions are not very restrictive and are always satisfied by suitably randomized decision rules. When they hold, the resulting DRA can be solved efficiently using gradient-based methods. This approach is demonstrated for an integrated capacity planning and inventory control problem.

3.2 Introduction

This chapter presents a new class of decision rules for formulating tractable approximations of nonlinear multistage stochastic programs (MSPs) with mixed-integer recourse decisions and very many stages (i.e., hundreds or thousands). Specifically, we consider a state-space MSP formulation with an expected-value objective function and stage-wise chance constraints over continuous random variables. Such MSPs commonly arise in problems where long-term investment decisions (e.g., design and expansion planning) must be integrated with operational decisions occurring on much shorter time scales and under significant uncertainty (e.g., scheduling, unit commitment, and control) [18, 35, 36, 43, 100]. This work is specifically motivated by the smart manufacturing and smart grid paradigms, which both emphasize the value of highly flexible systems that can optimally adapt to dynamic and uncertain operating environments. For systems such as microgrids, combined heat and power plants, multiproduct chemical plants, and biorefineries, such adaptability has tremendous potential to reduce costs and increase efficiency by exploiting real-time markets, leveraging variable renewable energy sources and feedstocks, and accommodating process variabilities and contingencies [25, 26]. For highly flexible systems, the integration of design and operational decisions is critical because the value of an investment in, e.g., additional production or storage capacity, is largely determined by the extent to which lower-level scheduling and control algorithms can capitalize on this capacity to achieve more efficient operation [88]. Technically, this leads to multistage stochastic programs (MSPs) with three uniquely challenging features. First, relevant operational decisions often occur on time-scales much shorter than the lifetime of an investment, resulting in MSPs with very many stages [15, 36–38]. For example, the value of an energy storage system with a lifetime of 10 years may depend critically on its ability to enhance responsiveness to hourly variations in electricity pricing or renewable power generation [36, 39]. Second, many critical operational decisions are discrete (e.g., adaptive scheduling and unit commitment) [10, 18, 36], resulting in MSPs with mixed-integer recourse. Third, several important uncertainties are best described by continuous random variables with significant variance, resulting in MSPs that are not easily approximated using few discrete scenarios (e.g., demands, natural resource availability, process yields, etc.) [40–42].

These features make such MSPs notoriously difficult to solve using scenario-based approximations (SBAs). In this approach, the continuous random variables (RVs) are approximated by a finite number of scenarios, which allows the recourse functions to be finitely parameterized by their values in each scenario. Unfortunately, enforcing non-anticipativity of the recourse decisions requires scenario trees that grow exponentially in the number of stages [121], leading to extremely large mixed-integer programs. For MSPs with few stages and a moderate number of scenarios, such SBAs can often be solved effectively using decomposition techniques. However, these techniques typically rely on strong duality arguments to ensure convergence, which fails for problems with integer recourse decisions or nonconvex models. A few rigorous decomposition methods have recently been developed for mixedinteger and nonconvex problems [48–50], but these are still nascent and have significant limitations (e.g., computational cost is relatively high; they only apply to two-stage models; the method in [48] requires purely integer first-stage decisions, etc.).
On the other hand, tractable approximations of MSPs arising in the integrated design and operation problems of interest here are often achieved through a variety of strategies that relax operational detail. These include scenario aggregation [67, 68]; decoupling consecutive stages using static process models [64, 69]; using coarse time grids [40, 64]; relaxing integrality of operational decisions [65, 66]; using linearized models [15, 37]; using deterministic or two-stage approximations [37, 65] that make operational decisions with perfect foresight rather than under uncertainty; etc. While these simplifications may be appropriate in some applications, they all degrade the original model in exactly the aspects that are most essential for assessing the value of adaptability in dynamic and uncertain environments. Thus, obscuring operational details through these simplifications may lead to system designs that are highly sub-optimal or even infeasible under real operating conditions.

A promising alternative to scenario-based approximation for MSPs with many stages is to use a decision-rule approximation (DRA). In this approach, the space of feasible recourse functions is restricted to a finitely parameterized family of decision rules (e.g., the piecewise affine functions with *n* pieces), which explicitly specify (sub-optimal) operational decisions for every realization of uncertainty. Decision rules (DRs) have huge potential to address problems with very many stages because they reduce the original MSP to a single-stage problem with dramatically fewer decisions, including only the original first-stage decisions and a (potentially) small number of rule parameters. In fact, for state-space MSP formulations of the type considered here, the number of decisions in the DRA can be made independent of the number of stages by considering static DRs that act on the state rather than the entire history of the uncertainty. Moreover, DRA formulations rigorously account for the feasibility and cost of recourse actions in every realization of uncertainty, either robustly or via expected costs and chance constraints. This can be a critical advantage over scenario-based approximations, which only model recourse in a finite number of scenarios that is often severely limited by computational considerations.

Decision rule approximation (DRA) has had tremendous success for linear prob-

lems with continuous recourse. For example, the use of affine decision rules for robust and chance-constrained instances of such problems results in DRAs that can be reformulated as standard-form linear or conic programs [81, 82, 122]. Thus, instances with more than fifty stages can be solved efficiently [82]. Various nonlinear decision rules have also been proposed and shown to result in tractable DRA reformulations (e.g., piecewise affine, polynomial, basis function expansions, etc.) [83–86]. In stark contrast, DRA has been much less successful for problems with mixed-integer recourse. The fundamental issue is that integer recourse decisions require discontinuous decision rules [90, 123]. The resulting DRA is therefore a discontinuous optimization problem, which proves to be highly problematic for devising efficient reformulations and solution procedures. The problem is made clear by considering an approximation of the DRA using a finite set of scenarios. In such an approximation, the action of the decision rules in each fixed scenario, and hence the cost and constraints in each scenario, are discontinuous function of the DRA decision variables (i.e., the original first-stage decisions plus the rule parameters). Reformulating this as a continuous problem requires the addition of integer variables describing the action of the decision rules in every scenario and every stage. This is clearly intractable for problems with many stages and largely obviates the key advantages of DRA relative to SBA¹.

For the class of MSPs considered in this chapter, no solution strategies using mixedinteger DRs have yet been proposed in the open literature. However, a few DRA approaches have been developed for linear multistage robust optimization problems with mixed-integer recourse, and the key problem outlined above is evident in these approaches too. The paper [90] proposes a highly flexible class of integer DRs based on the signs of piecewise affine threshold functions. However, the resulting DRA is a discontinuous robust optimization problem that is very difficult to solve. The article [123] proposes an alternative class of DRs described by linear combinations of discontinuous basis functions. A critical feature of this scheme is that the locations of the discontinuities are not decision-dependent (i.e., all

¹Although not entirely, since non-anticipativity is enforced by the DR structure rather than through constraints. As a consequence, the number of scenarios required to approximate DRA only depends on the variance of the objective and constraints and can be very much smaller than the exponential scenario tree required in standard SBA approaches.

admissible rules are piecewise constant on a fixed polyhedral partition of the uncertainty space), which is restrictive but provides significant computational advantages, particularly for basis functions corresponding to box partitions. Instead of using basis functions, several related approaches explicitly specify a partition of the uncertainty set and require the integer recourse decisions to be constant on each partition element. Fixed partitions are used in [124], while adaptive partitioning schemes are proposed for improved accuracy in [125, 126]. Despite their differences, all of these DR approaches ultimately require the solution of mixed-integer problems or subproblems, and critically, the number of integer variables again increases at least linearly (and often faster) with the number of stages², as well as something like the number of scenarios (i.e., worst-case candidate scenarios in [90], partition elements in [124–126], and basis functions in [123]).

For the state-space MSP formulation considered in this chapter, a fundamentally different approach is to cast the DRA as a simulation-optimization problem. This formulation, which we refer to as DRA-SO, consists of an 'outer' optimization problem over only the first-stage decisions (including DR parameters) and an 'inner' or 'embedded' stochastic simulation that (approximately) evaluates the objective and constraints. Specifically, this simulation uses the specified DR to make both continuous and discrete recourse decisions in all stages and for all simulated scenarios. Compared to the approaches discussed above, the critical advantage of DRA-SO is that it is scalable to problems with very many stages. In particular, when it is acceptable to use the same decision rule in every stage (formulated as a function of a state vector rather than the entire history of the uncertainty), the size of the outer optimization problem is completely independent of the number of stages, while the cost of the embedded simulation scales only linearly in the number of stages. Furthermore, DRA-SO offers tremendous modeling flexibility because it can readily accommodate nonlinear and nonconvex MSPs as well as nearly arbitrary decision rules. Notably, this includes

²Notably, the approach in [123] is unique in that the integer variables are used to parameterize the DR itself, rather than to represent its action in each stage and 'scenario'. In the latter case, an increase in integer variables with the number of stages is unavoidable regardless of the DR structure, while in [123] this growth occurs because the DR is permitted to depend on the entire history of the uncertainty, and to be different in each stage.

even implicit DRs that make very high-quality recourse decisions by solving a parameterized model predictive control (MPC) problem in each stage of the simulation. However, the obvious drawback of DRA-SO is that the outer optimization problem is highly complex despite being low-dimensional, and the need for discontinuous DRs introduces unique challenges in this context as well. In particular, such DRs make the simulated cost and constraint values discontinuous with respect to the outer optimization variables for any fixed scenario. For example, in integrated planning and scheduling problems, a perturbation of a design decision may induce a change in a discrete operational decision through the embedded DR, causing a discontinuity in the stage cost. Since this may occur in every stage and every simulated scenario, the number of such discontinuities can be huge, making the outer optimization problem extremely irregular and difficult to solve. Consequently, existing DRA-SO approaches treat the embedded simulation as a black box and solve the outer optimization problem using heuristic derivative-free algorithms [77, 78]. Unfortunately, these methods are not guaranteed to find optimal solutions finitely and often suffer from slow convergence compared to gradient-based algorithms [79, 80]. Thus, in practice, derivative-free methods often require prohibitive computational effort and may locate suboptimal solutions, particularly in high-dimensional problems [78].

The key takeaway from the preceding discussion is as follows. On one hand, DRs appear to have huge potential to address multistage problems with mixed-integer recourse in many stages by effectively eliminating a vast number of integer decisions. On the other hand, it is clear that this alone does not eliminate the overwhelming discrete character of these problems, since all existing strategies for solving the resulting DRA ultimately deal with auxiliary integer decisions or discontinuities that themselves scale at least linearly in the number of stages. The central contribution of this chapter is to develop a class of mixed-integer DRs that resolves this problem using the smoothing property of integration, specifically for state-space MSP formulations with expected-value objectives and chance constraints. The basic structure of the proposed DRs is very general, requiring only that binary decisions are made by checking the signs of a set of smooth threshold functions that may depend arbitrarily on the system state, the current uncertainty vector, and the first-stage decisions (including rule parameters). For any fixed state and uncertainty vector, these DRs are clearly discontinuous with respect to the first-stage decisions. However, the key insight in our approach is that such discontinuities can be smoothed by integration over random variables. Thus, the use of such DRs can potentially result in expected costs and chance constraints that are smooth functions of the decision variables. In this chapter, DRs with this property are referred to as smooth-in-expectation decision rules. This kind of smoothing is interesting because it mitigates the discrete character of the original problem in a fundamentally new way. In the context of DRO-SO, it implies that the embedded simulation returns stochastic estimates of smooth functions rather than discontinuous ones. Therefore, the outer optimization problem can be solved to first-order optimality using stochastic gradient-based techniques, which may significantly outperform heuristic approaches for high-dimensional problems. More fundamentally, smoothing actually endows the outer optimization problem with a meaningful concept of local optimality, thereby providing a potentially efficient means to locate high-quality solutions.

To formalize these ideas, the first concrete contribution of this chapter is a set of sufficient conditions under which the general class of DRs described above is guaranteed to result in continuously differentiable expected costs and chance constraints. These conditions are based on our prior results in Chapter 2 concerning the differentiability of expected costs associated with stochastic hybrid systems. In addition to adapting these conditions to state-space MSPs, we also provide important extensions to accommodate chance constraints and models with discrete state variables, neither of which is addressed in Chapter 2. The extension to discrete states is important because such states are often needed to enforce timing constraints such as minimum uptime/downtime constraints in unit commitment and scheduling problems. Although the resulting differentiability conditions are relatively mild, they are violated in some important cases. However, a key observation is that these conditions can always be satisfied by using a suitably randomized DR, and we provide a systematic method for achieving this by introducing a minimal number of additional random variables. Unfortunately, this randomization is undesirable in some cases because it can lead to violations of important operational constraints with a non-trivial probability. To address this, the second major contribution of this chapter is a second set of sufficient conditions that relaxes several problematic requirements in the first. This second set of conditions is much more likely to be satisfied in practice and is often easier to verify. Moreover, these conditions can always be satisfied by randomization, and this potentially requires many fewer additional random variables than the first set. Finally, we demonstrate the use of these results to solve an illustrative integrated design and operation problem with integer recourse decisions in 365 stages. Using the proposed class of mixedinteger DRs together with the developed differentiability conditions, we obtain a smooth DRA-SO formulation and demonstrate the advantages of differentiability by comparing the optimization performance of a basic stochastic trust-region algorithm [127] (which relies on differentiability) to that of a commercial gradient-free algorithm.

3.3 Problem Formulation

3.3.1 Notation

Scalars, vectors, and matrices are denoted without emphasis, bold font is used for sequences $\mathbf{x} = (x_0, \ldots, x_N)$, and $\mathbf{x}_{i:j}$ denotes the subsequence $(\mathbf{x}_i, \ldots, \mathbf{x}_j)$. For $S \subset \mathbb{R}^{n_s}$, the set of k-times continuously differentiable maps from S into \mathbb{R}^m is denoted by $C^k(S, \mathbb{R}^m)$, and the set of all essentially bounded measurable maps from S into \mathbb{R}^m is denoted by $L^{\infty}(S, \mathbb{R}^m)$. For $(\hat{s}, \hat{r}) \in S \times R$ with $R \subset \mathbb{R}^{n_r}$, the Jacobian matrix of $\ell(\hat{s}, \cdot)$ at \hat{r} is denoted by $\frac{\partial \ell}{\partial r}(\hat{s}, \hat{r})$ or $\nabla_r^{\mathrm{T}}\ell(\hat{s}, \hat{r})$.

3.3.2 General Model for State-Space Multistage Stochastic Programs

We consider a general state-space multistage stochastic program (MSP) with Kstages, affected by a sequence $\boldsymbol{\omega} = (w_0, \dots, w_K)$ of random variables $w_k \in \tilde{W} \subset \mathbb{R}^{n_w}$ revealed at each stage $k \in \mathcal{K} \equiv \{0, \dots, K\}$. Assumption 3.3.1. The random sequence $\boldsymbol{\omega}$ has a probability density $p: \tilde{\Omega} \to \mathbb{R}$ defined on the open set $\tilde{\Omega} \equiv \tilde{W} \times \cdots \times \tilde{W}$. Moreover, there exists a compact interval $W \equiv [w^L, w^U] \subset \tilde{W}$ such that p is zero outside of $\Omega \equiv W \times \cdots \times W$ and continuous on the interior of Ω .

The first-stage decisions of the MSP are denoted by $\theta \in \tilde{\Theta} \subset \mathbb{R}^{n_{\theta}}$ and the mixedinteger recourse decisions are denoted by $u_k(\omega) = (u_k^c(\omega), u_k^d(\omega))$ with $u_k^c(\omega) \in \tilde{U}^c \subset \mathbb{R}^{n_u^c}$ and $u_k^d(\omega) \in \tilde{U}^d \subset \{0,1\}^{n_u^d}$. The systems of interest are characterized by a state $x_k(\omega)$ which follows given nonlinear dynamics with a fixed initial state $x_0(\omega) = b_0$. We allow $x_k(\omega)$ to contain both continuous and discrete states, which we denote by $x_k(\omega) = (x_k^c(\omega), z_k^d(\omega))$ with $x_k^c(\omega) \in \tilde{X}^c \subset \mathbb{R}^{n_x^c}$ and $z_k^d(\omega) \in \tilde{X}^d \subset \mathbb{Z}^{n_x^d}$. Define the sets $\tilde{X} \equiv \tilde{X}^c \times \tilde{X}^d$ and $\tilde{U} \equiv \tilde{U}^c \times \tilde{U}^d$ and the functions $C : \tilde{\Theta} \to \mathbb{R}$, $f : \mathcal{K} \times \tilde{U} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \tilde{X}$, $\ell_S : \mathcal{K} \times \tilde{U} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \mathbb{R}$, and $g : \mathcal{K} \times \tilde{U} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \mathbb{R}^{n_g}$.

Assumption 3.3.2. The sets \tilde{U}^c , \tilde{X}^c , \tilde{W} , and $\tilde{\Theta}$ are open. Moreover, for each $k \in \mathcal{K}$, $u^d \in \tilde{U}^d$, and $z^d \in \tilde{X}^d$, the functions $C(\cdot)$, $f(k, (\cdot, u^d), (\cdot, z^d), \cdot, \cdot)$, $\ell_S(k, (\cdot, u^d), (\cdot, z^d), \cdot, \cdot)$, and $g(k, (\cdot, u^d), (\cdot, z^d), \cdot, \cdot)$ are continuously differentiable on $\tilde{U}^c \times \tilde{X}^c \times \tilde{W} \times \tilde{\Theta}$.

We consider the following state-space MSP model, where Θ is a compact subset of $\tilde{\Theta}$ and $\mathbb{E}[A]$ and $\mathbb{P}[A]$ denote the expected value and probability of A, respectively:

$$\begin{array}{l} \min_{\substack{\theta \in \Theta \\ x_k \in L^{\infty}(\Omega, \tilde{X}) \\ u_k \in L^{\infty}(\Omega, \tilde{U})}} & C(\theta) + \mathbb{E} \left[\sum_{k=0}^{K} \ell_S(k, u_k(\omega), x_k(\omega), w_k, \theta) \right] \\ \text{s.t.} & \mathbb{P} \left[g(k, u_k(\omega), x_k(\omega), w_k, \theta) \leq 0 \right] \geq 1 - \epsilon \\ & x_0(\omega) = b_0, \quad \forall \omega \in \Omega \\ & x_{k+1}(\omega) = f(k, u_k(\omega), x_k(\omega), w_k, \theta), \quad \forall \omega \in \Omega \\ & u_k \quad \text{nonanticipative} \\ & \forall k \in \{0, \dots, K\} \end{array}$$

$$(3.1)$$

The constraint $\mathbb{P}[g(k, u_k(\boldsymbol{\omega}), x_k(\boldsymbol{\omega}), w_k, \theta) \leq 0] \geq 1 - \epsilon$ is a general joint chance constraint specifying that $g(k, u_k(\boldsymbol{\omega}), x_k(\boldsymbol{\omega}), w_k, \theta) \leq 0$ must hold with probability $1 - \epsilon$, where $\epsilon \in (0, 1]$. Note that the case of $\epsilon = 0$, which corresponds to robust constraints, is not addressed by our solution method. However, cases when some of the constraints $g_i(k, u_k(\boldsymbol{\omega}), x_k(\boldsymbol{\omega}), w_k, \theta) \leq 0$ are required to hold robustly are discussed in §3.4.2. The *nonanticipativity* of u_k means that u_k must be decided at time k using only knowledge of w_j with $j \leq k$, and is required to model realistic operation of the system. This can be explicitly stated by the constraint $u_k(\boldsymbol{\omega}) = u_k(\hat{\boldsymbol{\omega}})$, for all $\boldsymbol{\omega}, \hat{\boldsymbol{\omega}} \in \Omega$ with $w_{0:k-1} = \tilde{w}_{0:k-1}$. Overall, the MSP (3.1) chooses the first stage decisions θ that simultaneously minimize the first-stage cost C and the expected value of the sum of the stage costs ℓ_S assuming optimal operations in each stage $k \in \mathcal{K}$.

3.3.3 Decision-Rule Approximation

The MSP (3.1) is intractable because, first, the sets of functions $L^{\infty}(\Omega, \tilde{X})$ and $L^{\infty}(\Omega, \tilde{U})$ are infinite dimensional, and second, the expected value \mathbb{E} and probability \mathbb{P} cannot be computed exactly except in very special cases. To address the first issue, a promising approach is to approximate the recourse decisions u_k with a *decision rule* $\kappa : \mathcal{K} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \tilde{U}$ as follows:

$$u_k(\boldsymbol{\omega}) = \kappa(k, x_k(\boldsymbol{\omega}), w_k, \theta). \tag{3.2}$$

The decision rule (DR) κ has a fixed structure, but can depend on parameters $\gamma \in \Gamma \subset \mathbb{R}^{n_{\gamma}}$ that can be co-optimized with the first-stage decisions θ . For simplicity of notation, we use θ henceforth to refer to the vector containing both the original first-stage decisions and the rule parameters γ . The advantage of using κ is that it eliminates the need to optimize over the infinite dimensional spaces $L^{\infty}(\Omega, \tilde{U})$ and $L^{\infty}(\Omega, \tilde{X})$ because, for each $(\omega, \theta) \in \tilde{\Omega} \times \tilde{\Theta}$, κ fixes the value of $u_k(\omega)$ and ensures that the value of $x_k(\omega)$ is uniquely determined by the dynamic model f. Moreover, κ directly enforces nonanticipativity of u_k , which eliminates the infinite number of nonanticipativity constraints in (3.1).

With a slight abuse of notation (recall that x_k and u_k are already defined as functions

of $\boldsymbol{\omega}$ only), define $x_k(\boldsymbol{\omega}, \theta)$ and $u_k(\boldsymbol{\omega}, \theta)$ for every $(\boldsymbol{\omega}, \theta) \in \tilde{\Omega} \times \tilde{\Theta}$ by the recursion:

$$x_0(\boldsymbol{\omega}, \boldsymbol{\theta}) \equiv b_0, \tag{3.3}$$

$$u_k(\boldsymbol{\omega}, \theta) \equiv \kappa(k, x_k(\boldsymbol{\omega}, \theta), w_k, \theta), \qquad (3.4)$$

$$x_{k+1}(\boldsymbol{\omega}, \theta) \equiv f(k, u_k(\boldsymbol{\omega}, \theta), x_k(\boldsymbol{\omega}, \theta), w_k, \theta).$$
(3.5)

Moreover, define $\ell(\boldsymbol{\omega}, \theta)$ and $\tau_k(\boldsymbol{\omega}, \theta)$ for each $(\boldsymbol{\omega}, \theta) \in \tilde{\Omega} \times \tilde{\Theta}$ by:

$$\ell(\boldsymbol{\omega}, \boldsymbol{\theta}) \equiv \sum_{k=0}^{K} \ell_S(k, u_k(\boldsymbol{\omega}, \boldsymbol{\theta}), x_k(\boldsymbol{\omega}, \boldsymbol{\theta}), w_k, \boldsymbol{\theta}),$$
(3.6)

$$\tau_k(\boldsymbol{\omega}, \theta) \equiv g(k, u_k(\boldsymbol{\omega}, \theta), x_k(\boldsymbol{\omega}, \theta), w_k, \theta).$$
(3.7)

Then, the *decision-rule approximation* (DRA) for (3.1) is given by:

$$\min_{\theta \in \Theta} \quad C(\theta) + \mathbb{E}\left[\ell(\boldsymbol{\omega}, \theta)\right]
s.t. \quad \mathbb{P}\left[\tau_k(\boldsymbol{\omega}, \theta) \le 0\right] \ge 1 - \epsilon, \quad \forall k \in \{0, \dots, K\}.$$
(3.8)

Problem (3.8) is a single-stage problem with a finite and potentially small number of decisions θ . This is a huge simplification of (3.1), particularly for problems where it is necessary to model short-time scale operations over a long horizon, leading to many stages in (3.1). Nevertheless, (3.8) is still intractable because $\mathbb{E}\left[\ell(\boldsymbol{\omega},\theta)\right]$ and $\mathbb{P}\left[\tau_k(\boldsymbol{\omega},\theta) \leq 0\right]$ are not be finitely computable in general.

In very special cases, the approximation (3.8) can be reformulated as an equivalent deterministic problem. For example, when (3.1) is linear and the recourse decisions $u_k(\omega)$ are purely continuous, a suitable DR (e.g., linear) can allow $\mathbb{E}[\ell(\omega, \theta)]$ and $\mathbb{P}[\tau_k(\omega, \theta) \leq 0]$ to be written explicitly in terms of θ . However, for the general case we consider here, a deterministic equivalent for (3.8) is very difficult to obtain because ℓ and τ_k may be nonlinear and are often highly discontinuous. The discontinuity of ℓ and τ_k arise because the definition of these functions involves κ , and κ must be discontinuous in order to model discrete recourse decisions. Prohibitively, the number of such discontinuities can be very large because they can be introduced at every stage and for each $\boldsymbol{\omega} \in \tilde{\Omega}$, making $\mathbb{E}\left[\ell(\boldsymbol{\omega}, \theta)\right]$ and $\mathbb{P}\left[\tau_k(\boldsymbol{\omega}, \theta) \leq 0\right]$ extremely hard to write explicitly.

A more general approach is to evaluate $\mathbb{E}\left[\ell(\boldsymbol{\omega}, \theta)\right]$ and $\mathbb{P}\left[\tau_k(\boldsymbol{\omega}, \theta) \leq 0\right]$ through stochastic simulations. For a given θ , this consists of simulating the recursion (3.3)–(3.5) for randomly generated sequences $\boldsymbol{\omega}$ to obtain $\ell(\boldsymbol{\omega}, \theta)$ and $\tau_k(\boldsymbol{\omega}, \theta)$, which are then used to estimate $\mathbb{E}\left[\ell(\boldsymbol{\omega}, \theta)\right]$ and $\mathbb{P}\left[\tau_k(\boldsymbol{\omega}, \theta) \leq 0\right]$. To emphasize this simulation approach, we define the following notation:

$$\mathcal{L}(\theta) \equiv \mathbb{E}\left[\ell(\boldsymbol{\omega}, \theta)\right],\tag{3.9}$$

$$\mathcal{P}_k(\theta) \equiv \mathbb{P}\left[\tau_k(\boldsymbol{\omega}, \theta) \le 0\right]. \tag{3.10}$$

Using this approach, it becomes natural to cast the approximation (3.8) as a simulationoptimization problem. This formulation, which we refer to as DRA-SO, consists of an 'outer' optimization problem over only θ and an 'inner' or 'embedded' stochastic simulation that evaluates $\mathcal{L}(\theta)$ and $\mathcal{P}_k(\theta)$. Thus, the DRA-SO problem can be written as follows:

$$\min_{\theta \in \Theta} \quad C(\theta) + \mathcal{L}(\theta)$$
s.t. $\mathcal{P}_k(\theta) \ge 1 - \epsilon, \quad \forall k \in \{0, \dots, K\}.$

$$(3.11)$$

It is not immediately clear that merely casting (3.8) as (3.11) resolves any of the key issues discussed above. Specifically, if ℓ and τ_k are discontinuous, then $\ell(\boldsymbol{\omega}, \cdot)$ and $\tau_k(\boldsymbol{\omega}, \cdot)$ may be discontinuous with respect to θ for each fixed $\boldsymbol{\omega}$. It follows that sample average approximations such as $\mathcal{L}(\theta) \approx M^{-1} \sum_{j=1}^{M} \ell(\boldsymbol{\omega}_j, \theta)$ will also be discontinuous with respect to θ , and therefore it seems very likely that \mathcal{L} and \mathcal{P}_k will also be discontinuous, making (3.11) difficult to solve. To the contrary, our primary interest in (3.11) is that the true expected value \mathcal{L} and probability \mathcal{P}_k can be smooth functions of θ even when sample average approximations are highly discontinuous, as shown by the following simple example.

Example 1. Consider a one-stage (i.e., K = 0) instance of (3.1) with w_0 uni-

formly distributed in [0,1], $\theta \in [0.1,0.8]$, $u_0(w_0) \in \{0,1\}$, $C(\theta) = 2(\theta - 0.7)^2$, $\ell_S(0, u_0(w_0), x_0(w_0), w_0, \theta) = u_0(w_0)$, and no chance constraints. Consider the DRA-SO approximation (3.11) for this instance with $u_0(w_0, \theta) = \kappa(0, x_0(w_0, \theta), w_0, \theta) = 0$ if $\theta \leq w_0$ and $u_0(w_0, \theta) = \kappa(0, x_0(w_0, \theta), w_0, \theta) = 1$ otherwise. By (3.6), this implies that $\ell(w_0, \theta) = 0$ if $\theta \leq w_0$ and $\ell(w_0, \theta) = 1$ otherwise. Thus, for any fixed sample w_0 , $\ell(w_0, \cdot)$ has one discontinuity at $\theta = w_0$, where it jumps from 0 to 1. In Fig. 3.1, the plot on the left shows an approximation of $C + \mathcal{L}$, where, for all θ , $\mathcal{L}(\theta) = \mathbb{E}[\ell(w_0, \theta)]$ is approximated by an average of $\ell(w_0, \theta)$ over 7 fixed samples (i.e., the same samples are used for every θ). Clearly, this function is discontinuous, and the number of discontinuities increases proportionally with the sample size. On the other hand, the plot on right shows $C + \mathcal{L}$ with $\mathcal{L}(\theta)$ computed



Figure 3.1: $C(\theta) + \mathcal{L}(\theta)$ vs. θ for Example 1 using a binary DR. Left: $\mathcal{L}(\theta)$ computed by sample average approximation with 7 samples. Right: $\mathcal{L}(\theta)$ computed exactly.

exactly as $\mathbb{E}[\ell(w_0, \theta)] = \theta$. The key observation is that, even though $\ell(w_0, \cdot)$ and the sample average approximation of \mathcal{L} are discontinuous, the true expected value function \mathcal{L} is smooth.

The key result of the preceding example is that the true expected value \mathcal{L} can be smooth even when ℓ is discontinuous, and hence even when sample average approximations are discontinuous for any finite number of samples. Although we used an explicit expression for \mathcal{L} to show this, it is not necessary to have such an expression in order to exploit this observation. Specifically, even when \mathcal{L} can only be approximated by stochastic simulations, it is possible to obtain stochastic estimates of $\nabla \mathcal{L}$ (e.g., by simple finite differencing) that are appropriate for use in stochastic gradient decent algorithms with probabilistic convergence to local minima for smooth problems [128, 129]. In contrast, if one replaces \mathcal{L} with a discontinuous sample average approximation based on some fixed set of samples chosen a priori, then any estimate of $\nabla \mathcal{L}$, such as a finite difference estimate, would be meaningless, and any descent algorithm based on it would likely fail. Thus, the knowledge that \mathcal{L} and \mathcal{P}_k are smooth, at least for some instances of (3.11), can potentially enable the use of efficient gradient-based techniques for solving (3.11) to local optimality, which is likely to have significant advantages over derivative-free approaches, especially when θ is high-dimensional. More subtly, it can be seen from Fig. 3.1 that the smoothness of \mathcal{L} actually endows (3.11) with a meaningful notion of local optimality that is absent in the discontinuous sampleaverage approximation (i.e., the discontinuities in the latter generate a profusion of highly suboptimal local minima). Moreover, even a global solution of the latter can be arbitrarily far from the solution of the smooth problem. Therefore, the use of decision rules that ensure smoothness of \mathcal{L} and \mathcal{P}_k , whenever it is practical to do so, may prove to be a powerful strategy for efficiently locating high-quality solutions of MSPs with mixed-integer recourse.

3.3.4 Objectives of the Chapter

The objectives of this chapter are to introduce a general class of mixed-integer decision rules, to establish a set of sufficient conditions under which such a rule is guaranteed to produce a DRA-SO approximation (3.11) with continuously differentiable objective \mathcal{L} and constraint functions \mathcal{P}_k , and to demonstrate that these conditions are practically useful. This is motivated by the hope that such a smoothness property will enable (3.11) to be solved efficiently using stochastic gradient descent methods, thereby providing a practical means to obtain high-quality solutions of otherwise intractable instances of the MSP (3.1). Although we demonstrate such an approach for one illustrative example, the development of a generally effective gradient descent algorithm for this class of problems is beyond the scope of this chapter. Moreover, in contrast to existing work on mixed-integer decision rules, the goal of this chapter is to provide a reformulation of (3.1) that is amenable to efficient *local* optimization. Thus, we neither claim nor attempt to arrange that (3.11) is convex or otherwise amenable to efficient global optimization.

3.4 Smooth-in-Expectation Decision Rules

In this section, we introduce a general class of mixed-integer decision rules and develop a first set of conditions under which such rules are guaranteed to give a smooth expected value function \mathcal{L} .

Definition 3.4.1. Let $S \equiv \{-1,1\}^{n_{\sigma}}$, let $\kappa_{\sigma} : \mathcal{K} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \tilde{U}$ be a collection of rules indexed by $\sigma \in S$, and let $h_i : \mathcal{K} \times S \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \mathbb{R}$ be a collection of *event* functions indexed by $i \in \{1, \ldots, n_{\sigma}\}$. Assume that, for every $k \in \mathcal{K}, z^d \in \tilde{X}^d$, and $\sigma \in S$, each $\kappa_{\sigma}(k, (\cdot, z^d), \cdot, \cdot)$ and $h_i(k, \sigma, (\cdot, z^d), \cdot, \cdot)$ is continuously differentiable on $\tilde{X}^c \times \tilde{W} \times \tilde{\Theta}$. Moreover, assume that each h_i is independent of all σ_j with $j \geq i$ and, with a slight abuse of notation, denote $h_i(k, \sigma_{1:i-1}, z, w, \theta) = h_i(k, \sigma, z, w, \theta)$. The class of DRs we consider is defined for each $(k, z, w, \theta) \in \mathcal{K} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ by

$$\sigma_{i} = \left\{ \begin{array}{cc} 1 & \text{if} \quad h_{i}(k, \sigma_{1:i-1}, z, w, \theta) \leq 0 \\ -1 & \text{otherwise} \end{array} \right\}, \quad \forall i \in \{1, \dots, n_{\sigma}\}$$
(3.12)

$$\kappa(k, z, w, \theta) = \kappa_{\sigma}(k, z, w, \theta). \tag{3.13}$$

In words, a DR satisfying Definition 3.4.1 makes decisions by first checking the sign of a sequence of event functions h_i to determine the binary vector σ , and then implementing a predetermined smooth decision rule κ_{σ} based on the value of σ . Note that each event function h_i can depend on the outcome σ_j of all previous event functions h_j with j < i. Thus, σ is determined by a binary decision tree. Moreover, the event functions h_i and rules κ_{σ} can depend arbitrarily on the current state, uncertainty, and first-stage decisions, provided that this dependence is smooth. In practice, these functions must be specified by the user, but they can be parameterized for flexibility by augmenting the first-stage decisions θ with the necessary rule parameters. In this way, the behavior of the rule will be co-optimized with the original first-stage decisions when solving (3.11). Note that each κ_{σ} makes both continuous and binary recourse decisions; i.e., $(u^c, u^d) = \kappa_{\sigma}(k, z, w, \theta)$. Since $\kappa_{\sigma}(k, (\cdot, z^d), \cdot, \cdot)$ is assumed to be continuously differentiable on $\tilde{X}^c \times \tilde{W} \times \tilde{\Theta}$ for every $k \in \mathcal{K}$, $z^d \in \tilde{X}^d$, and $\sigma \in S$, its binary output must be constant for each (k, z^d, σ) . Thus, each tuple (k, x^d, σ) yields a single binary outcome u^d . However, σ and u^d are not the same, and σ may be used to encode other non-smooth behaviors, such as piecewise affine policies for the continuous recourse decisions.

Definition 3.4.1 provides a general framework for modeling many decision rules found in the literature. These include exact recourse rules available from multiparametric programming [10], linear and nonlinear decision rules found in the robust optimization literature [81–86], and logic controllers such as energy management policies in microgrid systems, hedging rules in water resource management, and dispatching rules in flexible manufacturing [16, 74, 75]. The structure (3.12)–(3.13) is also closely related to the idea of uncertainty-set partitioning used in the robust optimization literature [124–126] in which a decision-rule is assigned to each partition element. In our case, once θ is fixed, the event functions h_i in (3.12) define a partition of the joint state and uncertainty set and a decision-rule κ_{σ} is used on each partition element. Notably, the structure of this partition can change with θ . Thus, the class of DRs satisfying Definition 3.4.1 is more flexible than classes based on fixed partitions (e.g., [123, 124]).

Definition 3.4.2. Let $\kappa : \mathcal{K} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \tilde{U}$ be a decision rule satisfying Definition 3.4.1 and define $\mathcal{L} : \tilde{\Theta} \to \mathbb{R}$ by (3.9) with (3.3)–(3.6). The rule κ is called *smooth-in-expectation* if $\mathcal{L} \in C^1(\tilde{\Theta}, \mathbb{R})$.

Remark 3.4.1. Although differentiability of \mathcal{L} seems like a property of both κ and the problem data (e.g., ℓ , f, etc.), the results in the next subsection show that it only depends on κ provided that Assumptions 3.3.1–3.3.2 hold. Thus, smoothness-in-expectation is truly a property of the decision rule, as the wording of Definition 3.2 suggests.

3.4.1 A First Set of Sufficient Conditions for Smoothness-in-Expectation

Let κ be a mixed-integer decision rule satisfying Definition 3.4.1. In this subsection, we establish a first set of conditions on κ that are sufficient to guarantee continuous differentiability of the expected-value \mathcal{L} .

To ease notation, we first define the sets $\mathcal{M}(k, \sigma, \theta)$, which partition the joint state and uncertainty set $\tilde{X} \times W$ at each k. For each fixed $k \in \mathcal{K}$ and $\theta \in \Theta$, these sets contain all $(z, w) \in \tilde{X} \times W$ consistent with a fixed discrete mode $\sigma \in \mathcal{S}$ according to (3.12). Note that we use the compact notation $\sigma_i h_i \leq 0$ to state that $h_i \leq 0$ if $\sigma_i = 1$ and $h_i \geq 0$ if $\sigma_i = -1$.

Definition 3.4.3. For every $k \in \mathcal{K}$, $\sigma \in \mathcal{S}$, and $\theta \in \tilde{\Theta}$, define the sets

$$\mathcal{M}(k,\sigma,\theta) \equiv \{(z,w) \in \tilde{X} \times W : \sigma_i h_i(k,\sigma,z,w,\theta) \le 0, \ \forall i\},\tag{3.14}$$

$$\partial_i \mathcal{M}(k,\sigma,\theta) \equiv \{(z,w) \in \mathcal{M}(k,\sigma,\theta) : h_i(k,\sigma,z,w,\theta) = 0\},\tag{3.15}$$

$$\partial_{ij}\mathcal{M}(k,\sigma,\theta) \equiv \left\{ (z,w) \in \mathcal{M}(k,\sigma,\theta) : \begin{array}{l} h_i(k,\sigma,z,w,\theta) = 0\\ h_j(k,\sigma,z,w,\theta) = 0 \end{array} \right\}.$$
(3.16)

The sufficient conditions for smoothness-in-expectation are stated below, followed by our main result (Theorem 3.4.1). A conceptual discussion of these conditions follows Theorem 3.4.1.

Condition 3.4.1. For any $k \in \mathcal{K}$, $\sigma \in \mathcal{S}$, $\theta \in \tilde{\Theta}$, and $i \in \{1, \ldots, n_{\sigma}\}$,

$$\frac{\partial h_i}{\partial w}(k,\sigma,z,w,\theta) \neq 0, \quad \forall (z,w) \in \partial_i \mathcal{M}(k,\sigma,\theta).$$

Condition 3.4.2. Choose any $k \in \mathcal{K}$, $\sigma \in \mathcal{S}$, $\theta \in \tilde{\Theta}$, and $i, j \in \{1, \ldots, n_{\sigma}\}$ with $i \neq j$. Then, the following condition holds:

$$\operatorname{rank} \begin{bmatrix} \frac{\partial h_i}{\partial w}(k, \sigma, z, w, \theta) \\ \frac{\partial h_j}{\partial w}(k, \sigma, z, w, \theta) \end{bmatrix} = 2, \quad \forall (z, w) \in \partial_{ij} \mathcal{M}(k, \sigma, \theta)$$

Condition 3.4.3. Choose any $k \in \mathcal{K}$, $\sigma \in \mathcal{S}$, $\theta \in \tilde{\Theta}$, $i \in \{1, \ldots, n_{\sigma}\}$, and $p \in \{1, \ldots, n_w\}$ and let e_p denote the unit vector with the 1 in the p^{th} position. Then, the following condition holds:

$$\operatorname{rank} \begin{bmatrix} \frac{\partial h_i}{\partial w}(k,\sigma,z,w,\theta) \\ e_p^{\mathrm{T}} \end{bmatrix} = 2, \forall (z,w) \in \partial_i \mathcal{M}(k,\sigma,\theta) \text{ with } w_p = w_p^L \text{ or } w_p = w_p^U.$$

Theorem 3.4.1. Under Condition 3.4.1, \mathcal{L} is continuous on $\tilde{\Theta}$. If Conditions 3.4.2–3.4.3 also hold, then $\mathcal{L} \in C^1(\tilde{\Theta}, \mathbb{R})$.

Theorem 3.4.1 is proven in the appendix of this dissertation by extending the main result in Chapter 2, which concerns the differentiability of expected-value costs associated with stochastic hybrid systems. The key idea is to apply this result to the dynamic system (3.3)-(3.6) with Definition 3.4.1. However, since this system is structurally different from that in Chapter 2, applying the result in Chapter 2 requires addressing several technical details. For brevity the proof is given in the appendix.

To conceptually understand Conditions 3.4.1–3.4.3, consider the following simple instance of (3.1) with K = 0, one-dimensional θ , w uniformly distributed in an interval $W \subset \mathbb{R}^2$, and purely binary recourse decisions $u_0(w) \in \tilde{U} = \{0, 1\}^2$:

$$\min_{\substack{\theta \in \Theta \\ u_0 \in L^{\infty}(W, \tilde{U})}} \mathbb{E} \left[u_{0,1}(w_0) + 2u_{0,2}(w_0) \right]$$
(3.17)

To form a DRA-SO approximation (3.11) of this instance, consider a decision rule κ satisfying Definition 3.4.1 with two event functions h_1 and h_2 determining $\sigma \in S = \{(1,1), (1,-1), (-1,1), (-1,-1)\}$, and with $\kappa_{\sigma}(w,\theta) = 0.5 + 0.5\sigma \in \{0,1\}^2$. According to (3.9), we have $\mathcal{L}(\theta) = \mathbb{E}[\kappa_1(w_0,\theta) + 2\kappa_2(w_0,\theta)]$. This situation is illustrated in Fig. 3.2, where the box represents the set W and the solid lines labeled $h_i(w,\theta) = 0$ are the subsets of W where h_i is active for the particular θ considered. For each fixed θ , the h_i 's partition the set W into regions $\mathcal{M}(\sigma,\theta)$ with $\sigma \in S$. Let $\mathbb{P}(\sigma,\theta) = \mathbb{P}[\mathcal{M}(\sigma,\theta)]$ denote the probability of observing $w \in \mathcal{M}(\sigma,\theta)$. This probability can be interpreted as



Figure 3.2: Illustration of situations that satisfy and violate Condition 3.4.1–3.4.3

the normalized area of the region $\mathcal{M}(\sigma, \theta)$. Then, $\mathcal{L}(\theta)$ can be rewritten as

$$\mathcal{L}(\theta) = \sum_{\sigma \in S} (\kappa_{\sigma,1}(w_0, \theta) + 2\kappa_{\sigma,2}(w_0, \theta)) \mathbb{P}(\sigma, \theta)$$

$$= \sum_{\sigma \in S} (1.5 + 0.5\sigma_1 + \sigma_2) \mathbb{P}(\sigma, \theta).$$
(3.18)

Thus, differentiability of \mathcal{L} depends on that of $\mathbb{P}(\sigma, \cdot)$ for each $\sigma \in \mathcal{S}$. Specifically, $\mathcal{L} \in C^1(\tilde{\Theta}, \mathbb{R})$ if and only if the probabilities $\mathbb{P}(\sigma, \theta)$ change smoothly upon perturbing θ . The effects of Conditions 3.4.1–3.4.3 on the smoothness of these probability changes is illustrated in Fig. 3.2. The top-left plot illustrates the case where Conditions 3.4.1–3.4.3 are satisfied, while the remaining three plots illustrate cases where each condition is violated. We discuss the violations first.

Condition 3.4.1 states that each h_i must have nontrivial dependence on w at all points where it is active (i.e., $h_i(w, \theta) = 0$). The top-right plot in Fig. 3.2 illustrates a case where Condition 3.4.1 is violated because h_2 is completely independent of w and $h_2(w,\theta) = h_2(\theta) = 0$ on the whole shaded area (i.e., the entire set W) for the specific value of θ shown in the figure. In this case $\sigma_2 = 1$ and there are only two possible values for σ determined by the sign of $h_1(w)$, namely $\sigma = (1,1)$ and $\sigma = (-1,1)$. Correspondingly, there are two regions $\mathcal{M}((1,1),\theta)$ and $\mathcal{M}((-1,1),\theta)$ and only two nonzero terms in (3.18). This situation can cause a discontinuity in \mathcal{L} because a perturbation $\delta \in \mathbb{R}$ such that $h_2(\theta+\delta) > 0$ will cause a switch from $\sigma_2 = 1$ to $\sigma_2 = -1$, shifting all of the probability discontinuously to the regions corresponding to $\sigma = (1, -1)$ and $\sigma = (-1, -1)$.

Condition 3.4.2 states that any two event functions must have linearly independent w-gradients at all points w where both of them are active. This requirement is clearly violated in the bottom-left plot in Fig. 3.2. In this case, the probabilities in (3.18) will change continuously with perturbations of θ by δ , but they may change non-smoothly. For example, suppose $\delta > 0$ causes h_2 to be translated to the right while $\delta < 0$ causes h_2 to translate left with h_1 fixed in both cases. Then, the region $\mathcal{M}((-1,1), \theta + \delta)$ will appear for $\delta > 0$ perturbations, but not for $\delta < 0$ perturbations. Critically, the degeneracy of $h_1(\cdot, \theta)$ and $h_2(\cdot, \theta)$ implies that the probability $\mathbb{P}((-1,1), \theta + \delta)$ will increase linearly w.r.t. $\delta > 0$ perturbations. Thus, $\mathbb{P}((-1,1), \theta + \delta)$ is constant for $\delta < 0$ and linear for $\delta > 0$, which makes $\mathbb{P}((-1,1), \cdot)$ nonsmooth at θ .

Condition 3.4.3 states that event functions must be non-degenerate with the boundaries of the interval W in the same sense that Condition 3.4.2 requires them to be nondegenerate with each other. The bottom-right plot in Fig. 3.2 illustrates a violation of this condition where $h_2(\cdot, \theta)$ is degenerate with the north boundary of W. As in the previous case, suppose that a perturbation $\delta > 0$ causes h_2 to be translated upward while a perturbation $\delta < 0$ causes h_2 to translate downward with h_1 fixed in both cases. Then, the degeneracy between $h_2(\cdot, \theta) = 0$ and the north boundary of W implies that the probability of, e.g., $\mathcal{M}((1,1), \theta + \delta)$ will increase linearly w.r.t δ as $\delta < 0$ increases while it will remain constant for $\delta > 0$ perturbations. Thus, $\mathbb{P}((1,1), \cdot)$ will be nonsmooth at θ .

Finally, the top-left plot illustrates a case where Conditions 3.4.2–3.4.3 are all satisfied. In this case, Theorem 3.4.1 ensures that the probabilities of all of the regions $\mathcal{M}(\sigma, \theta + \delta)$ will change smoothly with perturbations δ , therefore leading to smoothness of \mathcal{L} via (3.18).

A key consequence of Conditions 3.4.1–3.4.3 is that smoothness-in-expectation is only a property of the decision rule κ . This is important because it implies that any instance of (3.1) can potentially be made efficiently solvable via (3.11) by deliberately constructing DRs that are smooth-in-expectation. However, for (3.11) to be a useful approximation of (3.1), Conditions 3.4.1–3.4.3 have to allow DRs that are reasonably accurate. Fortunately, there are many applications where commonly used DRs naturally satisfy Conditions 3.4.1– 3.4.3. For example, in power systems and manufacturing, one common approach is to make discrete unit commitment decisions based on a random realization of uncertain quantities affecting the operation of the system, such as product demands, power loads, renewable resources, etc. [16, 74, 75]. This results in threshold functions of the form $h_i = w_k - b_i(k, x_k, \theta)$, which clearly satisfy Condition 3.4.1 and often satisfy Conditions 3.4.2–3.4.3 (although this is more difficult to show with simple examples because these conditions involve the whole set of h_i 's).

However, Conditions 3.4.1–3.4.3 rule out many other practically useful DRs. Examples include DRs that make discrete decisions based on thresholds on system states, such as product inventory levels, battery state of charge, or counter states required to enforce minimum up/down time constraints [20, 130]. This results in threshold functions of the form $h_i = x_k - b_i(k, \theta)$, which clearly violate Condition 3.4.1. Thus, Conditions 3.4.1–3.4.3 have some serious limitations. However, in the next section we show that any DR can be made to satisfy Conditions 3.4.1–3.4.3 by simply randomizing the event functions h_i , and we discuss cases where it is and is not desirable to perform such a randomization.

3.4.2 Satisfying Conditions 3.4.1–3.4.3 using Randomized Decision Rules

Let κ be any decision rule satisfying Definition 3.4.1 but violating one or more of Conditions 3.4.1–3.4.3. This subsection shows that there is always a simple modification of κ that is guaranteed to satisfy Conditions 3.4.1–3.4.3, and is therefore smooth-in-expectation. This modification consists of randomizing κ by adding new random variables to the event functions h_i as detailed in the following definition. This randomization does not affect the functions κ_{σ} .

Definition 3.4.4. Let κ be a decision rule satisfying Definition 3.4.1. For each $i \in \{1, \ldots, n_{\sigma}\}$, let $\xi_{1,i}$ and $\xi_{2,i}$ be random variables with a probability density $\rho : \tilde{\Xi} \to \mathbb{R}$, where $\tilde{\Xi}$ is open, ρ is zero outside of a compact interval $\Xi = [\xi^L, \xi^U] \subset \tilde{\Xi}$, and ρ is continuous on the interior of Ξ . Let $\check{W} \equiv W \times \Xi \times \cdots \times \Xi$, $\check{W} \equiv \tilde{W} \times \tilde{\Xi} \times \cdots \times \tilde{\Xi}$, and define $\check{\kappa}_{\sigma} : \mathcal{K} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \tilde{U}$ and $\check{h}_i : \mathcal{K} \times \mathcal{S} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \mathbb{R}$ as follows, where $\check{W} = (w, \xi_1, \xi_2) = (w, \xi_{1,1}, \ldots, \xi_{1,n_{\sigma}}, \xi_{2,1}, \ldots, \xi_{2,n_{\sigma}})$:

$$\check{h}_i(k,\sigma,z,\check{w},\theta) = h_i(k,\sigma,z,w,\theta) + \xi_{1,i} + \xi_{2,i}, \qquad (3.19)$$

$$\breve{\kappa}_{\sigma}(k, z, \breve{w}, \theta) = \kappa_{\sigma}(k, z, w, \theta).$$
(3.20)

Moreover, for every $\sigma \in \mathcal{S}$, define $\breve{\kappa} : \mathcal{K} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \tilde{U}$ by

$$\sigma_{i} = \left\{ \begin{array}{ccc} 1 & \text{if} & \check{h}_{i}(k, \sigma, z, \breve{w}, \theta) \leq 0 \\ -1 & \text{otherwise} \end{array} \right\}, \quad \forall i \in \{1, \dots, n_{\sigma}\}, \quad (3.21)$$

$$\breve{\kappa}(k, z, \breve{w}, \theta) = \breve{\kappa}_{\sigma}(k, z, \breve{w}, \theta).$$
(3.22)

Corollary 3.4.1. Let κ be any decision rule satisfying Definition 3.4.1. If $\check{\kappa}$ is constructed from κ as in Definition 3.4.4, then $\check{\kappa}$ satisfies Conditions 3.4.1–3.4.3 and is therefore smooth-in-expectation.

Proof It suffices to show that Conditions 3.4.1–3.4.3 are satisfied with \tilde{h}_i in place of h_i . Let \hat{e}_i^{T} be a unit vector of length n_{σ} with the 1 in the i^{th} position and let e_p^{T} be a unit vector of length $n_w + 2n_{\sigma}$ with the 1 in the p^{th} position. In the arguments below, we use the notation $\breve{\mathcal{M}}(k,\sigma,\theta)$ to denote $\mathcal{M}(k,\sigma,\theta)$ as defined in Definition 3.4.3 with the modified event functions \breve{h}_i . Accordingly, $\breve{\mathcal{M}}(k,\sigma,\theta)$ contains (z,\breve{w}) in the same way that $\mathcal{M}(k,\sigma,\theta)$ contains (z,w). Moreover, note that

$$\begin{bmatrix} \underline{\partial \check{h}_i} \\ \overline{\partial \check{w}} \end{bmatrix} = \begin{bmatrix} \underline{\partial \check{h}_i} & \underline{\partial \check{h}_i} & \underline{\partial \check{h}_i} \\ \overline{\partial w} & \overline{\partial \xi_1} & \overline{\partial \xi_2} \end{bmatrix}.$$
 (3.23)

To show Condition 3.4.1, choose any $k \in \mathcal{K}, \sigma \in \mathcal{S}, \theta \in \tilde{\Theta}, i \in \{1, \ldots, n_{\sigma}\}$, and $(z, \breve{w}) \in \partial_i \breve{\mathcal{M}}(k, \sigma, \theta)$. Applying (3.23) to (3.19), we have

$$\frac{\partial \check{h}_i}{\partial \check{w}}(k,\sigma,z,\check{w},\theta) = \begin{bmatrix} \frac{\partial h_i}{\partial w}(k,\sigma,z,w,\theta) & \hat{e}_i^{\mathrm{T}} & \hat{e}_i^{\mathrm{T}} \end{bmatrix} \neq 0.$$
(3.24)

To show Condition 3.4.2, choose any $k \in \mathcal{K}$, $\sigma \in \mathcal{S}$, $\theta \in \tilde{\Theta}$, $i, j \in \{1, \ldots, n_{\sigma}\}$ with $i \neq j$, and $(z, \breve{w}) \in \partial_{ij} \breve{\mathcal{M}}(k, \sigma, \theta)$. Applying (3.23) to (3.19), we have

$$\operatorname{rank} \begin{bmatrix} \frac{\partial \check{h}_i}{\partial \check{w}}(k, \sigma, z, \check{w}, \theta) \\ \frac{\partial \check{h}_j}{\partial \check{w}}(k, \sigma, z, \check{w}, \theta) \end{bmatrix} = \operatorname{rank} \begin{bmatrix} \frac{\partial h_i}{\partial w}(k, \sigma, z, w, \theta) & \hat{e}_i^{\mathrm{T}} & \hat{e}_i^{\mathrm{T}} \\ \frac{\partial h_j}{\partial w}(k, \sigma, z, w, \theta) & \hat{e}_j^{\mathrm{T}} & \hat{e}_j^{\mathrm{T}} \end{bmatrix} = 2.$$
(3.25)

Lastly, to show Condition 3.4.3, choose any $k \in \mathcal{K}, \sigma \in \mathcal{S}, \theta \in \tilde{\Theta}, i \in \{1, \ldots, n_{\sigma}\},$ $p \in \{1, \ldots, n_w + 2n_{\sigma}\}, \text{ and } (z, \breve{w}) \in \partial_i \breve{\mathcal{M}}(k, \sigma, \theta) \text{ with } \breve{w}_p = \breve{w}_p^L \text{ or } \breve{w}_p = \breve{w}_p^U.$ Applying (3.23) to (3.19), we have

$$\operatorname{rank} \begin{bmatrix} \frac{\partial \check{h}_i}{\partial \check{w}}(k, \sigma, z, \check{w}, \theta) \\ e_p^{\mathrm{T}} \end{bmatrix} = \operatorname{rank} \begin{bmatrix} \frac{\partial h_i}{\partial w}(k, \sigma, z, w, \theta) & \hat{e}_i^{\mathrm{T}} & \hat{e}_i^{\mathrm{T}} \\ e_p^{\mathrm{T}} & \end{bmatrix} = 2.$$
(3.26)

Remark 3.4.2. In practice, it is often only necessary to randomize a small subset of the event functions in order to satisfy Conditions 3.4.1-3.4.3 (see the example given in Section 6). However, in Definition 3.4.4, randomization is applied to all event functions h_i to simplify notation.

Corollary 3.4.1 implies that any potentially non-smooth decision rule approximation can be made smooth by simply randomizing the rule according to Definition 3.4.4. Importantly, this randomization does not change anything about the problem itself (i.e., the data f, ℓ_S , g, etc. defining the original MSP). Moreover, it does not need to change the decision rule very significantly either since there is no theoretical requirement on the size of the perturbations $\xi_{1,i}$ and $\xi_{2,i}$ used in Definition 3.4.4. Since the original rule κ only needs to satisfy Definition 3.4.1, which is very flexible, this result provides significant support for the claim that many MSPs of interest will admit decision rules that are simultaneously accurate (i.e., provide a good approximation of the true optimal recourse function) and smooth-in-expectation. Thus, the proposed use of gradient-based algorithms to efficiently solve smooth decision rule approximations should be broadly applicable.

However, achieving smoothness by randomization can be problematic when one is interested in satisfying some or all of the problem constraints robustly rather than in probability. Although robust constraints are strictly not allowed in the problem formulation (3.1), it is often both possible and desirable to design a decision rule that satisfies some or all of the constraints robustly (see the example in Section 6). Unfortunately, in these cases the randomization method in Definition 3.4.4 may cause a constraint that was satisfied robustly to be violated with some nonzero probability. This is particularly undesirable when the constraint models some aspect of the problem physics. For example, consider a constraint $g_j = x_k^d - x_{\max}^d \leq 0$ requiring that the number of time periods that some process has run (x_k^d) never exceeds a maximum value (x_{\max}^d) . In this case, a DR satisfying Definition 3.4.1 can be constructed such that the discrete decision to run or shut down the process is made using the threshold function $h_i = x_k^d - x_{\max}^d - 1$. Such a DR will enforce $g_j \leq 0$ robustly. However, this h_i violates Condition 3.4.1 and, unfortunately, randomizing it will lead to violation of the robust constraint $g_j \leq 0$ with non-zero probability (e.g., the process may run for longer than the allowed x_{\max}^d periods). Similar issues arise commonly with other constraints that are desirable to enforce robustly with the DR (e.g., exceeding a specified level of inventory, overcharging/discharging battery banks, etc.).

Fortunately, these limitations are not fundamental to the use of smooth-inexpectation decision rules. Rather, they reflect the fact that Conditions 3.4.1–3.4.3 are stronger than necessary. In the next section, we present a second, less restrictive set of sufficient conditions for smoothness-in-expectation that permits the use of some problematic event functions of the type discussed above without randomization. As a result, smoothnessin-expectation can be achieved in general with fewer additional random variables, and hopefully with none appearing where they might cause undesirable constraint violations with nonzero probability.

3.5 Relaxed Sufficient Conditions for Smoothness-in-Expectation

Let κ be a decision rule satisfying Definition 3.4.1. This section presents a new set of sufficient conditions for smoothness-in-expectation of κ that allow the derivative-based conditions in Conditions 3.4.1–3.4.3 to be violated in some important practical situations. Specifically, we show that they are only required to hold for the functions $h_i(k, \sigma, (\cdot, \overline{z}^d), \cdot, \cdot)$ corresponding to some choice of discrete quantities (k, σ, z^d) , but can be violated for others. Event functions that only depend on the discrete quantities (k, σ, z^d) are an important special case that satisfy these relaxed conditions. As a result, the new conditions developed in this section are more broadly applicable and often much easier to verify.

To state the new conditions, first consider the following generalization of the sets $\mathcal{M}(k,\sigma,\theta)$ defined in Definition 3.4.3.

Definition 3.5.1. For every $k \in \mathcal{K}$, $\sigma \in \mathcal{S}$, $\theta \in \tilde{\Theta}$, and $i, j, m \in \{1, \ldots, n_{\sigma}\}$ with $i \neq j$, define the sets

$$\mathcal{M}(k,\sigma_{1:m},\theta) \equiv \{(z,w) \in \tilde{X} \times W : \sigma_q h_q(k,\sigma,z,w,\theta) \le 0, \ \forall q \le m\},$$
(3.27)

$$\partial_i \mathcal{M}(k, \sigma_{1:m}, \theta) \equiv \{ (z, w) \in \mathcal{M}(k, \sigma_{1:m}, \theta) : h_i(k, \sigma, z, w, \theta) = 0 \},$$
(3.28)

$$\partial_{ij}\mathcal{M}(k,\sigma_{1:m},\theta) \equiv \left\{ (z,w) \in \mathcal{M}(k,\sigma_{1:m},\theta) : \begin{array}{l} h_i(k,\sigma,z,w,\theta) = 0\\ h_j(k,\sigma,z,w,\theta) = 0 \end{array} \right\}.$$
(3.29)

Note that the sets defined above satisfy:

$$\mathcal{M}(k, \sigma_{1:m}, \theta) \subset \mathcal{M}(k, \sigma_{1:q}, \theta), \quad \forall m \ge q,$$
(3.30)

$$\mathcal{M}(k,\sigma_{1:m},\theta) = \bigcup_{\{\hat{\sigma}\in\mathcal{S}:\hat{\sigma}_{1:m}=\sigma_{1:m}\}} \mathcal{M}(k,\hat{\sigma},\theta),$$
(3.31)

$$\partial_i \mathcal{M}(k, \sigma_{1:m}, \theta) = \bigcup_{\{\hat{\sigma} \in \mathcal{S}: \hat{\sigma}_{1:m} = \sigma_{1:m}\}} \partial_i \mathcal{M}(k, \hat{\sigma}, \theta),$$
(3.32)

$$\partial_{ij}\mathcal{M}(k,\sigma_{1:m},\theta) = \bigcup_{\{\hat{\sigma}\in\mathcal{S}:\hat{\sigma}_{1:m}=\sigma_{1:m}\}} \partial_{ij}\mathcal{M}(k,\hat{\sigma},\theta).$$
(3.33)

Remark 3.5.1. Condition 3.4.1 and 3.4.3 can be written equivalently on the sets $\partial_i \mathcal{M}(k, \sigma_{1:i-1}, \theta)$ and Condition 3.4.2 on the sets $\partial_{ij}\mathcal{M}(k, \sigma_{1:\max(i,j)-1}, \theta)$. On one hand, note that since the derivative requirements in Condition 3.4.1 and 3.4.3 are satisfied on $\partial_i \mathcal{M}(k, \hat{\sigma}, \theta)$ for any $\hat{\sigma}$, (3.32) implies that these requirements are satisfied on $\partial_i \mathcal{M}(k, \hat{\sigma}_{1:i-1}, \theta)$. Similarly, since the derivative requirement in Condition 3.4.2 is satisfied on $\partial_{ij}\mathcal{M}(k, \hat{\sigma}_{1:i-1}, \theta)$. Similarly, since the derivative requirement in Condition 3.4.2 is satisfied on $\partial_{ij}\mathcal{M}(k, \hat{\sigma}, \theta)$ for any $\hat{\sigma}$, (3.33) implies that this requirement is also satisfied on $\partial_{ij}\mathcal{M}(k, \hat{\sigma}_{1:\max(i,j)-1}, \theta)$. On the other hand, note that if the derivative requirements in Condition 3.4.1 and 3.4.3 are satisfied on the sets $\partial_i \mathcal{M}(k, \hat{\sigma}_{1:\max(i,j)-1}, \theta)$ for any $\hat{\sigma}$, then (3.30) implies that the derivative requirements Condition 3.4.1 and 3.4.3 are satisfied on $\partial_i \mathcal{M}(k, \hat{\sigma}, \theta)$ and the derivative requirement in Condition 3.4.2 is satisfied on $\partial_i \mathcal{M}(k, \hat{\sigma}, \theta)$ and the derivative requirement in Condition 3.4.2 is satisfied on the sets $\partial_{ij}\mathcal{M}(k, \hat{\sigma}_{1:\max(i,j)-1}, \theta)$ for any $\hat{\sigma}$, then (3.30) implies that the derivative requirement in Condition 3.4.2 is satisfied on the sets $\partial_{ij}\mathcal{M}(k, \hat{\sigma}_{1:\max(i,j)-1}, \theta)$ for any $\hat{\sigma}$, then $\partial_i \mathcal{M}(k, \hat{\sigma}, \theta)$ and the derivative requirement in Condition 3.4.2 is satisfied on the sets $\partial_{ij}\mathcal{M}(k, \hat{\sigma}_{1:\max(i,j)-1}, \theta)$ for any $\hat{\sigma}$, then (3.30) implies that the derivative requirement in Condition 3.4.2 is satisfied on the sets $\partial_{ij}\mathcal{M}(k, \hat{\sigma}_{1:\max(i,j)-1}, \theta)$ for any $\hat{\sigma}$, then $\partial_i \mathcal{M}(k, \hat{\sigma}, \theta)$ and the derivative requirement in Condition 3.4.2 is satisfied on $\partial_{ij}\mathcal{M}(k, \hat{\sigma}, \theta)$.

Next, recall that elements of the state space $z \in \tilde{X}$ have both continuous and discrete parts, denoted by $z = (z^c, z^d) \in \tilde{X}^c \times \tilde{X}^d$. The following definition partitions the sets $\mathcal{M}(k, \sigma_{1:i}, \theta)$ further based on the value of z^d .

Definition 3.5.2. For each fixed $k \in \mathcal{K}, \ \theta \in \tilde{\Theta}, \ \overline{z}^d \in \tilde{X}^d, \ \sigma \in \mathcal{S}, \ \text{and} \ i, j, m \in \{1, \dots, n_\sigma\}$

with $i \neq j$, define

$$\mathcal{M}(k,\sigma_{1:m},\theta,\overline{z}^d) \equiv \{(z,w) \in \mathcal{M}(k,\sigma_{1:m},\theta) : z^d = \overline{z}^d\},\tag{3.34}$$

$$\partial_i \mathcal{M}(k, \sigma_{1:m}, \theta, \overline{z}^d) \equiv \{(z, w) \in \partial_i \mathcal{M}(k, \sigma_{1:m}, \theta) : z^d = \overline{z}^d\},\tag{3.35}$$

$$\partial_{ij}\mathcal{M}(k,\sigma_{1:m},\theta,\overline{z}^d) \equiv \{(z,w)\in\partial_{ij}\mathcal{M}(k,\sigma_{1:m},\theta): z^d=\overline{z}^d\}.$$
(3.36)

Note that the sets defined above satisfy

$$\mathcal{M}(k,\sigma_{1:m},\theta) = \bigcup_{\overline{z}^d \in \tilde{X}^d} \mathcal{M}(k,\sigma_{1:m},\theta,\overline{z}^d), \qquad (3.37)$$

$$\partial_i \mathcal{M}(k, \sigma_{1:m}, \theta) = \bigcup_{\overline{z}^d \in \tilde{X}^d} \partial_i \mathcal{M}(k, \sigma_{1:m}, \theta, \overline{z}^d), \qquad (3.38)$$

$$\partial_{ij}\mathcal{M}(k,\sigma_{1:m},\theta) = \bigcup_{\overline{z}^d \in \tilde{X}^d} \partial_{ij}\mathcal{M}(k,\sigma_{1:m},\theta,\overline{z}^d).$$
(3.39)

Condition 3.5.1. For each fixed $k \in \mathcal{K}$, $\overline{z}^d \in \tilde{X}^d$, $\sigma \in \mathcal{S}$, and $i \in \{1, \ldots, n_\sigma\}$, at least one of the following conditions holds:

1. For each $\theta \in \tilde{\Theta}$,

$$\frac{\partial h_i}{\partial w}(k,\sigma,z,w,\theta) \neq 0, \quad \forall (z,w) \in \partial_i \mathcal{M}(k,\sigma_{1:i-1},\theta,\overline{z}^d).$$

2. $\exists \pi \in \mathbb{R}$ such that $h_i(k, \sigma, z, w, \theta) = \pi$ for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \mathcal{M}(k, \sigma_{1:i-1}, \theta, \overline{z}^d).$

Note that the nonzero *w*-derivative condition in Condition 3.5.1.1 (i.e., the first option in Condition 3.5.1) is identical to Condition 3.4.1. Thus, Condition 3.5.1 relaxes Condition 3.4.1 by allowing zero *w*-derivatives in the specific case when h_i depends only on the discrete quantities $(k, \sigma, \overline{z}^d)$. In this case, choosing any fixed $(k, \sigma, \overline{z}^d)$ results in a constant function $h_i(k, \sigma, (\cdot, \overline{z}^d), \cdot, \cdot) = \pi$. Therefore, $h_i(k, \sigma, \cdot, \cdot, \cdot)$ violates Condition 3.5.1.1 (provided that $\partial_i \mathcal{M}(k, \sigma, \theta, \overline{z}^d)$ is nonempty) but satisfies Condition 3.5.1.2 (i.e., the second option in Condition 3.5.1). Purely discrete event functions are a very important special case that arises, e.g., when enforcing minimum uptime/downtime constraints. Specifically, consider the function $h_i = x_k^d - x_{\max}^d - 1$ modeling a constraint prohibiting the counter state x_k^d from exceeding the upper threshold x_{\max} .

Condition 3.5.2. For each fixed $k \in \mathcal{K}$, $\overline{z}^d \in \tilde{X}^d$, $\sigma \in \mathcal{S}$, and $i, j \in \{1, \ldots, n_\sigma\}$ with i > j, at least one of the following conditions holds:

1. For each $\theta \in \tilde{\Theta}$,

$$\operatorname{rank}\left[\begin{array}{c}\frac{\partial h_{i}}{\partial w}(k,\sigma,z,w,\theta)\\\frac{\partial h_{j}}{\partial w}(k,\sigma,z,w,\theta)\end{array}\right] = 2, \quad \forall (z,w) \in \partial_{ij}\mathcal{M}(k,\sigma_{1:i-1},\theta,\overline{z}^{d})$$

- 2. $\exists \pi \in \mathbb{R}$ such that $h_i(k, \sigma, z, w, \theta) = \pi$ for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \mathcal{M}(k, \sigma_{1:i-1}, \theta, \overline{z}^d)$ or $h_j(k, \sigma, z, w, \theta) = \pi$ for for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \mathcal{M}(k, \sigma_{1:j-1}, \theta, \overline{z}^d)$.
- 3. $\exists \beta \neq 0$ such that $h_i(k, \sigma, z, w, \theta) = \beta h_j(k, \sigma, z, w, \theta)$ for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \mathcal{M}(k, \sigma_{1:i-1}, \theta, \overline{z}^d)$.

Condition 3.5.3. Choose any $k \in \mathcal{K}$, $\overline{z}^d \in \tilde{X}^d$, $\sigma \in \mathcal{S}$, $i \in \{1, \ldots, n_\sigma\}$, and $p \in \{1, \ldots, n_w\}$. Let e_p denote the unit vector with the 1 in the p^{th} position. Then, at least one of the following conditions holds:

- 1. For each $\theta \in \Theta$, $\operatorname{rank} \begin{bmatrix} \frac{\partial h_i}{\partial w}(k, \sigma, z, w, \theta) \\ e_p^{\mathrm{T}} \end{bmatrix} = 2, \quad \forall (z, w) \in \partial_i \mathcal{M}(k, \sigma_{1:i-1}, \theta, \overline{z}^d) \quad \text{with} \quad w_p = w_p^L \text{ or}$ $w_p = w_p^U.$
- 2. $\exists \pi \in \mathbb{R}$ such that $h_i(k, \sigma, z, w, \theta) = \pi$ for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \mathcal{M}(k, \sigma_{1:i-1}, \theta, \overline{z}^d).$
- 3. $\exists \alpha \neq 0$ such that $h_i(k, \sigma, z, w, \theta) = \alpha(w_p w_p^L)$ for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \mathcal{M}(k, \sigma_{1:i-1}, \theta, \overline{z}^d).$

4. $\exists \rho \neq 0$ such that $h_i(k, \sigma, z, w, \theta) = \rho(w_p - w_p^U)$ for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \mathcal{M}(k, \sigma_{1:i-1}, \theta, \overline{z}^d).$

Consider any fixed $(k, \sigma, \overline{z}^d)$ and note that derivative condition imposed on the functions $h_i(k, \sigma, (\cdot, \overline{z}^d), \cdot, \cdot)$ and $h_j(k, \sigma, (\cdot, \overline{z}^d), \cdot, \cdot)$ in Condition 3.5.2.1 is identical to that in Condition 3.4.2. However, Condition 3.5.2.2 allows Condition 3.5.2.1 to be violated if at least one of the functions $h_i(k, \sigma, (\cdot, \overline{z}^d), \cdot, \cdot)$ and $h_j(k, \sigma, (\cdot, \overline{z}^d), \cdot, \cdot)$ is constant. Additionally, Condition 3.5.2.3 allows Condition 3.5.2.1 to be violated if $h_i(k, \sigma, (\cdot, \overline{z}^d), \cdot, \cdot)$ is a constant multiple of $h_j(k, \sigma, (\cdot, \overline{z}^d), \cdot, \cdot)$. Similarly, note that the derivative condition imposed on $h_i(k, \sigma, (\cdot, \overline{z}^d), \cdot, \cdot)$ in Condition 3.5.3.1 is identical to that in Condition 3.4.3. However, Condition 3.5.3.2 allows Condition 3.5.3.1 to be violated if $h_i(k, \sigma, (\cdot, \overline{z}^d), \cdot, \cdot)$ is constant. Additionally, Conditions 3.5.3.3–3.5.3.4 allow Condition 3.5.3.1 to be violated if $h_i(k, \sigma, (\cdot, \overline{z}^d), \cdot, \cdot)$ is a constant multiple of either $w_p - w_p^L$ or $w_p - w_p^U$ is constant. In summary, it is clear that Condition 3.5.2 and Condition 3.5.3 relax Condition 3.4.2 and Condition 3.4.3, respectively, by allowing the derivative conditions in the latter to be violated for some $(k, \sigma, \overline{z}^d)$.

To prove that Conditions 3.5.1–3.5.3 are sufficient for κ to be smooth-in-expectation, we argue that if κ is defined by a set of event functions h_i satisfying Conditions 3.5.1–3.5.3, then κ can be transformed into a new decision rule which consists of replacing the set of h_i defining κ by an alternative set of event functions satisfying Conditions 3.4.1–3.4.3 and such that when the new rule is used in place of κ , the expected cost $\mathcal{L}(\theta)$ is not changed. This replacement idea is introduced in the next definition to first show that \mathcal{L} is continuous on all $\tilde{\Theta}$ under Condition 3.5.1. This result is formally given in Theorem 3.5.1 below which is established through the sequence of Lemmas 3.5.1–3.5.5 and Corollary 3.5.1.

Definition 3.5.3. Let κ be a decision rule satisfying Definition 3.4.1. For all $i \in \{1, \ldots, n_{\sigma}\}$, let $\hat{h}_i : \mathcal{K} \times \mathcal{S} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \mathbb{R}$. For each $k \in \mathcal{K}$, $\overline{z}^d \in \tilde{X}^d$, and $\sigma \in \mathcal{S}$, let $\hat{h}_i(k, \sigma, (\cdot, \overline{z}^d), \cdot, \cdot)$ be defined as follows:

(I) If $\exists \pi \in \mathbb{R}$ such that $h_i(k, \sigma, z, w, \theta) = \pi$ for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying

 $(z,w) \in \mathcal{M}(k,\sigma_{1:i-1},\theta,\overline{z}^d)$, then define

$$\hat{h}_i(k,\sigma,(z^c,\overline{z}^d),w,\theta) \equiv \left\{ \begin{array}{cc} -1 & \text{if} \quad \pi \le 0\\ 1 & \text{otherwise} \end{array} \right\}, \quad \forall (z^c,w,\theta) \in \tilde{X}^c \times \tilde{W} \times \tilde{\Theta}. \quad (3.40)$$

(II) Otherwise, define

$$\hat{h}_i(k,\sigma,(z^c,\overline{z}^d),w,\theta) \equiv h_i(k,\sigma,(z^c,\overline{z}^d),w,\theta), \quad \forall (z^c,w,\theta) \in \tilde{X}^c \times \tilde{W} \times \tilde{\Theta}.$$
(3.41)

Moreover, for every $\sigma \in \mathcal{S}$, define $\hat{\kappa}_{\sigma} : \mathcal{K} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \tilde{U}$ by

$$\hat{\kappa}_{\sigma}(k, z, w, \theta) \equiv \kappa_{\sigma}(k, z, w, \theta).$$
(3.42)

Finally, define $\hat{\kappa}: \mathcal{K} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \tilde{U}$ by

$$\sigma_i = \left\{ \begin{array}{cc} 1 & \text{if} \quad \hat{h}_i(k, \sigma_{1:i-1}, z, w, \theta) \le 0 \\ -1 & \text{otherwise} \end{array} \right\}, \quad \forall i \in \{1, \dots, n_\sigma\}, \qquad (3.43)$$

$$\hat{\kappa}(k, z, w, \theta) \equiv \hat{\kappa}_{\sigma}(k, z, w, \theta).$$
(3.44)

Remark 3.5.2. Recall that in Definition 3.4.1 h_i does not depend on $\sigma_{i:n_{\sigma}}$ and is written as a function of the entire sequence σ only for convenience of notation. Similarly, Definition 3.5.3 ensures that \hat{h}_i is also independent of $\sigma_{i:n_{\sigma}}$. Specifically, consider any (k, σ, z^d) and $(k, \overline{\sigma}, z^d)$ with $\sigma_{1:i-1} = \overline{\sigma}_{1:i-1}$. If $\hat{h}_i(k, \sigma, (\cdot, z^d), \cdot, \cdot)$ is defined by (I), then $h_i(k, \sigma, (\cdot, z^d), \cdot, \cdot)$ is constant on $\mathcal{M}(k, \sigma_{1:i-1}, \theta, z^d)$. Since, h_i is independent of $\sigma_{i:n_{\sigma}}$, it follows that $h_i(k, \sigma, (\cdot, z^d), \cdot, \cdot)$ is also constant on $\mathcal{M}(k, \overline{\sigma}_{1:i-1}, \theta, z^d)$, and hence $\hat{h}_i(k, \overline{\sigma}, (\cdot, z^d), \cdot, \cdot)$ is defined by (I). Since the same argument can be made starting with $\overline{\sigma}$, $\hat{h}_i(k, \sigma, (\cdot, z^d), \cdot, \cdot)$ is defined by (I) if and only if $\hat{h}_i(k, \overline{\sigma}, (\cdot, z^d), \cdot, \cdot)$ is defined by (I). Therefore, $\hat{h}_i(k, \sigma, (\cdot, z^d), \cdot, \cdot) = \hat{h}_i(k, \overline{\sigma}, (\cdot, z^d), \cdot, \cdot)$ for any (k, σ, z^d) and $(k, \overline{\sigma}, z^d)$ with $\sigma_{1:i-1} = \overline{\sigma}_{1:i-1}$. Moreover, note that (3.42) gives $\hat{\kappa}_{\sigma} = \kappa_{\sigma}$ and that $\hat{h}_i(k, \sigma, (\cdot, x^d), \cdot, \cdot)$ is continuously differentiable on $\tilde{X}^c \times \tilde{W} \times \tilde{\Theta}$, for each fixed $k \in \mathcal{K}$, $x^d \in \tilde{X}^d$ and $\sigma \in \mathcal{S}$. Thus, the modified decision rule $\hat{\kappa}$ satisfies Definition 3.4.1.

To show that Condition 3.5.1 is sufficient for continuity of \mathcal{L} on all of $\tilde{\Theta}$, we first use the next two Lemmas 3.5.1–3.5.2 to establish Lemma 3.5.3. The latter is important because, as per Theorem 3.4.1, it implies that using $\hat{\kappa}$ in place of κ results in an expected value that is continuous under Conditions 3.5.1. Thus, continuity of \mathcal{L} under Condition 3.5.1 is proven by showing that the expected value function that results from using $\hat{\kappa}$ is not different from \mathcal{L} , which is shown in the results following Lemma 3.5.3.

Lemma 3.5.1. Choose any $i \in \{1, ..., n_{\sigma}\}$, $(k, \tilde{\sigma}, \tilde{\theta}) \in \mathcal{K} \times \mathcal{S} \times \tilde{\Theta}$, and let $\hat{\mathcal{M}}(k, \sigma_{1:i}, \theta)$ denote the sets resulting from replacing h_i with \hat{h}_i in Definition 3.5.1. If $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i}, \tilde{\theta}) \cap \mathcal{M}(k, \tilde{\sigma}_{1:i-1}, \tilde{\theta})$, then $(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \tilde{\sigma}_{1:i}, \tilde{\theta})$.

Proof Assume $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i}, \tilde{\theta}) \cap \mathcal{M}(k, \tilde{\sigma}_{1:i-1}, \tilde{\theta})$. Note that $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i}, \tilde{\theta})$ implies that $\tilde{\sigma}_j \hat{h}_j(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \leq 0$, for all $j \in \{1, \ldots, i\}$ and $(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \tilde{\sigma}_{1:i-1}, \tilde{\theta})$ implies that $\tilde{\sigma}_j h_j(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \leq 0$, for all $j \in \{1, \ldots, i-1\}$. Hence, to show that $(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \tilde{\sigma}_{1:i}, \tilde{\theta})$, it suffices to show that $\tilde{\sigma}_i h_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \leq 0$.

Suppose $\hat{h}_i(k, \tilde{\sigma}, (\cdot, \tilde{z}^d), \cdot, \cdot)$ is defined by (3.40). Correspondingly, $\exists \pi \in \mathbb{R}$ such that $h_i(k, \tilde{\sigma}, z, w, \theta) = \pi$ for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \mathcal{M}(k, \tilde{\sigma}_{1:i-1}, \theta, \tilde{z}^d)$. Note that $(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \tilde{\sigma}_{1:i-1}, \tilde{\theta})$ implies that $(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \tilde{\sigma}_{1:i-1}, \theta, \tilde{z}^d)$. Thus, $h_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \pi$. Given that $\tilde{\sigma}_i \hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \leq 0$, if (3.40) gives $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = -1$, then we must have $h_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \pi \leq 0$ and $\tilde{\sigma}_i = 1$. Otherwise, we must have $h_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \pi > 0$ and $\tilde{\sigma}_i = -1$. In both cases, we have $\tilde{\sigma}_i h_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \tilde{\sigma}_i \pi \leq 0$. Next, suppose $\hat{h}_i(k, \tilde{\sigma}, (\cdot, \tilde{z}^d), \cdot, \cdot)$ is defined by (3.41). This implies that $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = h_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta})$. But, since $\tilde{\sigma}_i \hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \leq 0$, we must also have $\tilde{\sigma}_i h_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \leq 0$.

Lemma 3.5.2. For any $j \in \{1, ..., n_{\sigma}\}$ and $(k, \sigma, \theta) \in \mathcal{K} \times \mathcal{S} \times \tilde{\Theta}$, $\hat{\mathcal{M}}(k, \sigma_{1:j}, \theta) \subset \mathcal{M}(k, \sigma_{1:j}, \theta)$. Proof Choose any $j \in \{1, \ldots, n_{\sigma}\}, (k, \tilde{\sigma}, \tilde{\theta}) \in \mathcal{K} \times \mathcal{S} \times \tilde{\Theta}, \text{ and } (\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:j}, \tilde{\theta}).$ We must show that $(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \tilde{\sigma}_{1:j}, \tilde{\theta}).$

We first show that (\tilde{z}, \tilde{w}) satisfies the following implication, for any *i* with $1 \leq i \leq j$:

$$(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \tilde{\sigma}_{1:i-1}, \tilde{\theta}) \implies (\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \tilde{\sigma}_{1:i}, \tilde{\theta}).$$
 (3.45)

Choose any *i* with $1 \leq i \leq j$ and assume $(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \tilde{\sigma}_{1:i-1}, \tilde{\theta})$. Note that $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:j}, \tilde{\theta})$ implies that $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i}, \tilde{\theta})$ by Definition 3.5.1. Thus, $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i}, \tilde{\theta}) \cap \mathcal{M}(k, \tilde{\sigma}_{1:i-1}, \tilde{\theta})$. Hence, the implication in (3.45) holds by Lemma 3.5.1.

We now proceed with induction over *i*. First, note that $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:j}, \tilde{\theta})$ implies that $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:0}, \tilde{\theta}) = \tilde{X} \times W$ by Definition 3.5.1. For induction, choose some arbitrary i < j and assume $(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \tilde{\sigma}_{1:i-1}, \tilde{\theta})$. By (3.45), we must have $(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \tilde{\sigma}_{1:i}, \tilde{\theta})$. Thus, by induction on *i*, we must have $(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \tilde{\sigma}_{1:i}, \tilde{\theta})$, for all $i \leq j$. In particular, this implies $(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \tilde{\sigma}_{1:j}, \tilde{\theta})$ as desired.

Lemma 3.5.3. If Condition 3.5.1 holds for κ , then Condition 3.4.1 holds for $\hat{\kappa}$.

Proof Assume κ satisfies Condition 3.5.1. To show that $\hat{\kappa}$ satisfies Condition 3.4.1, choose any $i \in \{1, \ldots, n_{\sigma}\}, k \in \mathcal{K}, \sigma \in \mathcal{S}$, and $\theta \in \tilde{\Theta}$. We must show that

$$\frac{\partial \hat{h}_i}{\partial w}(k,\sigma,\tilde{z},\tilde{w},\theta) \neq 0, \quad \forall (\tilde{z},\tilde{w}) \in \partial_i \hat{\mathcal{M}}(k,\sigma_{1:i-1},\theta).$$
(3.46)

We first show that the following implication holds for any $(z, w) \in \tilde{X} \times \tilde{W}$:

$$\hat{h}_i(k,\sigma,z,w,\theta) = 0 \implies h_i(k,\sigma,(\cdot,z^d),\cdot,\cdot) = \hat{h}_i(k,\sigma,(\cdot,z^d),\cdot,\cdot) \text{ on } \tilde{X}^c \times \tilde{W} \times \tilde{\Theta}.$$
(3.47)

Choose any $(z,w) \in \tilde{X} \times \tilde{W}$ and assume $\hat{h}_i(k,\sigma,z,w,\theta) = 0$. By Definition 3.5.3, it is impossible to have $\hat{h}_i(k,\sigma,z,w,\theta) = 0$ if $\hat{h}_i(k,\sigma,(\cdot,z^d),\cdot,\cdot)$ is defined by (3.40). Hence, $\hat{h}_i(k,\sigma,(\cdot,z^d),\cdot,\cdot)$ must be defined by (3.41) which gives exactly $h_i(k,\sigma,(\cdot,z^d),\cdot,\cdot) = \hat{h}_i(k,\sigma,(\cdot,z^d),\cdot,\cdot)$ on $\tilde{X}^c \times \tilde{W} \times \tilde{\Theta}$.

To show (3.46), choose any $(\tilde{z}, \tilde{w}) \in \partial_i \hat{\mathcal{M}}(k, \sigma_{1:i-1}, \theta)$, which implies $\hat{h}_i(k, \sigma, \tilde{z}, \tilde{w}, \theta) = 0$ by definition. First, note that $\hat{h}_i(k, \sigma, \tilde{z}, \tilde{w}, \theta) = 0$ implies the following, by (3.47) and by noting that \tilde{W} is open:

$$\frac{\partial h_i}{\partial w}(k,\sigma,(z^c,\tilde{z}^d),w,\theta) = \frac{\partial \hat{h}_i}{\partial w}(k,\sigma,(z^c,\tilde{z}^d),w,\theta), \quad \forall (z^c,w,\theta) \in \tilde{X}^c \times \tilde{W} \times \tilde{\Theta}.$$
(3.48)

Second, note that $(\tilde{z}, \tilde{w}) \in \partial_i \hat{\mathcal{M}}(k, \sigma_{1:i-1}, \theta)$ means that $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \sigma_{1:i-1}, \theta)$, by definition. Hence, by Lemma 3.5.2, we must have $(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \sigma_{1:i-1}, \theta)$. Since $\hat{h}_i(k, \sigma, \tilde{z}, \tilde{w}, \theta) = 0$, we must have $h_i(k, \sigma, \tilde{z}, \tilde{w}, \theta) = 0$ by (3.47). But, since $(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \sigma_{1:i-1}, \theta), h_i(k, \sigma, \tilde{z}, \tilde{w}, \theta) = 0$ implies that $(\tilde{z}, \tilde{w}) \in \partial_i \mathcal{M}(k, \sigma_{1:i-1}, \theta)$ by definition. Using (3.35) in Definition 3.5.2, it is clear that $(\tilde{z}, \tilde{w}) \in \partial_i \mathcal{M}(k, \sigma_{1:i-1}, \theta)$ implies that $(\tilde{z}, \tilde{w}) \in \partial_i \mathcal{M}(k, \sigma_{1:i-1}, \theta, \tilde{z}^d)$. Thus, by the hypothesis that κ satisfies Condition 3.5.1, we must have $\frac{\partial h_i}{\partial w}(k, \sigma, \tilde{z}, \tilde{w}, \theta) \neq 0$ and hence $\frac{\partial \hat{h}_i}{\partial w}(k, \sigma, \tilde{z}, \tilde{w}, \theta) \neq 0$ by (3.48). Since the choice $(\tilde{z}, \tilde{w}) \in \partial_i \hat{\mathcal{M}}(k, \sigma_{1:i-1}, \theta)$ was arbitrary, (3.46) holds. \Box

Next, we use Definition 3.5.3 to show that using $\hat{\kappa}$ in place of κ in (3.3)–(3.5) leads to an expected value $\hat{\mathcal{L}}$ such that $\hat{\mathcal{L}}(\theta) = \mathcal{L}(\theta)$ for all $\theta \in \tilde{\Theta}$. For clarity of arguments, this result is established in Corollary 3.5.1 below using the definition of $\hat{\mathcal{L}}$, which is given first, and Lemmas 3.5.4–3.5.5 which are given next. To define $\hat{\mathcal{L}}(\theta)$, define $\hat{u}_k(\omega, \theta)$ and $\hat{x}_k(\omega, \theta)$ for every $(\omega, \theta) \in \tilde{\Omega} \times \tilde{\Theta}$ by the following recursion, which is analogous to (3.3)–(3.5):

$$\hat{x}_0(\boldsymbol{\omega}, \boldsymbol{\theta}) \equiv b_0, \tag{3.49}$$

$$\hat{u}_k(\boldsymbol{\omega}, \theta) \equiv \hat{\kappa}(k, \hat{x}_k(\boldsymbol{\omega}, \theta), w_k, \theta), \qquad (3.50)$$

$$\hat{x}_{k+1}(\boldsymbol{\omega}, \boldsymbol{\theta}) \equiv f(k, \hat{u}_k(\boldsymbol{\omega}, \boldsymbol{\theta}), \hat{x}_k(\boldsymbol{\omega}, \boldsymbol{\theta}), w_k, \boldsymbol{\theta}).$$
(3.51)

Note that the solution of this recursion exists because the modified decision rule $\hat{\kappa}$ still maps into \tilde{U} and the function f still maps into \tilde{X} . Moreover, define $\hat{\ell}(\theta, \omega)$ by

$$\hat{\ell}(\theta, \boldsymbol{\omega}) \equiv \sum_{k=0}^{K} \ell_S(k, \hat{u}_k(\boldsymbol{\omega}, \theta), \hat{x}_k(\boldsymbol{\omega}, \theta), w_k, \theta), \qquad (3.52)$$

and denote the expected value of $\hat{\ell}(\theta, \boldsymbol{\omega})$ by

$$\hat{\mathcal{L}}(\theta) \equiv \mathbb{E}[\hat{\ell}(\theta, \boldsymbol{\omega})].$$
(3.53)

Lemma 3.5.4. Choose any $i \in \{1, ..., n_{\sigma}\}$. For any $(k, \sigma, z, w, \theta) \in \mathcal{K} \times \mathcal{S} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ such that $(z, w) \in \mathcal{M}(k, \sigma_{1:i-1}, \theta, z^d)$, $h_i(k, \sigma, z, w, \theta) \leq 0 \iff \hat{h}_i(k, \sigma, z, w, \theta) \leq 0$.

Proof Choose any $(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) \in \mathcal{K} \times \mathcal{S} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ such that $(\overline{z}, \overline{w}) \in \mathcal{M}(k, \overline{\sigma}_{1:i-1}, \overline{\theta}, \overline{z}^d).$

Assume $h_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) \leq 0$. We must show that $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) \leq 0$. First, suppose $\exists \pi \in \mathbb{R}$ such that $h_i(k, \overline{\sigma}, z, w, \theta) = \pi$ for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \mathcal{M}(k, \overline{\sigma}_{1:i-1}, \theta, \overline{z}^d)$. This implies that $h_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \pi$. Moreover, according to Definition 3.5.3, this implies that $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta})$ is given by (3.40). Specifically, since $h_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) \leq 0$ by assumption, we must have that $\pi \leq 0$, which then implies that $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = -1 \leq 0$ as per (3.40). Second, suppose $\nexists \pi \in \mathbb{R}$ such that $h_i(k, \overline{\sigma}, z, w, \theta) = \pi$ for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \mathcal{M}(k, \overline{\sigma}_{1:i-1}, \theta, \overline{z}^d)$. According to Definition 3.5.3, this implies that $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = h_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) \leq 0$ as per (3.41).

Next, assume $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) \leq 0$. We must show that $h_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) \leq 0$. First, suppose $\hat{h}_i(k, \overline{\sigma}, (\cdot, \overline{z}^d), \cdot, \cdot)$ is defined by (3.40). Correspondingly, there must exist $\pi \in \mathbb{R}$ such that $h_i(k, \overline{\sigma}, z, w, \theta) = \pi$ for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \mathcal{M}(k, \overline{\sigma}_{1:i-1}, \theta, \overline{z}^d)$. By (3.40), the assumption $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) \leq 0$ holds only if $\pi \leq 0$. But, this implies that $h_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \pi \leq 0$. Second, suppose $\hat{h}_i(k, \overline{\sigma}, (\cdot, \overline{z}^d), \cdot, \cdot)$ is defined by (3.41). This implies directly that $h_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) \leq 0$ by assumption.

Lemma 3.5.5. For every $(k, z, w, \theta) \in \mathcal{K} \times \tilde{X} \times W \times \tilde{\Theta}$, $\kappa(k, z, w, \theta) = \hat{\kappa}(k, z, w, \theta)$.

Proof Choose any $(k, z, w, \theta) \in \mathcal{K} \times \tilde{X} \times W \times \tilde{\Theta}$ and let σ and $\hat{\sigma}$ be the binary sequences obtained by applying (3.12) and (3.43), respectively. To show that $\kappa(k, z, w, \theta) = \hat{\kappa}(k, z, w, \theta)$, it suffices to show that $\sigma = \hat{\sigma}$ according to (3.13), (3.42), and (3.44).

To show that $\sigma = \hat{\sigma}$, we use induction. Since σ satisfies (3.12), it follows that $(z,w) \in \mathcal{M}(k,\sigma_{1:i-1},\theta,z^d)$ for all $i \leq n_{\sigma}$. Hence, $(z,w) \in \mathcal{M}(k,\sigma_{1:0},\theta,z^d)$. But, this implies that $h_1(k,\sigma_{1:0},z,w,\theta)$ and $\hat{h}_1(k,\sigma_{1:0},z,w,\theta)$ have the same sign according to Lemma 3.5.4. However, note that $\sigma_{1:0}$ and $\hat{\sigma}_{1:0}$ are both empty and thus $\sigma_{1:0} = \hat{\sigma}_{1:0}$. Thus, $h_1(k,\sigma_{1:0},z,w,\theta)$ and $\hat{h}_1(k,\hat{\sigma}_{1:0},z,w,\theta)$ have the same sign. This implies that $\sigma_1 = \hat{\sigma}_1$. For induction, choose any $i \geq 1$ and assume $\sigma_{1:i-1} = \hat{\sigma}_{1:i-1}$. By Lemma 3.5.4, $h_i(k,\sigma_{1:i-1},z,w,\theta)$ and $\hat{h}_i(k,\sigma_{1:i-1},z,w,\theta)$ have the same sign. But, since $\sigma_{1:i-1} = \hat{\sigma}_{1:i-1}$, $h_i(k,\sigma_{1:i-1},z,w,\theta)$ and $\hat{h}_i(k,\hat{\sigma}_{1:i-1},z,w,\theta)$ must have the same sign, which implies that $\sigma_i = \hat{\sigma}_i$. Hence, $\sigma_{1:i} = \hat{\sigma}_{1:i}$. By induction on $i, \sigma_i = \hat{\sigma}_i$ for all $i \leq n_{\sigma}$. This gives $\sigma = \hat{\sigma}$ as desired.

Corollary 3.5.1. For any $\theta \in \tilde{\Theta}$, $\hat{\mathcal{L}}(\theta) = \mathcal{L}(\theta)$.

Proof Choose any $(\boldsymbol{\omega}, \theta) \in \Omega \times \hat{\Theta}$, let $u_{0:K}$ and $x_{0:K}$ be trajectories of the recursion (3.3)–(3.5), and let $\hat{u}_{0:K}$ and $\hat{x}_{0:K}$ be trajectories of the recursion (3.49)–(3.51). It is sufficient to show that $u_k = \hat{u}_k$ and $x_{k+1} = \hat{x}_{k+1}$, $\forall k \in \mathcal{K}$. Specifically, this implies that $\hat{\ell}(\boldsymbol{\omega}, \theta) = \ell(\boldsymbol{\omega}, \theta)$ by (3.6) and (3.52), leading to the desired result that $\hat{\mathcal{L}}(\theta) = \mathbb{E}[\hat{\ell}(\boldsymbol{\omega}, \theta)] = \mathbb{E}[\ell(\boldsymbol{\omega}, \theta)] = \mathcal{L}(\theta)$ since the choice of $(\boldsymbol{\omega}, \theta)$ is arbitrary.

To show that $u_k = \hat{u}_k$ and $x_{k+1} = \hat{x}_{k+1}$, $\forall k \in \mathcal{K}$, we first show that the following implication holds for any $k \in \mathcal{K}$:

$$x_k = \hat{x}_k \implies \left\{ \begin{array}{c} u_k = \hat{u}_k \\ x_{k+1} = \hat{x}_{k+1} \end{array} \right\}.$$
(3.54)

Assume $x_k = \hat{x}_k$. By Lemma 3.5.5, we immediately have $\kappa(k, x_k, w_k, \theta) = \hat{\kappa}(k, \hat{x}_k, w_k, \theta)$, which implies that $u_k = \hat{u}_k$ by (3.4) and (3.50). But, $x_k = \hat{x}_k$ and $u_k = \hat{u}_k$ leads to $x_{k+1} = \hat{x}_{k+1}$ by (3.5) and (3.51).

To finish the proof, we now proceed with finite induction over k. Noting that

 $x_0 = \hat{x}_0 = b_0 \in \tilde{X}$, a recursive application of (3.54) shows that $u_k = \hat{u}_k$ and $x_{k+1} = \hat{x}_{k+1}$ for all $k \in \mathcal{K}$.

Theorem 3.5.1. If κ satisfies Condition 3.5.1, then \mathcal{L} is continuous on $\tilde{\Theta}$.

Proof With Lemma 3.5.3, a direct application of Theorem 3.4.1 implies that $\hat{\mathcal{L}}$ is continuous on $\tilde{\Theta}$ under Condition 3.5.1. Thus, continuity of \mathcal{L} on $\tilde{\Theta}$ under Condition 3.5.1 follows by applying Corollary 3.5.1.

Finally, we show that $\mathcal{L} \in C^1(\tilde{\Theta}, \mathbb{R})$ under Conditions 3.5.1–3.5.3. This result is formally given in Theorem 3.5.2 below, which is established using the next definition, the sequence of Lemmas 3.5.6–3.5.13, and Corollary 3.5.3.

Definition 3.5.4. Let κ be a decision rule satisfying Definition 3.4.1 and let $\hat{\kappa}$ be defined as in Definition 3.5.3. For all $i \in \{1, \ldots, n_{\sigma}\}$ and $p \in \{1, \ldots, n_{w}\}$, let $\hat{h}_{i}: \mathcal{K} \times \mathcal{S} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \mathbb{R}$. For each $k \in \mathcal{K}, \overline{z}^{d} \in \tilde{X}^{d}$, and $\sigma \in \mathcal{S}$, let $\hat{h}_{i}(k, \sigma, (\cdot, \overline{z}^{d}), \cdot, \cdot)$ be defined in the first case that holds on the following list:

(a) If $\exists \beta \neq 0$ and some j < i such that $\hat{h}_i(k, \sigma, z, w, \theta) = \beta \hat{h}_j(k, \sigma, z, w, \theta)$, for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \hat{\mathcal{M}}(k, \sigma_{1:i-1}, \theta, \overline{z}^d)$, then define

$$\acute{h}_i(k,\sigma,(z^c,\overline{z}^d),w,\theta) \equiv -\beta\sigma_j, \quad \forall (z^c,w,\theta) \in \widetilde{X}^c \times \widetilde{W} \times \widetilde{\Theta}.$$
(3.55)

(b) If $\exists \alpha \neq 0$ such that $\hat{h}_i(k, \sigma, (z^c, \overline{z}^d), w, \theta) = \alpha(w_p - w_p^L)$, for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \hat{\mathcal{M}}(k, \sigma_{1:i-1}, \theta, \overline{z}^d)$, then define

$$\acute{h}_i(k,\sigma,(z^c,\overline{z}^d),w,\theta) \equiv \alpha, \quad \forall (z^c,w,\theta) \in \widetilde{X}^c \times \widetilde{W} \times \widetilde{\Theta}.$$
(3.56)

(c) If $\exists \rho \neq 0$ such that $\hat{h}_i(k, \sigma, (z^c, \overline{z}^d), w, \theta) = \rho(w_p - w_p^U)$, for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \hat{\mathcal{M}}(k, \sigma_{1:i-1}, \theta, \overline{z}^d)$, then define

$$\acute{h}_i(k,\sigma,(z^c,\overline{z}^d),w,\theta) \equiv -\rho, \quad \forall (z^c,w,\theta) \in \widetilde{X}^c \times \widetilde{W} \times \widetilde{\Theta}.$$
(3.57)

(d) Otherwise, define

$$\hat{h}_i(k,\sigma,(z^c,\overline{z}^d),w,\theta) \equiv \hat{h}_i(k,\sigma,(z^c,\overline{z}^d),w,\theta), \quad \forall (z^c,w,\theta) \in \tilde{X}^c \times \tilde{W} \times \tilde{\Theta}.$$
(3.58)

Additionally, for every $\sigma \in \mathcal{S}$, define $\dot{\kappa}_{\sigma} : \mathcal{K} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \tilde{U}$ by

$$\dot{\kappa}_{\sigma}(k, z, w, \theta) \equiv \kappa_{\sigma}(k, z, w, \theta).$$
(3.59)

Finally, define $\kappa : \mathcal{K} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \tilde{U}$ by

$$\sigma_{i} = \left\{ \begin{array}{cc} 1 & \text{if } \acute{h}_{i}(k, \sigma, z, w, \theta) \leq 0 \\ -1 & \text{otherwise} \end{array} \right\}, \quad \forall i \in \{1, \dots, n_{\sigma}\},$$
(3.60)

$$\dot{\kappa}(k, z, w, \theta) \equiv \dot{\kappa}_{\sigma}(k, z, w, \theta). \tag{3.61}$$

Remark 3.5.3. Recall that $\hat{\kappa}$ as defined in Definition 3.5.4 satisfies Definition 3.4.1 (Remark 3.5.2). Accordingly, Definition 3.5.4 ensures that $\hat{\kappa}$ satisfies Definition 3.4.1. In particular, following similar arguments as in Remark 3.5.2, it can be easily shown that Definition 3.5.4 ensures that \hat{h}_i depends only on $\sigma_{1:i-1}$ and the continuous differentiability requirements imposed on h_i and κ_{σ} in Definition 3.4.1 are ensured by Definition 3.5.4 for \hat{h}_i and $\hat{\kappa}_{\sigma}$.

We first use the next three Lemmas 3.5.6–3.5.8 to establish Lemma 3.5.9 which, as per Theorem 3.4.1, implies that using κ in place of κ results in an expected value that is continuously differentiable under Conditions 3.5.1–3.5.3. Thus, continuous differentiability of \mathcal{L} under Conditions 3.5.1–3.5.3 is proven by showing that the expected value function that results from using κ is not different from \mathcal{L} , which is shown in the results following Lemma 3.5.9.

Lemma 3.5.6. Choose any $i \in \{1, ..., n_{\sigma}\}$, $(k, \tilde{\sigma}, \tilde{\theta}) \in \mathcal{K} \times \mathcal{S} \times \tilde{\Theta}$, and let $\dot{\mathcal{M}}(k, \sigma_{1:i}, \theta)$ denote the sets resulting from replacing h_i with \dot{h}_i in Definition 3.5.1. If

$$(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \tilde{\sigma}_{1:i}, \tilde{\theta}) \cap \mathcal{M}(k, \tilde{\sigma}_{1:i-1}, \tilde{\theta}), \text{ then } (\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \tilde{\sigma}_{1:i}, \tilde{\theta}).$$

Proof Assume $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i}, \tilde{\theta}) \cap \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i-1}, \tilde{\theta})$. This implies that $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i-1}, \theta, \tilde{z}^d)$, that $\tilde{\sigma}_q \hat{h}_q(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \leq 0$ for all $q \in \{1, \ldots, i\}$, and that $\tilde{\sigma}_q \hat{h}_q(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \leq 0$, for all $q \in \{1, \ldots, i-1\}$. Hence, to show that $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i}, \tilde{\theta})$, it suffices to show that

$$\tilde{\sigma}_i \hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \le 0.$$
(3.62)

We must show (3.62) in all of the following cases:

Case 1: Suppose $\hat{h}_i(k, \tilde{\sigma}, (\cdot, \tilde{z}^d), \cdot, \cdot)$ is defined by (3.55). Correspondingly, $\exists \beta \neq 0$ and some j < i, such that $\hat{h}_i(k, \sigma, z, w, \theta) = \beta \hat{h}_j(k, \sigma, z, w, \theta)$, for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i-1}, \theta, \tilde{z}^d)$. Recall that $\tilde{\sigma}_i \hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \leq 0$ and $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i-1}, \theta, \tilde{z}^d)$. This implies $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \beta \hat{h}_j(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta})$ and $\tilde{\sigma}_j \hat{h}_j(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \leq 0$. Consider the following sub-cases:

Case 1 (a): Suppose (3.55) gives $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = -\beta \tilde{\sigma}_j < 0$. In this situation, $\tilde{\sigma}_i \hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \leq 0$ implies that $\tilde{\sigma}_i = 1$. Consider the following sub-cases:

Case 1 (a)(i): $\hat{h}_j(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = 0$. In this situation, we have $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \beta \hat{h}_j(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = 0$ for any β . Case 1 (a)(ii): $\hat{h}_j(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) < 0$. In this situation, $\tilde{\sigma}_j \hat{h}_j(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \leq 0$ requires $\tilde{\sigma}_j = 1$ and so $-\beta \tilde{\sigma}_j < 0$ implies that $\beta > 0$, leading to $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \beta \hat{h}_j(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) < 0$. Case 1 (a)(iii): $\hat{h}_j(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) > 0$. In this situation, $\tilde{\sigma}_j \hat{h}_j(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \leq 0$ requires $\tilde{\sigma}_j = -1$, and so $-\beta \tilde{\sigma}_j < 0$ implies that $\beta < 0$, which leads to $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \beta \hat{h}_j(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) < 0$.

Since all of the Cases 1 (a)(i)–(iii) give $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \leq 0$ and $\tilde{\sigma}_i = 1$ in Case 1 (a), (3.62) holds.

Case 1 (b): Suppose (3.55) gives $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = -\beta \tilde{\sigma}_j > 0$. In this situation,
$\tilde{\sigma}_i \dot{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \leq 0$ implies that $\tilde{\sigma}_i = -1$. Consider the following sub-cases:

Case 1 (b)(i): $\hat{h}_j(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = 0$. This situation is exactly similar to Case 1 (a)(i), which gives $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \beta \hat{h}_j(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = 0$. Case 1 (b)(ii): $\hat{h}_j(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) < 0$. This implies $\tilde{\sigma}_j = 1$ as in Case 1 (a)(ii). But, since $-\beta \tilde{\sigma}_j > 0$, we must have $\beta < 0$, which leads to $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \beta \hat{h}_j(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) > 0$. Case 1 (b)(iii): $\hat{h}_j(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) > 0$. This implies $\tilde{\sigma}_j = -1$ as in Case 1 (a)(iii). But, since $-\beta \tilde{\sigma}_j > 0$, we must have $\beta > 0$, which leads to $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \beta \hat{h}_j(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) > 0$.

Since all of the Cases 1 (b)(i)-(iii) give $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \geq 0$ and $\tilde{\sigma}_i = -1$ in Case 1 (b), (3.62) holds.

Case 2: Suppose $\hat{h}_i(k, \tilde{\sigma}, (\cdot, \tilde{z}^d), \cdot, \cdot)$ is defined by (3.56). Correspondingly, $\exists \alpha \neq 0$ such that $\hat{h}_i(k, \tilde{\sigma}, (z^c, \tilde{z}^d), w, \theta) = \alpha(w_p - w_p^L)$, for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i-1}, \theta, \tilde{z}^d)$. Recall that $\tilde{\sigma}_i \hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \leq 0$ and $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i-1}, \theta, \tilde{z}^d)$. The latter implies $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \alpha(\tilde{w}_p - w_p^L)$. If (3.56) gives $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \alpha < 0$, then we must have $\tilde{\sigma}_i = 1$. But, since $(\tilde{w}_p - w_p^L) \geq 0$, we have $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \alpha(\tilde{w}_p - w_p^L) \leq 0$. Otherwise, (3.56) gives $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \alpha > 0$, which requires $\tilde{\sigma}_i = -1$. This leads to $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \alpha(\tilde{w}_p - w_p^L) \geq 0$. In either situation, (3.62) holds.

Case 3: Suppose $\hat{h}_i(k, \tilde{\sigma}, (\cdot, \tilde{z}^d), \cdot, \cdot)$ is defined by (3.57). Correspondingly, $\exists \rho \neq 0$ such that $\hat{h}_i(k, \tilde{\sigma}, (z^c, \tilde{z}^d), w, \theta) = \rho(w_p - w_p^U)$, for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i-1}, \theta, \tilde{z}^d)$. Recall that $\tilde{\sigma}_i \hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \leq 0$ and $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i-1}, \theta, \tilde{z}^d)$. The latter implies $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \alpha(\tilde{w}_p - w_p^U)$. If (3.57) gives $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = -\rho < 0$, then we must have $\tilde{\sigma}_i = 1$ and $\rho > 0$. But, since $(\tilde{w}_p - w_p^U) \leq 0$, this leads to $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \rho(\tilde{w}_p - w_p^U) \leq 0$. Otherwise, (3.57) gives $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = -\rho > 0$, which requires $\tilde{\sigma}_i = -1$ and $\rho < 0$, leading to $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \rho(\tilde{w}_p - w_p^U) \ge 0.$ In either situation, (3.62) holds.

Case 4: Suppose $\hat{h}_i(k, \tilde{\sigma}, (\cdot, \tilde{z}^d), \cdot, \cdot)$ is defined by (3.58). This implies that $\hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) = \hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta})$. But, since $\tilde{\sigma}_i \hat{h}_i(k, \tilde{\sigma}, \tilde{z}, \tilde{w}, \tilde{\theta}) \leq 0$, (3.62) holds.

Lemma 3.5.7. For any $j \in \{1, \ldots, n_{\sigma}\}$ and $(k, \sigma, \theta) \in \mathcal{K} \times \mathcal{S} \times \tilde{\Theta}$, $\hat{\mathcal{M}}(k, \sigma_{1:j}, \theta) \subset \hat{\mathcal{M}}(k, \sigma_{1:j}, \theta)$.

Proof Choose any $j \in \{1, \ldots, n_{\sigma}\}, (k, \tilde{\sigma}, \tilde{\theta}) \in \mathcal{K} \times \mathcal{S} \times \tilde{\Theta}, \text{ and } (\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \tilde{\sigma}_{1:j}, \tilde{\theta}).$ We must show that $(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \tilde{\sigma}_{1:j}, \tilde{\theta}).$

We first show that (\tilde{z}, \tilde{w}) satisfies the following implication, for any i with $1 \leq i \leq j$:

$$(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i-1}, \tilde{\theta}) \implies (\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i}, \tilde{\theta}).$$
 (3.63)

Choose any i with $1 \leq i \leq j$ and assume $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i-1}, \tilde{\theta})$. Note that $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:j}, \tilde{\theta})$ implies that $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i}, \tilde{\theta})$ by Definition 3.5.1. Thus, $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i}, \tilde{\theta}) \cap \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i-1}, \tilde{\theta})$. Hence, the implication in (3.63) holds by Lemma 3.5.6.

We now proceed with induction over *i*. First, note that $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:j}, \tilde{\theta})$ implies that $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:0}, \tilde{\theta}) = \tilde{X} \times W$, by Definition 3.5.1. For induction, choose some arbitrary $i \leq j$ and assume $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i-1}, \tilde{\theta})$. By (3.63), we must have $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i}, \tilde{\theta})$. Thus, by induction on *i*, we must have $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:i}, \tilde{\theta})$, for all $i \leq j$. In particular, this implies $(\tilde{z}, \tilde{w}) \in \hat{\mathcal{M}}(k, \tilde{\sigma}_{1:j}, \tilde{\theta})$ as desired.

Lemma 3.5.8. Choose any $(k, \sigma, z^d) \in \mathcal{K} \times \mathcal{S} \times \tilde{X}^d$. If $\exists (z^c, w, \theta) \in \tilde{X}^c \times \tilde{W} \times \tilde{\Theta}$ such that $\hat{h}_i(k, \sigma, z, w, \theta) = 0$, then the following conditions hold:

(i)
$$\hat{h}_i(k,\sigma,(\cdot,z^d),\cdot,\cdot) = \hat{h}_i(k,\sigma,(\cdot,z^d),\cdot,\cdot) = h_i(k,\sigma,(\cdot,z^d),\cdot,\cdot)$$
 on all of $\tilde{X}^c \times \tilde{W} \times \tilde{\Theta}$.

$$(ii) \quad \frac{\partial \dot{h}_i}{\partial w}(k,\sigma,(\cdot,z^d),\cdot,\cdot) = \frac{\partial \hat{h}_i}{\partial w}(k,\sigma,(\cdot,z^d),\cdot,\cdot) = \frac{\partial h_i}{\partial w}(k,\sigma,(\cdot,z^d),\cdot,\cdot) \text{ on all of } \tilde{X}^c \times \tilde{W} \times \tilde{\Theta}.$$

(iii) $\hat{h}_i(k,\sigma,(\cdot,z^d),\cdot,\cdot)$ does not satisfy the hypotheses in cases (a)–(c) of Definition 3.5.4.

(iv) $h_i(k, \sigma, (\cdot, z^d), \cdot, \cdot)$ is not constant on $\mathcal{M}(k, \sigma_{1:i-1}, \theta, z^d)$.

Proof Assume $\exists (z^c, w, \theta) \in \tilde{X}^c \times \tilde{W} \times \tilde{\Theta}$ such that $\hat{h}_i(k, \sigma, z, w, \theta) = 0$. This implies that $\hat{h}_i(k, \sigma, (\cdot, z^d), \cdot, \cdot)$ is not defined by any of (3.55)–(3.57) in Definition 3.5.4 because this would contradict $\hat{h}_i(k, \sigma, z, w, \theta) = 0$. Thus, conclusion (iii) holds. Moreover, $\hat{h}_i(k, \sigma, (\cdot, z^d), \cdot, \cdot)$ must be defined by (3.58). Specifically, we have $\hat{h}_i(k, \sigma, (\cdot, z^d), \cdot, \cdot) = \hat{h}_i(k, \sigma, (\cdot, z^d), \cdot, \cdot)$, which means that $\hat{h}_i(k, \sigma, z, w, \theta) = 0$. Suppose $h_i(k, \sigma, (\cdot, z^d), \cdot, \cdot)$ is constant on $\mathcal{M}(k, \sigma_{1:i-1}, \theta, z^d)$. This implies that $\hat{h}_i(k, \sigma, (\cdot, z^d), \cdot, \cdot)$ is defined by (3.40) in Definition 3.5.3. Specifically, (3.40) gives $\hat{h}_i(k, \sigma, (\cdot, z^d), \cdot, \cdot) = \pm 1$. But, since this contradicts $\hat{h}_i(k, \sigma, z, w, \theta) = 0$, $h_i(k, \sigma, (\cdot, z^d), \cdot, \cdot)$ cannot be constant on $\mathcal{M}(k, \sigma_{1:i-1}, \theta, z^d)$. Thus, conclusion (iv) holds. Moreover, it implies that $\hat{h}_i(k, \sigma, (\cdot, z^d), \cdot, \cdot)$ is defined by (3.41) in Definition 3.5.3. Specifically, (3.41) gives $\hat{h}_i(k, \sigma, (\cdot, z^d), \cdot, \cdot) = h_i(k, \sigma, (\cdot, z^d), \cdot, \cdot)$ on $\tilde{X}^c \times \tilde{W} \times \tilde{\Theta}$. Thus, conclusion (i) holds. Finally, conclusion (ii) follows from conclusion (i) since \tilde{W} is open.

Lemma 3.5.9. If Conditions 3.5.1–3.5.3 hold for κ , then Conditions 3.4.1–3.4.3 hold for κ .

Proof Assume κ satisfies Conditions 3.5.1–3.5.3 and note that, for any $i \in \{1, \ldots, n_{\sigma}\}$ and $(k, \sigma, \theta) \in \mathcal{K} \times \mathcal{S} \times \tilde{\Theta}$, $\mathcal{M}(k, \sigma_{1:i}, \theta) \subset \mathcal{M}(k, \sigma_{1:i}, \theta)$ by Lemma 3.5.2 and Lemma 3.5.7. Moreover, note that $(\tilde{z}, \tilde{w}) \in \partial_i \mathcal{M}(k, \sigma_{1:i-1}, \theta)$ implies that $(\tilde{z}, \tilde{w}) \in \partial_i \mathcal{M}(k, \sigma_{1:i-1}, \theta, \tilde{z}^d)$.

To show that κ satisfies Condition 3.4.1, choose any $i \in \{1, \ldots, n_{\sigma}\}, k \in \mathcal{K}, \sigma \in \mathcal{S}$, and $\theta \in \tilde{\Theta}$. We must show that

$$\frac{\partial \dot{h}_i}{\partial w}(k,\sigma,\tilde{z},\tilde{w},\theta) \neq 0, \quad \forall (\tilde{z},\tilde{w}) \in \partial_i \dot{\mathcal{M}}(k,\sigma_{1:i-1},\theta).$$
(3.64)

Choose any $(\tilde{z}, \tilde{w}) \in \partial_i \dot{\mathcal{M}}(k, \sigma_{1:i-1}, \theta)$. First, this implies that $\dot{h}_i(k, \sigma, \tilde{z}, \tilde{w}, \theta) = 0$, by definition. Hence, $h_i(k, \sigma, \tilde{z}, \tilde{w}, \theta) = 0$ by Lemma 3.5.8. Second, it implies that $(\tilde{z}, \tilde{w}) \in \dot{\mathcal{M}}(k, \sigma_{1:i-1}, \theta) \subset \mathcal{M}(k, \sigma_{1:i-1}, \theta)$, which means that $(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \sigma_{1:i-1}, \theta, \tilde{z}^d)$. Hence, $h_i(k, \sigma, \tilde{z}, \tilde{w}, \theta) = 0$ implies that $(\tilde{z}, \tilde{w}) \in \partial_i \mathcal{M}(k, \sigma_{1:i-1}, \theta, \tilde{z}^d)$ by definition. Note that Conclusion (iv) in Lemma 3.5.8 combined with the hypothesis that κ satisfies Condition 3.5.1 implies that h_i satisfies Condition 3.5.1.1. Hence, with Conclusion (ii) in Lemma 3.5.8 and $(\tilde{z}, \tilde{w}) \in \partial_i \mathcal{M}(k, \sigma_{1:i-1}, \theta, \tilde{z}^d)$, we must have

$$\frac{\partial \hat{h}_i}{\partial w}(k,\sigma,\tilde{z},\tilde{w},\theta) = \frac{\partial h_i}{\partial w}(k,\sigma,\tilde{z},\tilde{w},\theta) \neq 0.$$
(3.65)

Since the choice $(\tilde{z}, \tilde{w}) \in \partial_i \mathcal{M}(k, \sigma_{1:i-1}, \theta)$ was arbitrary, (3.64) holds.

To show that κ satisfies Condition 3.4.2, choose any $i, j \in \{1, \ldots, n_{\sigma}\}$ with i > j, $k \in \mathcal{K}, \sigma \in \mathcal{S}$, and $\theta \in \tilde{\Theta}$. We must show that

$$\operatorname{rank}\left[\begin{array}{c}\frac{\partial \dot{h}_{i}}{\partial w}(k,\sigma,z,w,\theta)\\\frac{\partial \dot{h}_{j}}{\partial w}(k,\sigma,z,w,\theta)\end{array}\right] = 2, \quad \forall (z,w) \in \partial_{ij} \dot{\mathcal{M}}(k,\sigma_{1:i-1},\theta).$$
(3.66)

 $\in \partial_{ij} \mathcal{M}(k, \sigma_{1:i-1}, \theta).$ (\tilde{z}, \tilde{w}) Choose any First, implies this that Thus, all of the By Conclusion (i) of conclusions of Lemma 3.5.8 hold for *i* and *j*. Lemma 3.5.8, $h_i(k,\sigma,\tilde{z},\tilde{w},\theta) = h_j(k,\sigma,\tilde{z},\tilde{w},\theta) = 0.$ Second, it implies that $(\tilde{z}, \tilde{w}) \in \acute{\mathcal{M}}(k, \sigma_{1:i-1}, \theta) \subset \mathcal{M}(k, \sigma_{1:i-1}, \theta)$, which means that $(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \sigma_{1:i-1}, \theta, \tilde{z}^d)$. Hence, $h_i(k,\sigma,\tilde{z},\tilde{w},\theta) = h_j(k,\sigma,\tilde{z},\tilde{w},\theta) = 0$ implies that $(\tilde{z},\tilde{w}) \in \partial_{ij}\mathcal{M}(k,\sigma_{1:i-1},\theta,\tilde{z}^d)$ by definition. Recall that κ satisfies Condition 3.5.2 by hypothesis. Conclusion (iv) in Lemma 3.5.8 implies that h_i and h_j do not satisfy Condition 3.5.2.2. Conclusion (iii) of Lemma 3.5.8 similarly implies that $hi(k, \sigma, (\cdot, \tilde{z}_d), \cdot, \cdot)$ does not satisfy Condition 3.5.2.3. Specifically, by Conclusion (iii), there does not exist $\beta \neq 0$ such that $\hat{h}_i(k,\sigma,z,w,\theta) = \beta \hat{h}_j(k,\sigma,z,w,\theta) \text{ for all } (z^c,w,\theta) \text{ such that } (z,w) \in \hat{\mathcal{M}}(k,\sigma_{1:i-1},\theta,\tilde{z}^d).$ But, by Conclusion (i) of Lemma 3.5.8, it follows that there does not exist $\beta \neq 0$ such that $h_i(k,\sigma,z,w,\theta) = \beta h_j(k,\sigma,z,w,\theta)$ for all (z^c,w,θ) such that $(z,w) \in \hat{\mathcal{M}}(k,\sigma_{1:i-1},\theta,\tilde{z}^d)$. Finally, since $\hat{\mathcal{M}}(k, \sigma_{1:i-1}, \theta, \tilde{z}^d) \subset \mathcal{M}(k, \sigma_{1:i-1}, \theta, \tilde{z}^d)$ by Lemma 3.5.2, there cannot be $\beta \neq 0$ such that $h_i(k,\sigma,z,w,\theta) = \beta h_j(k,\sigma,z,w,\theta)$ for all (z^c,w,θ) such that $(z,w) \in \mathcal{M}(k,\sigma_{1:i-1},\theta,\tilde{z}^d)$. This implies that Condition 3.5.2.3 cannot hold for the chosen i and j. Therefore, Condition 3.5.2.1 must hold. Hence, with Conclusion (ii) in Lemma 3.5.8 and $(\tilde{z}, \tilde{w}) \in \partial_{ij} \mathcal{M}(k, \sigma_{1:i-1}, \theta, \tilde{z}^d)$, we must have

$$\operatorname{rank}\left[\begin{array}{c}\frac{\partial \hat{h}_{i}}{\partial w}(k,\sigma,\tilde{z},\tilde{w},\theta)\\\frac{\partial \hat{h}_{j}}{\partial w}(k,\sigma,\tilde{z},\tilde{w},\theta)\end{array}\right] = \operatorname{rank}\left[\begin{array}{c}\frac{\partial h_{i}}{\partial w}(k,\sigma,\tilde{z},\tilde{w},\theta)\\\frac{\partial h_{j}}{\partial w}(k,\sigma,\tilde{z},\tilde{w},\theta)\end{array}\right] = 2.$$
(3.67)

Since the choice $(\tilde{z}, \tilde{w}) \in \partial_{ij} \dot{\mathcal{M}}(k, \sigma_{1:i-1}, \theta)$ was arbitrary, (3.66) holds.

Lastly, to show that κ satisfies Condition 3.4.3, choose any $i \in \{1, \ldots, n_{\sigma}\}$, $p \in \{1, \ldots, n_w\}, k \in \mathcal{K}, \sigma \in \mathcal{S}$, and $\theta \in \tilde{\Theta}$. We must to show that

$$\operatorname{rank}\left[\begin{array}{c}\frac{\partial \hat{h}_{i}}{\partial w}(k,\sigma,z,w,\theta)\\e_{p}^{T}\end{array}\right] = 2, \quad \forall (z,w) \in \partial_{i} \hat{\mathcal{M}}(k,\sigma_{1:i-1},\theta) \text{ with } w_{p} = w_{p}^{L} \text{ or } w_{p} = w_{p}^{U}.$$

$$(3.68)$$

Choose any $(\tilde{z}, \tilde{w}) \in \partial_i \dot{\mathcal{M}}(k, \sigma_{1:i-1}, \theta)$ with $w_p = w_p^L$ or $w_p = w_p^U$. First, this implies that $\hat{h}_i(k,\sigma,\tilde{z},\tilde{w},\theta) = 0$ by definition. Hence, all of the conclusions of Lemma 3.5.8 hold. By Conclusion (i) of Lemma 3.5.8, $h_i(k,\sigma,\tilde{z},\tilde{w},\theta) = 0$. Second, it implies that $(\tilde{z}, \tilde{w}) \in \acute{\mathcal{M}}(k, \sigma_{1:i-1}, \theta) \subset \mathcal{M}(k, \sigma_{1:i-1}, \theta),$ which means that $(\tilde{z}, \tilde{w}) \in \mathcal{M}(k, \sigma_{1:i-1}, \theta, \tilde{z}^d).$ Hence, $h_i(k,\sigma,\tilde{z},\tilde{w},\theta) = 0$ implies that $(\tilde{z},\tilde{w}) \in \partial_i \mathcal{M}(k,\sigma_{1:i-1},\theta,\tilde{z}^d)$ by definition. Recall that κ satisfies Condition 3.5.3 by hypothesis. Thus, Conclusion (iv) in Lemma 3.5.8 implies that h_i does not satisfy Condition 3.5.3.2. Conclusion (iii) of Lemma 3.5.8 similarly implies that $hi(k, \sigma, (\cdot, \tilde{z}_d), \cdot, \cdot)$ satisfies neither Condition 3.5.3.3 nor 3.5.3.4. Specifically, first note that by Conclusion (iii), there does not exist $\alpha \neq 0$ such that $\hat{h}_i(k,\sigma,z,w,\theta) = \alpha(w_p - w_p^L)$ for all (z^c,w,θ) such that $(z,w) \in \hat{\mathcal{M}}(k,\sigma_{1:i-1},\theta,\tilde{z}^d)$. But, by Conclusion (i) of Lemma 3.5.8, it follows that there does not exist $\alpha \neq 0$ such that $h_i(k,\sigma,z,w,\theta) = \alpha(w_p - w_p^L)$ for all (z^c,w,θ) such that $(z,w) \in \hat{\mathcal{M}}(k,\sigma_{1:i-1},\theta,\tilde{z}^d)$. But, since $\hat{\mathcal{M}}(k, \sigma_{1:i-1}, \theta, \tilde{z}^d) \subset \mathcal{M}(k, \sigma_{1:i-1}, \theta, \tilde{z}^d)$ by Lemma 3.5.2, there cannot be $\alpha \neq 0$ such that $h_i(k, \sigma, z, w, \theta) = \alpha(w_p - w_p^L)$ for all (z^c, w, θ) such that $(z, w) \in \mathcal{M}(k, \sigma_{1:i-1}, \theta, \tilde{z}^d)$. This implies that Condition 3.5.3.3 cannot hold. Second, note that by Conclusion (iii), there does not exist $\rho \neq 0$ such that $\hat{h}_i(k, \sigma, z, w, \theta) = \rho(w_p - w_p^U)$ for all (z^c, w, θ) such that $(z,w) \in \hat{\mathcal{M}}(k,\sigma_{1:i-1},\theta,\tilde{z}^d)$. But, by Conclusion (i) of Lemma 3.5.8, it follows that there does not exist $\rho \neq 0$ such that $h_i(k,\sigma,z,w,\theta) = \rho(w_p - w_p^U)$ for all (z^c,w,θ) such that $(z,w) \in \hat{\mathcal{M}}(k,\sigma_{1:i-1},\theta,\tilde{z}^d)$. But, since $\hat{\mathcal{M}}(k,\sigma_{1:i-1},\theta,\tilde{z}^d) \subset \mathcal{M}(k,\sigma_{1:i-1},\theta,\tilde{z}^d)$ by Lemma 3.5.2, there cannot be $\rho \neq 0$ such that $h_i(k,\sigma,z,w,\theta) = \rho(w_p - w_p^U)$ for all (z^c,w,θ) such that $(z,w) \in \mathcal{M}(k,\sigma_{1:i-1},\theta,\tilde{z}^d)$. This implies that Condition 3.5.3.4 cannot hold. Therefore, Condition 3.5.3.1 must hold. Thus, with Conclusion (ii) in Lemma 3.5.8 and $(\tilde{z},\tilde{w}) \in \partial_i \mathcal{M}(k,\sigma_{1:i-1},\theta,\tilde{z}^d)$, we must have

$$\operatorname{rank} \begin{bmatrix} \frac{\partial \hat{h}_i}{\partial w}(k, \sigma, \tilde{z}, \tilde{w}, \theta) \\ e_p^T \end{bmatrix} = \operatorname{rank} \begin{bmatrix} \frac{\partial h_i}{\partial w}(k, \sigma, \tilde{z}, \tilde{w}, \theta) \\ e_p^T \end{bmatrix} = 2.$$
(3.69)

Since the choice $(\tilde{z}, \tilde{w}) \in \partial_i \dot{\mathcal{M}}(k, \sigma_{1:i-1}, \theta)$ was arbitrary, (3.68) holds.

Next, we use Definition 3.5.4 to show that using κ in place of κ in (3.3)–(3.5) leads to an expected value \mathcal{L} such that $\mathcal{L}(\theta) = \mathcal{L}(\theta)$ for all $\theta \in \tilde{\Theta}$. This result is established in Corollary 3.5.3 below, and for clarity of arguments, we first define \mathcal{L} and then establish the sequence of Lemmas 3.5.10–3.5.11, Corollary 3.5.2 and Lemmas 3.5.12–3.5.5. To define $\mathcal{L}(\theta)$, first define $\hat{u}_k(\omega, \theta)$ and $\hat{x}_k(\omega, \theta)$ for every $(\omega, \theta) \in \tilde{\Omega} \times \tilde{\Theta}$ by the following recursion, which is analogous to (3.3)–(3.5):

$$\dot{x}_0(\boldsymbol{\omega}, \boldsymbol{\theta}) \equiv b_0, \tag{3.70}$$

$$\acute{u}_k(\boldsymbol{\omega}, \theta) \equiv \acute{\kappa}(k, \acute{x}_k(\boldsymbol{\omega}, \theta), w_k, \theta), \qquad (3.71)$$

$$\dot{x}_{k+1}(\boldsymbol{\omega},\boldsymbol{\theta}) \equiv f(k, \dot{u}_k(\boldsymbol{\omega},\boldsymbol{\theta}), \dot{x}_k(\boldsymbol{\omega},\boldsymbol{\theta}), w_k, \boldsymbol{\theta}).$$
(3.72)

Note that the solution of this recursion exists because the modified decision rule $\hat{\kappa}$ still maps into \tilde{U} and the function f still maps into \tilde{X} . Moreover, define $\hat{\ell}(\theta, \omega)$ by

$$\acute{\ell}(\theta, \boldsymbol{\omega}) \equiv \sum_{k=0}^{K} \ell_{S}(k, \acute{u}_{k}(\boldsymbol{\omega}, \theta), \acute{x}_{k}(\boldsymbol{\omega}, \theta), w_{k}, \theta), \qquad (3.73)$$

and denote the expected value of $\ell(\theta, \omega)$ by

$$\hat{\mathcal{L}}(\theta) \equiv \mathbb{E}[\hat{\ell}(\theta, \boldsymbol{\omega})]. \tag{3.74}$$

We first establish Corollary 3.5.2 using the next two Lemmas 3.5.10–3.5.11.

Lemma 3.5.10. For any $i \in \{1, ..., n_{\sigma}\}$ and $(k, \sigma, z, w, \theta) \in \mathcal{K} \times \mathcal{S} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ such that $(z, w) \in \hat{\mathcal{M}}(k, \sigma_{1:i-1}, \theta)$ and w is in the interior of W, the following implications hold:

$$\hat{h}_i(k,\sigma,z,w,\theta) < 0 \implies \hat{h}_i(k,\sigma,z,w,\theta) < 0, \tag{3.75}$$

$$\hat{h}_i(k,\sigma,z,w,\theta) > 0 \implies \hat{h}_i(k,\sigma,z,w,\theta) > 0.$$
(3.76)

Proof Choose any $i \in \{1, \ldots, n_{\sigma}\}$ and $(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) \in \mathcal{K} \times \mathcal{S} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ such that $(\overline{z}, \overline{w}) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \overline{\theta}), \overline{w}$ is in the interior of W, and $\hat{h}_j(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) \neq 0$ for all $j \in \{1, \ldots, i-1\}$. Note that \overline{w} in the interior of W implies that $(\overline{w}_p - w_p^L) > 0$ and $(\overline{w}_p - w_p^U) < 0$. We must show (3.75)–(3.76) in all of the following cases which correspond to each definition of \hat{h}_i in Definition 3.5.4.

1: Suppose $\exists \beta \neq 0$ and some j i, Case< suchthat $\hat{h}_i(k,\overline{\sigma},z,w,\theta) = \beta \hat{h}_i(k,\overline{\sigma},z,w,\theta), \text{ for all } (z,w,\theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta} \text{ satisfying}$ $(z,w) \in \hat{\mathcal{M}}(k,\overline{\sigma}_{1:i-1},\theta,\overline{z}^d)$. Correspondingly, $\hat{h}_i(k,\overline{\sigma},\overline{z},\overline{w},\overline{\theta})$ will be given by (3.55) in Definition 3.5.4. Since $(\overline{z}, \overline{w}) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \overline{\theta})$, and hence $(\overline{z}, \overline{w}) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \overline{\theta}, \overline{z}^d)$, we have $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \beta \hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta})$. To show (3.75), assume $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) < 0$. This implies $\beta \hat{h}_j(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) < 0$. Recall that $(\overline{z}, \overline{w}) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \overline{\theta})$ which implies that $\overline{\sigma}_j \hat{h}_j(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) \leq 0$. If $\hat{h}_j(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) < 0$, then we must have $\beta > 0$ and $\overline{\sigma}_j = 1$. Otherwise, we must have $\beta < 0$ and $\overline{\sigma}_j = -1$. In both of these situations, (3.55) gives $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = -\beta \overline{\sigma}_j < 0$. Thus, (3.75) holds. To show (3.76), assume $\hat{h}_i(k,\overline{\sigma},\overline{z},\overline{w},\overline{\theta}) > 0.$ This implies $\beta \hat{h}_j(k,\overline{\sigma},\overline{z},\overline{w},\overline{\theta}) > 0.$ If $\hat{h}_j(k,\overline{\sigma},\overline{z},\overline{w},\overline{\theta}) < 0$, then we must have $\beta < 0$ and $\overline{\sigma}_j = 1$. Otherwise, we must have $\beta > 0$ and $\overline{\sigma}_j = -1$. In both of these situations, (3.55) gives $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = -\beta \overline{\sigma}_j > 0$. Hence, (3.76) holds.

Case 2: Suppose Case 1 does not hold, but $\exists \alpha \neq 0$ such that $\hat{h}_i(k, \overline{\sigma}, z, w, \theta) = \alpha(w_p - w_p^L)$ for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \theta, \overline{z}^d)$. Correspondingly, $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta})$ is given by (3.56) in Definition 3.5.4. Since $(\overline{z}, \overline{w}) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \overline{\theta})$, and hence $(\overline{z}, \overline{w}) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \overline{\theta}, \overline{z}^d)$, we have $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \alpha(\overline{w}_p - w_p^L)$. To show (3.75), assume $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \alpha(\overline{w}_p - w_p^L) < 0$. Since \overline{w} is in the interior of W, implying $(\overline{w}_p - w_p^L) > 0$, we must have $\alpha < 0$, which gives $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \alpha(\overline{w}_p - w_p^L) > 0$. This assumption requires $\alpha > 0$, which leads to $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \alpha > 0$ as required.

Case 3: Suppose Cases 1-2 do not hold, but $\exists \rho \neq 0$ such that $\hat{h}_i(k, \overline{\sigma}, z, w, \theta) = \rho(w_p - w_p^U)$ for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \theta, \overline{z}^d)$. Correspondingly, $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta})$ is given by (3.57) in Definition 3.5.4. Since $(\overline{z}, \overline{w}) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \overline{\theta})$, and hence $(\overline{z}, \overline{w}) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \overline{\theta}, \overline{z}^d)$, we have $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \rho(\overline{w}_p - w_p^U)$. To show (3.75), assume $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \rho(\overline{w}_p - w_p^U) < 0$. Since \overline{w} is in the interior of W, implying $(\overline{w}_p - w_p^U) < 0$, we must have $\rho > 0$, which gives $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = -\rho < 0$ as required. To show (3.76), assume $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \rho(\overline{w}_p - w_p^U) > 0$. This assumption requires $\rho < 0$. Hence, $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = -\rho > 0$ as required.

Case 4: Suppose Cases 1–3 do not hold. This implies that $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta})$ is given by (3.58) in Definition 3.5.4. Specifically, we have $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta})$. Hence, the implications in (3.75)–(3.76) hold.

Lemma 3.5.11. For any $i \in \{1, ..., n_{\sigma}\}$ and $(k, \sigma, z, w, \theta) \in \mathcal{K} \times \mathcal{S} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ such that $(z, w) \in \hat{\mathcal{M}}(k, \sigma_{1:i-1}, \theta)$, w is in the interior of W, and $\hat{h}_j(k, \sigma, z, w, \theta) \neq 0$ for all

 $j \in \{1, \ldots, i-1\}$, the following implications hold:

$$\hat{h}_i(k,\sigma,z,w,\theta) < 0 \implies \hat{h}_i(k,\sigma,z,w,\theta) < 0, \tag{3.77}$$

$$\hat{h}_i(k,\sigma,z,w,\theta) > 0 \implies \hat{h}_i(k,\sigma,z,w,\theta) > 0.$$
(3.78)

Proof Choose any $i \in \{1, \ldots, n_{\sigma}\}$ and $(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) \in \mathcal{K} \times \mathcal{S} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ such that $(\overline{z}, \overline{w}) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \overline{\theta}), \overline{w}$ is in the interior of W, and $\hat{h}_j(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) \neq 0$ for all $j \in \{1, \ldots, i-1\}$. Note that \overline{w} in the interior of W implies that $(\overline{w}_p - w_p^L) > 0$ and $(\overline{w}_p - w_p^U) < 0$. We must show the implications in (3.77)–(3.78) in all the following cases which cover all possible definitions of \hat{h}_i in Definition 3.5.4:

Case 1: Suppose $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta})$ is given by (3.55). Correspondingly, $\exists \beta \neq 0$ and some j < i, such that $\hat{h}_i(k, \overline{\sigma}, z, w, \theta) = \beta \hat{h}_j(k, \overline{\sigma}, z, w, \theta)$, for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \theta, \overline{z}^d)$. Since $(\overline{z}, \overline{w}) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \overline{\theta})$, and hence $(\overline{z}, \overline{w}) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \overline{\theta}, \overline{z}^d)$, we have $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \beta \hat{h}_j(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta})$ and we must have $\overline{\sigma}_j \hat{h}_j(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) \leq 0$ by definition of $\hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \overline{\theta})$. To show (3.77), assume $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = -\beta \hat{\sigma}_j < 0$. If $\hat{h}_j(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) < 0$, we must have $\overline{\sigma}_j = 1$. Hence, with $-\beta \overline{\sigma}_j < 0$, we must have $\beta > 0$, which gives $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \beta \hat{h}_j(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) < 0$ as desired. Otherwise, $\hat{h}_j(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) > 0$ and we must have $\overline{\sigma}_j = -1$ and $\beta < 0$, which gives $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \beta \hat{h}_j(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) < 0$ as desired. To show (3.78), assume $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = -\beta \overline{\sigma}_j > 0$. With similar reasoning as above, if $\hat{h}_j(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) < 0$, then we have $\overline{\sigma}_j = 1$ leading to $\beta < 0$. Otherwise, we have $\overline{\sigma}_j = -1$ leading to $\beta > 0$. Either situation leads to $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \beta \hat{h}_j(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) > 0$ as desired.

Case 2: Suppose $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta})$ is given by (3.56). Correspondingly, $\exists \alpha \neq 0$ such that $\hat{h}_i(k, \overline{\sigma}, z, w, \theta) = \alpha(w_p - w_p^L)$ for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \theta, \overline{z}^d)$. Since $(\overline{z}, \overline{w}) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \overline{\theta})$, and hence $(\overline{z}, \overline{w}) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \overline{\theta}, \overline{z}^d)$, we have $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \alpha(\overline{w}_p - w_p^L)$. To show (3.77), assume (3.56) gives $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \alpha < 0$. Since $(\overline{w}_p - w_p^L) > 0$, we must have $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \alpha(\overline{w}_p - w_p^L) < 0$ as desired. To show (3.78), assume (3.56) gives $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \alpha > 0.$ In this case, we have $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \alpha(\overline{w}_p - w_p^L) > 0$ as desired.

Case 3: Suppose $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta})$ is given by (3.57). Correspondingly, $\exists \rho \neq 0$ such that $\hat{h}_i(k, \overline{\sigma}, z, w, \theta) = \rho(w_p - w_p^U)$ for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ satisfying $(z, w) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \theta, \overline{z}^d)$. Since $(\overline{z}, \overline{w}) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \overline{\theta})$, and hence $(\overline{z}, \overline{w}) \in \hat{\mathcal{M}}(k, \overline{\sigma}_{1:i-1}, \overline{\theta}, \overline{z}^d)$, we have $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \rho(\overline{w}_p - w_p^U)$. To show (3.77), assume (3.57) gives $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = -\rho < 0$. Since $(\overline{w}_p - w_p^U) < 0$, we must have $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \rho(\overline{w}_p - w_p^U) < 0$ as desired. To show (3.78), assume (3.57) gives $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = -\rho > 0$. In this case, we must have $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \rho(\overline{w}_p - w_p^U) > 0$ as desired.

Case 4: Suppose $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta})$ is given by (3.58). In this case, we have $\hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta}) = \hat{h}_i(k, \overline{\sigma}, \overline{z}, \overline{w}, \overline{\theta})$. Hence, the implications in (3.77)–(3.78) hold.

Corollary 3.5.2. For any $i \in \{1, ..., n_{\sigma}\}$ and $(k, \sigma, z, w, \theta) \in \mathcal{K} \times \mathcal{S} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ such that $(z, w) \in \hat{\mathcal{M}}(k, \sigma_{1:i-1}, \theta)$, w is in the interior of W, and $\hat{h}_j(k, \sigma, z, w, \theta) \neq 0$ for all $j \in \{1, ..., i-1\}$, the following implications hold:

$$\hat{h}_i(k,\sigma,z,w,\theta) < 0 \iff \hat{h}_i(k,\sigma,z,w,\theta) < 0, \tag{3.79}$$

$$\hat{h}_i(k,\sigma,z,w,\theta) > 0 \iff \hat{h}_i(k,\sigma,z,w,\theta) > 0.$$
(3.80)

Proof A direct combination of Lemmas 3.5.10 and 3.5.11 gives this result. \Box

Next, Corollary 3.5.2 is used to establish the next Lemma 3.5.12, which is then used by Lemma 3.5.13 stating that for each θ , $\hat{\ell}(\theta, \omega) = \hat{\ell}(\theta, \omega)$ everywhere except on a set of ω 's which, in order to conclude that $\hat{\mathcal{L}}(\theta) = \hat{\mathcal{L}}(\theta)$, is shown to be of measure-zero in Corollary 3.5.3. The latter is used to establish the main result of this section, which is finally given in Theorem 3.5.2.

Lemma 3.5.12. Choose any $(k, z, w, \theta) \in \mathcal{K} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta}$ and let $\hat{\sigma} \in S$ be the binary sequence obtained by applying (3.43). If w is in the interior of W and $\hat{h}_i(k, \hat{\sigma}, z, w, \theta) \neq 0$

for all $i \in \{1, \ldots, n_{\sigma}\}$, then $\hat{\kappa}(k, z, w, \theta) = \hat{\kappa}(k, z, w, \theta)$.

Proof Let (k, z, w, θ) and $\hat{\sigma}$ the hypothesis of the lemma. Let $\hat{\sigma}$ be the binary sequence obtained by applying (3.60) with (k, z, w, θ) . To show that $\hat{\kappa}(k, z, w, \theta) = \hat{\kappa}(k, z, w, \theta)$, it suffices to show that $\hat{\sigma} = \hat{\sigma}$ according to (3.42), (3.44), (3.59), and (3.61). Since $\hat{\sigma}$ satisfies (3.43), it follows that $(k, \hat{\sigma}, z, w, \theta)$ satisfies all of the hypotheses in Corollary 3.5.2.

To show that $\hat{\sigma} = \hat{\sigma}$, we use induction. To begin, first note that $\hat{\sigma}_{1:0} = \hat{\sigma}_{1:0}$ since both of $\hat{\sigma}_{1:0}$ and $\hat{\sigma}_{1:0}$ are empty sequences. For induction, choose any i with $0 < i \leq n_{\sigma}$ and assume that $\hat{\sigma}_{1:i-1} = \hat{\sigma}_{1:i-1}$. By Corollary 3.5.2, $\hat{h}_i(k, \hat{\sigma}_{1:i-1}, z, w, \theta)$ and $\hat{h}_i(k, \hat{\sigma}_{1:i-1}, z, w, \theta)$ have the same sign. But, since $\hat{\sigma}_{1:i-1} = \hat{\sigma}_{1:i-1}$, $\hat{h}_i(k, \hat{\sigma}_{1:i-1}, z, w, \theta)$ and $\hat{h}_i(k, \hat{\sigma}_{1:i-1}, z, w, \theta)$ must have the same sign. Hence, $\hat{\sigma}_{1:i} = \hat{\sigma}_{1:i}$. By induction on $i, \hat{\sigma} = \hat{\sigma}_{1:n_{\sigma}} = \hat{\sigma}_{1:n_{\sigma}} = \hat{\sigma}$. \Box

Lemma 3.5.13. Choose any $(\boldsymbol{\omega}, \theta) \in \tilde{\Omega} \times \tilde{\Theta}$, let $\hat{u}_{0:K}$ and $\hat{x}_{0:K}$ be the input and state trajectories of the recursion (3.49)–(3.51), and let $\hat{u}_{0:K}$ and $\hat{x}_{0:K}$ be the input and state trajectories of the recursion (3.70)–(3.72). Moreover, let $\hat{\sigma}_{0:K}$ and $\hat{\sigma}_{0:K}$ be the binary trajectories obtained by applying (3.43) and (3.60), respectively, at each $k \in \mathcal{K}$. If w_k is in the interior of W and $\hat{h}_i(k, \hat{\sigma}_{k,1:i-1}, \hat{x}_k, w_k, \theta) \neq 0$ for all $i \in \{1, \ldots, n_\sigma\}$ and $k \in \mathcal{K}$, then $\hat{\ell}(\theta, \boldsymbol{\omega}) = \hat{\ell}(\theta, \boldsymbol{\omega})$.

Proof To show that $\hat{\ell}(\theta, \omega) = \hat{\ell}(\theta, \omega)$, it is sufficient to show that $\hat{u}_k = \hat{u}_k$ and $\hat{x}_{k+1} = \hat{x}_{k+1}, \forall k \in \mathcal{K}$. Specifically, this implies that $\hat{\ell}(\omega, \theta) = \hat{\ell}(\omega, \theta)$ by (3.52) and (3.73).

To show that $\hat{u}_k = \hat{u}_k$ and $\hat{x}_{k+1} = \hat{x}_{k+1}, \forall k \in \mathcal{K}$, we first show that the following implication holds for any $k \in \mathcal{K}$:

$$\hat{x}_{k} = \acute{x}_{k} \implies \left\{ \begin{array}{c} \hat{u}_{k} = \acute{u}_{k} \\ \hat{x}_{k+1} = \acute{x}_{k+1} \end{array} \right\}.$$
(3.81)

Assume $\hat{x}_k = \acute{x}_k$. By Lemma 3.5.12, we immediately have $\hat{\kappa}(k, \hat{x}_k, w_k, \theta) = \acute{\kappa}(k, \hat{x}_k, w_k, \theta)$. But, by the assumption, we must have $\hat{\kappa}(k, \hat{x}_k, w_k, \theta) = \acute{\kappa}(k, \acute{x}_k, w_k, \theta)$. This implies that $\hat{u}_k = \acute{u}_k$ by (3.50) and (3.71). Then, $\hat{x}_k = \hat{x}_k$ and $\hat{u}_k = \hat{u}_k$ leads to $\hat{x}_{k+1} = \hat{x}_{k+1}$ by (3.51) and (3.72).

To finish the proof, we now proceed with finite induction over k. Noting that $\hat{x}_0 = \hat{x}_0 = b_0$, a recursive application of (3.81) shows that $\hat{u}_k = \hat{u}_k$ and $\hat{x}_{k+1} = \hat{x}_{k+1}$ for all $k \in \mathcal{K}$.

Corollary 3.5.3. If κ satisfies Condition 3.5.1, then $\acute{\mathcal{L}}(\theta) = \mathcal{L}(\theta)$ for any $\theta \in \tilde{\Theta}$.

Proof Assume κ satisfies Condition 3.5.1. Choose any $\theta \in \tilde{\Theta}$. By Corollary 3.5.1, $\hat{\mathcal{L}}(\theta) = \mathcal{L}(\theta)$, so it suffices to show that $\hat{\mathcal{L}}(\theta) = \hat{\mathcal{L}}(\theta)$. Recall that $\hat{\mathcal{L}}(\theta) = \mathbb{E}[\hat{\ell}(\theta, \omega)]$ and $\hat{\mathcal{L}}(\theta) = \mathbb{E}[\hat{\ell}(\theta, \omega)]$. Thus, it sufficed to show that $\hat{\ell}(\cdot, \omega)$ and $\hat{\ell}(\cdot, \omega)$ only differ on the set of Lebesgue measure zero. To do this, we first construct the sets on which $\hat{\ell}(\cdot, \omega)$ and $\hat{\ell}(\cdot, \omega)$ disagree according to Lemma 3.5.13. These sets are given as follows for each $k \in \mathcal{K}$ and $i \in \{1, \ldots, n_{\sigma}\}$ where, for each $\omega \in \Omega$, $\hat{x}_k(\omega, \theta)$ is as defined in (3.51) and $\hat{\sigma}_k(\omega, \theta)$ denotes the binary sequence obtained by applying (3.43) with $(k, \hat{x}_k(\omega, \theta), w_k, \theta)$:

$$\partial_{ki}\Omega(\theta) \equiv \{ \boldsymbol{\omega} \in \Omega : \hat{h}_i(k, \hat{\sigma}_{k,1:i-1}(\boldsymbol{\omega}, \theta), \hat{x}_k(\boldsymbol{\omega}, \theta), w_k, \theta) = 0 \}, \quad \forall k, \forall i,$$
(3.82)

$$\partial_k^L \Omega(\theta) \equiv \{ \boldsymbol{\omega} \in \Omega : w_k = w^L \}, \tag{3.83}$$

$$\partial_k^U \Omega(\theta) \equiv \{ \boldsymbol{\omega} \in \Omega : w_k = w^U \}.$$
(3.84)

Since κ satisfies Condition 3.5.1, $\hat{\kappa}$ satisfies Condition 3.4.1 by Lemma 3.5.3. By Lemma 3.9.4 (see appendix), this implies that $\mu(\partial_{ki}\Omega(\theta)) = 0$, for all $k \in \mathcal{K}$ and $i \in \{1, \ldots, n_{\sigma}\}$. Moreover, it is easy to see that $\mu(\partial_{k}^{L}\Omega(\theta)) = 0$ and $\mu(\partial_{k}^{U}\Omega(\theta)) = 0$ for every $k \in \mathcal{K}$. By Lemma 3.5.13, $\hat{\ell}(\theta, \omega) \neq \hat{\ell}(\theta, \omega)$ is possible only if $\omega \in \partial_{ki}\Omega(\theta), \omega \in \partial_{k}^{L}\Omega(\theta)$, or $\omega \in \partial_{k}^{U}\Omega(\theta)$, for some $k \in \mathcal{K}$. Since these sets are all of Lebesgue measure zero, it follows that $\hat{\mathcal{L}}(\theta) = \hat{\mathcal{L}}(\theta)$. But, since $\hat{\mathcal{L}}(\theta) = \mathcal{L}(\theta)$ by Lemma 3.5.1, we must have $\hat{\mathcal{L}}(\theta) = \mathcal{L}(\theta)$. \Box

Theorem 3.5.2. If κ satisfies Condition 3.5.1, then \mathcal{L} is continuous on $\tilde{\Theta}$. If κ satisfies Conditions 3.5.2–3.5.3 also, then $\mathcal{L} \in C^1(\tilde{\Theta}, \mathbb{R})$; i.e., κ is smooth-in-expectation.

Proof Theorem 3.5.1 gives continuity of \mathcal{L} . With Lemma 3.5.9, a direct application of

Theorem 3.4.1 gives $\hat{\mathcal{L}} \in C^1(\tilde{\Theta}, \mathbb{R})$. Hence, with Corollary 3.5.3, we have $\mathcal{L} \in C^1(\tilde{\Theta}, \mathbb{R})$. \Box

3.6 Continuous Differentiability of Chance Constraints \mathcal{P}_k

In this section, we show that the results from the previous section concerning the continuous differentiability of the expected-value cost function \mathcal{L} can be applied to analyze continuous differentiability of chance constraints \mathcal{P}_k as given by (3.10). Even though differentiability of probability functions is a known subject in the literature, the function \mathcal{P}_k differs from probability functions treated in the literature by the fact that $\mathcal{P}_k(\theta)$ is subject to the recursion (3.3)–(3.5) which involves the decision rule κ satisfying Definition 3.4.1. Accordingly, the results presented here are a new contribution.

In order to apply the results from the previous sections, we use the fact that $\mathcal{P}_k(\theta)$ can be equivalently expressed as an expected value of an indicator function. To show this clearly, consider the following definition.

Definition 3.6.1. Let κ be a decision rule satisfying Definition 3.4.1. Let $\check{S} \equiv S \times \{-1, 1\}^{n_g}$. For each $k \in \mathcal{K}$ and $\check{\sigma} \in \check{S}$, let $\check{g} : \mathcal{K} \times \check{S} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \mathbb{R}^{n_g}$ be defined as follows, for all $(z, w, \theta) \in \tilde{X} \times \tilde{W} \times \tilde{\Theta}$:

$$\check{g}(k,\check{\sigma},z,w,\theta) \equiv g(k,\kappa_{\check{\sigma}_{1:n_h}}(k,z,w,\theta),z,w,\theta).$$
(3.85)

Moreover, for each $q \in \{1, \ldots, n_h + n_g\}$, $k \in \mathcal{K}$ and $\check{\sigma} \in \check{S}$, let $\check{h}_q : \mathcal{K} \times \check{S} \times \check{X} \times \check{W} \times \check{\Theta} \to \mathbb{R}$ be defined as follows, for all $(z, w, \theta) \in \check{X} \times \check{W} \times \check{\Theta}$:

(a) If $q > n_h$, then define

$$\check{h}_{q}(k,\check{\sigma},z,w,\theta) \equiv \check{g}_{q-n_{h}}(k,\check{\sigma},z,w,\theta).$$
(3.86)

(b) Otherwise, define

$$\dot{h}_{q}(k,\check{\sigma},z,w,\theta) \equiv h_{q}(k,\check{\sigma}_{1:n_{h}},z,w,\theta).$$
(3.87)

Moreover, define $\check{\kappa} : \mathcal{K} \times \tilde{X} \times \tilde{W} \times \tilde{\Theta} \to \tilde{U} \times \{-1, 1\}^{n_g}$ by

$$\check{\sigma}_q = \left\{ \begin{array}{cc} 1 & \text{if} & \check{h}_q(k, \check{\sigma}_{1:q-1}, z, w, \theta) \le 0 \\ -1 & \text{otherwise} \end{array} \right\}, \quad \forall q \in \{1, \dots, n_{\check{\sigma}}\}, \qquad (3.88)$$

$$\check{\kappa}(k, z, w, \theta) \equiv (\kappa_{\check{\sigma}_{1:n_h}}(k, z, w, \theta), \check{\sigma}_{k, n_h + 1:n_{\check{\sigma}}}).$$
(3.89)

Remark 3.6.1. Since κ satisfies Definition 3.4.1, it can be easily shown that Definition 3.6.1 satisfies Definition 3.4.1. In particular, the functions \check{h}_q satisfy the same continuous differentiability requirement on h_i in Definition 3.4.1. This is true because, for every $k \in \mathcal{K}$, $z^d \in \tilde{X}^d$, and $\check{\sigma} \in \check{S}$, the function $\check{g}(k,\check{\sigma},(\cdot,z^d),\cdot,\cdot)$ is continuously differentiable on $\tilde{X}^c \times \tilde{W} \times \tilde{\Theta}$ by Assumption 3.3.2, Definition 3.4.1, and by the fact that \check{g} is defined as the composition of g and $\kappa_{\check{\sigma}_{1:n_h}}$ and the composition of two continuously differentiable functions is also continuously differentiable.

To write $\mathcal{P}_k(\theta)$ as an expected value of an indicator function, consider the following recursion, which is similar to (3.3)–(3.5):

$$x_0(\boldsymbol{\omega}, \boldsymbol{\theta}) \equiv b_0, \tag{3.90}$$

$$\check{u}_k(\boldsymbol{\omega}, \theta) \equiv \check{\kappa}(k, x_k(\boldsymbol{\omega}, \theta), w_k, \theta), \tag{3.91}$$

$$x_{k+1}(\boldsymbol{\omega}, \theta) \equiv f(k, \check{u}_{k,1:n_u}(\boldsymbol{\omega}, \theta), x_k(\boldsymbol{\omega}, \theta), w_k, \theta).$$
(3.92)

Moreover, define the indicator function $\psi(\boldsymbol{\omega}, \theta)$ for each $(\boldsymbol{\omega}, \theta) \in \tilde{\Omega} \times \tilde{\Theta}$ by:

$$\psi(\boldsymbol{\omega}, \boldsymbol{\theta}) \equiv \left\{ \begin{array}{ll} 1, & \text{if } \check{u}_{k, n_u + j}(\boldsymbol{\omega}, \boldsymbol{\theta}) = 1, \forall j \in \{1, \dots, n_g\} \\ 0, & \text{otherwise} \end{array} \right\}.$$
(3.93)

According to (3.85)–(3.92), $\check{u}_{k,n_u+j}(\boldsymbol{\omega},\theta) = 1$ for $j \in \{1,\ldots,n_g\}$ indicates that $g(k, u_k(\boldsymbol{\omega},\theta), x_k(\boldsymbol{\omega},\theta), w_k, \theta) \leq 0$, as per (3.7). Thus, noting that $\check{u}_{k,1:n_u}(\boldsymbol{\omega},\theta) = u_k(\boldsymbol{\omega},\theta)$, we must have the following, by (3.7), (3.10) and the fact that a chance constraint can be

written as an expected value of an indicator function:

$$\mathcal{P}_k(\theta) = \mathbb{P}\left[\tau_k(\boldsymbol{\omega}, \theta) \le 0\right] \tag{3.94}$$

$$= \mathbb{P}\left[g(k, u_k(\boldsymbol{\omega}, \theta), x_k(\boldsymbol{\omega}, \theta), w_k, \theta) \le 0\right]$$
(3.95)

$$= \mathbb{E}\left[\psi(\boldsymbol{\omega}, \boldsymbol{\theta})\right]. \tag{3.96}$$

Now that $\mathcal{P}_k(\theta)$ is expressed as an expected-value, we next prove the following result for continuous differentiability of $\mathcal{P}_k(\theta)$.

Theorem 3.6.1. If $\check{\kappa}$ satisfies Condition 3.5.1, then \mathcal{P}_k is continuous on $\tilde{\Theta}$. If $\check{\kappa}$ satisfies Conditions 3.5.2–3.5.3 also, then $\mathcal{P}_k \in C^1(\tilde{\Theta}, \mathbb{R})$.

Proof Theorem 3.6.1 holds by Theorem 3.5.2 because 1) $\check{\kappa}$ satisfies Definition 3.4.1, 2) \mathcal{P}_k is an expected value of ψ which is constant, and thus continuously differentiable on $\tilde{\Omega} \times \tilde{\Theta}$, for each fixed $k \in \mathcal{K}$, $\check{u}_k^d = (u_k^d, \check{u}_{k,n_u:nu+n_g})$, and $z^d \in \tilde{X}^d$ (this is a similar requirement for ℓ_S in Assumption 3.3.2).

Remark 3.6.2. Note that applying Conditions 3.5.1–3.5.3 to $\check{\kappa}$ involves checking the derivatives $\frac{\partial \check{h}_q}{\partial w}(k,\check{\sigma},z,w,\theta)$, which involve the derivatives $\frac{\partial \check{g}_i}{\partial w}(k,\check{\sigma},z,w,\theta)$ as given by

$$\frac{\partial \check{g}_i}{\partial w}(k,\check{\sigma},z,w,\theta) = \frac{\partial g_i}{\partial w} + \frac{\partial g_i}{\partial \kappa_{\check{\sigma}_{1:n_h}}} \frac{\partial \kappa_{\check{\sigma}_{1:n_h}}}{\partial w},\tag{3.97}$$

where the derivatives of g_i are evaluate at $(k, \kappa_{\check{\sigma}}(k, z, w, \theta), z, w, \theta)$ and $\frac{\partial \kappa_{\check{\sigma}}}{\partial w}$ at (k, z, w, θ) .

3.7 An Illustrative Example: Optimization of an Inventory System

This section considers an illustrative integrated design and operation problem for a two-product inventory system that is operated daily over a year. We first present an MSP model of the form (3.1), then develop a decision rule approximation and show that it is differentiable using the results from §3.5. Finally, we solve the smooth decision rule approximation using a gradient-based approach and compare with gradient-free algorithms.

3.7.1 MSP Model for the Inventory Example

We consider the optimization of the inventory system illustrated in Figure 3.3. The



Figure 3.3: A simple two-product inventory system

system consists of two processes, Process 1 and Process 2, which are run on a daily basis for a year (i.e., K = 364) to produce two products, Prod.1 (produced by Process 1 only) and Prod.2 (produced by both processes). These products are stored in two tanks with capacities C_1^{St} and C_2^{St} , from which uncertain daily demands $D_{k,1}$ and $D_{k,2}$ are supplied. The demands $D_{k,i}$ are non-stationary and are modeled by a time-varying deterministic sequence perturbed by random variables $w_k = (\xi_k, \lambda_k)$, as described in detail in the appendix:

$$D_{k,i} = D_{k,i}^{det} + \xi_{k,i} + \lambda_{k,i}, \quad \forall i \in \{1,2\}.$$
(3.98)

The MSP model for this system has mixed-integer operational decisions $u_k = (s_{k,1}, s_{k,2}, P_{k,1}^u, P_{k,2}^u, P_{k,1}^d, P_{k,2}^d, y_{k,1}, y_{k,2})$ taking values in $\tilde{U} \equiv \mathbb{R}^6 \times \{0, 1\}^2$, system states $x_k = (x_{k,1}^c, x_{k,2}^c, \overline{x}_{k,1}^d, \overline{x}_{k,2}^d, \underline{x}_{k,1}^d, \underline{x}_{k,2}^d)$ taking values in $\tilde{X} \equiv \mathbb{R}^2 \times \mathbb{Z}^4$, and design decisions $\theta = (C_1^{St}, C_2^{St})$ taking values in $\Theta \equiv [\theta^L, \theta^U]$, with $\theta^L = (10^{-3}, 10^{-3})$ and $\theta^L = (20, 20)$. The components of u_k, x_k , and θ are defined in Table 3.1. The MSP we consider is as follows, where j is used for indexing processes and i for indexing products, and the values of the cost coefficients and other constants are given in Table 3.2:

$$\min_{\substack{\theta \in \Theta \\ x_k \in L^{\infty}(\Omega, \tilde{X}) \\ u_k \in L^{\infty}(\Omega, \tilde{U})}} \beta^T C^{st} + \mathbb{E} \left[\sum_{k=0}^{364} \begin{pmatrix} c_y^T y_k(\boldsymbol{\omega}) - c_s^T s_k(\boldsymbol{\omega}) + c_u^T P_k^u(\boldsymbol{\omega}) \\ + c_d^T P_k^d(\boldsymbol{\omega}) + c_x^T x_{k+1}^c(\boldsymbol{\omega}) \end{pmatrix} \right]$$
(3.99)

subject to :

$$x_{k+1,i}^{c}(\boldsymbol{\omega}) = x_{k,i}^{c}(\boldsymbol{\omega}) - s_{k,i}(\boldsymbol{\omega}) + \sum_{j=1}^{2} (\mu_{i,j} y_{k,j}(\boldsymbol{\omega}) C_{j}^{Pr}) - P_{k,i}^{d}(\boldsymbol{\omega}), \quad \forall i$$
(3.100)

$$\overline{x}_{k+1,j}^d(\boldsymbol{\omega}) = y_{k,j}(\boldsymbol{\omega})(\overline{x}_{k,j}^d(\boldsymbol{\omega}) + 1), \quad \forall j$$
(3.101)

$$\underline{x}_{k+1,j}^d(\boldsymbol{\omega}) = (1 - y_{k,j}(\boldsymbol{\omega}))(\underline{x}_{k,j}^d(\boldsymbol{\omega}) + 1), \quad \forall j$$
(3.102)

$$x_{0,i}^c(\boldsymbol{\omega}) = 0.75C_i^{st}, \quad \forall i$$
(3.103)

$$\overline{x}_{0,j}^d(\boldsymbol{\omega}) = \overline{M}_j, \quad \forall j \tag{3.104}$$

$$\underline{x}_{0,j}^d(\boldsymbol{\omega}) = 0, \quad \forall j \tag{3.105}$$

$$s_{k,i}(\boldsymbol{\omega}) \le x_{k,i}^c(\boldsymbol{\omega}), \quad \forall i$$

$$(3.106)$$

$$D_{k,i}(\boldsymbol{\omega}) = s_{k,i}(\boldsymbol{\omega}) + P_{k,i}^u(\boldsymbol{\omega}), \quad \forall i$$
(3.107)

$$0 \le x_{k+1,i}^c(\boldsymbol{\omega}) \le C_i^{St}, \quad \forall i$$
(3.108)

$$(1 \le \underline{x}_{k,j}^d(\boldsymbol{\omega}) \le \underline{M}_j - 1) \implies (y_{k,j}(\boldsymbol{\omega}) = 0), \quad \forall j$$
 (3.109)

$$(1 \le \overline{x}_{k,j}^d(\boldsymbol{\omega}) \le \overline{M}_j - 1) \implies (y_{k,j}(\boldsymbol{\omega}) = 1), \quad \forall j$$
(3.110)

$$s_{k,i}(\boldsymbol{\omega}), P_{k,i}^u(\boldsymbol{\omega}), P_{k,i}^d(\boldsymbol{\omega}) \ge 0, \quad \forall i$$

$$(3.111)$$

y_k, s_k, P_k^u, P_k^d nonanticipative (3.112)

$\forall k \in \{0, \dots, K\}, \forall \boldsymbol{\omega} \in \Omega$

The first term in the objective function is the storage investment cost, where β_i is the cost of a unit of storage capacity C_i^{st} . The second term is the expected value of the sum of daily operational costs,

$$\ell_S(k, u_k, x_k, w_k, \theta) = c_y^T y_k - c_s^T s_k + c_u^T P_k^u + c_d^T P_k^d + c_x^T x_{k+1}^c, \qquad (3.113)$$

Operational decisions u_k	Description				
$y_{k,j}$	On/off status of process j on day k (binary)				
$s_{k,i}$	Amount of product i sold in day k (continuous)				
$P_{k,i}^u$	Unmet demand for product i in day k (continuous)				
$P_{k,i}^d$	Amount of product i dumped in day k (continuous)				
System states x_k	Description				
$x_{k,i}^c$	Storage level for product i at the beginning of day k (contin-				
,	uous)				
$\overline{x}_{k,j}^d$	Number of days prior to day k that process j has been running				
	including the day it was last turned on (integer)				
$\underline{x}_{k,i}^d$	Number of days prior to day k that process j has been off				
	including the day it was last turned off (integer)				
Random variables w_k	Description				
$\xi_{k,i}$ and $\lambda_{k,i}$	Random perturbations on demand for product i in day k				
Design decisions θ	Description				
C_i^{St}	Capacity of storage tank for product i				

Table 3.1: Description of operational decisions u_k , system states x_k , random variables w_k , and design decisions θ for the MSP in (3.99)–(3.112)

Table 3.2: Values for cost coefficients and other constants in (3.99)-(3.112)

Constant	$c_{y,j}$	$c_{s,i}$	$c_{u,i}$	$c_{d,i}$	$c_{x,i}$	β_i	\overline{M}_{j}	\underline{M}_{j}	C_j^{Pr}	$\mu_{1,j}$	$\mu_{2,j}$
i or j = 1	12	3	60	0.3	0.06	50	2	1	1	4	0
i or j = 2	14.4	6	120	0.6	0.12	50	1	1	1	1.33	4

where $c_{y,j}$ is the cost for running processes j and $c_{s,i}$, $c_{u,i}$, $c_{d,i}$, and $c_{x,i}$ are, respectively, the selling price, the cost penalty for unmet demand, the cost of dumping, and the storage cost per unit of product i. Note that x_{k+1}^c is used in ℓ_S as a short-hand for the right hand side of (3.100). Thus, ℓ_S depends on x_k as in (3.1). Constraints (3.100)–(3.102) specify how the system state is updated and define the function f in (3.1). Constraint (3.100) states that the amount (storage level) of product i at the end of the day depends on the amount $x_{k,i}^c$ available at beginning of that day, the amount $s_{k,i}$ sold, the amount produced during the day (the summation term), and the amount dumped. In the summation term, which is non-zero if $y_{k,j} = 1$ (process j is run), $\mu_{i,j}$ denotes the amount of product i produced for each unit of capacity C_i^{Pr} of process j. We assume that both processes run at their full capacity or not at all. Thus, dumping excess product is permitted with an associated cost penalty to avoid overfilling the storage tanks. We also assume that new products from Processes 1 and 2 become available only at the end of the day, so demands must be supplied entirely from storage $x_{k,i}^c$ (constraint (3.106)). Consequently, there may be unmet demands (constraint (3.107)), which are associated with large penalty costs. Constraint (3.108) requires the storage level to remain between zero and the storage capacity C_i^{St} . To avoid frequent and costly process start-ups and shutdowns, $\overline{x}_{k,j}^d$ and $\underline{x}_{k,j}^d$ (see Table 3.1) are recorded and updated according to (3.101) and (3.102). Once process j is turned on, it is allowed to be shut down only if it has reached its minimum uptime (constraint (3.110)), and once it is shut down, it is allowed to be turned on only if it has reach its minimum downtime (constraint (3.109)). Note that the logical constraints (3.109)-(3.110) admit a big-M-type reformulation into integer linear constraints. However, this reformulation is not performed here for convenience of notation. Finally, constraints (3.103)-(3.105) specify the initial conditions, where $\overline{x}_{0,j}^d$ and $\underline{x}_{0,j}^d$ are chosen so that $y_{0,j}$ is free.

Note that all constraints in the MSP above are required to hold robustly. Strictly to match the form of the general MSP (3.1), constraints (3.106)-(3.111) should be written as chance constraints. However, it is clearly desirable to enforce them robustly because they encode some aspects of the problem physics, such as the impossibility of filling a storage

tank beyond its capacity. In general, the methods developed in this chapter do not address robust constraints. However, we will show in the next section that it is possible in this case to formulate an effective decision rule that satisfies (3.106)-(3.111) robustly.

3.7.2 Decision Rule Approximation

The decision rule approximation of (3.99)-(3.112) is obtained by replacing u_k with the decision rule κ presented in Fig.'s 3.4–3.5, which is parametrized by parameters γ . When γ and $\theta = (C_1^{St}, C_2^{St})$ are fixed, the rule makes operational decisions $u_k = (s_k, P_k^u, P_k^d, y_k)$ in each stage k while also enforcing the robust constraints (3.106)–(3.111). Since the binary decisions y_k affect how some of the continuous decisions s_k , P_k^u , and P_k^d are made (Fig. 3.5), the rule decides y_k first (Fig. 3.4). In relation to Definition 3.4.1, the expressions in the \diamond blocks in both Fig. 3.4 and Fig. 3.5 are for checking the event functions $h_i \leq 0$ as in (3.12).

For each process $j \in \{1,2\}$, the binary decision $y_{k,j}$ is made first using Fig. 3.4. Since process j has a minimum up-time \overline{M}_j and minimum down-time \underline{M}_j , the rule first determines if $y_{k,j}$ is fixed by the constraints (3.109)–(3.110). For example, suppose $\overline{x}_{k,j}^d = 0$, which means that process j is not running. If $\underline{x}_{k,j}^d < \underline{M}_j$, then process j has not reached its minimum down-time and cannot be started $(y_{k,j} = 0)$. Otherwise, the process can be started again. In all cases where $y_{k,j}$ is not fixed by (3.109)–(3.110), the rule determines $y_{k,j}$ using the following threshold function parametrized by γ :

$$b_{k,j} = \gamma_{j,1} + \gamma_{j,2}(x_{k,1}^c - D_{k,1}) + \gamma_{j,3}(x_{k,2}^c - D_{k,2}) + \eta_{k,j}, \qquad (3.114)$$

where $\eta_{k,j}$ is a small random perturbation that is added to randomize the rule. If $b_{k,j} \leq 0$, then process j is turned on $(y_{k,j} = 1)$. Otherwise, the process is turned off $(y_{k,j} = 0)$.

Next, continuous decisions $s_{k,i}$, $P_{k,i}^u$, and $P_{k,i}^d$ are made using Fig. 3.5. These decisions are made such that constraint (3.106)–(3.108) are robustly satisfied. The strategy is to first sell as much product as possible without violating constraint (3.106). If $x_{k,i}^c \leq D_{k,i}$, then all of the stored product *i* is sold $(s_{k,i} = x_{k,i}^c)$ and there is an unmet de-



Figure 3.4: Decision rule making binary operational decisions $y_{k,j}$.



Figure 3.5: Decision rule making continuous decisions $P_{k,i}^u$, $s_{k,i}$, and $P_{k,i}^d$

mand $P_{k,i}^u = D_{k,i} - x_{k,i}^c$. Otherwise, the demand is fully supplied $(s_{k,i} = D_{k,i})$ and $P_{k,i}^u = 0$. It is easy to see that this strategy ensures that (3.107) is satisfied. Next, the rule decides whether or not it is necessary to dump excess products at the end of the day to enforce constraint (3.108). This decision is made based on $\dot{x}_{k,i}^c$, which denotes the storage level at the end of the day assuming no dumping. If $\dot{x}_{k,i}^c \leq C_i^{St}$, then no dumping is needed $(P_{k,i}^d = 0)$. Otherwise, $P_{k,i}^d = \dot{x}_{k,i}^c - C_i^{St}$. This ensures that (3.108) will be satisfied at k+1.

The decision rule approximation obtained by replacing u_k in (3.99)–(3.112) with the decision rule in Fig.'s 3.4–3.5 can be cast as the following simulation-optimization problem:

$$\min_{\theta \in \Theta, \gamma \in \Gamma} \quad C(\theta) + \mathcal{L}(\theta, \gamma) \quad , \tag{3.115}$$

where $C(\theta) = \beta^T C^{st}$ and $\mathcal{L}(\theta, \gamma) = \mathbb{E}[\ell(\boldsymbol{\omega}, (\theta, \gamma))]$, with $\ell(\boldsymbol{\omega}, (\theta, \gamma))$ evaluated through simulation. For any fixed $\boldsymbol{\omega}$, γ , and $\theta = (C_1^{St}, C_2^{St})$, a simulation consists of recursively evaluating f as defined in (3.100) and the decision rule in Fig.'s 3.4–3.5 to obtain the system states $x_k(\boldsymbol{\omega}, (\theta, \gamma))$ and operational decisions $u_k(\boldsymbol{\omega}, (\theta, \gamma))$ that are used to compute $\ell(\boldsymbol{\omega}, (\theta, \gamma))$ as follows:

$$\ell(\boldsymbol{\omega},(\boldsymbol{\theta},\boldsymbol{\gamma})) = \sum_{k=0}^{364} \ell_S(k, u_k(\boldsymbol{\omega},(\boldsymbol{\theta},\boldsymbol{\gamma})), x_k(\boldsymbol{\omega},(\boldsymbol{\theta},\boldsymbol{\gamma})), w_k,(\boldsymbol{\theta},\boldsymbol{\gamma})).$$
(3.116)

Note that in relation to the general simulation-optimization problem (3.11), problem (3.115) does not have chance constraints since all constraints in (3.99)-(3.112) are robustly enforced by the rule in Fig.'s 3.4-3.5. In the next subsection, we show that the rule in Fig.'s 3.4-3.5 makes (3.115) is smooth-in-expectation, allowing its solution using gradient-based approaches.

3.7.3 Verification of Smoothness of the Decision Rule Approximation

In this subsection, we show that the decision rule in Fig.'s 3.4–3.5 satisfies Definition 3.4.1 and is smooth-in-expectation. Fig.'s 3.4–3.5 obey Definition 3.4.1 with the event functions h_i in (3.12) defined as the expressions inside the \diamond blocks. We denote the event functions in Fig.'s 3.4–3.5 using the indexing scheme $h_{1:3}^{(j)}$ (Fig. 3.4) and $h_{4:5}^{(i)}$ (Fig. 3.5) with $i, j \in \{1, 2\}$ corresponding to the values $\sigma_{k,1:3}^{(j)}$ and $\sigma_{k,4:5}^{(i)}$ shown in the figures. To relate this indexing scheme to Definition 3.4.1, we can define $h_q = h_n^{(r)}$ where q = 2(n-1) + r, $r \in \{1, 2\}$, and $n \in \{1, \dots, 5\}$. For clarity, the event functions $h_{1:3}^{(j)}$ and $h_{4:5}^{(i)}$ are given explicitly in Table 3.3. The functions κ_{σ} are too numerous to write explicitly, but are evident from Fig.'s 3.4–3.5.

We first argue that the decision rule defined by Fig.'s 3.4–3.5 satisfies Definition 3.4.1. First, note that Definition 3.4.1 allows each h_q to depend on $k, x_k, w_k, (\theta, \gamma)$, and

Table 3.3: Event functions corresponding to Fig.'s 3.4–3.5

Figure	Event functions $h_{1:3}^{(j)}$ and $h_{4:5}^{(i)}$
Fig. 3.4	
Fig. 3.5	$ h_{4}^{(i)} = x_{k,i}^{c} - D_{k,i} $ $ h_{5}^{(i)} = \begin{cases} \sum_{j=1}^{2} y_{k,j}(\mu_{i,j}C_{j}^{Pr}) - C_{i}^{St} & \text{if } \sigma_{k,4}^{(i)} = 1 \\ x_{k,i}^{c} - C_{i}^{St} - D_{k,i} + \sum_{j=1}^{2} y_{k,j}(\mu_{i,j}C_{j}^{Pr}) & \text{otherwise} \end{cases} $

 $\sigma_{1:q-1}$. Every h_q defined in Table 3.3 depends only on these quantities with the exception of $h_5^{(i)}$, which also depends on y_k and hence on the input vector u_k . However, with more cumbersome notation, the dependence of $h_5^{(i)}$ on y_k could be replaced with dependence on $\sigma_{k,1:3}^{(i)}$, which uniquely determines y_k via Fig.3.4. Therefore, this requirement is satisfied. Second, it is easy to see from Table 3.3 that all of the $h_{1:3}^{(j)}$ and $h_{4:5}^{(i)}$ are continuously differentiable w.r.t. x_k^c , $w_k = (\xi_k, \lambda_k, \eta_k)$, $\theta = (C_1^{St}, C_2^{St})$, and γ , for any fixed k, $x_k^d \equiv (\underline{x}_k^d, \overline{x}_k^d)$, and $\sigma_k \equiv (\sigma_{k,1:5}^{(1)}, \sigma_{k,1:5}^{(2)})$, as required by Definition 3.4.1.

To show that the decision rule defined by Fig.'s 3.4–3.5 is smooth-in-expectation, we apply Conditions 3.5.1–3.5.3 to the event functions in Table 3.3. Specifically, we show that Conditions 3.5.1–3.5.3 hold provided that the following assumptions hold for every $(\theta, \gamma) \in \tilde{\Theta} \times \tilde{\Gamma}$:

$$C_i^{St} > \sum_{j=1}^2 \mu_{i,j} C_j^{Pr}, \quad \forall i \in \{1, 2\},$$
(3.117)

$$\gamma_{j,2} \neq 0 \text{ or } \gamma_{j,3} \neq 0, \quad \forall j \in \{1,2\}.$$
 (3.118)

Assumption (3.117) means that the maximum amount of product *i* that can be produced in a single day is smaller than the maximum storage capacity. Assumption (3.118) means that the two coefficients $\gamma_{j,2}$ and $\gamma_{j,3}$ cannot be both zero. Recalling that $w_k = (\xi_k, \lambda_k, \eta_k)$ and that $D_{k,i}$ has a non-trivial dependence on both $\xi_{k,i}$ and $\lambda_{k,i}$ via (3.98), assumption (3.118) ensures that the event function determining $y_{k,j}$ in Fig. 3.4 (i.e., $h_3^{(j)}$ in Table 3.3) is a nontrivial function of w_k and x_k . Showing that Conditions 3.5.1–3.5.3 hold under (3.117)– (3.118) verifies that \mathcal{L} is smooth at each θ for which (3.117)–(3.118) hold. Unfortunately, (3.117)–(3.118) rule out smoothness of \mathcal{L} on the whole $(n_{\theta} + n_{\gamma})$ -dimensional space of decisions (θ, γ) . Specifically, (3.117) and (3.118) describe $(n_{\theta} + n_{\gamma} - 1)$ and $(n_{\theta} + n_{\gamma} - 2)$ dimensional surfaces of potential discontinuities, respectively, in the $(n_{\theta} + n_{\gamma})$ -dimensional space, which is, however, unlikely to cause major problems for a gradient-based solver. Moreover, the number of discontinuities described by (3.117)–(3.118) is significantly much smaller relative to the number of discontinuities in the case where Conditions 3.5.1–3.5.3 do not hold at all.

For simplicity of notation in the arguments that follow, we use θ to refer to (θ, γ) . Moreover, for any choice of q corresponding to (n, r) with $n \in \{1, \dots, 5\}$ and $r \in \{1, 2\}$ and any choice of k, σ_k , and x_k^d , we refer to h_q as follows, where $h_n^{(r)}$ are as given in Table 3.3:

$$h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot) = h_n^{(r)}(k, \sigma_{k,n-1}^{(r)}, (\cdot, (\overline{x}_k^d, \underline{x}_k^d)), \cdot, \cdot).$$
(3.119)

To verify Condition 3.5.1, choose any q corresponding to (n, r) with $n \in \{1, \dots, 5\}$ and $r \in \{1, 2\}$, and choose any k, σ_k , and x_k^d . We must show that at least one of Conditions 3.5.1.1–3.5.1.2 holds for $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot)$. First, suppose $n \in \{1, 2\}$. From Table 3.3 and using (3.119), it is easy to see that $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot)$ satisfies Condition 3.5.1.2 because, with the integer state x_k^d fixed, $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot)$ is constant. Next, suppose $n \in \{3, 4, 5\}$. Consider the case with n = 5 and $\sigma_{k,4}^{(r)} = 1$. Recalling that y_k can be determined from knowledge of $\sigma_{k,1:3}^{(r)}$, then y_k in $h_5^{(r)}$ is fixed since σ_k is fixed. Condition 3.5.1.1 holds trivially in this case because, as per (3.117), it is impossible to have $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot) = 0$ at any point (x_k^c, w_k, θ) . Finally, with assumption (3.118) ensuring that $h_3^{(r)}$ is a non-trivial function of w_k , all other cases are the cases in which $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot)$ is a non-trivial function of w_k (e.g., h_q depends either on $\xi_{k,i}$ and $\lambda_{k,i}$ through $D_{k,i}$ or directly on $\eta_{k,i}$). This justifies that Condition 3.5.1.2 holds for these cases.

To verify Condition 3.5.2, choose any q corresponding to (n, r) with $n \in \{1, \dots, 5\}$ and $r \in \{1, 2\}$, any v corresponding to (m, s) with $m \in \{1, \dots, 5\}$ and $s \in \{1, 2\}$ such that $v \neq q$, and choose any k, σ_k , and x_k^d . We must show that at least one of Conditions 3.5.2.1– 3.5.2.3 holds for $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot)$ and $h_v(k, \sigma_{k,1:v-1}, (\cdot, x_k^d), \cdot, \cdot)$. First, suppose that either $n \in \{1, 2\}$ or $m \in \{1, 2\}$. From Table 3.3 and using (3.119), it is easy to see that Condition 3.5.2.2 holds because, with the integer state x_k^d fixed, $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot)$ or $h_v(k, \sigma_{k,1:v-1}, (\cdot, x_k^d), \cdot, \cdot)$ is constant. Next, suppose that $n, m \in \{3, 4, 5\}$. Consider the following cases: Case 1: n = 5 and $\sigma_{k,4}^{(r)} = 1$ or m = 5 and $\sigma_{k,4}^{(s)} = 1$. In this case, Condition 3.5.2.1 holds trivially because, as per (3.117), it is impossible to have $h_q(k,\sigma_{k,1:q-1},(\cdot,x_k^d),\cdot,\cdot) = h_v(k,\sigma_{k,1:v-1},(\cdot,x_k^d),\cdot,\cdot) = 0 \text{ at any point } (x_k^c,w_k,\theta). \quad Case \ 2:$ r = s with either n = 5 and m = 4 or n = 4 and m = 5. Since r = s, we have $\sigma_{k,4}^{(r)} = \sigma_{k,4}^{(s)}$ Condition 3.5.2.1 holds trivially in this case too because, as per (3.117), it is impossible to have $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot) = h_v(k, \sigma_{k,1:v-1}, (\cdot, x_k^d), \cdot, \cdot) = 0$ at any point (x_k^c, w_k, θ) . With assumption (3.118) ensuring that $h_3^{(r)}$ is a nontrivial function of w_k , all other cases are cases in which $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot)$ is a non-trivial function of at least one element of w_k that is different from all other elements of w_k of which $h_v(k, \sigma_{k,1:v-1}, (\cdot, x_k^d), \cdot, \cdot)$ is a non-trivial function. This means that Condition 3.5.1.1 holds because the following holds at all points (x_k^c, w_k, θ) , where the arguments $(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot)$ and $(k, \sigma_{k,1:v-1}, (\cdot, x_k^d), \cdot, \cdot)$ are omitted for brevity of notation:

$$\operatorname{rank} \begin{bmatrix} \frac{\partial h_q}{\partial w} \\ \frac{\partial h_v}{\partial w} \end{bmatrix} = \operatorname{rank} \begin{bmatrix} \frac{\partial h_q}{\partial \xi} & \frac{\partial h_q}{\partial \lambda} & \frac{\partial h_q}{\partial \eta} \\ \frac{\partial h_v}{\partial \xi} & \frac{\partial h_v}{\partial \lambda} & \frac{\partial h_v}{\partial \eta} \end{bmatrix} = 2.$$
(3.120)

To elaborate, first consider n = m = 3 and $r \neq s$. In this case $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot)$ depends on $\eta_{k,r}$, but $h_v(k, \sigma_{k,1:v-1}, (\cdot, x_k^d), \cdot, \cdot)$ depends $\eta_{k,s}$ and it does not depend on $\eta_{k,r}$. Second, consider n = m = 4 and $r \neq s$. In this case, through $D_{k,r}$ and $D_{k,s}$, $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot)$ depends on both $\xi_{k,r}$ and $\lambda_{k,r}$, but $h_v(k, \sigma_{k,1:v-1}, (\cdot, x_k^d), \cdot, \cdot)$ depends on $\xi_{k,s}$ and $\lambda_{k,s}$ and it does not depend on $\xi_{k,r}$ and $\lambda_{k,r}$. Third, consider $(n,m) \in \{(3,4), (4,3), (3,5), (5,3)\}$. In this case, we can have two situations. In the first situation, we have that $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot)$ depends on both $\xi_{k,r}$ and $\lambda_{k,r}$ through $D_{k,r}$, but $h_v(k, \sigma_{k,1:v-1}, (\cdot, x_k^d), \cdot, \cdot)$ depends on $\eta_{k,s}$ and not on $\xi_{k,r}$ and $\lambda_{k,r}$. The reverse situation where r and s are switched is similar. Lastly, consider $(n,m) \in \{(4,5), (5,4)\}$ with $r \neq s$. In this case, $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot)$ depends on both $\xi_{k,r}$ and $\lambda_{k,r}$ through $D_{k,r}$, but $h_v(k, \sigma_{k,1:v-1}, (\cdot, x_k^d), \cdot, \cdot)$ depends on $\xi_{k,s}$ and $\lambda_{k,s}$ through $D_{k,s}$ and it does not depend on $\xi_{k,r}$ and $\lambda_{k,r}$.

Finally, to verify Condition 3.5.3, choose any q corresponding to (n,r) with $n \in \{1, \dots, 5\}$ and $r \in \{1, 2\}$, and choose any $p \in \{1, \dots, n_w\}$, k, σ_k , and x_k^d . We must show that at least one of Conditions 3.5.2.1–3.5.3.4 holds for $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot)$. First, consider the case with $n \in \{1, 2\}$. From Table 3.3 and using (3.119), it is easy to see that $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot)$ is constant because the integer state x_k^d is fixed. Thus, $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot)$ satisfies Condition 3.5.3.2. Next, consider the case with $n \in \{3, 4, 5\}$. If n = 5 and $\sigma_{k,4}^{(r)} = 1$, then Condition 3.5.3.1 holds trivially because, as per (3.117), it is impossible to have $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot) = 0$ at any point (x_k^c, w_k, θ) . With assumption (3.118) ensuring that $h_3^{(r)}$ is a non-trivial function of w_k , all other cases are cases in which $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot)$ is a nontrivial function of at least two elements of w_k . Specifically, with (3.118), $h_q(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot)$ depends non-trivially on $\xi_{k,r}$ and $\lambda_{k,r}$ through $D_{k,r}$. This means that Condition 3.5.1.1 holds because the following holds at all points (x_k^c, w_k, θ) , where the arguments $(k, \sigma_{k,1:q-1}, (\cdot, x_k^d), \cdot, \cdot)$ are omitted for brevity of notation:

$$\operatorname{rank} \begin{bmatrix} \frac{\partial h_q}{\partial w} \\ e_p^T \end{bmatrix} = \operatorname{rank} \begin{bmatrix} \frac{\partial h_q}{\partial \xi} & \frac{\partial h_q}{\partial \lambda} & \frac{\partial h_q}{\partial \eta} \\ & e_p^T \end{bmatrix} = 2.$$
(3.121)

Although Conditions 3.5.1-3.5.3 are shown to hold with assumptions (3.117)-(3.118), Fig. 3.6 shows that \mathcal{L} is smooth at every point where (3.117)-(3.118) hold. This happens because, in this case, the rule in Fig.'s 3.4-3.5 obeys Conditions 3.5.1-3.5.3 as



Figure 3.6: Cost ℓ with $\boldsymbol{\omega}$ fixed (*left column*) and cost \mathcal{L} estimated with average of ℓ over 10^5 random $\boldsymbol{\omega}$'s (*right column*) vs $\gamma_{1,1}(top \ row)$ and $C_2^{St}(bottom \ row)$

shown above. Nonetheless, as we show in the next section, smoothness of \mathcal{L} enable us to solve problem (3.115) with gradient-based approaches that are much more efficient than gradient-free approaches.

3.7.4 Optimization Results

In this section, we demonstrate that exploiting differentiability of \mathcal{L} is advantageous for solving (3.115). We consider $(\theta, \gamma) = (C_1^{St}, C_2^{St}, \gamma_{1,1}, \gamma_{1,2}, \gamma_{1,3}, \gamma_{2,1}, \gamma_{2,2}, \gamma_{2,3})$ with feasible set $\Theta \times \Gamma = [\theta^L, \theta^U] \times [\gamma^L, \gamma^U]$, where $\theta^L = (5.33, 4), \ \theta^U = (20, 20), \ \gamma^L = (-10, 10, -25, -25, -10, -5)$ and $\gamma^U = (9, 30, -5, -7, 10, 16)$. To determine these bounds, a one sample approximation of problem (3.115), which is discontinuous, was solved on an unrestricted space of decisions (θ, γ) (i.e., the bounds were made very large) using a particle swarm optimization algorithm (PSO). Then, an appropriate vector of positive constants was used to perturb the PSO solution to obtained the specified bounds. Specifically, (θ^L, γ^L) was obtained by a perturbation on the left and (θ^U, γ^U) was obtained by a perturbation on the right. Clearly, the way these bounds were constructed is non-restrictive. Importantly, note that these bounds enforce (3.117) and (3.118) for j = 1, making the original problem (3.115) smooth on the whole space of decisions (θ, γ) defined by these bounds

except at points where (3.118) with j = 2 does not hold, which is very unlikely to happen during the optimization process.

Even though problem (3.115) has only 8 decision variables, and thus might seem simple, the MSP model (3.99)–(3.112) requires mixed-integer operational decisions $u_k = (y_k, s_k, P_k^u, P_k^d)$ and $x_k = (x_k^c, x_k^d, x_k^d)$ at each stage $k \in \{0, \dots, 364\}$ and for each scenario $\boldsymbol{\omega}$. In fact, a single scenario $\boldsymbol{\omega}$ gives an a MILP that takes Gurobi 7.5.1 more than 16h³ to solve, although constraints (3.109)–(3.110) were excluded. In contrast, we solve (3.115) using an implementation of a stochastic trust-region algorithm adapted from [127]. Our primary motivation for considering the stochastic trust-region approach is that it relies on the assumption that the problem is at least continuously differentiable, a property that is established for \mathcal{L} in §3.7.3 above. However, note that we implemented the algorithm in [127] with some modifications to suit our problem. Specifically, a rectangular trust-region intersected with feasible region $\Theta \times \Gamma$ was used, and this was done both to enforce bounds on (θ, γ) and to simplify generation of candidate designs (θ, γ) for local model construction. For the linear model, a 2_{III}^{10-4} fractional factorial design was used, and for the quadratic model, a central composite design was used. Let N_s denote the number of samples $\boldsymbol{\omega}^s$ of $\boldsymbol{\omega}$ used in the approximation of $\mathcal{L}(\theta, \gamma)$ as follows:

$$\mathcal{L}(\theta,\gamma) \approx \sum_{s=1}^{N_s} \ell(\boldsymbol{\omega}^s,(\theta,\gamma)).$$
(3.122)

Another important modification that had to be made is on how N_s is computed because the suggestions in [127] could not efficiently handle the deleterious effects of the noise in the approximation (3.122) on the algorithm. Through trial-and-error, we found that using $N_s = 6$ for model construction and $N_s = 100$ for performing the ratio-comparison and sufficient-reduction tests was adequate when the algorithm is in the inner-loop. On the other hand, when the algorithm is in the outer-loop, N_s was computed as suggested in [127], but imposing $N_s < 30$ for model construction and $N_s < 300$ for the ratio-comparison

³Dell Precision T3600, 3.0 GHz Intel Xeon, 8GB RAM, Windows 7, MATLAB R2015a

n_0	n_d	Δ_0	$\tilde{\Delta}$	η_0	η_1	γ_1	γ_2	α_k
N_s	N_s	3.15	1	0.05	1.5	0.5	2	$0.5 imes 0.98^k$

Table 3.4: Considered modifications for parameters in Table 2 in [127]

and sufficient-reduction tests. Furthermore, the values of the remaining parameters for the algorithm, as described in [127] and given in Table 2 there, were tuned for our example and are given in Table 3.4. Finally, the algorithm was terminated when the trust region radius has shrunk to 0.05, which is small enough to justify that the algorithm was not making significant progress.

Recall that we consider the minimization of the expected-value $\mathcal{L}(\theta, \gamma)$. The stochastic trust region algorithm implementation we consider, as referred to as STRONG in [127]. is compared with the particle swarm optimization (PSO) code particleswarm and the genetic algorithm (GA) code ga in MATLAB R2015a with default settings for both. The PSO and GA algorithms we consider are, in our experience, unstable when the objective function they are dealing with is stochastic. Therefore, N_s and the samples ω^s used in the approximation (3.122) were fixed before each of their runs so that the objective function is deterministic. Fig. 3.8 shows the optimization results obtained by PSO and GA for different values of N_s . For each N_s , 100 runs were considered, where a different batch of ω^s was used for each run. The histograms show the percentage of solutions $(\theta_{\min}, \gamma_{\min})$ found versus their corresponding expected cost $\mathcal{L}(\theta_{\min}, \gamma_{\min})$ which is approximated with (3.122) using $N_s = 3 \times 10^3$. From the histograms, it is easy to see that both PSO and GA find scattered solutions with $N_s = 1$ as indicated by the different bars in the histograms. As N_s is increased, the number of bars becomes smaller and smaller towards one obviously dominating bar. In the PSO case, the dominating bar contains the value $\mathcal{L}(\theta_{\min}, \gamma_{\min}) = -1535$, where $(\theta_{\min}, \gamma_{\min}) = (9.3, 7.5, -9.04, 11.29, -5.68, -24.96, -0.28, 7.42)$ is the best value of (θ, γ) found. However, for both PSO and GA the dominating bar contains different solutions but with similar costs $\mathcal{L}(\theta_{\min}, \gamma_{\min}) \in [-1535 - 1510]$. Notably, with $N_s = 30$, PSO reliably finds these solutions 97% of the time and GA 70% of the time. This behavior indicates that for PSO to be qualified as solving the expected-value minimization problem, at least



Figure 3.7: Percentage of solutions found by STRONG versus the corresponding expected costs (in dollars)

 $N_s = 30$ is required. This is because, with this N_s , varying the batches of ω^s does not have any effect on the range of the cost corresponding to PSO solutions. Consequently, the performance of PSO with $N_s = 30$ is considered as a benchmark for comparison with STRONG.

On the other hand, STRONG was initiated at 100 initial guesses and $\mathcal{L}(\theta_{\min}, \gamma_{\min})$ is also approximated with 3×10^3 samples. As shown in Fig. 3.7, approximately 65% of the time STRONG terminated at solutions with cost values in the same range as those in the dominating bar in the PSO and GA histograms with $N_s = 30$. However, STRONG also found other solutions which were graphically confirmed to be local minima. This is expected because STRONG is a local solver. More importantly, STRONG achieves a $20 \times$ computational speed-up over PSO and $33 \times$ over GA. This is measured in terms of the number of function evaluations since the latter dominates the total computational time spent by the solvers until termination. Specifically, PSO uses an average of 4×10^5 function evaluations, GA uses an average of 6.7×10^5 , and STRONG uses only an average of 2×10^4 which translates to an average CPU time of 7 mins⁴. For this rather small example we considered, this showcases that even though STRONG is not optimally tuned and needs significant improvements, it outperforms the much more mature PSO (≈ 2.3 h) and $GA(\approx 3.5h)$ algorithms. This demonstrates the great advantages of exploiting differentiability of decision-rule approximation problems, allowing optimization with gradient-based methods which are expected to perform even much better in higher dimensional problems in which derivative-free approaches are highly inefficient.

⁴Dell Precision T3600, 3.0 GHz Intel Xeon, 8GB RAM, Windows 7, MATLAB R2015a



Figure 3.8: Percentage of solutions found by PSO and GA versus the corresponding expected costs (in dollars)

3.8 Conclusions

In this chapter, a novel approach was presented for efficiently solving very large multistage stochastic programs (MSPs) with mixed-integer recourse decisions. Such MSPs arise as very effective models for formulating the problem of integrated design and operation of manufacturing and energy systems that must adapt to highly dynamic and uncertain operating conditions. However, such MSPs are notoriously difficult to solve by any other means currently available in the literature. For our first contribution, a new general class of mixed-integer decision rules was proposed for deriving accurate decision-rule approximation (DRA) of such MSPs. However, the standard sample average approximation (SAA) of the DRA problem is highly discontinuous. In this case, reformulating the DRA as a standard mathematical program is intractable for the type of MPS we consider because it requires reintroducing very many binary variables (i.e., for each scenario and stage). In contrast, this chapter proposes formulating the DRA as a simulation-optimization (DRA-SO) problem. Note that the SAA of this DRA-SO is still highly discontinuous. However, our second contribution provides a novel set of sufficient conditions (imposed on the proposed class of decisions rules) that guarantees that the true expected value over all possible scenarios is smooth. Moreover, our third contribution provides an extension that allows the application of these conditions to analyze smoothness of chance constraints in the DRA-SO problem. The significance of these conditions is that when they hold, the DRA-SO problem is smooth, enabling its solution using gradient-based optimization algorithms which are far more efficient than the commonly used gradient-free approaches. Furthermore, our fourth contribution provides a randomization strategy that ensures that the sufficient conditions can be made to hold for all decision rules of the proposed class. Therefore, these conditions can be applied more broadly towards the efficient solution of general MSP problems. The application of these contributions was demonstrated on a MSP model of an integrated design and operation example problem for an inventory system. For this example problem, significant improvements in the optimization results were obtained with a stochastic trustregion algorithm (which relies on smoothness of the problem) relative to two state-of-the-art gradient-free approaches. Overall, this example problem illustrates that the contributions of this chapter address the limitations of solving the MSPs using the standard scenario-based approach. Moreover, it illustrates that the contributions address the well-known limitations of gradient-free approaches which are commonly used to solve the highly discontinuous SAA of the DRA-SO problem. However, although the results presented in this chapter show huge potential, the proposed class of mixed-integer decision rules does not cover highly advanced decision rules, such as model predictive control. Such decision rules are expected to provide more accurate DRAs for MSPs since they are based on the solution of an auxiliary optimization problem to approximate mixed-integer recourse decisions. Our future work will explore the application of the results developed in this chapter in cases where an advanced decision rule is used to approximate MSPs. Since such cases are closely related to multilevel stochastic programs that also arise in smart manufacturing and energy systems, the aim of our future work will be to help develop a tractable solution approach for multilevel stochastic programs with mixed-integer recourse decisions.

3.9 Appendix

3.9.1 Proof of Theorem 3.4.1

The proof of Theorem 3.4.1 consists of applying Theorem 2.4.1 in Chapter 2. However, the latter applies to expected value functions subject to discrete time stochastic hybrid systems (DTSHS), which differ from the recursion (3.3)–(3.6) used here in some technical details. The first difference between the DTSHS considered in Chapter 2 and the recursion (3.3)-(3.6) is that the functions f and ℓ_S in (3.3)-(3.6) depend on an input u_k , which is determined by a decision rule κ satisfying Definition 3.4.1. In contrast, the functions f and ℓ_S in Chapter 2 do not depend on an input, but instead depend directly on a binary sequence σ that is analogous to the σ used in Definition 3.4.1 here. The second technical difference is that the formulation in Chapter 2 assumes that the set $\tilde{X} \times \tilde{W} \times \tilde{\Theta}$, on which the functions h_i , f and ℓ_S are defined, is open. But, this does not hold here specifically because $\tilde{X}^d \subset \mathbb{Z}^{n_x^d}$, and hence $\tilde{X} = \tilde{X}^c \times \tilde{X}^d$, is not open. Consequently, in order to apply Theorem 2.4.1 in Chapter 2, we must translate (3.3)-(3.6) into a DTSHS of the form analyzed in Chapter 2. To do this, we first establish Definition 3.9.1 in which we begin by extending \tilde{X} to a new open set $\check{\tilde{X}} \supset \tilde{X}$. Then, we define new functions \check{h}_i , \check{f} and $\check{\ell}_S$ on the open set $\check{\tilde{X}} \times \tilde{W} \times \tilde{\Theta}$. These definitions embed the decision rule κ , and therefore no longer depend on an input u_k . This allows us to construct a DTSHS of the form analyzed in Chapter 2 with a corresponding expected value function $\check{\mathcal{L}}$. The defined DTSHS enables a direct application of Theorem 2.4.1 in Chapter 2 to conclude that $\check{\mathcal{L}}$ is continuously differentiable provided that the new event functions h_i satisfy Conditions 3.4.1–3.4.3. Next, we establish Lemma 3.9.1 in which we show that $\check{\mathcal{L}}(\theta) = \mathcal{L}(\theta)$ for any θ . This allows us to directly establish continuous differentiability of \mathcal{L} through $\dot{\mathcal{L}}$.

Definition 3.9.1. For any $x^d \in \tilde{X}^d$, let $B_{\delta}(x^d)$ be the n_x^d -dimensional open ball of radius $\delta > 0$ around x^d . Choose any $\delta > 0$ such that

$$B_{\delta}(\overline{x}) \bigcap B_{\delta}(\underline{x}) = \emptyset, \quad \forall \overline{x}, \underline{x} \in \tilde{X}^d, \tag{3.123}$$

and define

$$\tilde{\tilde{X}} \equiv \tilde{X}^c \times \bigcup_{\overline{x} \in \tilde{X}^d} B_{\delta}(\overline{x}).$$
(3.124)

Moreover, define $\check{h}_i : \mathcal{K} \times \mathcal{S} \times \check{\tilde{X}} \times \tilde{W} \times \tilde{\Theta} \to \mathbb{R}$, $\check{f} : \mathcal{K} \times \mathcal{S} \times \check{\tilde{X}} \times \tilde{W} \times \tilde{\Theta} \to \check{\tilde{X}}$, and $\check{\ell}_S : \mathcal{K} \times \mathcal{S} \times \check{\tilde{X}} \times \tilde{W} \times \tilde{\Theta} \to \mathbb{R}$, for all $(k, \sigma, (x^c, x^*), w, \theta) \in \mathcal{K} \times \mathcal{S} \times \check{\tilde{X}} \times \tilde{W} \times \tilde{\Theta}$ as follows, where x^d is the unique element of \tilde{X}^d such that $x^* \in B_{\delta}(x^d)$:

$$\check{h}_i(k,\sigma,(x^c,x^*),w,\theta) \equiv h_i(k,\sigma,(x^c,x^d),w,\theta), \qquad (3.125)$$

$$\check{f}(k,\sigma,(x^c,x^*),w,\theta) \equiv f(k,\kappa_{\sigma}(k,(x^c,x^d),w,\theta),(x^c,x^d),w,\theta),$$
(3.126)

$$\check{\ell}_S(k,\sigma,(x^c,x^*),w,\theta) \equiv \ell_S(k,\kappa_\sigma(k,(x^c,x^d),w,\theta),(x^c,x^d),w,\theta).$$
(3.127)

Furthermore, define the following recursion, where $\check{x}_0 = x_0 = b_0$:

$$\check{\sigma}_{k,i} = \left\{ \begin{array}{cc} 1 & \text{if } \check{h}_i(k, \check{\sigma}_{k,1:i-1}, \check{x}_k, w_k, \theta) \le 0\\ -1 & \text{otherwise} \end{array} \right\}, \quad \forall i \in \{1, \dots, n_\sigma\}, \tag{3.128}$$

$$\check{x}_{k+1} = \check{f}(k, \check{\sigma}_k, \check{x}_k, w_k, \theta).$$
(3.129)

For any given $(\boldsymbol{\omega}, \theta) \in \tilde{\Omega} \times \tilde{\Theta}$, define the solutions of (3.128)–(3.129) at stage k by $\check{\sigma}_k(\boldsymbol{\omega}, \theta) \equiv \check{\sigma}_k$ and $\check{x}_k(\boldsymbol{\omega}, \theta) \equiv \check{x}_k$. Finally, define the total cost of a trajectory of (3.128)–(3.129) by

$$\check{\ell}(\boldsymbol{\omega},\boldsymbol{\theta}) \equiv \sum_{k=0}^{K} \check{\ell}_{S}(k, \check{\sigma}_{k}(\boldsymbol{\omega},\boldsymbol{\theta}), \check{x}_{k}(\boldsymbol{\omega},\boldsymbol{\theta}), w_{k}, \boldsymbol{\theta}), \qquad (3.130)$$

and the expected cost associated with (3.128)-(3.130) by

$$\check{\mathcal{L}}(\theta) \equiv \mathbb{E}[\check{\ell}(\boldsymbol{\omega},\theta)]. \tag{3.131}$$

The dynamic system (3.128)-(3.130) has exactly the same structure as the DTSHS

analyzed in Chapter 2. Moreover, (3.128)–(3.130) is equivalent to (3.3)–(3.6) in the sense of the following result.

Lemma 3.9.1. For any $\theta \in \tilde{\Theta}$, $\check{\mathcal{L}}(\theta) = \mathcal{L}(\theta)$.

Proof Choose any $(\boldsymbol{\omega}, \theta) \in \tilde{\Omega} \times \tilde{\Theta}$. Using κ as defined in (3.12)–(3.13), let $\sigma_{0:K}$, $u_{0:K}$, and $x_{0:K}$ be the trajectories of the recursion (3.3)–(3.5), and let $\check{\sigma}_{0:K}$ and $\check{x}_{0:K}$ be the trajectories of the recursion (3.128)–(3.129). It is sufficient to show that $\sigma_k = \check{\sigma}_k$ and $x_{k+1} = \check{x}_{k+1}, \forall k \in \mathcal{K}$. If this holds, then, $\forall k \in \mathcal{K}$,

$$\check{\ell}_S(k,\check{\sigma}_k,\check{x}_k,w_k,\theta) = \check{\ell}_S(k,\sigma_k,x_k,w_k,\theta)$$
(3.132)

$$= \ell_S(k, \kappa_{\sigma_k}(k, x_k, w_k, \theta), x_k, w_k, \theta)$$
(3.133)

$$=\ell_S(k, u_k, x_k, w_k, \theta). \tag{3.134}$$

But, (3.134) implies directly that $\check{\ell}(\omega, \theta) = \ell(\omega, \theta)$ by (3.130) and (3.6), which then implies that $\check{\mathcal{L}}(\theta) = \mathbb{E}[\ell(\omega, \theta)] = \mathbb{E}[\ell(\omega, \theta)] = \mathcal{L}(\theta)$ since the choice of (ω, θ) was arbitrary.

To show that $\sigma_k = \check{\sigma}_k$ and $x_{k+1} = \check{x}_{k+1}, \forall k \in \mathcal{K}$, we first show that the following implication holds for any $k \in \mathcal{K}$:

$$x_{k} = \check{x}_{k} \implies \left\{ \begin{array}{c} \sigma_{k} = \check{\sigma}_{k} \\ x_{k+1} = \check{x}_{k+1} \end{array} \right\}.$$
(3.135)

Assume $x_k = \check{x}_k$. It is trivial to see that the following implication holds for any $i \in \{1, \ldots, n_\sigma\}$:

$$\check{h}_i(k, \check{\sigma}_{k,1:i-1}, \check{x}_k, w_k, \theta) = h_i(k, \sigma_{k,1:i-1}, x_k, w_k, \theta) \implies \check{\sigma}_{k,i} = \sigma_{k,i}.$$
(3.136)

We show by induction that

$$\check{h}_{i}(k, \check{\sigma}_{k,1:i-1}, \check{x}_{k}, w_{k}, \theta) = h_{i}(k, \sigma_{k,1:i-1}, x_{k}, w_{k}, \theta), \quad \forall i.$$
(3.137)
By the assumption that $x_k = \check{x}_k$, we have the following, by (3.125):

$$\check{h}_{i}(k, \check{\sigma}_{k,1:i-1}, \check{x}_{k}, w_{k}, \theta) = h_{i}(k, \check{\sigma}_{k,1:i-1}, x_{k}, w_{k}, \theta), \quad \forall i.$$
(3.138)

Thus, showing (3.137) is equivalent to showing that

$$h_i(k, \check{\sigma}_{k,1:i-1}, x_k, w_k, \theta) = h_i(k, \sigma_{k,1:i-1}, x_k, w_k, \theta), \quad \forall i.$$
(3.139)

Because h_1 does not depend on σ_k or $\check{\sigma}_k$, (3.139) holds trivially for i = 1. For induction, choose an arbitrary $i \ge 1$ and assume that (3.139) holds for all $j \le i$. By (3.136), this implies directly that $\sigma_{k,1:i} = \check{\sigma}_{k,1:i}$. But, the latter together with $x_k = \check{x}_k$, leads to $h_{i+1}(k, \check{\sigma}_{k,1:i}, \check{x}_k, w_k, \theta) = h_{i+1}(k, \sigma_{k,1:i}, x_k, w_k, \theta)$, showing that (3.139) holds for all i by induction. Correspondingly, (3.137) holds as desired.

To show (3.135), we proceed by combining (3.137) with (3.136) and noting that this gives $\sigma_{k,i} = \check{\sigma}_{k,i}$ for all $i \in \{1, \ldots, n_{\sigma}\}$, meaning that $\sigma_k = \check{\sigma}_k$. With this and by the assumption that $x_k = \check{x}_k$, we have

$$\check{f}(k,\check{\sigma}_k,\check{x}_k,w_k,\theta) = \check{f}(k,\sigma_k,x_k,w_k,\theta)$$
(3.140)

$$= f(k, \kappa_{\sigma_k}(k, x_k, w_k, \theta), x_k, w_k, \theta)$$
(3.141)

$$= f(k, u_k, x_k, w_k, \theta).$$
 (3.142)

But, (3.142) implies directly that $\check{x}_{k+1} = x_{k+1}$, by (3.129) and (3.5). Therefore, (3.135) holds.

To finish the proof, we now proceed with induction over k. Noting that $\check{x}_0 = x_0 = b_0 \in \tilde{X}$, a recursive application of (3.135) shows that $\sigma_k = \check{\sigma}_k$ and $x_{k+1} = \check{x}_{k+1}$ for all $k \in \mathcal{K}$.

Lemma 3.9.2. For each fixed $k \in \mathcal{K}$ and $\sigma \in S$, the functions $\check{f}(k, \sigma, \cdot, \cdot, \cdot)$, $\check{\ell}_S(k, \sigma, \cdot, \cdot, \cdot)$, and $\check{h}_i(k, \sigma, \cdot, \cdot, \cdot)$ for all $i \in \{1, \ldots, n_\sigma\}$, are continuously differentiable on the extended set $\check{X} \times \tilde{W} \times \tilde{\Theta}$. Proof Choose any $k \in \mathcal{K}, \sigma \in \mathcal{S}, i \in \{1, \ldots, n_{\sigma}\}$, and $((x^c, x^*), w, \theta) \in \check{X} \times \tilde{W} \times \tilde{\Theta}$. By (3.124), $x^* \in B_{\delta}(x^d)$ for some $x^d \in \check{X}^d$. The function $\check{h}_i(k, \sigma, (\cdot, x^*), \cdot, \cdot)$ is continuously differentiable at (x^c, w, θ) by (3.125) and Definition 3.4.1. Moreover, the functions $\check{f}(k, \sigma, (\cdot, x^*), \cdot, \cdot)$ and $\check{\ell}_S(k, \sigma, (\cdot, x^*), \cdot, \cdot)$ are continuously differentiable at (x^c, w, θ) by (3.126)–(3.127), Assumption 3.3.2, and by the fact that the composition of two continuously differentiable functions is also continuously differentiable. On the other hand, (3.125)–(3.126) imply that the functions $\check{f}(k, \sigma, (x^c, \cdot), w, \theta)$, $\check{\ell}_S(k, \sigma, (x^c, \cdot), w, \theta)$, and $\check{h}_i(k, \sigma, (x^c, \cdot), w, \theta)$ are constant on $B_{\delta}(x^d)$, and hence in the neighborhood of x^* , and are therefore trivially continuously differentiable at x^* . Thus, by Theorem 6.2 in [120], $\check{f}(k, \sigma, \cdot, \cdot, \cdot)$, $\check{\ell}_S(k, \sigma, \cdot, \cdot, \cdot)$, and $\check{h}_i(k, \sigma, \cdot, \cdot, \cdot)$ are continuously differentiable at $((x^c, x^*), w, \theta)$, and are therefore continuously differentiable on $\check{X} \times \check{W} \times \check{\Theta}$ since $((x^c, x^*), w, \theta)$ was arbitrary chosen from $\check{X} \times \check{W} \times \check{\Theta}$.

Recall that the interest here is to prove continuous differentiability of \mathcal{L} under Conditions 3.4.1–3.4.3. To easily prove this result, we next establish Lemma 3.9.3 which allows us to apply Theorem 2.4.1 in Chapter 2 to show continuous differentiability of $\check{\mathcal{L}}$ under Conditions 3.4.1–3.4.3. To establish Lemma 3.9.3, consider the following definition.

Definition 3.9.2. For every $k \in \mathcal{K}$, $\sigma \in \mathcal{S}$, and $\theta \in \tilde{\Theta}$, define the sets

$$\check{\mathcal{M}}(k,\sigma,\theta) \equiv \{(z,w) \in \check{\tilde{X}} \times W : \sigma_i \check{h}_i(k,\sigma,z,w,\theta) \le 0, \ \forall i\}.$$
(3.143)

$$\partial_i \check{\mathcal{M}}(k,\sigma,\theta) \equiv \{(z,w) \in \check{\mathcal{M}}(k,\sigma,\theta) : \check{h}_i(k,\sigma,z,w,\theta) = 0\}.$$
(3.144)

$$\partial_{ij}\check{\mathcal{M}}(k,\sigma,\theta) \equiv \left\{ (z,w) \in \check{\mathcal{M}}(k,\sigma,\theta) : \begin{array}{l} \check{h}_i(k,\sigma,z,w,\theta) = 0\\ \\ \check{h}_j(k,\sigma,z,w,\theta) = 0 \end{array} \right\}.$$
(3.145)

Lemma 3.9.3. If the functions h_i satisfy Conditions 3.4.1–3.4.3, then Conditions 3.4.1– 3.4.3 are also satisfied by the functions \check{h}_i with the sets $\mathcal{M}(k,\sigma,\theta)$ replaced by the sets $\check{\mathcal{M}}(k,\sigma,\theta)$.

Proof Assume the functions h_i satisfy Conditions 3.4.1–3.4.3. To begin, first note

that, for any $k \in \mathcal{K}$, $\sigma \in \mathcal{S}$, $i \in \{1, \ldots, n_{\sigma}\}$, and $z^{d} \in \tilde{X}^{d}$, (3.125) implies that

$$\check{h}_i(k,\sigma,(\cdot,z^*),\cdot,\cdot) = h_i(k,\sigma,(\cdot,z^d),\cdot,\cdot), \quad \forall z^* \in B_\delta(z^d).$$
(3.146)

Since \tilde{W} is open, this implies that

$$\frac{\partial \dot{h}_i}{\partial w}(k,\sigma,(\cdot,z^*),\cdot,\cdot) = \frac{\partial h_i}{\partial w}(k,\sigma,(\cdot,z^d),\cdot,\cdot), \quad \forall z^* \in B_{\delta}(z^d).$$
(3.147)

Next, we show that the following implication holds for any $k \in \mathcal{K}$, $\sigma \in \mathcal{S}$, and $\theta \in \Theta$, where z^d is the unique element of \tilde{X}^d such that $z^* \in B_{\delta}(z^d)$:

$$((z^c, z^*), w) \in \check{\mathcal{M}}(k, \sigma, \theta) \implies ((z^c, z^d), w) \in \mathcal{M}(k, \sigma, \theta).$$
(3.148)

Choose any $((z^c, z^*), w) \in \check{\mathcal{M}}(k, \sigma, \theta)$ and let $z^d \in \tilde{X}^d$ be such that $z^* \in B_{\delta}(z^d)$. By Definition 3.9.2, this implies that $\sigma_i \check{h}_i(k, \sigma, (z^c, z^*), w, \theta) \leq 0$ for all *i*. By the definition of \check{h}_i in (3.125), this implies that $\sigma_i h_i(k, \sigma, (z^c, z^d), w, \theta) \leq 0$ for all *i*. By Definition 3.4.3, this implies that $((z^c, z^d), w) \in \mathcal{M}(k, \sigma, \theta)$ as desired.

To show that the functions \check{h}_i satisfy Condition 3.4.1, choose any $i \in \{1, \ldots, n_{\sigma}\}$, $k \in \mathcal{K}, \sigma \in \mathcal{S}$, and $\theta \in \Theta$. We must show that

$$\frac{\partial h_i}{\partial w}(k,\sigma,(z^c,z^*),w,\theta) \neq 0, \quad \forall ((z^c,z^*),w) \in \partial_i \check{\mathcal{M}}(k,\sigma,\theta).$$
(3.149)

Choose any $((z^c, z^*), w) \in \partial_i \check{\mathcal{M}}(k, \sigma, \theta)$. By (3.144), it follows that $\check{h}_i(k, \sigma, (z^c, z^*), w, \theta) = 0$. But, since $z^* \in B_{\delta}(z^d)$ for some $z^d \in \check{X}^d$, we must have $h_i(k, \sigma, (z^c, z^d), w, \theta) = 0$ by (3.146). Moreover, since $((z^c, z^*), w) \in \partial_i \check{\mathcal{M}}(k, \sigma, \theta)$ implies that $((z^c, z^*), w) \in \check{\mathcal{M}}(k, \sigma, \theta)$, (3.148) implies that $((z^c, z^d), w) \in \mathcal{M}(k, \sigma, \theta)$. Thus, $h_i(k, \sigma, (z^c, z^d), w, \theta) = 0$ implies that $((z^c, z^d), w) \in \partial_i \mathcal{M}(k, \sigma, \theta)$. Consequently, by the hypothesis that h_i satisfies Condition 3.4.1, we must have $\frac{\partial h_i}{\partial w}(k, \sigma, (z^c, z^d), w, \theta) \neq 0$. Hence, by (3.147), we must have $\frac{\partial \check{h}_i}{\partial w}(k, \sigma, (z^c, z^*), w) \in \partial_i \check{\mathcal{M}}(k, \sigma, \theta)$ was arbitrary, (3.149) holds.

To show that the functions \check{h}_i satisfy Condition 3.4.2, choose any $i, j \in \{1, \ldots, n_\sigma\}$ with $i \neq j, k \in \mathcal{K}, \sigma \in \mathcal{S}$, and $\theta \in \Theta$. We must show that

$$\operatorname{rank}\left[\begin{array}{c}\frac{\partial \check{h}_{i}}{\partial w}(k,\sigma,(z^{c},z^{*}),w,\theta)\\\frac{\partial \check{h}_{j}}{\partial w}(k,\sigma,(z^{c},z^{*}),w,\theta)\end{array}\right] = 2, \quad \forall ((z^{c},z^{*}),w) \in \partial_{ij}\check{\mathcal{M}}(k,\sigma,\theta).$$
(3.150)

Choose any $((z^c, z^*), w) \in \partial_{ij} \check{\mathcal{M}}(k, \sigma, \theta)$. By (3.145), we have $\check{h}_i(k, \sigma, (z^c, z^*), w, \theta) = \check{h}_j(k, \sigma, (z^c, z^*), w, \theta) = 0$. But, since $z^* \in B_{\delta}(z^d)$ for some $z^d \in \check{X}^d$, we must have $h_i(k, \sigma, (z^c, z^d), w, \theta) = h_j(k, \sigma, (z^c, z^d), w, \theta) = 0$ by (3.146). Moreover, since $((z^c, z^*), w) \in \check{\mathcal{M}}(k, \sigma, \theta)$, (3.148) implies that $((z^c, z^d), w) \in \mathcal{M}(k, \sigma, \theta)$. Thus, $((z^c, z^d), w) \in \partial_{ij} \mathcal{M}(k, \sigma, \theta)$ by (3.148). Consequently, by the hypothesis that h_i and h_j satisfy Condition 3.4.2, we must have rank $\left[\frac{\partial h_i}{\partial w}(k, \sigma, (z^c, z^d), w, \theta) \right] = 2$. Hence, by (3.147), we have rank $\left[\frac{\partial \tilde{h}_i}{\partial w}(k, \sigma, (z^c, z^*), w, \theta) \right] = 2$. Since the choice $((z^c, z^*), w) \in \partial_{ij} \check{\mathcal{M}}(k, \sigma, \theta)$ was arbitrary, (3.150) holds.

Lastly, to show that the functions h_i satisfy Condition 3.4.3, choose any $i \in \{1, \ldots, n_\sigma\}, k \in \mathcal{K}, \sigma \in \mathcal{S}, \theta \in \tilde{\Theta}, \text{ and } p \in \{1, \ldots, n_w\}, \text{ and let } e_p \text{ denote the unit vector with the 1 in the } p^{th} \text{ position.}$ We must show that the following holds, for all $((z^c, z^*), w) \in \partial_i \check{\mathcal{M}}(k, \sigma, \theta) \text{ with } w_p = w_p^L \text{ or } w_p = w_p^U$:

$$\operatorname{rank} \begin{bmatrix} \frac{\partial \check{h}_i}{\partial w}(k, \sigma, (z^c, z^*), w, \theta) \\ e_p^T \end{bmatrix} = 2.$$
(3.151)

Choose any $((z^c, z^*), w) \in \partial_i \check{\mathcal{M}}(k, \sigma, \theta)$. By (3.144), we have $\check{h}_i(k, \sigma, (z^c, z^*), w, \theta) = 0$. But, since $z^* \in B_{\delta}(z^d)$ for some $z^d \in \check{X}^d$, we must have $h_i(k, \sigma, (x^c, x^d), w, \theta) = 0$ by (3.125). Moreover, since $((z^c, z^*), w) \in \check{\mathcal{M}}(k, \sigma, \theta)$, (3.148) implies that $((z^c, z^d), w) \in \mathcal{M}(k, \sigma, \theta)$. Thus, $((z^c, z^d), w) \in \partial_i \mathcal{M}(k, \sigma, \theta)$. Consequently, by the hypothesis that h_i satisfies Condition 3.4.3, we must have rank $\begin{bmatrix} \frac{\partial h_i}{\partial w}(k, \sigma, (z^c, z^d), w, \theta) \\ e_p^T \end{bmatrix} = 2$. Hence, by (3.147), we have $\operatorname{rank} \begin{bmatrix} \frac{\partial \tilde{h}_i}{\partial w}(k,\sigma,(z^c,z^*),w,\theta) \\ e_p^T \end{bmatrix} = 2. \text{ Therefore, since the choice } ((z^c,z^*),w) \in \partial_i \check{\mathcal{M}}(k,\sigma,\theta) \text{ was}$ arbitrary, (3.151) holds.

Finally, we provide the proof of Theorem 3.4.1, which we re-state here for clarity.

Theorem 3.9.1. If κ satisfies Condition 3.4.1, then \mathcal{L} is continuous on $\tilde{\Theta}$. If Conditions 3.4.2–3.4.3 also hold, then $\mathcal{L} \in C^1(\tilde{\Theta}, \mathbb{R})$.

Proof By Lemma 3.9.1, it is sufficient to show that $\check{\mathcal{L}} \in C^1(\check{\Theta}, \mathbb{R})$. For this, Theorem 2.4.1 from Chapter 2 will be applied. Note that the latter applies to the hybrid system in (3.128)–(3.130) and requires the functions $\check{h}_i(k, \sigma, \cdot, \cdot, \cdot)$, $\check{f}(k, \sigma, \cdot, \cdot, \cdot)$ and $\check{\ell}_S(k, \sigma, \cdot, \cdot, \cdot)$ to be continuously differentiable on the open set $\check{X} \times \tilde{W} \times \check{\Theta}$ for each fixed $k \in \mathcal{K}$ and $\sigma \in \mathcal{S}$. Under these requirements and Assumption 3.3.1, Theorem 2.4.1 in Chapter 2 says that $\check{\mathcal{L}} \in C^1(\check{\Theta}, \mathbb{R})$ provided that Conditions 3.4.1–3.4.3 are satisfied with h_i replaced by \check{h}_i and the sets $\mathcal{M}(k, \sigma, \theta)$ replaced by the sets $\check{\mathcal{M}}(k, \sigma, \theta)$. Since all of these requirements are satisfied by Lemmas 3.9.2–3.9.3, $\check{\mathcal{L}} \in C^1(\check{\Theta}, \mathbb{R})$.

3.9.2 A Supplemental Result Used to Prove Corollary 3.5.3 in §3.5

The main result of this sub-section is Lemma 3.9.4 below. This result is important because it is needed to justify the conclusion of Corollary 3.5.3. However, Lemma 3.9.4 is given here for its relevance to the results from the previous sub-section. To state Lemma 3.9.4, we first give the following definition.

Using the definition of κ in (3.12)–(3.13), let $x_k(\boldsymbol{\omega}, \theta)$ be as defined in (3.3)–(3.5), and let $\sigma_k(\boldsymbol{\omega}, \theta)$ denote the solution of (3.12) for a given $(\boldsymbol{\omega}, \theta)$.

Definition 3.9.3. For every $k \in \mathcal{K}$, $i \in \{1, \ldots, n_{\sigma}\}$, and $\theta \in \tilde{\Theta}$, define the sets $\partial_{ki}\Omega(\theta)$ as follows:

$$\partial_{ki}\Omega(\theta) \equiv \{ \boldsymbol{\omega} \in \Omega : h_i(k, \sigma_{k,1:i-1}(\boldsymbol{\omega}, \theta), x_k(\boldsymbol{\omega}, \theta), w_k, \theta) = 0 \}.$$
(3.152)

Lemma 3.9.4. If the functions h_i satisfy Condition 3.4.1, then the Lebesgue measure μ of the set $\partial_{ki}\Omega(\theta)$ is zero (i.e., $\mu(\partial_{ki}\Omega(\theta)) = 0$), for all $k \in \mathcal{K}$, $i \in \{1, \ldots, n_{\sigma}\}$, and $\theta \in \tilde{\Theta}$.

Proof For this proof, Lemma 2.3.3 in Chapter 2 will be applied. However, it cannot be applied directly because the sets $\partial_{ki}\Omega(\theta)$ correspond to the dynamic system (3.3)–(3.5), but Lemma 2.3.3 in Chapter 2 applies to the sets defined for the hybrid system in (3.128)– (3.129). Therefore, we first define sets corresponding to (3.128)–(3.129).

For every $k \in \mathcal{K}$, $i \in \{1, ..., n_{\sigma}\}$, and $\theta \in \tilde{\Theta}$, define the following set, where $\check{\sigma}_k(\boldsymbol{\omega}, \theta)$ and $\check{x}_k(\boldsymbol{\omega}, \theta)$ denote the solutions of (3.128)–(3.129) for a given $(\boldsymbol{\omega})$, respectively:

$$\partial_{ki} \hat{\Omega}(\theta) \equiv \{ \boldsymbol{\omega} \in \Omega : \check{h}_i(k, \check{\sigma}_{k,1:i-1}(\boldsymbol{\omega}, \theta), \check{x}_k(\boldsymbol{\omega}, \theta), w_k, \theta) = 0 \}.$$
(3.153)

Furthermore, for any $(\boldsymbol{\omega}, \theta) \in \tilde{\Omega} \times \tilde{\Theta}$, $k \in \mathcal{K}$, and $\boldsymbol{\sigma} \in \mathcal{S}^{K+1}$, let $\check{x}_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta)$ denote the solution x_k resulting from applying the recursion in (3.129) with $\boldsymbol{\sigma}$ fixed (i.e., (3.128) is not used) up to k. For every $\theta \in \tilde{\Theta}$, and $\boldsymbol{\sigma} \in \mathcal{S}^{K+1}$, define the set $\check{\Omega}^{dl}(\boldsymbol{\sigma}, \theta)$ as follows:

$$\check{\Omega}^{dl}(\boldsymbol{\sigma},\boldsymbol{\theta}) \equiv \{\boldsymbol{\omega} \in \Omega : \sigma_{k,i}\check{h}_i(k,\sigma_{k,1:i-1},\check{x}_k^{dl}(\boldsymbol{\sigma},\boldsymbol{\omega},\boldsymbol{\theta}),w_k,\boldsymbol{\theta}) \le 0, \quad \forall k,\forall i\},$$
(3.154)

and define the set $\partial_{ki}\check{\Omega}^{dl}(\boldsymbol{\sigma},\theta)$ as follows, for very $k \in \mathcal{K}$ and $i \in \{1,\ldots,n_{\sigma}\}$:

$$\partial_{ki} \tilde{\Omega}^{dl}(\boldsymbol{\sigma}, \theta) \equiv \{ \boldsymbol{\omega} \in \check{\Omega}^{dl}(\boldsymbol{\sigma}, \theta) : \check{h}_i(k, \sigma_{k,1:i-1}, \check{x}_k^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_k, \theta) = 0 \}.$$
(3.155)

Moreover, define the following set for very $k \in \mathcal{K}$ and $i \in \{1, \ldots, n_{\sigma}\}$:

$$\partial_{ki} \check{\Omega}^{dl}(\theta) \equiv \bigcup_{\boldsymbol{\sigma} \in \mathcal{S}^{K+1}} \partial_{ki} \check{\Omega}^{dl}(\boldsymbol{\sigma}, \theta).$$
(3.156)

Since the functions \dot{h}_i satisfy Condition 3.4.1 by Lemma 3.9.3, applying Lemmas 2.3.3 and 2.4.1 in Chapter 2 shows that $\mu(\partial_{ki}\check{\Omega}^{dl}(\boldsymbol{\sigma},\theta)) = 0$ for all $\theta \in \tilde{\Theta}, i \in \{1,\ldots,n_{\sigma}\}, k \in \mathcal{K}$, and $\boldsymbol{\sigma} \in \mathcal{S}^{K+1}$. Hence, by (3.156), $\mu(\partial_{ki}\check{\Omega}^{dl}(\theta)) = 0$ for all $\theta \in \tilde{\Theta}, i \in \{1,\ldots,n_{\sigma}\}$, and $k \in \mathcal{K}$. Next, we show that

$$\partial_{ki} \check{\Omega}(\theta) \subset \partial_{ki} \check{\Omega}^{dl}(\theta), \quad \forall i \in \{1, \dots, n_{\sigma}\}, \quad \forall k \in \mathcal{K}, \quad \forall \theta \in \tilde{\Theta}.$$
(3.157)

Choose any $k \in \mathcal{K}$, $i \in \{1, ..., n_{\sigma}\}$, $\theta \in \tilde{\Theta}$, and $\omega \in \partial_{ki}\check{\Omega}(\theta)$. By definition, $\check{h}_i(k, \check{\sigma}_{k,1:i-1}(\omega, \theta), \check{x}_k(\omega, \theta), w_k, \theta) = 0$. To show (3.157), we need to show that $\omega \in \partial_{ki}\check{\Omega}^{dl}(\theta)$. By the definition of $\partial_{ki}\check{\Omega}^{dl}(\theta)$ in (3.155), we must show that $\exists \sigma \in \mathcal{S}^{K+1}$ such that the following holds:

$$\check{h}_i(k,\sigma_{k,1:i-1},\check{x}_k^{dl}(\boldsymbol{\sigma},\boldsymbol{\omega},\boldsymbol{\theta}),w_k,\boldsymbol{\theta}) = 0, \qquad (3.158)$$

$$\sigma_{k,j}\check{h}_j(k,\sigma_{k,1:i-1},\check{x}_k^{dl}(\boldsymbol{\sigma},\boldsymbol{\omega},\theta),w_k,\theta) \le 0, \quad \forall k,j.$$
(3.159)

For the chosen $(\boldsymbol{\omega}, \theta)$, let $\check{x}_{0:K}(\boldsymbol{\omega}, \theta)$ and $\check{\sigma}_{0:K}(\boldsymbol{\omega}, \theta)$ denote, respectively, the entire trajectory of of the recursion (3.128)–(3.129). By setting $\boldsymbol{\sigma} = \check{\sigma}_{0:K}(\boldsymbol{\omega}, \theta)$, it can be easily verified that $\check{x}_{k}^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta) = \check{x}_{k}(\boldsymbol{\omega}, \theta)$. Therefore, $\check{h}_{i}(k, \check{\sigma}_{k,1:i-1}(\boldsymbol{\omega}, \theta), \check{x}_{k}(\boldsymbol{\omega}, \theta), w_{k}, \theta) = \check{h}_{i}(k, \sigma_{k,1:i-1}, \check{x}_{k}^{dl}(\boldsymbol{\sigma}, \boldsymbol{\omega}, \theta), w_{k}, \theta) = 0$. This shows (3.158). Moreover, (3.159) holds by (3.129).

Since $\mu(\partial_{ki}\check{\Omega}^{dl}(\theta)) = 0$ for all $\theta \in \check{\Theta}$, $i \in \{1, \ldots, n_{\sigma}\}$, and $k \in \mathcal{K}$, (3.157) implies that $\mu(\partial_{ki}\check{\Omega}(\theta)) = 0$ for all $\theta \in \check{\Theta}$, $i \in \{1, \ldots, n_{\sigma}\}$, and $k \in \mathcal{K}$. Moreover, from the proof of Lemma 3.9.1, we have shown that $\sigma_k(\omega, \theta) = \check{\sigma}_k(\omega, \theta)$ and $x_k(\omega, \theta) = \check{x}_k(\omega, \theta)$ for all $k \in \mathcal{K}$ and any $(\omega, \theta) \in \check{\Omega} \times \check{\Theta}$. This is important because then (3.125) gives directly that $\check{h}_i(k, \check{\sigma}_{k,1:i-1}(\omega, \theta), \check{x}_k(\omega, \theta), w_k, \theta) = h_i(k, \sigma_{k,1:i-1}(\omega, \theta), x_k(\omega, \theta), w_k, \theta)$. This implies that $\partial_{ki}\check{\Omega}(\theta) = \partial_{ki}\Omega(\theta)$. Since $\mu(\partial_{ki}\check{\Omega}(\theta)) = 0$, it follows that $\mu(\partial_{ki}\Omega(\theta)) = 0$.

3.9.3 Supplemental Material for §3.7: Demand Profile Generation

This section provides details on how the product demand profiles given by (3.98) in §3.7 were synthesized.

The yearly profiles for product demand $D_{k,i}$ consists of a deterministic part $D_{k,i}^{det}$ and two random components $\xi_{k,i}$ and $\lambda_{k,i}$ as follows, where $\xi_{k,1}$ and $\lambda_{k,1}$ are generated from a truncated normal distribution with mean 0 and standard deviation 0.0564, and $\xi_{k,2}$ and $\lambda_{k,2}$ from a truncated normal distribution with mean 0 and standard deviation 0.0571:

$$D_{k,i} = D_{k,i}^{det} + \xi_{k,i} + \lambda_{k,i}.$$
(3.160)

The deterministic part $D_{k,i}^{det}$ is given by

$$D_{k,i}^{det} = D_{k,i}^{l} + D_{k,i}^{s} + D_{k,i}^{m}, aga{3.161}$$

where $D_{k,i}^{l}$ represents a linear trend (increase/decrease), $D_{k,i}^{s}$ is a periodic component representing a seasonal trend, and $D_{k,i}^{m}$ is a periodic component representing a monthly trend. These are given by

$$D_{k,i}^{l} = a_i + b_i \frac{k}{K-1}, (3.162)$$

$$D_{k,i}^{s} = \left| r_{i}^{s} \sin\left(\hat{r}_{i}^{s} + \hat{r}_{i}^{s} \pi \frac{k}{K-1} \right) \right|, \qquad (3.163)$$

$$D_{k,i}^{m} = \left| r_{i}^{m} \sin\left(\hat{r}_{i}^{m} + \hat{r}_{i}^{m} \pi \frac{k}{K-1} \right) \right|, \qquad (3.164)$$

where $a_i, b_i, r_i^s, \hat{r}_i^s, \hat{r}_i^s, r_i^m, \hat{r}_i^m$, and \hat{r}_i^m are constants whose values are given in Table 3.5. A sample of demand profiles $D_{k,i}$ is given in Fig. 3.9.

Table 3.5: Constants $a_i, b_i, r_i^s, \hat{r}_i^s, \hat{r}_i^s, r_i^m, \hat{r}_i^m$, and \hat{r}_i^m used in (3.162)–(3.164)

Constants	a_i	b_i	r_i^s	\hat{r}^s_i	\acute{r}^s_i	r_i^m	\hat{r}_i^m	\acute{r}^m_i
i = 1	0.5	2	1	0	2	0	20	12
i=2	1.5	-1.5	2	$\pi/2$	1	0	40	12



Figure 3.9: A sample of demand profiles $D_{k,1}$ (left) and $D_{k,2}$ (right)

Chapter 4

Conclusions and Future Work

4.1 Concluding Remarks

The work in this dissertation provided novel and rigorous theoretical results that enable the use of effective optimization algorithms to solve complex optimization problems called integrated design and operation under uncertainty. Such problems were considered in the interest of addressing the design of flexible energy and manufacturing systems. Flexible systems are critical in advancing the application of smart manufacturing and energy technologies and were defined as systems that are able to make discrete and continuous changes in their operations in order to optimally react to the uncertain fluctuations in their operating environments over short-time scales. The integrated design and operation problem under uncertainty results because designing flexible systems requires considering these operational details and uncertainty in the early design stage of the system. This makes the integrated problem highly complex because the operational details involve mixed-integer operational decisions that must made over many operational time periods (e.g., hundreds or thousands) and under huge uncertainties. Unfortunately, these features make standard scenario-based mathematical programing formulations of such an integrated problem highly intractable. Tractable mathematical programming formulations are usually achieved using major simplifications of the operational details and uncertainty. Moreover, standard simulation-based optimization formulations are usually highly discontinuous due to mixed-integer operational decisions, leading to their solutions using inefficient gradient-free approaches. These simplifications and inefficiencies often lead to sub-optimal system designs.

In this dissertation, we developed novel strategies that address these issues. This was done for two representative models for the type of integrated design and operation problems considered. Specifically, Chapter 2 addressed the issue of discontinuities in a representative simulation-optimization (SO) model and Chapter 3 developed a highly tractable solution approach for a representative mathematical programming model, namely a general nonlinear multistage stochastic program (MSP) model. In relation to existing solution approaches for these models, this dissertation did not assume simplifications of operational details for the MSP model. Moreover, this dissertation did not use gradient-free approaches for the SO problem. Instead, we developed novel theoretical results that guarantee that the SO model is free of discontinuities, allowing use of gradient-based approaches which achieve major improvements in both the computational time and quality of system designs.

Chapter 2 considered an SO model representative of SO models usually used for the optimal sizing of microgrid energy systems that are operated using a type of decision rule (DR) called energy management policy (EMP) and under uncertainty in power demands and renewable energy resources. In this model, the integrated design and operation problem was formulated as a minimization problem that seeks to determine a microgrid system design that simultaneously minimizes the investment cost and the expected operational cost that is determined through stochastic time-series simulations of the system over its lifetime. Note that this SO model is extremely scalable in the number of operational time periods and uncertainty scenarios, both of which are necessary for modeling operational details over the lifetime of the system. This scalability is due to the fact that the operational details are evaluated by the simulation through the embedded EMP. The EMP is a DR whose primary responsibility is to determine mixed-integer operational decisions in each operational time period and for every simulated uncertainty scenario. Thus, the SO model takes a decision-rule-embedded simulation-optimization (DR-SO) formulation. Since the EMP is a discontinuous DR (i.e., its output include integer decisions), the DR-SO formulation considered is inevitably highly discontinuous with the commonly used sample average approximation. This leads to its solution using gradient-free algorithms which are well-known to be computationally inefficient with no guarantees of finding an optimal design. The main contributions to address this issue were two sets of sufficient conditions imposed solely on the EMP rule to guarantee continuous differentiability of the expected cost, despite its sample average approximation being highly discontinuous. Continuous differentiability under these conditions was shown through rigorous mathematical proofs. Moreover, we demonstrated the verification of these two sets on representative EMPs. We found that these conditions are non-restrictive and thus more likely to hold for many EMPs of interest in applications. Notably, although the two sets of conditions are independent, we found that the first set is much easier to verify. Importantly, these conditions allow use of gradient-based approaches to solve the DR-SO problem more efficiently relative to standard gradient-free approaches. Through illustrative examples of microgrid system design and capacity expansion planning, we showed that a custom gradient-based algorithm that was not even optimized outperformed state-of-the-art gradient-free algorithms.

Chapter 3 considered a general nonlinear state-space multistage stochastic program (MSP) model for the integrated design and operation problem. Recall that, for energy and manufacturing systems of interest in this dissertation, the integrated design and operation problem contains mixed-integer operational decisions which must be made over many operational time periods and under huge uncertainties. Thus, the MSP formulation considered is characterized by very many stages (e.g., hundreds or thousands), resulting in a huge number of mixed-integer decisions, each of which is a function of the uncertainty. Thus, the standard scenario-based approximation of this MSP becomes highly intractable. However, we introduced a new type of decision rules (DRs), referred to as *smooth-in-expectation*, that leads to highly efficient solutions of such MSPs. To develop this type of DRs, we first proposed a general class of mixed-integer DRs that provides a framework for modeling many DRs found in the literature, including the EMPs considered in Chapter 2. Using this class, the general MSP was transformed into a DR approximation (DRA) problem which has extremely fewer decisions relative to the original MSP which, for the applications of interest in this dissertation, could have hundreds of thousands with the standard scenario-based approach. The DRA was then cast as a decision-rule embedded simulation-optimization (DR-SO) problem similar to the DR-SO problem analyzed in Chapter 2. However, due to the generality of the class of DRs proposed, major extensions of the results in Chapter 2 were made to address the issue of discontinuities in this more general DR-SO problem. First, we defined a *smooth-in-expectation* decision rule as any decision rule that makes the expected value function of the DR-SO problem smooth. Then, we developed a new set of sufficient conditions that guarantees that the proposed class of mixed-integer DRs is smooth-in-expectation. The new set of conditions involves major extensions of the first set of conditions developed in Chapter 2 which were made to accommodate state-space MSPs with chance constraints and discrete state variables, neither of which was possible with the results developed in Chapter 2. The extension to discrete states is important because such states are often needed to enforce timing constraints such as minimum uptime/downtime constraints for process units, which can often be achieved by a suitably constructed DR. Finally, a strategy was developed that is able to transform any given decision rule of the proposed class into a smooth-in-expectation decision rule, allowing the new conditions to be broadly applicable. These results are important because smoothness enables the general DR-SO problem to be efficiently solved using gradient-based approaches. The significance of these results was demonstrated using an inventory optimization problem for which we obtained major optimization performance improvements using a trust-region algorithm (which depends on the DR-SO problem smoothness) relative to gradient-free approaches.

4.2 **Recommendations for Future Work**

The success of solving the integrated design and operation problems considered in this dissertation can partly be attributed to the overall theme of using DR-SO formulations in which stochastic simulations use a DR to evaluate the expected operational cost of the system over long-term operation. However, this dissertation leaves significant improvements that need to be made in order to devise more accurate DR-SO formulations and more efficient implementations of gradient-based approaches.

First, although Chapter 3 proposed a class of mixed-integer decision rules that is flexible enough to model many decision rules in the literature, this class can only model explicit control strategies that are defined by a set of threshold functions. Unfortunately, such strategies are often criticized for being sub-optimal. This issue is accentuated by the complexity of system operations in the energy and manufacturing systems of interest in this dissertation because it makes it practically difficult to devise explicit control strategies that can compute high-quality operational decisions. Thus, although such explicit control strategies are computational efficient and can be parametrized and optimized along with the design decisions, the number of parameters needed can be significantly large, increasing the size of the corresponding DR-SO problem. In cases there is not enough parameterization, the DR-SO formulation is likely to provide conservative designs. However, in applications, it is becoming an increasingly common practice to make operational decisions using advanced control strategies that involve solving an optimization problem [43, 47]. For example, model predictive control (MPC) is widely regarded as an advanced control strategy for operating energy systems such as microgrid and combined heat and power systems [43–45] and for the dynamic control of complex chemical processes [36, 46, 47]. Such advanced control strategies are often easy to formulate (e.g. standard MILP formulation) and they offer much more freedom in modeling system operations and economical benefits relative to explicit control strategies [70, 131]. Accordingly, there is a huge interest in incorporating advanced control strategies in the problems of integrated planning and scheduling [59, 132, 133], scheduling and control [57, 134, 135], and design and control [63, 136–138]. Importantly, for integrated design and operation problems considered in this dissertation, modeling the operational details with an advanced control strategy potentially leads to more economical designs relative to explicit control laws [71]. Thus, a potentially significant future work can explore the application of the results developed in Chapter 3 to cases where an advanced control law is used to approximate MSPs, which is likely to give more accurate DR-SO formulations. Since such cases are closely related to stochastic multilevel programs (SMLPs) that also arise in smart manufacturing and energy systems, the main focus could be placed on developing a tractable solution approach for SMLPs with mixed-integer recourse decisions, which, as in the case of MSPs, are intractable by any other existing approaches (see Chapter 1 for details).

Second, although this dissertation lays the theoretical groundwork for the application of gradient-based approaches to solve DR-SO problems, it leaves a number of implementation challenges to be addressed. To lay out these challenges, first recall that the DR-SO problems of interest in this dissertation involve seeking design decisions θ that minimize an expected value defined as follows, where $\ell(\omega, \theta)$ is the operational cost evaluated through a decision-rule-embedded stochastic simulation for any fixed θ and uncertainty scenario ω :

$$\mathcal{L}(\theta) \equiv \mathbb{E}\left[\ell(\boldsymbol{\omega}, \theta)\right]. \tag{4.1}$$

The DR-SO problem can be loosely stated (i.e., excluding constraints and investment cost) as follows:

$$\min_{\theta \in \Theta} \quad \mathcal{L}(\theta). \tag{4.2}$$

In general, provided that they are smooth, problems similar to (4.2) are most commonly solved using stochastic approximation (SA), which is essentially the application of the standard steepest-descent algorithm with stochastic gradient estimates of $\mathcal{L}(\theta)$ [139–141]. Since smoothness of (4.2) is guaranteed by the theoretical results developed in this dissertation, the gradient algorithms used in this dissertation were of SA-type. However, although more impressive results were obtained relative to gradient-free approaches, the following challenges were faced and need to be addressed for more efficient implementation of these approaches:

(i) Recall that for any fixed uncertainty scenario ω , $\ell(\omega, \cdot)$ is a highly discontinuous func-

tion of θ due to discontinuous decision rules determining mixed-integer decisions in the simulation of $\ell(\boldsymbol{\omega}, \theta)$. As a consequence, the standard finite difference (FD) approach based on direct Monte Carlo sampling leads to very high variance estimates of $\nabla \mathcal{L}(\theta) = \nabla \mathbb{E} \left[\ell(\boldsymbol{\omega}, \theta) \right]$ due to artificial *rare events* created by the differencing scheme (i.e., small perturbations) [142]. Critically, compensating for this high variance required a very large number of samples, which significantly deteriorates the performance of SA.

- (ii) Although SA guarantees convergence in probability [139], its convergence rate depends critically on many parameters (e.g., step size for iterate update and scaling matrix for hessian approximation to avoid ill-conditioning) that have to be tuned. In our experience with DR-SO problems, this tuning was very strenuous, even for cases with a modest number of decision variables. Moreover, SA struggled to terminate because the noise in gradient estimates was magnified in the neighborhood of the local solution. Unfortunately, we struggled to find an efficient sampling technique to could help with this issue.
- (iii) As discussed above, more accurate DR-SO approximations could be obtained using advanced decision rules which are based on the solution of auxiliary optimization problems (e.g., model predictive control) to obtain more accurate operational decisions. Unfortunately, such rules will make simulations very slow due to the repetitive solution of the auxiliary problems, making the optimization process and the diagnosis of Challenges (i)–(ii) very time-consuming.

4.2.1 Efficient Computation of Unbiased and Low-Variance Gradient Estimates

To address Challenge (i), standard variance reduction techniques, such as the use of common random numbers, control variates, importance sampling, and conditional expectation can be adapted to gradient estimation. Note that although these techniques will

help reduce the variance of stochastic estimates of $\nabla \mathbb{E}[\ell(\boldsymbol{\omega}, \theta)]$, specifically by reducing the variance of stochastic estimates of $\mathbb{E}\left[\ell(\omega, \theta)\right]$, the effect of the differencing scheme will not entirely be eliminated and this can possibly be the bottleneck for these techniques. However, recall that $\nabla \mathcal{L}(\theta) = \nabla \mathbb{E}[\ell(\boldsymbol{\omega}, \theta)]$. A common way to get around the differencing scheme is to use sample path estimators which compute $\nabla \ell(\boldsymbol{\omega}, \boldsymbol{\theta})$ directly. Unfortunately, since $\ell(\boldsymbol{\omega}, \cdot)$ is a discontinuous function of θ , $\nabla \mathcal{L}(\theta) = \nabla \mathbb{E}\left[\ell(\boldsymbol{\omega}, \theta)\right] \neq \mathbb{E}\left[\nabla \ell(\boldsymbol{\omega}, \theta)\right]$, making sample path estimators, such as infinitesimal perturbation analysis (IPA) and smoothed IPA, inappropriate [143]. However, let $\nabla \mathcal{G}(\theta) = \nabla \mathbb{E} \left[\ell(\boldsymbol{\omega}, \theta) \right] - \mathbb{E} \left[\nabla \ell(\boldsymbol{\omega}, \theta) \right]$ denote the IPA error. Accordingly, $\nabla \mathcal{L}(\theta)$ can be written as $\nabla \mathcal{L}(\theta) = \mathbb{E} \left[\nabla \ell(\boldsymbol{\omega}, \theta) \right] + \nabla \mathcal{G}(\theta)$. The work in Chapter 2 (see appendix) showed that the IPA term $\mathbb{E}\left[\nabla \ell(\boldsymbol{\omega}, \theta)\right]$ can be written as a volume integral and the IPA error $\nabla \mathcal{G}(\theta)$ can be expressed as a sum of surface integrals along the discontinuities of $\ell(\boldsymbol{\omega}, \cdot)$. Thus, one promising approach is to develop a sampling technique to estimate this error. Another alternative is to apply a change-of-variables (COV) to transform the surface integrals into volume integrals which can then be sampled along with $\nabla \ell(\boldsymbol{\omega}, \boldsymbol{\theta})$. In fact, some of these ideas have been tried (e.g., conditional expectation, the IPA and COV techniques) on a specific DR-SO problem and significant reduction were obtained in the variance of the estimates compared to the standard FD, leading to very substantial speed-ups in the overall optimization process. However, these ideas were abandoned because their extension to a much general class of DR-SO problems seemed to be out of scope of the intended time frame. Additionally, the variance of the COV estimates did not seem to improve very much over FD. Thus, it would be worthwhile revisiting these techniques and explore how they can be combined or improved to further reduce their variance and increase their broader applicability.

4.2.2 Accelerating SA Through Adaptive Techniques

To address Challenge (ii), efforts may be focused on the development of advanced stochastic gradient descent algorithms that achieve much faster and more reliable convergence through adaptive techniques that automatically generate scaling matrices, step sizes, and regularization parameters, and adaptive sampling techniques that effectively focus computational effort near the optimal solution. Note that some of these techniques are available for smooth deterministic problems. For example, automatic generation of step sizes can be achieved with line-search and trust-region methods and adaptive estimation of the scaling matrix (e.g. Hessian estimation) can be achieved with quasi-Newton methods. Although the adaptation of these methods to stochastic problems is still a nascent area of research, some effort has already been made. Specifically, it would be worthwhile exploring the application of existing stochastic gradient methods predominantly designed for machine learning problems to DR-SO problems [144] or to devise more effective adaptive strategies for the existing stochastic trust-region methods [127, 145].

4.2.3 Accelerating Simulations which Embed Auxiliary Optimization Problems

To address Challenge (iii), research efforts may be directed towards the development of advanced explicit mixed-integer decision rules which consist of simple function evaluations. Notably, to ensure smoothness of DR-SO problems, such decision rules will need to be expressed in the mathematical forms proposed in Chapters 2 and 3. Moreover, effective methods for parameterizing such rules will be needed to ensure comparative performance with rules that are based on solution of an optimization problem. For example, to obtain an explicit decision rule whose performance is comparable to that of a model predictive control (MPC), the explicit rule will need to have parameters that model the predictive capabilities of MPC. As a starting point, it would be worthwhile exploring possible improvements that could be made on existing application-specific decision rules that are based on priority lists [16, 146, 147]. Alternatively, multi-parametric programming techniques could be pursued for deriving exact explicit decision rules corresponding to the implicit decision rules based on solution of an optimization problem [148]. However, note that multi-parametric programming techniques may give a very large number of expressions that define the explicit decision rule, especially for large instances of the original optimization problem [10, 63]. Nonetheless, it would be interesting to explore the difference between the computational cost of simulations with repetitive solution of an optimization problem and that of simulations with the explicit multi-parametric programming rule.

Chapter 5

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