Abstract

DILLARD, KAREN EDNA MICHELE. An Application of Implicit Filtering to Water Resources Management. (Under the direction of C.T. Kelley.)

We introduce the concept of a water market, the buying and selling of water as prices fluctuate based on supply and demand, applied to a region in southern Texas. The water market provides different alternatives for a municipality to acquire water. The water resources problem is to determine the combination of alternatives that results in minimum cost. To accomplish this, we link a one-year stochastic simulation that randomly selects from historical data to an optimizer called implicit filtering. We find that a municipality can lower expected costs while meeting the water demand by allowing a portfolio with cost variability. The stochastics create low amplitude, high frequency perturbations, called noise, in the optimization landscape. We apply a variance reduction method to reduce the noise. We select the control variate method to reduce the variance. This method does reduce the variance and the computational cost as well. Variance reduction also makes it possible to expand to a multi-year model. A multi-year model is more useful to the water resources manager since municipalities will not change the portfolio every year. Municipalities look at longer time horizons that account for such factors as growth in demand. Last, we design

a methodology in which the model adapts the number of realizations to control the estimated level of noise. The model uses information from the optimizer about the current location and increases the number of realizations in the noisier areas of the landscape. We find that the benefit of applying the adaptive model is the reduction in the average realizations per function call.

An Application of Implicit Filtering to Water Resources Management

BY

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Biography

Karen Dillard was born in Thailand, but she grew up in upstate New York with her parents, sister, brother, grandparents, aunts, uncles, and cousins. She attended elementary, middle, and high school in the same small town. She graduated from Rensselaer Polytechnic Institute and was commissioned as a second lieutenant in the United States Air Force. Her duties in the Air Force have taken her to Massachusetts, Colorado, New Mexico, South Korea, North Carolina...just to name a few. Her most rewarding duty thus far has been teaching and mentoring the cadets at the Air Force Academy Preparatory School and the Air Force Academy. Upon graduation, the Air Force will send her to Ohio.

Acknowledgments

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The views expressed in this article are those of the author and do not reflect the official policy or position of the United States Air Force, Department of Defense, or the U.S. Government.

Chapter 1

Introduction

1.1 Historical View

Is water a commodity that can be traded in a water market, just as stocks in a stock market or is it a public resource that all people share? The answer to this question depends on the region. Factors such as population growth, water scarcity, past water policies, and public perspective can affect the evolution of water policies. The following section provides an overview of general water policies in the United States. Different regions manage their water resources according to their needs and so many variations of these policies can exist [29].

Throughout history, [1], water policies varied: from riparian doctrine to government control of water to trading water for capital gain. There was a time during the gold rush of the mid-nineteenth century, when miners in the West would buy and sell their water rights freely. The State governments allowed these water transfers without interference. Over the next century, this free water trade was replaced by two differing positions. Water markets, the buying and selling of water, were not

promoted in either policy. One position treated water as a public resource where government ensured its equitable distribution. The second position viewed water as a local resource where the original communities of the area had claim to it. (This is riparian doctrine.) See section 1.1.2 for more. In the next few paragraphs, I describe the historical views and where the United States is moving toward today.

1.1.1 Arguments For Water Markets

Proponents of water markets claim there are economic and environmental benefits [16], [63]. One benefit occurs while regions of low water supply, high demand/high-value use, purchase water from lower-value uses instead of building expensive and environmentally damaging structures to gain water [62]. Municipal use is considered high-value and agricultural use is considered low-value. For example, if an agricultural user was given the opportunity to sell water for a higher price than he paid, then he might conserve water use on his crops and allow a portion to be sold. Then the urban areas could purchase the water instead of building expensive, intrusive structures. Another benefit of water prices responding to supply and demand, is the potential for increased conservation. Studies have shown if prices become high enough, there is a decrease in agricultural and municipal use [2],[23]. As mentioned already, when the agricultural community reduces water consumption, more water is available for municipal use. In fact, it is estimated that if five percent of agricultural water was transferred to the municipalities, then the water demand due to urban growth in the western United States would be met for the next twenty-five years [58]. This provides an idea of how much water the agricultural community consumes. During times of

drought, water markets could trigger reduced consumption since high water costs have an affect on people's actions more so than government pleas for conservation. Transferring water to high-value uses to avert a drought could be accomplished [1], [62]. Lastly, water markets would encourage private industry to compete and develop efficient water management processes to supply their customers.

1.1.2 Arguments Against Water Markets

Even with the state government outward approval of water transfers as mentioned above, there is still public skepticism [62]. Water markets have not been the norm. It is difficult for people to change, move past common practices and accept what is written into law or believe the law will not change later. People have seen the regulations change to meet a current crisis [53], [62]. There have been bans on wasting water and if the water waste continued for a number of years, the government saw fit to reallocate the water to another user. The following examples illustrate the reason for skepticism. If the agricultural user sells water a few times, it may appear he doesn't need it and therefore is wasting water. Then he fears the government will see this as a forfeiture of his water [62], [63]. If a municipality buys water on a temporary basis and then comes to rely on those purchases in the future, the government may regulate that they receive that water permanently. In the end, the water is again taken away from another entity that apparently had too much. Basically, if the government regulates through water transfers now in order to increase the water market activity, what guarantees the government won't change the regulation again? Another reason the public is cautious is the fear that a monopoly will become established. The belief

is that water should be owned by the people and controlled by the people. The following describes two philosophies on water ownership that impede the transition to water markets.

Public Resource Position

The public resource position was predominant in the western United States. Government organizations and tiers of authority developed to control the water and promote development in the West. Much of the West was divided into public agencies and irrigation districts that control the water in their particular region. The debate over water markets continued and at one time all water transfers were banned from ten states. Today, those ten states either repealed the bans or have allowed exceptions. Though, the mindset is still in favor of government control [62].

Local Resource Position

The second position, the local resource position, was based on riparian doctrine which gave water rights to the landowners along a water source. This view grew primarily in the eastern United States. So indeed it was difficult to incorporate water transfers in this type of domain. Water belongs to the local group and should not be given to any outsiders. Congress and federal courts recognized the local authorities and allowed areas to protect their share of water by preventing its transportation outside their region [62], [48].

1.1.3 Water Banks

Within the last fifteen to twenty years, more state governments have tried to increase the activity of water markets through the regulation process, temporary trials of water transfers, and the institution of water banks. Water banks are highly regulated, government-operated agencies. The water bank is the middle man for water transfers. Those who won't use all their water can sell to the water bank who then sells the water to a buyer. Since the water banks are government-run, the purchase and sale prices are regulated and have a tendency not to fluctuate with supply and demand. Sometimes, the water bank will prioritize who it sells water to. Municipalities with owner rights have the highest priority, then agricultural users with irrigation policies, and last to agricultural users who don't irrigate. Some state/local governments set up water banks only during times of drought to help control the water market [62].

Benefits have emerged from the institution of water banks. Transaction costs have decreased. Because of the government's agenda to increase water transfers, the water banks are equipped to handle transfers faster and easier, thus reducing costs [26]. The water banks provide added assurance that water rights will not be forfeited by a seller. Sales will not be scrutinized to determine if water rights have been allocated appropriately. The water prices are controlled and can allow profit or no profit during transfers. Different terminology is used to give the perception that water is still allocated for all to use and not a resource to profit from. For example, water is contributed or deposited to the bank, not sold to the bank. The result is that the water banks have gained the public trust which is a difficult feat for a government agency as described above in section 1.1.2.

1.1.4 Summary

So, water at one time was a commodity to be traded in the private sector. Then water distribution was controlled by the state governments with shifts from banning water transfers to allowing water transfers to encouraging water transfers. Currently, water markets are seen sporadically around the nation. Some areas have developed more active markets than others [41],[42], [12], [16], [52]. There have been predictions that the fresh water supply will not meet the exponential growth in demand [49]. People change their habits when the price of water changes (i.e., conserve water when the price increases)[1]. People might invest in water-efficient appliances, wash their cars less frequently, and stop watering their lawns. Agricultural users might invest in alternative irrigation techniques or make different crop decisions. Research on how a water market might assist with water resource management has been on-going [8], [14], [17].

1.2 Means of Water Transfers

Given a water supply for a region, water is allocated to its users. There are three means of acquiring water that are considered in this problem: permanent rights, spot market leases, and option contracts.

1.2.1 Permanent Rights

Permanent rights represent the volume of water the city is entitled to each year. In reality, the city never receives its total volume of water at the start of each year.

Instead, the city receives its share of new water flowing into the region. If the city owns 10% of the total volume of permanent rights for the region, then the city receives 10% of the new water. New water is defined as the water added to the region (through precipitation for example) minus the water lost through evaporation or drainage into the ground. The new water is allocated at the end of each month and can be used in any subsequent month. Permanent rights are transferable but due to a lengthy approval process, the city's volume of permanent rights is assumed to be constant throughout the year. The price of the city's permanent rights (p_R) is an annualized cost which includes the cost of buying a permanent right [13].

1.2.2 Leases

The lease is a method of temporarily transferring water. The city purchases water from a lessor according to the current prices of water. A lessor could be someone in the agricultural community, a government agency such as a local water district or water bank, a private company such as a power or water company, or another municipality within the region or outside the region [1]. The lessor comes in many different forms depending on the organization of the water allocation system and the available private resources. For this study, the assumption is that the lessor most likely comes from the agricultural community. (See section 1.3 for more explanation.) The water is purchased at the end of the month to be used in any subsequent month. The lease approval process takes only days. Lease prices ($\hat{p_{L_t}}$) are considered random variables associated with low or high reservoir water levels [13]. See section 2.1 below for an explanation of this linkage.

1.2.3 Option Contracts

Option contracts are purchased at the start of the year. These contracts allow the city to exercise the option, meaning purchase water, at a later date and at an agreed upon price. Both the date and price are set at the time the option contract is made. Here, a European call option is used (versus an American call option which allows an option to be exercised anytime up to the option call date) where the exercise date is the last day of a specified month (t_X). (The European method simplifies the model and is still representative of market conditions.) After the option has been exercised, the water can be used in any subsequent month. Options that are not exercised on the call date are no longer valid. Option prices (p_O) and exercise option prices (p_X) are based on the lease prices ($\hat{p_{L_t}}$) in the exercise month [13].

1.3 Optimization Problem, Version I

The objective of this first problem is to identify the number of permanent rights, leases, and options that minimize the expected annual cost of meeting a city's annual water demand subject to reliability and cost variability constraints. Reliability is an indicator of how often the city will be able to meet its demand. (See Failures, Critical Failures, and Reliability in section 2.1.7.) Cost variability is an indicator of the risk for very high annual portfolio costs. (See Cost Variability in section 2.1.8.)

To evaluate the objective function (expected annual cost), Jocelyn Ramsey and Brian Kirsch created a stochastic water market model [13], [51], that simulates hydrologic and water market conditions using randomly sampled historical data. (See

section 2.1.) Then, the decision parameters are optimized using implicit filtering to minimize expected annual cost while meeting the reliability and cost variability constraints. (See section 2.2 and chapter 4.)

There are many assumptions in this problem. This paragraph provides a preview. Chapter 2 includes more details. The model simulates a 12-month cycle where one city located in the western United States receives its entire water supply from a reservoir, and its allocation of water is governed by a system of water rights. The water market is active with many other municipalities purchasing water and agriculturalists selling water. Since the city is only one of many involved in the water market, it has no ability to affect the market price of water and therefore accepts the water price [13]. Since most of the water is used for irrigation which is considered to be of low value, it is assumed that the city will always be able to purchase water within the market [13]. The city holds a number of permanent water rights assumed to be constant throughout the year. Some fraction of the water owned is distributed at the beginning of the year. The remaining water rights are distributed throughout the year as water becomes available. And it is possible that the city does not receive its entire amount of water rights.

1.4 Optimization Problem, Version II

Version I of the optimization problem involves a one-year cycle that is repeated many times. Randomly sampling the historical data and repeating the annual cycle can provide a realistic simulation. However, this introduces noise (small peaks and valleys) into the solution surface. Many simulation runs can help reduce the noise but at a

higher computational cost. Another way to reduce the noise is by applying a variance reduction technique which is described in chapter 6. Version II of the optimization problem involves the application of a variance reduction technique. The variance of an estimate is a measure of its accuracy. The smaller the variance, the more accurate the estimate.

1.5 Thesis Goals

The following is a general description of my thesis goals.

Goal 1: Simulate a one-year water market for a city and use an optimization technique called implicit filtering to find the scenario of least annual cost. First, solve version I of this optimization problem. Then, apply variance reduction.

Goal 2: Expand the simulation to a multi-year water market and apply variance reduction.

Goal 3: Design a methodology where the simulation adapts the number of runs to the level of noise. So, the number of simulation runs would increase in areas where noise is more prominent.

We start by providing background information on the overarching water resources problem in chapter 2. Specifically, details of the stochastic water market model, the optimization framework, and the study region are described. Then, we review some mathematical concepts relating to unconstrained optimization and bound constrained optimization in chapter 3. Details of implicit filtering are in chapter 4.

More discussion of the goals, results, and conclusions follow in the next chapters. We provide results of solving the optimization problem, version I (without variance

reduction), in chapter 5. We describe the optimization problem, version II (with variance reduction), the selected variance reduction method, and results in chapter 6. We apply variance reduction to the expanded multi-year water market simulation in chapter 7. We describe the adaptive model in chapter 8.

We also provide appendices with water resources terms, mathematical terms, and statistical information. There are references to the appendices when necessary.

Chapter 2

Methodology

2.1 Stochastic Water Market Model

Characklis et al [13] describe the model parameters, constraints, and assumptions used to build a 12-month water market model, as well as the optimization formulation and the study region as follows.

The model simulates a 12-month water market that begins on December 31st ($t = 0$). At $t = 0$, the city holds a number of permanent rights (N_{R_T}) and options (N_O). The reservoir storage (R_0) and the amount of water the city has carried over from the previous year (N_{r_0}) are set as initial conditions. For $t = 1, ..., 11$, the model simulates the hydrologic and water market conditions for the given study region. (See section 2.3 below for more details on the given study region.) Then, each month, the model decides whether or not to purchase water and if so, how much to purchase. The output of the model is expected annual cost. The following is a detailed description of the model [13].

2.1.1 Data Sets Defined

To simulate the hydrologic and water market conditions, the model randomly samples from historical data. There is monthly data from 1970 - 2002 on inflows, losses, new water, reservoir variation, and demand. There is monthly data from 1994 - 2002 on lease prices for low-level and high-level reservoirs. Inflows refer to the additional water flowing into the region. Most of the inflows the study region receives comes from precipitation hundreds of miles from it. Losses account for occurrences such as, evaporation and seepage into the ground. New water is the difference between inflows and losses. Reservoir variation is the difference in reservoir water level from month t to month $t + 1$ which takes into account outflows (water that is released from the reservoir due to city usage or excess spillage) as well as inflows and losses. Demand is the city's water consumption.

In this study region, there are two data sets for lease prices. One data set is for a reservoir of low water level. The second is for a reservoir of high water level. The reservoir water level is defined to be low when the water level is less than 1.43 million acre-feet and high when it is greater than 1.43 million acre-feet. At first glance, one might conjecture that as reservoir water levels increase, lease prices decrease. Through some analysis by Ramsey [51], it was found that this is not entirely accurate. A more accurate scheme is to separate lease prices into two populations: one when the reservoir water level is low and the second when the reservoir water level is high as defined above. And as expected, the lease prices are generally lower when the reservoir water level is high.

2.1.2 Obtain Input Data by Random Sampling

The model obtains the input data by randomly sampling with replacement from a data set.

Ramsey [51] found that the data sets for losses, inflows, reservoir variation, and high/low lease prices do not fit a standard statistical distribution. So, the model obtains the 12 inputs directly from each of these data sets by randomly sampling with replacement. One data point is randomly sampled from January, one point from February, and so on until each month has been sampled for each of the data sets mentioned.

Ramsey [51] set demand as a normally distributed continuous variable using monthly mean demand data with associated monthly standard deviations. Brian Kirsch used this information to develop a demand data set with a discrete set of numbers for each month. After randomly selecting 100 points from the distribution, Kirsch identified all points within two standard deviations of the mean to be in the set. This was completed for each month. Then, the model obtains the monthly demand value by randomly sampling with replacement from these new data sets. Note that all random variables are denoted by a "^".

2.1.3 Annual Cost

Since the city pays for water via permanent rights, options, exercised options, and leases purchased in month t, the annual cost of water is the sum of all units multiplied

by the corresponding price:

$$\text{Annual Cost} = N_{R_T} p_R + N_O p_O + E[\hat{N}_X] p_X + E\left[\sum_{t=0}^{11} \hat{N}_{L_t} \hat{p}_{L_t}\right] \tag{2.1}$$

where,

N_{R_T} = total volume of permanent rights held by the city (ac-ft)

p_R = annualized price of permanent water rights (dollars/ac-ft)

N_O = volume of options purchased at the beginning of the year (ac-ft)

p_O = price of options (dollars/ac-ft)

$\hat{N}_X$ = volume of exercised options (ac-ft)

p_X = exercise price of options (dollars/ac-ft)

$\hat{N}_{L_t}$ = volume of leases purchased at the end of each month t (ac-ft)

$\hat{p}_{L_t}$ = lease price in month t (dollars/ac-ft).

Here, E[Y] represents the expected or mean value of random variable Y. The number of exercised options, the number of leases purchased, and the price of leases are random variables.

2.1.4 Simulation Constraints

The simulation is subject to the following constraints:

$\hat{N}_X \leq N_O$ = The city cannot exercise more options than it buys at $t = 0$;

$\sum_{t=0}^{11} \hat{N}_{r_t} \leq N_{R_T}$ = The sum of water allocations each month cannot exceed the number of permanent rights the city holds, where $\hat{N}_{r_t}$ is the new allocation of water to the city in month t (ac-ft);

$R_{Max} \geq R_t \geq R_{Min}$ = The reservoir level at month t (R_t) must remain within specified bounds of storage capacity where R_{Max} is the maximum storage level and R_{Min} is the minimum storage level;

Each of these simulation constraints is monitored within the simulation. The maximum volume of options that can be exercised is equal to the volume of options purchased at the start of the year. If the city requires more water, the city must purchase leases to fill the gap. See section 2.1.6 for more details. The simulation does not allow any more monthly allocations once the number of permanent rights the city holds is reached. If the reservoir level dips below the minimum storage level R_{Min}, the simulation sets it to R_{Min}. If the level becomes greater than the maximum

storage level R_{Max}, it is set to R_{Max}.

2.1.5 Calculating Supply

The simulation maintains a water balance such that the reservoir level at month t is equal to the reservoir level from the previous month (at month $t-1$) plus the inflows (i_t) and minus the outflows (o_t) and losses (l_t):

$$R_t = R_{t-1} + i_t - o_t - l_t. \tag{2.2}$$

Recall from above that the model samples data from the reservoir variation data set. Reservoir variation is equal to the inflows minus the outflows and losses.

The city's monthly allocation of water ($\hat{N}_{r_t}$) is calculated from the new water available ($\hat{n}_t$) each month as seen below in equation 2.4. First, the random variable $\hat{n}_t$ is calculated using monthly inflows ($\hat{i}_t$), monthly losses ($\hat{l}_t$), and an instream loss factor (l_I) as follows:

$$\hat{n}_t = (\hat{i}_t - \hat{l}_t) \cdot (1 - l_I).$$

The instream loss factor is due to the geography and the assumptions of this particular study region. The study region has two reservoirs that are separated by more than 350 miles but are connected by a river [55]. (See section 2.3 below for more details on the given study region.) The assumption is that the two reservoirs act as one reservoir for this model. So, the instream loss factor is used to account for water loss between the two reservoirs. The instream loss factor (l_I) for these two reservoirs is

0.175 and the computation for the new reservoir inflows becomes:

$$\hat{n}_t = (\hat{i}_t - \hat{l}_t) \cdot (0.825). \tag{2.3}$$

Now, the city's monthly allocation of water ($\hat{N}_{r_t}$) can be calculated as follows:

$$\hat{N}_{r_t} = \hat{n}_t \cdot \left(\frac{N_{R_T}}{\bar{N}_R} \right). \tag{2.4}$$

Recall that N_{R_T} is the total volume of permanent water rights for the city. Let $\bar{N}_R$ be the total volume of water rights for the entire study region. So, if the city owns 10% of the total volume of permanent water rights for the region, then the city will be allocated 10% of the new water each month.

The city's water supply for month t is calculated at the end of month $t-1$. This calculation is different depending on whether month t is before or after the exercise month (t_X). Recall that in month t_X, options are exercised on the last day. In this simulation, we let $t_X = 5$, so options are exercised on May 31st. (May 31st was selected due to the agricultural season. At this point in the year, the agricultural community has plenty of water to lease. If the date were in September, for instance, the agricultural community may not have as much water to lease because of irrigating crops over the summer months.) For months prior to t_X ($t < t_X$), the city's available water supply for month $t+1$ (S_{t+1}) is calculated using the city's monthly allocations of water ($\hat{N}_{r_t}$) and purchased leases ($\hat{N}_{L_t}$) minus the city's water usage in month t (u_t) as follows:

$$S_{t+1} = \sum_{i=0}^{t} \hat{N}_{r_i} + \sum_{i=0}^{t-1} \hat{N}_{L_i} - \sum_{i=1}^{t} u_i, \qquad \text{for } \; t = 0, 1, 2, \ldots, t_X - 1. \tag{2.5}$$

For month t_X or months after t_X ($t \geq t_X$), the calculation accounts for the volume of exercised options ($\hat{N}_X$). In this case, the city's available water supply for month $t+1$ (S_{t+1}) is:

$$S_{t+1} = \sum_{i=0}^{t} \hat{N}_{r_i} + \sum_{i=0}^{t-1} \hat{N}_{L_i} - \sum_{i=1}^{t} u_i + \hat{N}_X, \qquad \text{for } \; t = t_X, t_X + 1, \ldots, 11. \tag{2.6}$$

Notice that in equations 2.5 and 2.6 the summation of the purchased leases ($\hat{N}_{L_i}$) starts at $i = 0$ and ends at $i = t - 1$. The decision whether or not to purchase leases in month t has not been made yet so that volume of water is not included in these calculations.

The leasing decision in month t is based on the city's available water supply (S_{t+1}) and the allocation of water the city expects to receive in the future months. So, now the city's expected water supply ($S_{E_{t+1}}$) over the remainder of the year is calculated as the sum of the current water supply and the expected water allocations from month $t+1$ to month $t = 11$ as follows:

$$S_{E_{t+1}} = S_{t+1} + \sum_{i=t+1}^{11} E[\hat{N}_{r_i}], \qquad \text{for } \; t = 0, 1, \ldots, 10.$$

This calculation of the expected water supply ($S_{E_{t+1}}$) is only valid for months $t = 0$ to $t = 10$. Recall from equations 2.5 and 2.6 that the monthly allocation of water ($\hat{N}_{r_t}$) is used to determine the city's water supply (S_{t+1}) in the following month. So, the November allocation of water ($\hat{N}_{r_{11}}$) is used to calculate the city's available water supply in December ($S_{11+1} = S_{12}$). The December allocation of water ($\hat{N}_{r_{12}}$) is transferred to the following year. Therefore, when $t = 11$, the December's expected water supply ($S_{E_{11+1}} = S_{E_{12}}$) will not include a calculation of the December expected water allocation ($\hat{N}_{r_{12}}$). So, December's available water supply (S_{12}) and expected water supply ($S_{E_{12}}$) are the same. The expected water allocations come from equation 2.4.

2.1.6 Purchase Decisions - When and How Much?

Now that the city's expected water supply ($S_{E_{t+1}}$) is calculated, the city can make decisions regarding lease purchases and option exercises. For months prior to t_X and after t_X, the city considers purchasing leases only. For month t_X, the city considers purchasing leases and exercising options. The decision entails whether or not to purchase water and if yes, then how much water to purchase. The answer to both questions lies in a ratio of expected supply-to-expected demand.

First, the city needs to make the purchase decision by comparing the ratio of expected supply-to-expected demand to a threshold value referred to as α. The following condition prompts the city to purchase water:

$$\text{If } \frac{S_{E_{t+1}}}{\sum_{i=t+1}^{12} E[\hat{d}_i]} \leq \alpha, \quad \text{for } t = 0, 1, 1, \ldots, 11, \quad \text{then the city will purchase water.}$$

where,

$$\hat{d}_t = \text{city's water demand in month t (ac-ft).}$$

Values for α tend to range from 0.7 to 2.0. For example, $\alpha = 1.2$ means that the model purchases water if the expected supply is 1.2 times the expected demand. A value of $\alpha > 1$ means the model purchases water before the supply becomes less than demand. A value of $\alpha < 1$ is more risky since the model only purchases water if the expected supply is less than the expected demand.

Next, the city determines how much water to lease and/or exercise by comparing another ratio of expected supply-to-expected demand to a threshold value referred to as β. The city continues to purchase leases and/or exercise options until the following condition holds:

$$\frac{(\hat{N}_{L_t} + \hat{N}_X) + S_{E_{t+1}}}{\sum_{i=t+1}^{12} E[\hat{d}_i]} = \beta, \qquad \text{for} \qquad t = 0, 1, 2, \ldots, 11. \tag{2.7}$$

($\hat{N}_{L_t}$ is the volume of leases purchased at the end of each month t in ac-ft and $\hat{N}_X$ is the volume of options exercised on May 31st, t=5 in ac-ft.) The numerator which represents the total expected water supply to date consists of the volume of leases purchased in month t, options exercised, and expected water supply for the remainder of the year ($S_{E_{t+1}}$). Values for β tend to range from 0.8 to 2.5. A value of $\beta = 2$ means that the model buys enough leases to ensure the supply is twice as large as the demand.

Since options can only be exercised in month t_X, $\hat{N}_X = 0$ in every month except

t_X. Then, the volume of leases to purchase is:

$$\hat{N}_{L_t} = \beta \left(\sum_{i=t+1}^{12} E[\hat{d}_i] \right) - S_{E_{t+1}}, \qquad \text{for} \qquad t \neq t_X. \tag{2.8}$$

During the option exercise month t_X, the city considers exercising options before purchasing leases. First, the city compares the exercise price (p_X) to the lease price ($\hat{p}_{L_t}$) of the current month t. If the lease price is less than the exercise price, then the city will purchase leases as calculated in equation 2.8. If the exercise price is less than the lease price, then the city will exercise options. The volume of options exercised is determined by the following conditions:

$$\text{If} \qquad \beta \left(\sum_{i=t+1}^{12} E[\hat{d}_i] \right) - S_{E_{t+1}} \leq N_O, \tag{2.9}$$

$$\text{then} \qquad \hat{N}_X = \beta \left(\sum_{i=t+1}^{12} E[\hat{d}_i] \right) - S_{E_{t+1}}, \tag{2.10}$$

$$\text{otherwise} \qquad \hat{N}_X = N_O. \tag{2.11}$$

(N_O is the volume of options purchased at the beginning of the year in ac-ft.) If the city needs less water than the volume of options purchased at the beginning of the year, then the water requirement can be met by exercising the volume of options equivalent to the need as in equation 2.10. On the other hand, notice that when condition 2.9 is not met, the volume of water required by the city is greater than the volume of options the city purchased early (N_O). If this occurs, then the volume of options exercised is set equal to the volume of options purchased at the beginning of the year as represented by equation 2.11. This is because the city cannot exercise

Table 2.1: How Much Water to Purchase when $t \neq t_X$

Condition	Action	Volume of Leases	Volume of Exercised Options
If $\frac{\hat{N}_{L_t}+S_{E_{t+1}}}{\sum_{i=t+1}^{12} E[\hat{d}_i]} < \beta$ ($\hat{N}_X = 0$ here.)	Purchase Leases	$\beta\left(\sum_{i=t+1}^{12} E[\hat{d}_i]\right) - S_{E_{t+1}}$	None

more options than it purchased at $t = 0$. In this situation, options alone won't meet the condition in equation 2.7 so the city will need to purchase leases. The volume of leases to purchase is determined by subtracting the volume of options exercised from the total volume of water required so condition 2.7 is met:

$$\hat{N}_{L_t} = \beta\left(\sum_{i=t+1}^{12} E[\hat{d}_i]\right) - S_{E_{t+1}} - \hat{N}_X, \qquad \text{for} \qquad t = t_X. \tag{2.12}$$

Table 2.1 and Table 2.2 provide a summary of the conditions needed to make decisions on how much water to lease or options to exercise.

Now that the number of leases to purchase has been calculated, we can incorporate leases for month t into the calculation of supply for month t. We rewrite equations 2.5 and 2.6 to account for the change in index from $t+1$ to t and the lease purchases of month t:

$$S_t = \sum_{i=0}^{t-1} \hat{N}_{r_i} + \sum_{i=0}^{t-1} \hat{N}_{L_i} - \sum_{i=1}^{t-1} u_i, \qquad \text{for} \quad t = 1, 2, \ldots, t_X. \tag{2.13}$$

Table 2.2: How Much Water to Purchase when $t = t_X$

Condition	Action	Volume of Leases	Volume of Exercised Options
If $\hat{p}_{L_t} < p_X$	Purchase Leases	$\beta\left(\sum_{i=t+1}^{12} E[\hat{d}_i]\right) - S_{E_{t+1}}$	None
If $\hat{p}_{L_t} > p_X$	Exercise Options as follows		
	Until $\frac{\hat{N}_X + S_{E_{t+1}}}{\sum_{i=t+1}^{12} E[\hat{d}_i]} = \beta$ or $\hat{N}_X = N_O$	None	$\beta \sum_{i=t+1}^{12} E[\hat{d}_i] - S_{E_{t+1}}$ or N_O
	If $\hat{N}_X = N_O$ and $\frac{\hat{N}_X + S_{E_{t+1}}}{\sum_{i=t+1}^{12} E[\hat{d}_i]} < \beta$ Then Purchase Leases until $\frac{\hat{N}_{L_t} + \hat{N}_X + S_{E_{t+1}}}{\sum_{i=t+1}^{12} E[\hat{d}_i]} = \beta$	$\beta\left(\sum_{i=t+1}^{12} E[\hat{d}_i]\right) - S_{E_{t+1}} - \hat{N}_X$	N_O

or as:

$$S_t = \sum_{i=0}^{t-1} \hat{N}_{r_i} + \sum_{i=0}^{t-1} \hat{N}_{L_i} - \sum_{i=1}^{t-1} u_i + \hat{N}_X, \qquad \text{for } t = t_X + 1, t_X + 2, \ldots, 12. \quad (2.14)$$

There can be different values of α and β associated with different periods of time throughout the year, such as with each season or with each month. In this simulation, there are two sets of these threshold values: (α_1, β_1) and (α_2, β_2). The first set is used for the months up until options can be exercised which are months $t = 0$ to $t = t_X - 1$. The second set is used for the rest of the year, months $t = t_X$ to $t = 11$.

2.1.7 Failures, Critical Failures, and Reliability

Now, the city's available water supply for month t (S_t) accounts for the allocation of water and the lease purchases/exercised options minus the city's usage up until the previous month (month $t-1$). This value for water supply is compared to the city's water demand in month t ($\hat{d}_t$) which is randomly sampled. The comparison signals if a failure or critical failure occurred. A failure is a water shortfall for the month (i.e. $S_t < \hat{d}_t$). At any given month, when the city's available water supply cannot meet the demand, then the city's usage is equal to the supply ($u_t = S_t$) and there is a shortfall of $\hat{d}_t - S_t$. A critical failure is a water shortfall for the month and $\frac{S_t}{\hat{d}_t} \leq 0.6$. (This is a reasonable definition for critical failure. A supply to demand ratio above 0.6 represents the voluntary conservation of water by not watering lawns or washing cars. A ratio below 0.6 represents the point at which an economic impact could occur and businesses may need to reduce operating hours or shut down.) Otherwise, supply can meet the demand ($S_t \geq \hat{d}_t$), then usage equals demand ($u_t = \hat{d}_t$). The simulation keeps track of the number of failures and critical failures.

During a 12-month run, the simulation will calculate the city's monthly allocation of water, the monthly water supply before and after lease purchase/option exercise decisions are made, the expected water supply for the remainder of the year, and the volumes of leases to purchase and options to exercise, as well as keep track of failures and critical failures. Given a scenario with initial conditions and decision variables defined, each realization of the model outputs the cost and reliability of a city's water portfolio. Recall that the initial conditions are: reservoir level at $t = 0$ (R_0) and the amount of water the city has carried over from the previous year (N_{r_0}).

The decision variables are: volume of permanent rights (N_{R_T}), volume of options purchased at $t = 0$ (N_O), and threshold values one and two to make decisions on lease purchases/options exercised and amount of water to purchase/exercise (α_1, β_1, α_2, β_2). This process repeats year after year. The expected annual cost and expected reliability (defined for the first time below) are determined after n realizations of the simulation.

$$\begin{aligned} E[\text{Annual Cost}] &= \frac{1}{n}\sum_{i=1}^{n}\left(N_{R_T}p_R + N_O p_O + E[\hat{N}_X]p_X + E\left[\sum_{t=0}^{11}\hat{N}_{L_t}\hat{p}_{L_t}\right]\right)_i \\ E[r_f] &= 1 - \left(\frac{\text{failures}}{12\cdot\text{years}}\right) \end{aligned} \tag{2.15}$$

where,

$$\begin{aligned} \text{failures} &= \text{number of months when } S_t < \hat{d}_t \\ r_f &= \text{monthly reliability against a failure;} \\ \text{years} &= \text{number of simulated years (i.e. annual runs).} \end{aligned}$$

After the computations, reliability is a number between 0 and 1 which indicates the ratio of the number of months that the city's water supply is greater than or equal to its demand to the number of simulated years times 12 months/year. In other words, reliability is an indicator of how often the city will be able to meet its demand.

Acceptable reliability ranges from .995 (which is one failure every 16.7 years) to .98 (which is one failure every 4.2 years). In [13], we applied the three values: .98, .99, .995 (see section 5.3). Expected reliability with respect to critical failures ($E[r_{cf}]$) is calculated similarly:

$$E[r_{cf}] = 1 - \left(\frac{\text{critical failures}}{12 \cdot \text{years}} \right) \tag{2.16}$$

where,

$$\begin{aligned} \text{critical failures} &= \text{number of months when } S_t < \hat{d}_t \text{ and } \frac{S_t}{\hat{d}_t} \leq 0.6 \\ r_{cf} &= \text{monthly reliability against a critical failure;} \\ \text{years} &= \text{number of simulated years (i.e. annual runs).} \end{aligned}$$

Acceptable reliability with respect to critical failures is .995.

2.1.8 Cost Variability

After many simulation runs of the 12-month cycle, the result is a distribution of the annual portfolio costs as mentioned above. This next paragraph focuses on the cost variability aspect. Cost variability is an indicator of the risk associated with very high portfolio costs.

A few definitions of terms are required here: Value at Risk and Conditional Value at Risk. These financial terms are used in the electricity and natural gas industries, among others, and have a similar application here. Generally speaking, Value at Risk (VAR) is the total risk in a portfolio of financial assets. A financial manager can be

X% certain that the highest dollar amount to lose is no more than the VAR measure. In this application, VAR is defined as the maximum amount of money a portfolio will cost 95% of the time. Now assume that the $(100 - X)\%$ worst-case event occurred. The next thought is to ask how much is the expected loss. Conditional Value at Risk (CVAR) is the average amount lost when the worse scenario happens. In this application, CVAR is defined as the expected dollar amount a portfolio will cost if the VAR measure is exceeded. So, given the distribution of annual portfolio costs, CVAR is calculated as the mean of the annual costs falling above the 95th percentile [13], [32] .

2.1.9 Alternatives Studied

This section briefly defines the alternatives studied for this first problem. Strategy A involves permanent rights only. There is only one decision variable, the total volume of permanent rights (N_{R_T}). Strategy B includes permanent rights and options. When strategy B is studied, there are four decision variables: the total volume of permanent rights (N_{R_T}), volume of options purchased before the start of the year (N_O), and the threshold values for purchasing decisions and water volume decisions (α_2, β_2) after option exercise month t_X. Strategy C includes all three means of water transfers: permanent rights, options, and leases. The analysis of this alternative includes six decision variables. They include the same four from Strategy B with the addition of two others: the threshold values for purchasing decisions and water volume decisions (α_1, β_1) before option exercise month t_X.

2.2 Optimization

The output of the above model is an expected annual cost. The prices for permanent rights p_R, options p_O, and exercised options p_X remain constant. Since N_{R_T} and N_O are inputs, the model can calculate the first two terms ($N_{R_T} \cdot p_R + N_O \cdot p_O$) of the cost function. The model randomly selects the lease price ($\hat{p}_{L_t}$) in month t from lease price data. The model also determines the volume of exercised options ($\hat{N}_X$) and purchased leases ($\hat{N}_{L_t}$) by using the expected supply-to-expected demand ratio and threshold values α and β as mentioned earlier. Because $\hat{N}_X$, $\hat{N}_{L_t}$, and $\hat{p}_{L_t}$ are random variables, the last two terms ($E[\hat{N}_X] \cdot p_X + E\left[\sum_{t=1}^{12} \hat{N}_{L_t} \cdot \hat{}_{L_t}\right]$) vary from one model run to the next. So, the model runs many times, say 10,000 times. The model computes the average of the annual costs from the 10,000 runs and also outputs expected reliability, expected critical reliability, and CVAR. Now that the model can evaluate the cost function, the second step is to identify the strategy resulting in least cost. So, for n realizations of the model, we want to minimize the expected annual cost ($x = N_{R_T}, N_O, \alpha_1, \beta_1, \alpha_2, \beta_2$):

$$\begin{aligned}
\text{Minimize } Z &= \min_x E[\text{Annual Cost}] \\
&= \min_x \frac{1}{n} \sum_{i=1}^{n} (\text{Annual Cost})_i \\
&= \min_x \frac{1}{n} \sum_{i=1}^{n} \left(N_{R_T} p_R + N_O p_O + E[\hat{N}_X] p_X + E\left[\sum_{t=0}^{11} \hat{N}_{L_t} \hat{p}_{L_t} \right] \right)_i
\end{aligned}$$

such that:

$$\begin{aligned} E[r_f] &\geq \text{monthly reliability threshold, } \in [0,1]; \\ E[r_{cf}] &\geq \text{monthly critical reliability threshold, } \in [0,1]. \\ \frac{\text{CVAR}}{E[\text{Annual Cost}]} &\leq \text{cost risk threshold, } \in [1,\infty). \end{aligned}$$

The expected annual cost is minimized. The objective function can be represented by an optimization landscape where expected annual cost is plotted against permanent rights and options ($\alpha_1, \beta_1, \alpha_2, \beta_2$ are held constant). The average of the 10,000 cost evaluations is plotted for one pair of values of permanent rights and options. The model runs again with the same set of initial conditions but a different pair of values for permanent rights and options. The result of repeating this process is a mesh of expected annual costs that generates the optimization landscape.

The feasible region is determined by the chosen values for permanent rights and options to build the optimization landscape and the reliability and CVAR constraints which can be set by the user. In [13], we set the reliability to three different values: .98, .99, .995. We studied strategies in which we set the CVAR constraint to 1.1 and other strategies in which we didn't use the CVAR constraint. (See section 5.3.) The values used for permanent rights were in the range of 20,000 acre-feet to 50,000 acre-feet. The values used for options were in the range of 0 acre-feet to 10,000 acre-feet.

The randomness appears in the lease price and in the determination of the expected volumes of options exercised and leases purchased. This is noise (small oscillations in function values) in the optimization landscape and can be seen when the use of exercised options and purchased leases in the portfolio are large. Otherwise, when these volumes are small and the portfolio relies mostly on permanent rights, the landscape is relatively smooth.

The reliability constraints (as defined in Failures, Critical Failures, and Reliability in section 2.1.7) affect whether a certain data point for an expected annual cost is part of the feasible region. The expected reliability and critical reliability for each expected annual cost data point is calculated and compared to the required threshold. If the calculated reliability is less than the required reliability threshold (which is set by the user), then the associated expected annual cost is not in the feasible region. This could cause gaps in the optimization landscape, which, if not treated with careful consideration, could result in the optimizer pointing to a non-minimum cost.

The ratio of CVAR to the expected annual cost (defined in Cost Variability in section 2.1.8) is another constraint in which the threshold is set by the user. When this ratio is close to 1, the risk for variability in the expected annual cost becomes less. In other words, the risk for very high annual costs to actually occur becomes less. So, for portfolios with only permanent rights, there is no variability in cost. The introduction of options and leases into the portfolio causes variability in cost due to the randomness mentioned above.

2.3 Study Region

The given study region is the United States side of the Lower Rio Grande Valley (LRGV) located in the southern tip of Texas. See figure 2.1. The region's water supply comes mostly from the Rio Grande River which flows into the Falcon and Amistad reservoirs. The Treaty of 1944 provides for the distribution of water between the United States and Mexico [54]. The two reservoirs are treated as one system. So, the collection of data and calculation of variables is conducted under the assumption there is one reservoir. There is an instream loss factor (see Calculating Supply in section 2.1.5) which accounts for the loss of water between the two reservoirs because they are separated by approximately 350 miles [55]. The LRGV consists of nearly 1600 water rights owners. Water allocations and transfers are controlled by the Rio Grande Watermaster's Office [13]. The Rio Grande Watermaster's Office is part of a state environmental agency called the Texas Commission on Environmental Quality.

2.3.1 Hydrologic Data

The collection of the hydrologic data, as mentioned in section 2.1, occurred from 1970 - 2002, after the completion of the Amistad dam in 1968 [13].

One might expect that outflows would be related to and depend on inflows. But in the LRGV, Ramsey [51] found that reservoir inflows and outflows are poorly correlated and considered them independent. This poor correlation and independence may exist because the inflows that are used by the water rights holders of the LRGV originate from precipitation that occurs in north central Mexico located hundreds of miles away [13].

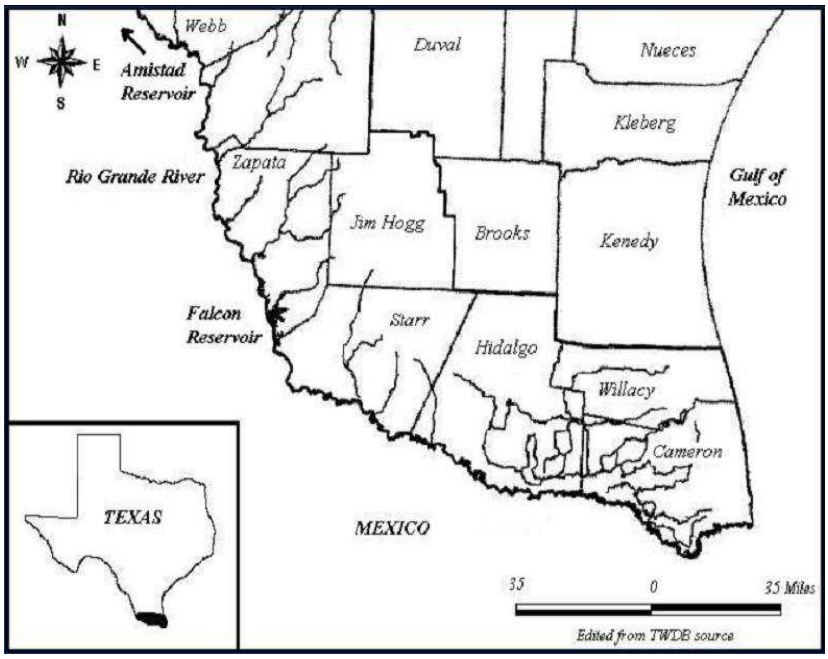

Figure 2.1: Lower Rio Grande Valley

Also, one might expect the inflows data collected to represent some rainfall distribution. But, it is difficult to estimate illegal water use (human interference not in accordance with the treaty) before it reaches the LRGV. This would certainly affect the volume of water flowing downstream that the LRGV receives. And there is the matter of having only 33 data points. These reasons foreshadow that a standard statistical distribution does not exist for the hydrologic data. Ramsey [51] tested the data sets for inflows, outflows, and losses to find out how well they fit an expected set of data. The test showed no approximation to a statistical distribution [51]. Therefore the values required by the simulation were sampled directly from the data sets [13].

2.3.2 Initial Conditions

The initial reservoir storage, R_0, and the city's initial allocation of water, N_{r_0} are set at $t = 0$ as mentioned in section 2.1. The initial reservoir storage ranges from 0.8 to 2.2 million acre-feet. The initial allocation is calculated as:

$$N_{r_0} = f_{R_0} \cdot N_{R_T},$$

where

f_{R_0} = fraction of permanent water rights allocated at the beginning of the year;

N_{R_T} = total volume of permanent water rights held by the city.

Three values were chosen for f_{R_0} (0.1, 0.3, 0.5) and R_0 (0.8, 1.5, 2.2 million acre-feet). The different combinations represent the possible range of initial conditions from low to normal to high. A high (or low) initial reservoir level doesn't necessarily correspond to a high (or low) initial allocation of water. The LRGV receives most of its inflows during the Fall resulting in the city's ability to carry over a large volume of water as its initial allocation for the following year. This situation can occur even if the reservoir level is low. So, the different pairs of f_{R_0} and R_0 considers these potential events [13].

2.3.3 Supply and Demand in the LRGV

Supply is calculated as described in equations 2.5 and 2.6 in section 2.1. Recall that the city's monthly allocation of water ($\hat{N}_{r_t}$) needs to be determined (equation 2.4) using the total volume of regional water rights, $\bar{N}_R$, and the new water, $\hat{n}_t$. For the LRGV region, $\bar{N}_R$ is 1.9 million acre-feet. As in equation 2.3, new water is calculated using the instream loss factor for the LRGV ($l_I = 0.175$). On average, the model allocates about 0.725 acre-feet of water for every 1 acre-foot of water rights since the regional water rights out numbers the new water flowing into the reservoir system [13].

The water use by municipalities increased from 7% to 13% of the LRGV region's total during the data collection period. Even though there was an increase in municipal use, the patterns in average annual usage and monthly usage did not change. The water demand for the city referred to throughout the study is based on the usage records for Brownsville, Texas which has a population of 120,000 and an average

demand of approximately 21,000 acre-feet per year [13].

2.3.4 Water Market in the LRGV

The municipal population in the LRGV is growing and is expected to double by 2050. The agricultural community accounts for 85% of the LRGV region's water use and utilizes most of this water towards the low-value irrigation of crops such as cotton. There is a large economic motivation for the agriculturalists to transfer water to the high-valued urban use [13],[12], [27].

In recent years, the LRGV water market has operated relatively efficiently and allows permanent rights transfers from the agriculturalists to the municipalities [12], [27]. Even though permanent rights transfers are usually approved, the approval process can take more than a year due to the critical regulatory process. Lease transfers undergo less scrutiny because there tends to be less impacts on third parties. So, the approval process for the lease transfers is much simpler and occurs in a few days [28]. The Watermaster only requires the seller and buyer to send a one page document with their account numbers and volume of water to be transferred (and price information is optional). This simplified process promotes high water market activity. In fact, the Rio Grande Watermaster's Office has logged an average of 70,000 acre-feet of water in lease transfers per year from 1994-2002 [47].

Current regulation in the LRGV water market allows permanent rights to be transferred from the agricultural community to the municipalities, but lease transfers are only allowed between similar user types. This means that only urban users can transfer water via leases to other urban users and the same for the agricultural

community, resulting in two lease markets [14]. The municipal market is less active than the agricultural market which logged 1514 lease transfers from 1994–2002 with an average price of $22.60 per acre-foot. Cities tend to prefer to hold onto their water rights, even if the demand falls way below the supply. The South Central Texas Regional Water Planning Group 2000 is attempting to change the current legislation to allow leasing between the agricultural community and municipalities. When this occurs, the lease market is expected to behave similar to the agricultural market. So, this study assumes that the lease prices from the agricultural market represent the agricultural-to-urban market [13].

2.3.5 Lease Prices in the LRGV

As mentioned in Data Sets Defined in section 2.1.1, analysis was conducted to investigate the relationship between the lease prices and certain hydrologic parameters: reservoir level, inflows, and outflows. Analysis showed there are two populations of lease data: one when the reservoir level is below 1.43 million acre-feet and another when the level is above 1.43 million acre-feet. So the monthly lease prices which are separated into the data set for high reservoir levels tend to be lower than those in the set for low reservoir levels [51].

2.3.6 Option Contracts in the LRGV

Currently, the LRGV does not incorporate option contracts into their water market, but the LRGV water planning group is considering to add option contracts. The

model uses the European call option where the option contract is purchased on December 31st ($t = 0$) and exercised on May 31st ($t = 5$). This date was chosen since it occurs before the heavy usage months for both the agricultural community and the municipalities. Summer is the time of year for growing crops and gardens, watering lawns, washing cars, filling pools, etc.

A risk-neutral approach is used in pricing options [6]. So, the expected value an option provides relative to a lease, does not exceed the option's price [31]. The price of a European call option (p_O) is calculated by discounting the option's expected value on the call date back to the point at which the option is purchased, such that

$$p_O = e^{-rT} \cdot E[max(\hat{p}_{L_t} - p_X, 0)] \tag{2.17}$$

where,

$$\begin{aligned} r &= \text{discount rate (monthly);} \\ T &= \text{period between purchase and exercise date (months).} \end{aligned}$$

In this simulation of the LRGV water market, the conditional probability of the reservoir level in May (R_5) being above or below 1.43 million acre-feet (MAF) is computed given the initial reservoir level (R_0). This information is used to determine the option price subject to R_0 and equation 2.17 becomes:

$$
\begin{aligned}
p_{O|R_0} &= e^{-r5} \cdot P[R_5 \geq 1.43\text{MAF}|R_0] \cdot E[max(\hat{p}^a_{L_5} - p_X, 0)] \\
&\quad + e^{-r5} \cdot P[R_5 < 1.43\text{MAF}|R_0] \cdot E[max(\hat{p}^b_{L_5} - p_X, 0)]
\end{aligned}
$$

where,

$\hat{p}^a_{L_5}$ = spot market lease price for May when reservoir level is below 1.43 MAF;

$\hat{p}^b_{L_5}$ = spot market lease price for May when reservoir level is above 1.43 MAF.

The exercise price of options (p_X) is constant at \$15 per ac-ft. This results in option prices of \$13.26, \$11.36, and \$2.18 per ac-ft when the initial reservoir levels are 0.8, 1.5, and 2.2 MAF respectively.

2.3.7 Annualized Price of Permanent Rights in the LRGV

The annualized price of permanent rights (p_R) is \$22.60 per ac-ft. As mentioned above in Supply and Demand in the LRGV (section 2.3.3), only about 0.725 ac-ft of the permanent rights are allocated on average, so the annualized price becomes \$31.17 per ac-ft.

2.4 Summary of Variables

User Specified Parameters (These variables are specified by the user to define the scenario.)

R_0 = reservoir level at beginning of the year, t=0 (ac-ft);

f_{R_0} = fraction of permanent water rights allocated at the beginning of the year;

N_{r_0} = initial allocation of water at the beginning of the year (ac-ft) which is equivalent to $f_{R_0} * N_{R_T}$.

Known Parameters (These are constant values.)

p_R = annualized price for permanent water rights (dollars/ac-ft);

p_X = exercise price of options (dollars/ac-ft);

t_X = the month that options are exercised on;

$\bar{N}_R$ = total volume of regional water rights (ac-ft).

Decision Variables (These variables are optimized.)

N_{R_T} = total volume of permanent water rights held by the city (ac-ft);

N_O = volume of options purchased before the start of the year, t=0 (ac-ft);

α_1, α_2 = Purchase decision factor;

β_1, β_2 = Water volume decision factor.

Random Variables

$\hat{i}_t$ = volume of reservoir inflows in month t (ac-ft)
(This is a historical data set.);

$\hat{l}_t$ = volume of reservoir losses in month t (ac-ft)
(This is a historical data set.);

$\hat{o}_t$ = volume of reservoir outflows in month t based on historical data (ac-ft);

$\hat{p}_{L_t}$ = lease price at the end of month t (dollars/ac-ft)
(This is a historical data set;)

$\hat{d}_t$ = city's water demand in month t based on historical data (ac-ft).

Random Variables (These random variables are calculated as functions of the above random variables. Equations to calculate these variables are referenced.)

$\hat{n}_t$ = new inflows available for distribution in month t to all permanent rights holders of the study region (ac-ft) (Equation 2.3);

$\hat{N}_{r_t}$ = new allocation of water to the city in month t (ac-ft) (Equation 2.4);

$\hat{N}_{L_t}$ = volume of leases purchased at the end of the month t (ac-ft) (Tables 2.1 and 2.2);

$\hat{N}_X$ = volume of options exercised on May 31st, t=5 (ac-ft) (Tables 2.1 and 2.2);

Calculated Values (Equations to calculate these variables are referenced.)

R_t = reservoir level at the end of month t (ac-ft) (Equation 2.2);

S_{t+1} = volume of water available for the city's use in month t+1 (ac-ft) (Equations 2.5 and 2.6);

$S_{E_{t+1}}$ = the city's expected water supply over the remainder of the year (ac-ft) (Equation 2.7);

u_t = city's water usage in month t (ac-ft) which is determined from comparing supply S_t (Equations 2.13 and 2.14) to demand $\hat{d}_t$;

p_O = price of options (dollars/ac-ft) (Equation 2.17).

Chapter 3

Review of Mathematical Concepts

The purpose of this chapter is to review mathematical concepts required to understand the optimization technique called implicit filtering when applied to a bound constrained problem. First, we review fundamentals in unconstrained optimization: necessary and sufficient conditions for local minima, line search methods, method of steepest descent, quasi-Newton methods, and the convergence theories for these methods. Then, we review constrained optimization. In particular, we focus on bound constrained optimization. This requires new definitions of necessary and sufficient conditions for local minima. Bound constrained problems also use the methods discussed in the unconstrained section, with modifications. We also review convergence theory.

3.1 Fundamentals in Unconstrained Optimization

3.1.1 Introduction

The goal of unconstrained optimization is to minimize a function $f(x)$, also referred to as the objective function, for all $x \in \mathbb{R}^n$:

$$\min_x f(x). \tag{3.1}$$

This means that the solution to 3.1 is a point $x^* = (x_1, x_2, ...x_n)^T$ such that

$$f(x^*) \leq f(x) \quad \text{for all } x \in \mathbb{R}^n. \tag{3.2}$$

Equation 3.2 defines a global minimizer whereas a local minimizer is the solution x^* to 3.1 such that

$$f(x^*) \quad \leq \quad f(x) \quad \text{for } x \text{ near } x^*.$$

Formal definitions follow:

Definition 3.1. *The function $f(x)$ has a global minimum at x^* if*

$$f(x^*) \leq f(x)$$

for all $x \in \mathbb{R}^n$.

Definition 3.2. *The function $f(x)$ has a local minimum at x^* if there exists an $\varepsilon > 0$ such that*

$$f(x^*) \leq f(x)$$

for all points such that $0 \leq \|x^* - x\| < \varepsilon$.

3.1.2 Necessary and Sufficient Conditions

Necessary Conditions

Let $f(x) \in \mathbb{C}^2$, meaning $f(x)$ is twice continuously differentiable. For x^* to be a local minimum, it is necessary that the gradient of $f(x)$ is zero at x^* and the Hessian matrix of $f(x)$ at x^*, denoted as $\nabla^2 f(x^*)$, is positive semidefinite:

$$\begin{aligned} &(1) \quad \nabla f(x^*) = 0; \\ &(2) \quad y^T \nabla^2 f(x^*) y \geq 0, \text{for all nonzero } y \in \mathbb{R}^n. \end{aligned}$$

This can be shown, as Murray did [45], using the Taylor expansion of $f(x)$ about x^*. To show condition (1), let $f(x) \in \mathbb{C}^1$, then

$$\begin{aligned} f(x^* + \varepsilon y) &= f(x^*) + \varepsilon \nabla f(x^*)^T y + O(\varepsilon^2) \\ f(x^* + \varepsilon y) - f(x^*) &= \varepsilon \nabla f(x^*)^T y + O(\varepsilon^2) \end{aligned} \tag{3.3}$$

where $y \in \mathbb{R}^n$ is given and ε is sufficiently small.

For ε sufficiently small and x^* a local minimum,

$$f(x^* + \varepsilon y) \geq f(x^*) \tag{3.4}$$

$$f(x^* + \varepsilon y) - f(x^*) \geq 0 \tag{3.5}$$

Use 3.3 to obtain:

$$\varepsilon \nabla f(x^*)^T y + O(\varepsilon^2) \geq 0$$

$$\nabla f(x^*)^T y + O(\varepsilon) \geq 0 \tag{3.6}$$

Let $\varepsilon = 0$ and choose $y = -\nabla f(x^*)$. Equation 3.6 becomes:

$$-\nabla f(x^*)^T \nabla f(x^*) \geq 0$$

$$\|\nabla f(x^*)\|^2 = 0$$

which implies that $\nabla f(x^*) = 0$.

To show condition (2), let $f(x) \in \mathbb{C}^2$, then

$$f(x^* + \varepsilon y) = f(x^*) + \varepsilon \nabla f(x^*)^T y + \frac{1}{2}\varepsilon^2 y^T \nabla^2 f(x^*) y + O(\varepsilon^3)$$

Knowing that $\nabla f(x^*) = 0$,

$$\begin{aligned} f(x^* + \varepsilon y) &= f(x^*) + \frac{1}{2}\varepsilon^2 y^T \nabla^2 f(x^*) y + O(\varepsilon^3) \\ f(x^* + \varepsilon y) - f(x^*) &= \frac{1}{2}\varepsilon^2 y^T \nabla^2 f(x^*) y + O(\varepsilon^3) \end{aligned} \tag{3.7}$$

Equations 3.4 and 3.5 apply here, so equation 3.7 continues:

$$\begin{aligned} \frac{1}{2}\varepsilon^2 y^T \nabla^2 f(x^*) y + O(\varepsilon^3) &\geq 0 \\ \frac{1}{2} y^T \nabla^2 f(x^*) y + O(\varepsilon) &\geq 0 \end{aligned}$$

Let $\varepsilon = 0$:

$$\frac{1}{2} y^T \nabla^2 f(x^*) y \geq 0$$

which indicates that $\nabla^2 f(x^*)$ is positive semidefinite.

Sufficient Conditions

Let $f(x) \in \mathbb{C}^2$ and $\nabla f(x^*) = 0$. For x^* to be a local minimum, it is sufficient that $\nabla^2 f(x^*)$ is positive definite:

$$y^T \nabla^2 f(x^*) y > 0 \text{ for all nonzero } y \in \mathbb{R}^n.$$

Nocedal and Wright [46] show this as follows. Since the Hessian is continuous and positive definite at x^*, choose a radius $r > 0$ and define an open ball $\mathcal{B} =$

$\{x|\ \|x - x^*\| < r\}$ such that $\nabla^2 f(x^*)$ is positive definite for all x. Choose a nonzero vector y such that $\|y\| < r$ and $x^* + y \in \mathcal{B}$, for some $\varepsilon \in (0, 1)$.

$$f(x^* + y) \quad = \quad f(x^*) + y^T \nabla f(x^*) + \frac{1}{2} y^T \nabla^2 f(x^* + \varepsilon y) y$$

Since $\nabla f(x^*) = 0$,

$$f(x^* + y) \quad = \quad f(x^*) + \frac{1}{2} y^T \nabla^2 f(x^* + \varepsilon y) y.$$

Knowing $x^* + \varepsilon y \in \mathcal{B}$ implies that $y^T \nabla^2 f(x^* + \varepsilon y) y > 0$, then

$$f(x^* + y) \quad > \quad f(x^*)$$

and x^* is a minimum.

Summary

If x^* is a local minimizer of $f \in \mathbb{C}^2$, then $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*)$ is positive semidefinite. The converse need not be true. It is possible for $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*)$ to be positive semidefinite, and x^* not to be a minimizer. Consider $f(x) = -x^4$ in which the necessary conditions hold at $x^* = 0$ but it is a maximizer. A strictly positive second derivative will ensure a minimizer. So, if $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*)$ is positive definite for $f \in \mathbb{C}^2$, then x^* is a local minimizer of f. Since positive definiteness is a sufficient condition, it is possible for x^* to be a minimizer and fail this sufficient condition. Consider $f(x) = x^4$ where $x^* = 0$ is a minimizer, yet $\nabla^2 f(x^*) = 0$ and is not positive definite.

3.1.3 Line Search Methods

Now that we understand the conditions for a local minimum, we look at ways to find the minimum of an objective function $f(x)$ given a starting point. This section discusses the general class of methods that uses a line search to find the minimum. Line search methods move from one point to another searching for the x that possibly gives the lowest function value. Line search methods are defined as an iterative process.

As described in [45], [50], and [34], the following iterative process can be used to solve the minimization problem posed in 3.1:

$$x_+ = x_c + \lambda_c d_c \tag{3.8}$$

where,

$$\begin{aligned} x_+ &= \text{the new iteration;} \\ x_c &= \text{the current iteration;} \\ \lambda_c &= \text{the step length in the direction } d_c \\ &\quad \text{which is chosen to minimize } f(x_c + \lambda_c d_c) \text{ with respect to } \lambda_c; \\ d_c &= \text{the direction from } x_c \text{ to move in.} \end{aligned}$$

Line search methods choose a direction d_c then search along this direction from the current iterate x_c for a new iterate x_+ with a lower function value. The method needs to determine how far (called the step length λ_c) to move along that direction. The

line search applies a step length $\lambda_c > 0$ found by solving the following minimization problem:

$$\min_{\lambda>0} f(x_c + \lambda d_c). \tag{3.9}$$

Solving equation 3.9 exactly can be time-consuming and unnecessary so line search methods may opt to find an approximation to equation 3.9. Once the new iterate is found, a new direction and step length are computed and the process repeats.

There are various ways to construct the direction d_c and determine the step length λ_c, each with different convergence results and calculation time. In general, the idea to move in a direction in which the function decreases makes sense in order to find a minimum x^* within a specific accuracy.

Determine the Direction

Nocedal and Wright [46] indicate that most line search methods require d_c to be a descent direction, one in which $d_c^T \nabla f(x_c) < 0$. A choice of d_c in this manner will reduce the function assuming the step length is sufficiently small as shown next. It is known that

$$d_c^T \nabla f(x_c) = \|d_c\| \|\nabla f(x_c)\| \cos\theta_c. \tag{3.10}$$

When d_c is a descent direction, the angle θ_c between d_c and $\nabla f(x_c)$ has $\cos\theta_c < 0$ and so

$$d_c^T \nabla f(x_c) < 0. \tag{3.11}$$

From Taylor's theorem (see theorem B.2),

$$f(x_c + \lambda d_c) = f(x_c) + \lambda d_c^T \nabla f(x_c) + O(\lambda^2). \tag{3.12}$$

Using condition 3.11 and equation 3.12, observe that

$$f(x_c + \lambda d_c) < f(x_c)$$

for all sufficiently small $\lambda > 0$. Indeed, the function f is reduced along the direction chosen to meet condition 3.11.

The search directions can be of the form

$$d_c = -B_c^{-1} \nabla f(x_c), \tag{3.13}$$

where B_c is a symmetric, nonsingular matrix. This direction does meet condition 3.11 when B_c is positive definite:

$$\begin{aligned} d_c^T \nabla f(x_c) &= (-B_c^{-1} \nabla f(x_c))^T \nabla f(x_c) \\ &= -\nabla f(x_c)^T B_c^{-1^T} \nabla f(x_c) \\ &= -\nabla f(x_c)^T B_c^{T^{-1}} \nabla f(x_c) \\ &= -\nabla f(x_c)^T B_c^{-1} \nabla f(x_c) \\ &< 0 \end{aligned}$$

The method of steepest descent which is described below in section 3.1.4 uses the

Identity matrix I for B_c. In quasi-Newton methods (see section 3.1.5), B_c is an approximation to the Hessian that is updated every iteration.

Determine the Step Length

The step length should be chosen so that the function value sufficiently decreases to ensure the iterations make progress towards the minimum. Some line search methods use the Armijo condition [46] to define sufficient decrease in the function:

$$f(x_c + \lambda_c d_c) - f(x_c) < \alpha \lambda_c \nabla f(x_c)^T d_c, \tag{3.14}$$

where $0 < \alpha < 1$. Nocedal and Wright [46] mention that in general, line search methods test a sequence of possible step length values to find the one meeting the specified condition.

3.1.4 Method of Steepest Descent

The method of steepest descent is a line search method that uses direction $d_c = -\nabla f(x_c)$. So, from the iterative process of equation 3.8, the steepest descent method is:

$$x_+ = x_c - \lambda_c \nabla f(x_c). \tag{3.15}$$

Steepest Descent Direction

The direction of steepest descent is $d = -\nabla f(x)$. Nocedal and Wright [46] verify this by first looking at Taylor's theorem. From Taylor's theorem, for any search direction

d and step length λ, and for some $\varepsilon \in (0,1)$,

$$f(x_c + \lambda d) \quad = \quad f(x_c) + \lambda d^T \nabla f(x_c) + \frac{1}{2}\lambda^2 d^T \nabla^2 f(x_c + \varepsilon d) d.$$

The rate of change in f along the direction d at x_c is the coefficient of λ which is $d^T \nabla f(x_c)$. Now, to find the unit direction d with the fastest decrease (the steepest negative slope), solve

$$\min_d d^T \nabla f(x_c), \qquad \text{where } \|d\| = 1.$$

From equation 3.10, the problem to solve is

$$\min_d \|d\| \|\nabla f(x_c)\| \cos\theta,$$

where $\|d\| = 1$ and θ is the angle between d and $\nabla f(x_c)$. So to solve

$$\min_d \|\nabla f(x_c)\| \cos\theta,$$

$\cos\theta$ must attain its minimum value of -1, meaning $\theta = \pi$ radians is the angle between d and $\nabla f(x_c)$. This occurs when the unit direction is

$$d = -\frac{\nabla f(x_c)}{\|\nabla f(x_c)\|}.$$

Step Length

Next, the step length is determined. Backtracking is an approach where the sufficient decrease condition is tested with a choice of λ. If the condition fails, then λ is reduced. The process continues until a λ is found to meet the condition.

One way to reduce λ is described by Kelley [34]. Let $\lambda = \beta^m$, where $\beta \in (0, 1)$ and $m \geq 0$ is the smallest nonnegative integer such that the sufficient decrease condition for $f(x)$ holds:

$$f(x_+) - f(x_c) < -\alpha\lambda\|\nabla f(x_c)\|^2 \tag{3.16}$$

where $0 < \alpha < 1$ is an arbitrarily chosen constant. According to Kelley [34], $\alpha = 10^{-4}$ is normal for this parameter. The following steps are used to determine λ_c, assuming x_c is known:

1. Start with a λ such that $\lambda = \beta^m$, where $\beta \in (0, 1)$ and $m \geq 0$.
2. Calculate $\nabla f(x_c),\ x_+,\ f(x_c),\ f(x_+)$.
3. Check the sufficient decrease condition 3.16.
4. If 3.16 holds, then take $\lambda = \lambda_c$.
5. If 3.16 does not hold, then reduce λ until 3.16 does hold.

This approach can require too many stepsize reductions for the sufficient decrease condition to hold if β is too large or can prohibit progress of the entire method if β is too small. So the manner of stepsize reduction can affect the algorithm.

Kelley [34] describes a general strategy to reduce the step length. If condition

3.16 fails for the current step length, λ_c, then choose λ_+ such that

$$\lambda_+ \in [\beta_{low}\lambda_c, \beta_{high}\lambda_c],$$

where $0 < \beta_{low} \leq \beta_{high} < 1$.

Algorithm for the Method of Steepest Descent

Kelley [34] provides an algorithm for the method of steepest descent:

1. For iteration $k = 1, 2, ..., k_{max}$

   (a) Calculate $f(x)$ and $\nabla f(x_c)$.

   (b) Test termination criteria such as:

$$\|\nabla f(x_c)\| \leq \tau_r \|\nabla f(x_0)\| + \tau_a$$

   where,

$$\begin{aligned} x_0 &= \text{initial iterate;} \\ \tau_r &= \text{relative error tolerance;} \\ \tau_a &= \text{absolute error tolerance.} \end{aligned}$$

   (c) Start with $\lambda = 1$ and choose a method to reduce λ until 3.16 holds.

(d) Update $x_+ = x_c + \lambda d$.

2. If iteration $k = k_{max}$ and termination test failed, then method failed within certain constraints.

Convergence of Steepest Descent Method

The goal of this section is to show, as in [34], that the steepest descent method is globally convergent, meaning that the gradient norms, $\|\nabla f(x_k)\|$, will converge to zero with any choice of an initial iterate. This is the strongest global convergence result that can be proved. The method does not guarantee convergence to a minimizer.

Kelley [34] proves this for a general line search method that uses the Armijo sufficient decrease condition 3.14. The following lemmas and theorem proves convergence for general line search methods, so it also applies to the method of steepest descent. Recall that the method of steepest descent is a line search method where symmetric positive definite B_c in equation 3.13 is taken to be the Identity matrix.

Specifically, Kelley [34] shows that if the condition numbers (see definition B.13) of the matrices B and the sequence of iterates $\{x_k\}$ produced by the line search-Armijo method remain bounded, then every limit point (see definition B.4) is a stationary point (see definition B.12). The limit point need not be unique. So, if the sequence of function values $\{f(x_k)\}$ is bounded from below, then any limit point of the sequence $\{x_k\}$ converges to a point x^* such that $\nabla f(x^*) = 0$. Kelley [34] uses the following lemmas to show this.

Lemma 3.1. *Let B be symmetric positive definite with its largest and smallest eigenvalues satisfying, $\lambda_{max} > \lambda_{min} > 0$. Then for all $z \in \mathbb{R}^n$,*

$$\frac{1}{\lambda_{max}}\|z\|^2 \leq z^T B^{-1} z \leq \frac{1}{\lambda_{min}}\|z\|^2.$$

Lemma 3.2. *Let ∇f be Lipschitz continuous with Lipschitz constant L (see definition B.5). Let $\alpha \in (0,1), x \in \mathbb{R}^n$, and B be symmetric positive definite. Let $\lambda_{max} \geq \lambda_{min} > 0$ where λ_{max} is the largest eigenvalue of B and λ_{min} is the smallest eigenvalue of B. Let $d = -B^{-1}\nabla f(x)$. Assume that $\nabla f(x) \neq 0$. Then the Armijo condition 3.14 holds for any λ such that*

$$0 < \lambda \leq \frac{2\lambda_{min}(1-\alpha)}{L\kappa(B)}, \tag{3.17}$$

where $\kappa(B)$ is the condition number of B.

This lemma states that for the given assumptions, the objective function will obtain sufficient decrease for a step length that satisfies 3.17 and the line search will terminate. In fact, the step lengths that do meet the sufficient decrease condition are bounded away from zero.

Lemma 3.3. *Let ∇f be Lipschitz continuous with Lipschitz constant L. Let the line search-Armijo method produce the sequence of iterates $\{x_k\}$ with symmetric positive matrices B_k satisfying*

$$\kappa(B_k) \leq \bar{\kappa}$$

for all k. Then the line search-Armijo iteration

$$x_{k+1} = x_k + \lambda_k d_k = x_k - \lambda_k B_k^{-1} \nabla f(x_k)$$

satisfies

$$\lambda_k \geq \bar{\lambda} = \frac{2\beta_{low}\lambda_{min}(1-\alpha)}{L\bar{\kappa}}$$

and at most

$$m = \log\left(\frac{2\lambda_{min}(1-\alpha)}{L\bar{\kappa}}\right) / \log(\beta_{high})$$

stepsize reductions will be required.

This lemma indicates there is a lower bound for the step length and that the sufficient decrease condition is met in a finite number of steps.

Theorem 3.1. *Let ∇f be Lipschitz continuous with Lipschitz constant L. Assume that for symmetric positive definite matrices B_k, there exists a $\bar{\kappa}$ and λ_{max} such that $\kappa(B_k) \leq \bar{\kappa}$ and $\|B_k\| \leq \lambda_{max}$ for all k. Then either $f(x_k)$ is unbounded from below or*

$$\lim_{k\to\infty} \nabla f(x_k) = 0$$

and any limit point of the sequence produced by the line search-Armijo method is a stationary point.

Meaning, if $f(x_k)$ is bounded from below and $x_{k_i} \to x^*$ is any convergent subsequence of $\{x_k\}$, then

$$\nabla f(x^*) = 0.$$

Proof. The sufficient decrease condition ensures that the sequence of function values $\{f(x_k)\}$ is a decreasing sequence. If $\{f(x_k)\}$ is bounded from below, then $\lim_{k\to\infty} f(x_k)$ exists and

$$\lim_{k\to\infty} f(x_{k+1}) - f(x_k) = 0. \tag{3.18}$$

The result of lemma 3.1:

$$\begin{aligned} \frac{1}{\lambda_{max}}\|z\|^2 &\leq z^T B^{-1} z \leq \frac{1}{\lambda_{min}}\|z\|^2 \\ -\frac{1}{\lambda_{max}}\|z\|^2 &\geq -z^T B^{-1} z \geq -\frac{1}{\lambda_{min}}\|z\|^2 \end{aligned}$$

can be used in the Armijo condition 3.14:

$$\begin{aligned} f(x_{k+1}) - f(x_k) &\leq -\alpha\lambda_k \nabla f(x_k)^T B_k^{-1} \nabla f(x_k) \\ &\leq -\alpha\lambda_k \frac{1}{\lambda_{max}}\|\nabla f(x_k)\|^2 \end{aligned}$$

Then apply lemma 3.3 to obtain:

$$\begin{aligned} f(x_{k+1}) - f(x_k) &\leq -\alpha\bar{\lambda}\frac{1}{\lambda_{max}}\|\nabla f(x_k)\|^2 \\ \|\nabla f(x_k)\|^2 &\leq \frac{\lambda_{max}(f(x_{k+1}) - f(x_k))}{-\alpha\bar{\lambda}} \end{aligned}$$

Using 3.18, the right hand side approaches 0 as $k \to \infty$ and so

$$\lim_{k\to\infty} \|\nabla f(x_k)\|^2 = 0$$
$$\lim_{k\to\infty} \nabla f(x_k) = 0.$$

The theorem is proved.

Let $B_k = I$ and theorem 3.1 can be applied to the method of steepest descent. So, given the above assumptions, the gradient norms converge to zero regardless of the initial iterate.

3.1.5 Quasi-Newton Methods

Quasi-Newton methods have search directions of the form

$$d_c = -B_c^{-1}\nabla f(x_c), \tag{3.19}$$

where B_c is a symmetric positive definite matrix that is an approximation to the exact Hessian matrix of $f(x)$. This matrix B_c is updated each iteration by a quasi-Newton formula which uses information from the new iterate in the update process. Basically,

1. Compute the search direction, d_c as given above in equation 3.19.
2. Find the next iterate $x_+ = x_c + \lambda_c d_c$ where the step length ensures sufficient decrease (see the Armijo condition 3.14).
3. Use a quasi-Newton formula and x_c, x_+, B_c to obtain B_+ (the updated B_c).

Two quasi-Newton formulas are described below.

Broyden, Fletcher, Goldfarb, Shanno (BFGS) Method

Kelly [34] and Nocedal and Wright [46] describe the BFGS method [9], [21], [25], [56] as follows. It satisfies the following condition, called the secant equation:

$$B_+ s_c = y_c,$$

where

$$\begin{aligned} B_+ &= \text{The matrix B at the new iterate;} \\ s_c &= x_+ - x_c; \\ y_c &= \nabla f(x_+) - \nabla f(x_c). \end{aligned}$$

The BFGS method, is defined by the formula:

$$\begin{aligned} B_+ &= B_c - \frac{B_c s_c s_c^T B_C}{s_c^T B_c s_c} + \frac{y_c y_c^T}{y_c^T s_c} \\ &= B_c - \frac{(B_c s_c)(B_c s_c)^T}{s_c^T B_c s_c} + \frac{y_c y_c^T}{y_c^T s_c}. \end{aligned} \tag{3.20}$$

Observe that the difference between B_+ and B_c is a rank-two matrix. The BFGS formula generates a symmetric positive definite matrix whenever the initial B_0 is symmetric positive definite and $y_c^T s_c > 0$.

Lemma 3.4. *Let B_c be symmetric positive definite, $y^T s > 0$, and B_+ is defined by equation 3.20. Then B_+ is symmetric positive definite.*

When the BFGS method computes the search direction using equation 3.19, the inverse of the approximate Hessian, B^{-1}, is needed and is given as follows.

Lemma 3.5. *Let B_c be symmetric positive definite, $y^T s \neq 0$, and B_+ is defined by equation 3.20. Then B_+^{-1} is nonsingular and*

$$B_+^{-1} = \left(I - \frac{sy^T}{y^T s}\right) B_c^{-1} \left(I - \frac{ys^T}{y^T s}\right) + \frac{ss^T}{y^T s}. \tag{3.21}$$

Local Convergence of the BFGS Method

Local convergence refers to the convergence of a method when the initial iterate is close to a local minimizer x^*. The rate of convergence can be measured. One rate of convergence is next.

Definition 3.3 (q-Superlinear Convergence)**.** *Let $\{x_n\} \subset \mathbb{R}^N$ and local minimizer $x^* \in \mathbb{R}^N$. If $x_n \to x^*$ and there is a $K > 0$ such that*

$$\|x_{n+1} - x^*\| \leq K\|x_n - x^*\|^\alpha \tag{3.22}$$

for n sufficiently large, then x_n converges to x^* q-superlinearly with q-order $\alpha > 1$. Furthermore, $x_n \to x^*$ q-superlinearly if

$$\lim_{n\to\infty} \frac{\|x_{n+1} - x^*\|}{\|x_n - x^*\|} = 0.$$

The next theorem requires the standard assumptions which are defined below.

Definition 3.4 (Standard Assumptions)**.** *The standard assumptions are:*

1. *f is twice Lipschitz continuously differentiable with Lipschitz constant $L > 0$, meaning*

$$\|\nabla^2 f(x) - \nabla^2 f(y)\| \leq L\|x - y\|.$$

2. $\nabla f(x^*) = 0$.

3. $\nabla^2 f(x^*)$ *is positive definite.*

If these standard assumptions hold, then as mentioned in *Necessary and Sufficient Conditions*, section 3.1.2, x^* is a local minimizer of f.

Kelley [34] states the following local convergence theorem for the BFGS method:

Theorem 3.2. *Let the standard assumptions hold. Then there is a δ such that if*

$$\|x_0 - x^*\| \leq \delta \text{ and } \|B_0 - \nabla^2 f(x^*)\| \leq \delta,$$

then the BFGS iterates are defined and converge q-superlinearly to x^*.

So, local convergence depends on how accurate the initial iterate is to x^* and the initial approximation of the Hessian matrix is to $\nabla^2 f(x^*)$.

Global Convergence of the BFGS Method

Byrd and Nocedal [10] proved the global convergence of the BFGS method for a wide variety of line search methods and Kelley [34] stated the theorem specifying the Armijo line search as follows:

Theorem 3.3. *Let the set*

$$D = \{x | f(x) \leq f(x_0)\}$$

be convex and f be Lipschitz twice continuously differentiable in D. There exists $\lambda_+ \geq \lambda_- > 0$ such that

$$\sigma(\nabla^2 f(x)) \subset [\lambda_-, \lambda_+]$$

for all $x \in D$. Let B_0 be symmetric positive definite. Then the BFGS iterates that satisfy the Armijo condition 3.14 converge q-superlinearly to x^*.

Note that global, q-superlinear convergence of the BFGS method applies to functions that have convex level curves. It is the strong assumptions of theorem 3.3, specifically that the level set D is convex, f is Lipschitz twice continuously differentiable in D, and $\nabla^2 f(x)$ has all positive eigenvalues for all $x \in D$, that imply that f has a unique minimizer x^* in D.

Symmetric Rank One (SR1)

Another formula for updating the Hessian approximation, B_c, is the SR1 formula which is a rank-one update:

$$B_+ = B_c + \frac{(y_c - B_c s_c)(y_c - B_c s_c)^T}{(y_c - B_c s_c)^T s_c}. \tag{3.23}$$

Quasi-Newton methods require the inverse of a symmetric positive definite matrix in computing the search direction. The inverse of B_+ in the SR1 formula 3.23 can be determined directly by using the Sherman-Morrison formula (B.2). But the SR1 formula does not guarantee the new matrix is positive definite. Fiacco and McCormick [20] show that the SR1 method converges in finitely many iterations for a convex quadratic objective function.

3.2 Fundamentals in Bound Constrained Optimization

3.2.1 General Constrained Optimization

Nocedal and Wright [46] describe a general constrained optimization problem which is the minimization of a function subject to constraints on the variables:

$$\min_{x \in \mathbb{R}^n} f(x)$$

subject to

$$\begin{aligned} c_i(x) &= 0,\ i \in \mathcal{E} \\ c_i(x) &\geq 0,\ i \in \mathcal{N}, \end{aligned}$$

where

- f is the smooth, real-valued objective function;
- c_i are smooth, real-valued functions;
- $\mathcal{N}$ and $\mathcal{E}$ are two finite sets of indices;
- c_i for $i \in \mathcal{E}$ are the equality constraints;
- c_i for $i \in \mathcal{N}$ are the inequality constraints.

Nocedal and Wright [46] discuss the necessary and sufficient conditions for a solution to the general constrained optimization problem. The constraints add another challenge since the solution is required to remain feasible, meaning that the solution must meet all the constraints. And as in the unconstrained case, the conditions still involve properties of the gradients and hessians.

3.2.2 Bound Constrained Optimization

Bound constrained optimization problems are a subset of the general constrained problems because the constraints can be represented more simply as bounds on each variable, rather than functions. Kelley [34] writes the problem as follows and uses the following notation:

$$\min_{x \in \Omega} f(x), \tag{3.24}$$

where

$$\Omega = \{x \in \mathbb{R}^n | L_i \leq (x)_i \leq U_i\}$$

and $\{L_i\}_{i=1}^n$ and $\{U_i\}_{i=1}^n$ are sequences of real numbers such that $-\infty < L_i < U_i < \infty$. The objective function f is minimized over all x in the feasible set, Ω. The local minimizer x^* is the point in Ω such that

$$f(x^*) \leq f(x) \text{ for all } x \in \Omega \text{ near } x^*.$$

The constraints which are upper and lower bounds for each component of x can be defined as active or inactive.

Definition 3.5 (Active Constraint)**.** *The ith constraint is called active at $x \in \Omega$ if an equality constraint holds: $(x)_i = L_i$ or $(x)_i = U_i$.*

Definition 3.6 (Inactive Constraint)**.** *The constraint is called inactive if it is not active.*

Definition 3.7 (Active Set)**.** *The active set, $\mathcal{A}(x)$, is the set of all indices i where the ith constraint is active.*

Definition 3.8 (Inactive Set)**.** *The inactive set, $\mathcal{I}(x)$, is the set of all indices i where the ith constraint is inactive.*

3.2.3 Necessary and Sufficient Conditions for Bound Constrained Optimization

Bound constrained optimization adds new cases for consideration when determining optimality of a point. The bounds created by the feasible set, Ω can complicate matters. For example, in the one-dimensional case, it is possible for the minimum to occur at one of the endpoints and for the derivative at this point to not equal zero. So, the necessary conditions for bound constrained optimization need to address this.

First, we need a definition for a stationary point in a bound constrained optimization problem. Recall that Ω defines the feasible region constrained by simple bounds:

$$\Omega = \{x \in \mathbb{R}^n | L_i \leq (x)_i \leq U_i\}$$

Definition 3.9 (Stationary Point for Bound Constrained Optimization)**.** *The point $x^* \in \Omega$ is a stationary point for the bound constrained optimization problem $\min_{x\in\Omega} f(x)$ if*

$$\nabla f(x^*)^T(x - x^*) \geq 0$$

for all $x \in \Omega$.

Necessary Conditions

Kelley [34] states three necessary conditions:

Theorem 3.4. *Let f be continuously differentiable on Ω and x^* be a minimizer for the constrained minimization problem $\min_{x\in\Omega} f(x)$. Then x^* is a stationary point.*

So, x^* being a minimizer implies that x^* is a stationary point. This is true in the unconstrained problem.

Theorem 3.5. *Let f be twice Lipschitz continuously differentiable and x^* be the minimizer for the constrained minimization problem $\min_{x\in\Omega} f(x)$. Then the reduced Hessian $\nabla_R^2 f(x^*)$ is positive semidefinite where the entries of the reduced Hessian matrix are:*

$$\nabla_R^2 f(x^*))_{ij} = \begin{cases} \delta_{ij} & \text{if } i \in \mathcal{A}(x^*) \text{ or } j \in \mathcal{A}(x^*), \\ (\nabla^2 f(x^*))_{ij} & \text{otherwise.} \end{cases}$$

(See definition B.1 for the definition of δ_{ij}.) The theorem indicates that the second partial derivatives associated with the inactive constraints must be nonnegative at the minimizer x^*:

$$\frac{\partial^2 f(x^*)}{\partial x_i \partial x_j} \geq 0 \text{ for } i, j \in \mathcal{I}(x).$$

Theorem 3.6. *Let f be continuously differentiable. A point $x^* \in \Omega$ is a stationary point for the constrained minimization problem $\min_{x\in\Omega} f(x)$ if and only if*

$$x^* = \mathcal{P}(x^* - \lambda \nabla f(x^*))$$

for all $\lambda \geq 0$, *where* $\mathcal{P}$ *is defined as:*

$$\mathcal{P}(x)_i = \begin{cases} L_i & \text{if } (x)_i \leq L_i, \\ (x)_i & \text{if } L_i < (x)_i < U_i, \\ U_i & \text{if } (x)_i \geq U_i. \end{cases}$$

The iterative process that is used to find the new x_+ could produce a point that lies outside the bound constraints. The projection $\mathcal{P}$ onto Ω maps x_+ to its nearest point in Ω. So, when $x_+ = x^* - \lambda \nabla f(x^*)$ is mapped to x^* by the projection $\mathcal{P}$ defined above, then x^* is a stationary point for the constrained minimization problem. Theorem 3.6 states the converse is true as well.

Sufficient Conditions

Kelley [34] states the sufficient condition in theorem 3.7 below. First, theorem 3.7 requires the definition of a nondegenerate stationary point.

Definition 3.10 (Nondegenerate Stationary Point)**.** *A point* $x^* \in \Omega$ *is a nondegenerate stationary point for the constrained minimization problem* $\min_{x \in \Omega} f(x)$ *if* x^* *is a stationary point and*

$$(\nabla f(x^*))_i \neq 0 \text{ for all } i \in A(x^*).$$

If x^* is a solution to $\min_{x \in \Omega} f(x)$ then x^* is called a nondegenerate local minimizer.

Theorem 3.7. *Let $x^* \in \Omega$ be a nondegenerate stationary point for the constrained minimization problem $\min_{x\in\Omega} f(x)$. Let f be twice differentiable in a neighborhood of x^*. Let the reduced Hessian at x^* be positive definite. Then x^* is a nondegenerate local minimizer of $\min_{x\in\Omega} f(x)$.*

3.2.4 Gradient Projection Method

Bertsekas [4] describes a gradient projection method for bound constrained problems with convergence results that are similar to those of the steepest descent method for unconstrained minimization. Bertsekas [4] also shows that the method can be combined with a quasi-Newton method to achieve a faster convergence rate.

An iteration of the gradient projection method results in the projection of a vector $x_c - \lambda\nabla f(x_c)$ on Ω:

$$x_+ = \mathcal{P}(x_c - \lambda\nabla f(x_c)), \tag{3.25}$$

where

$$\begin{aligned} x_+ &= \text{new iterate;} \\ x_c &= \text{current iterate;} \\ \lambda &= \text{step length that meets the sufficient decrease condition 3.26;} \\ \mathcal{P} &= \text{projection as defined in theorem 3.6.} \end{aligned}$$

In the unconstrained case, the steepest descent method required the step length to meet the Armijo condition 3.14 for sufficient decrease. In the bound constrained

case, the gradient projection method requires the step length to meet the following sufficient decrease condition:

$$f(x(\lambda)) - f(x) \leq \frac{-\alpha}{\lambda}\|x - x(\lambda)\|^2 \tag{3.26}$$

where

$$\begin{aligned} x(\lambda) &= \mathcal{P}(x - \lambda\nabla f(x)); \\ \alpha &= 10^{-4}. \text{ This is a normal value for this parameter according to} \\ &\quad \text{Dennis and Schnabel [18].} \end{aligned}$$

Convergence of Gradient Projection Method

Bertsekas [4] stated the following lemma showing that the step lengths meeting the sufficient decrease condition 3.26 are bounded away from zero:

Lemma 3.6. *Assume that ∇f is Lipschitz continuous with Lipschitz constant L. Then for any point $x \in \Omega$ and any scalar $\alpha \in (0, 1)$, the sufficient decrease condition 3.26 is satisfied for all λ such that*

$$0 < \lambda \leq \frac{2(1-\alpha)}{L}.$$

Bertsekas [4] also showed there is a lower bound for the step length and the step length can be determined in a finite number of function evaluations in order to prove theorem 3.8 below. These points and a result similar to the above lemma 3.6 were

also used to prove the convergence result for the steepest descent method. See section 3.1.4.

Bertsekas [4] proved the following convergence result for the gradient projection method.

Theorem 3.8. *Assume that ∇f is Lipschitz continuous with Lipschitz constant L and let $\{x_k\}$ be a sequence generated by the iteration 3.25 of the gradient projection method, where λ meets the sufficient decrease condition 3.26. Then every limit point of $\{x_k\}$ is a stationary point.*

Kelley [34] states in the following theorem that the gradient projection method identifies the active set of x^* in finitely many iterations.

Theorem 3.9. *If f is Lipschitz continuously differentiable and the gradient projection iterates $\{x_n\}$ converge to a nondegenerate local minimizer x^*, then there is n_0 such that $\mathcal{A}(x_n) = \mathcal{A}(x^*)$ for all $n \geq n_0$.*

Scaled Gradient Projection Method

Consider an iteration in which the gradient is scaled by the inverse of a symmetric positive definite matrix, H_c:

$$x_+ = \mathcal{P}(x_c - \lambda H_c^{-1} \nabla f(x_c)). \tag{3.27}$$

Kelley [34] uses an example to show that the theory for the gradient projection method cannot be applied to iterations of the form in 3.27. We show this using the following example.

Let $f(x) = (x_1 - 2)^2 + x_2^2$ where $0 \leq x_1 \leq 1$ and $-1 \leq x_2 \leq 1$. Define the minimization problem in terms of the notation used in section 3.2.2 as:

$$\min_{x \in \Omega} (x_1 - 2)^2 + x_2^2, \tag{3.28}$$

where $\Omega = \{x \in \mathbb{R}^2 | L_i \leq (x)_i \leq U_i\}$ and $\{L_i\}_{i=1}^2 = \{0, -1\}$ and $\{U_i\}_{i=1}^2 = \{1, 1\}$.

The solution to problem 3.28 is $x^* = (1, 0)^T$ and $\mathcal{A}(x^*) = \{1\}$. To make the point, choose an x known not to be the minimizer: $x_0 = (1, 2/3)^T$. The gradient is: $\nabla f(x) = (2x_1 - 4, 2x_2)^T$. The gradient at x_0 is: $\nabla f(x_0) = (-2, 4/3)^T$. Let H_c be symmetric positive definite such that:

$$H_0^{-1} = \begin{pmatrix} 3 & 2 \\ 2 & 3 \end{pmatrix}.$$

Now, for $\lambda > 0$,

$$\begin{aligned}
\mathcal{P}(x_0 - \lambda H_0^{-1}\nabla f(x_0)) &= \mathcal{P}\left(\begin{pmatrix} 1 \\ 2/3 \end{pmatrix} - \lambda \begin{pmatrix} 3 & 2 \\ 2 & 3 \end{pmatrix} \begin{pmatrix} -2 \\ 4/3 \end{pmatrix}\right) \\
&= \mathcal{P}\left(\begin{pmatrix} 1 \\ 2/3 \end{pmatrix} - \lambda \begin{pmatrix} -10/3 \\ 0 \end{pmatrix}\right) \\
&= \mathcal{P}\begin{pmatrix} 1 + (10/3)\lambda \\ 2/3 \end{pmatrix} \\
&= \begin{pmatrix} 1 \\ 2/3 \end{pmatrix} = x_0.
\end{aligned}$$

Observe that $x_0 = \mathcal{P}(x_0 - \lambda H_0^{-1}\nabla f(x_0))$. If the theorems for the gradient projection method did apply here, we would expect that the minimizer was found. But we know x_0 is not the minimizer. The above example shows that the symmetric positive definite matrix H_0^{-1} scaled the gradient so that the search direction became $d = -H_0^{-1}\nabla f(x_0) = ((10/3), 0)^T$. This means that the search direction points entirely in the horizontal direction and is perpendicular to the vertical descent direction of the inactive constraint. The problem can be thought of as unconstrained in the inactive directions. So in the unconstrained problem, the positive definiteness of the matrix alone does not ensure movement towards the minimizer [34].

The iteration $x_+ = \mathcal{P}(x_c - \lambda H_c^{-1}\nabla f(x_c))$ can fail, as shown above, while using the model Hessian. The reduced model Hessian, $R(H)_{ij}$, should be used in the iteration

instead, where

$$R(H)_{ij} = \begin{cases} \delta_{ij} & \text{if } i \in \mathcal{A}(x) \text{ or } j \in \mathcal{A}(x), \\ H_{ij} & \text{otherwise.} \end{cases}$$

But Bertsekas [5] states this may not improve convergence either and suggests enlarging the active set by a certain amount to steer the iterates toward the solution.

Bertsekas [5] shows that overestimating the active set and modeling the reduced Hessian does work. Kelley [34] defines the ϵ-active set at $x \in \Omega$ as:

$$\mathcal{A}^{\epsilon}(x) = \{i | U_i - (x)_i \leq \epsilon \text{ or } (x)_i - L_i \leq \epsilon\},$$

where $0 \leq \epsilon < \min(U_i - L_i)/2$. Then the ϵ-inactive set, $\mathcal{I}^{\epsilon}(x)$, is the complement of $\mathcal{A}^{\epsilon}(x)$. Observe that now, if $(x)_i$ is within ϵ of the upper or lower bounds, then the ith constraint will be in the ϵ-active set for x.

So, the reduced Hessian can be modeled by $\mathcal{R}(x_c, \epsilon_c, H_c)$ which depends on x_c, ϵ_c, and H_c:

$$(\mathcal{R}_c)_{ij} = \begin{cases} \delta_{ij} & \text{if } i \in \mathcal{A}_c^{\epsilon}(x_c) \text{ or } j \in \mathcal{A}_c^{\epsilon}(x_c), \\ (H_c)_{ij} & \text{otherwise.} \end{cases} \tag{3.29}$$

Now, the iteration for the scaled gradient projection method becomes:

$$x_+ = \mathcal{P}(x_c - \lambda \mathcal{R}(x_c, \epsilon_c, H_c)^{-1} \nabla f(x_c)). \tag{3.30}$$

The following example illustrates how the use of ϵ improves convergence. Let $f(x) = (x_1 - 2)^2 + x_2^2$ where $0 \leq x_1 \leq 1$ and $1 \leq x_2 \leq 2$. The minimization problem

Table 3.1: Scaled Gradient Projection Iterates without ϵ

Iterate	Component 1	Component 2	Active Set	f(x)
x_0	0.750	1.50		3.8250
x_1	0.750	1.00	2	2.5625
x_2	1.000	1.20	1	2.4400
x_3	0.900	1.00	2	2.2100
x_4	1.000	1.08	1	2.1664
x_5	0.980	1.00	2	2.0404
x_6	1.000	1.01	1	2.0201
x_7	0.991	1.00	2	2.0181
$\vdots$				

Table 3.2: Scaled Gradient Projection Iterates with ϵ

Iterate	Component 1	Component 2	Active Set	f(x)
x_0	0.75	1.5	1	3.825
x_1	1.00	1.0	1,2	2.000

is:

$$\min_{x\in\Omega}(x_1-2)^2+x_2^2, \tag{3.31}$$

where $\Omega = \{x \in \mathbb{R}^2 | L_i \leq (x)_i \leq U_i\}$ and $\{L_i\}_{i=1}^2 = \{0,1\}$ and $\{U_i\}_{i=1}^2 = \{1,2\}$. The solution to problem 3.31 is $x^* = (1,1)^T$ and $\mathcal{A}(x^*) = \{1,2\}$. Table 3.1 shows the components, active sets, and function values of each iterate. The iterates were determined by: $x_+ = \mathcal{P}(x_c - H_c^{-1}\nabla f(x_c))$.

Now, let $\epsilon = .25$, form the ϵ-active set, and construct $\mathcal{R}_c$. Table 3.2 shows that the solution was determined in one iteration. The iterates were determined by: $x_+ = \mathcal{P}(x_c - \mathcal{R}(x_c, \epsilon_c, H_c)^{-1}\nabla f(x_c))$.

Convergence of Scaled Gradient Projection Method

The step length must meet the following sufficient decrease condition for sufficiently small λ:

$$f(x^{H,\epsilon}(\lambda)) - f(x) \leq -\alpha \nabla f(x)^T (x - x^{H,\epsilon}(\lambda)), \tag{3.32}$$

where $x^{H,\epsilon}(\lambda) = \mathcal{P}(x - \lambda \mathcal{R}(x, \epsilon, H)^{-1} \nabla f(x)$.

Kelley [34] states this in the next lemma:

Lemma 3.7. *Let $x \in \Omega$, $0 < \epsilon < \min(U_i - L_i)/2$, and H be symmetric positive definite with smallest and largest eigenvalues $0 < \lambda_{min} \leq \lambda_{max}$. Let ∇f be Lipschitz continuous on Ω. Then there is $\overline{\lambda}(\epsilon, H)$ such that sufficient decrease condition 3.32 holds for all*

$$\lambda \leq \overline{\lambda}(\epsilon, H).$$

Kelley [34] states the following theorem on the convergence of the scaled gradient projection method and notes the similarity with theorem 3.1, convergence of the steepest descent method. The assumptions are the same, except the theorem below needs an additional assumption to guarantee the step lengths are bounded away from zero. (Theorem 3.1 used the result of lemma 3.2 to do this.) The proof of the above lemma 3.7, [34], shows a direct relationship between λ and ϵ. So, if ϵ_k is bounded away from zero, then so are the iterates λ_k.

Theorem 3.10. *Let ∇f be Lipschitz continuous with Lipschitz constant L. Assume that for symmetric positive definite matrices H_k, there exists a $\bar{\kappa}$ and λ_{max} such*

that $\kappa(H_k) \leq \bar{\kappa}$ *and* $\|H_k\| \leq \lambda_{max}$ *for all* k. *Assume there is* $\bar{\epsilon} > 0$ *such that* $\bar{\epsilon} \leq \epsilon_k < \min(U_i - L_i)/2$ *for all* k. *Then*

$$\lim_{k\to\infty} \|x_k - \mathcal{P}(x_k - \mathcal{R}(x_k, \epsilon, H)^{-1}\nabla f(x_k))\| = 0$$

and hence any limit point of the sequence of iterates produced by the scaled gradient projection method is a stationary point.
Meaning, if $x_{k_l} \to x^*$ *is any convergent subsequence of* $\{x_k\}$, *then* $x^* = \mathcal{P}(x^* - \mathcal{R}(x^*, \epsilon, H)^{-1}\nabla f(x^*))$. *If* x_k *converges to a nondegenerate local minimizer* x^*, *then the active set of* x_k *is the same as that of* x^* *after finitely many iterations.*

Note that the scaled projected gradients , $x_k - \mathcal{P}(x_k - \mathcal{R}(x_k, \epsilon, H)^{-1}\nabla f(x_k)) = x_k - x_k^{H,\epsilon}(1)$, converge to zero, just as in the convergence theorem for the steepest descent method (theorem 3.1).

Bertsekas [5] states that if the active set of x^* is identified in a finite number of iterations so that the constraints that are frozen at the boundary will be known, then the problem will eventually be reduced to an unconstrained problem. Then it is possible to obtain superlinear convergence. The next two subsections explain how the convergence theory for Newton methods show this.

3.2.5 Projected Newton Method

Kelley [34] reiterates that the projected Newton method can be applied once the active set of x^* is identified implying that the current iterate x_c is close to x^* and the reduced Hessians, $\nabla_R^2 f(x_c)$, are symmetric positive definite.

The projected Newton iterate is the scaled gradient projection iterate 3.30 where $H_c = \nabla^2_R f(x_c)$ as follows:

$$x_+ = \mathcal{P}(x_c - \lambda \mathcal{R}(x_c, \epsilon_c, \nabla^2_R f(x_c))^{-1} \nabla f(x_c)). \tag{3.33}$$

Bertsekas [5] and Kelley [34] make a point to choose an ϵ_c that changes in such a way that quadratic convergence can be obtained from using the projected Newton iterate. Let

$$\epsilon_c = \min\{\|x_c - x_c(1)\|,\ \min(U_i - L_i)/2\}.$$

When the original problem is constrained and the iterate x_c is far from a stationary point, as long as the model reduced Hessians remain symmetric positive definite, then convergence theorem 3.10 for the scaled gradient projection method holds. The ϵ_c will be chosen, as required by that theorem, to be bounded away from zero. As the iterations progress, the norm of the scaled gradient becomes smaller. If the problem is reduced to an unconstrained problem and x_c converges to a nondegenerate local minimizer x^*, then the scaled gradient, $x_c - x_c(1)$, will become small enough so ϵ_c can be set to the norm of the scaled gradient which is converging to zero.

The choice of ϵ impacts which indices i are in the ϵ-active set. If ϵ_c is converging to zero, then the indices in the ϵ-active set must also be the indices in the active set for x_c and x^*. ($\mathcal{A}(x_c) = \mathcal{A}(x^*)$ because of the assumption that the active set has been identified for x^*.) This leads to the following convergence theorem for the projected Newton method.

Theorem 3.11. *Let x^* be a nondegenerate local minimizer. Then if x_0 is sufficiently near to x^* and $\mathcal{A}(x_0) = \mathcal{A}(x^*)$, then the projected Newton iteration 3.33, with $\epsilon_c = \|x_c - x_c(1)\|$, will converge q-quadratically to x^*.*

The q-quadratic convergence rate is defined next.

Definition 3.11 (q-Quadratic Convergence)**.** *Let $\{x_n\} \subset \mathbb{R}^N$ and local minimizer $x^* \in \mathbb{R}^N$. If $x_n \to x^*$ and there is a $K > 0$ such that*

$$\|x_{n+1} - x^*\| \leq K\|x_n - x^*\|^2$$

for n sufficiently large, then x_n converges to x^* q-quadratically.

3.2.6 Projected BFGS-Armijo Method

The name projected BFGS-Armijo suggests that superlinear convergence can be obtained because of the previous results in section 3.1.5. The theorems in this section will show similar local and global convergence results.

The following notation is used throughout this section: Let $\mathcal{S}$ be any set of indices, then

$$(\mathcal{P}_{\mathcal{S}}x)_i = \begin{cases} (x)_i & \text{if } i \in \mathcal{S}, \\ 0 & \text{if } i \notin \mathcal{S}. \end{cases}$$

The reduced Hessian can be determined by computing one part and approximating another part. Kelley [34] explains that the projected BFGS-Armijo method models

the reduced Hessian in this manner, where the approximation is determined by a projected BFGS update. Let the model reduced Hessian be:

$$\mathcal{R} = \mathcal{C}(x) + A,$$

where $\mathcal{C}(x) = \mathcal{P}_{\mathcal{A}^{\epsilon(x)}}$ is the computed part and A is the approximation to the model Hessian that is acting on the ϵ-inactive set. Since the secant equation $R_+ s = y$ must hold, the update to A must satisfy $A_+ s = y - C(x)s$ [19].

A BFGS update can be applied to A according to the following formula from [19]:

$$A_+ = A_c + \frac{y^\sharp y^{\sharp T}}{y^{\sharp T} s} - \frac{(A_c s)(A_c s)^T}{s^T A_c s},$$

where $s = x_+ - x_c$ and $y^\sharp = y - C(x)s$ when the ϵ-active set does not change. But until the active set has been identified, the approximation A needs to include the information from the changing active set. Kelley [34] gives a projected BFGS update of A to do this:

$$A_+ = \mathcal{P}_{\mathcal{I}_+} A_c \mathcal{P}_{\mathcal{I}_+} + \frac{y^\sharp y^{\sharp T}}{y^{\sharp T} s} - \mathcal{P}_{\mathcal{I}_+} \frac{(A_c s)(A_c s)^T}{s^T A_c s} \mathcal{P}_{\mathcal{I}_+}, \tag{3.34}$$

where

$$\begin{aligned} \mathcal{I}_+ &= \mathcal{I}^{\epsilon_+}(x_+), \text{ the } \epsilon\text{-inactive set for the new iterate,} \\ y^\sharp &= \mathcal{P}_{\mathcal{I}_+}(\nabla f(x_+) - \nabla f(x_c)), \\ s &= x_+ - x_c. \end{aligned}$$

The following theorems from [34] state the superlinear convergence results.

Theorem 3.12. *Let x^* be a nondegenerate local minimizer. Then if x_0 is sufficiently near to x^* and $\mathcal{A}(x_0) = \mathcal{A}(x^*)$, and A_0 sufficiently near to $\mathcal{P}_{\mathcal{I}(x^*)}\nabla^2 f(x^*)\mathcal{P}_{\mathcal{I}(x^*)}$, then the projected BFGS iteration 3.34, with $\epsilon_c = \|x_c - x_c(1)\|$, will converge q-superlinearly to x^*.*

This local theorem requires good data for the initial iterate, good data for the initial approximation to the reduced Hessian, and the identification of the active set in order for the projected BFGS-Armijo method to converge superlinearly.

Theorem 3.13. *Let ∇f be Lipschitz continuous on Ω. Assume that the matrices H_k are constructed with the projected BFGS method and satisfy the assumptions of the scaled gradient projection convergence theorem 3.10, then*

$$\lim_{k\to\infty} \|x_k - \mathcal{P}(x_k - \mathcal{R}(x_k, \epsilon, H)^{-1}\nabla f(x_k))\| = 0$$

and hence any limit point of the sequence of iterates produced by the projected BFGS

method is a stationary point.

If x^* is a nondegenerate local minimizer such that there is k_0 such that $\mathcal{A}(x_k) = \mathcal{A}(x^*)$ for all $k \geq k_0$, H_{k_0} is symmetric positive definite, and the set $D = \{x | f(x) \leq f(x_{k_0})$ and $\mathcal{A}(x) = \mathcal{A}(x^*)\}$ is convex, then the projected BFGS-Armijo method converges q-superlinearly to x^*.

This theorem indicates global convergence and note the assumptions that are needed. Just as in section 3.1.5, global convergence requires strict assumptions such as identification of the active set for x^* and convex set $\mathcal{D}$.

Chapter 4

Implicit Filtering

The purpose of this chapter is to describe implicit filtering which is the method we use to optimize our problem (chapters 5 and 6).

Implicit filtering which originated in [61], [64], [65], and described by Kelley in [34], is a sampling method that can be used to optimize smooth functions with low-amplitude, high-frequency perturbations, referred to as noise. Sampling methods use evaluations of the objective function at some set of points (called a stencil) to determine the next stencil. The stencil varies in size throughout the optimization process. The idea is that the local minima created by the noise do not trap the iteration and the noise is filtered out. Implicit filtering uses finite difference gradients to determine the direction of descent. Faster convergence can be obtained by using a quasi-Newton update of the model Hessian [34]. Since we have a bound constrained problem, we apply the projected quasi-Newton method.

4.1 Introduction

4.1.1 Objective Function

Implicit filtering can be used for objective functions of the following form:

$$f(x) = f_s(x) + \phi(x), \tag{4.1}$$

where a smooth function $f_s(x)$ has small perturbations represented by $\phi(x)$ [34]. The perturbations produced by $\phi(x)$ are referred to as noise and cause $f(x)$ to have many local minima. The objective function could also be discontinuous or undefined. It might be impossible or too expensive to determine the derivatives of f.

In our problem, we run a model to evaluate the objective function. We build the optimization landscape by graphing discrete inputs and the corresponding functional values. Due to the randomness in the model, we do not expect to obtain the same functional value for two realizations with the same inputs. So, we take the average of a large number of realizations to be the functional value. The result is an optimization landscape that looks relatively smooth. But a closer look on a finer mesh reveals high-frequency, low amplitude noise.

We also observe points in the landscape with no value for the function. These points tend to form a gap where the function is undefined. It is possible for the model to return *NaN* instead of a numerical evaluation. When the model does not return a value, then one of the constraints within the model was not met. We consider a reliability and a cost variability constraint. If one or both constraints are not met, we disregard the functional value because it has no meaning to us. We only care

about the inputs that meet both constraints.

So, we do not have an explicit formula for the smooth function and the noisy part. And we do not need it. Implicit filtering only requires function evaluations. We do not even need derivatives. Implicit filtering uses function evaluations to estimate derivatives as well.

4.1.2 Coordinate Search

Implicit filtering starts with the very basic coordinate search [35]. Let $x \in \mathbb{R}^N$. The idea is to search along the positive and negative coordinate directions a length (or scale) h from the current point x_c. These $2N$ points form what we refer to as a stencil:

$$\mathcal{S}(x_c, h) = \{z|\ z = x_c \pm he_i, \quad 1 \leq i \leq N\}, \tag{4.2}$$

where e_i is the unit vector in the ith coordinate direction.

The search requires the function evaluations of these $2N$ points which are compared to the function's value at the current point. The algorithm takes the point with the least function value as the next iterate. If the least function value occurs at the current point, a stencil failure occurs and we shrink the stencil by reducing h (by one-half for example). Coordinate search terminates after the maximum number of function evaluations is used.

4.1.3 Steepest Descent Augments Coordinate Search

Implicit filtering augments coordinate search with steepest descent. Implicit filtering begins with coordinate search. If stencil failure occurs, h is reduced. If a point on the stencil does have a lower function value than the base point, then the algorithm tests the termination criterion and performs a line search until sufficient decrease is met (or the maximum number of steplength reductions achieved). The function evaluations performed during the coordinate search are used again in calculating the finite difference gradient for the line search. If the line search fails, the algorithm takes the point on the stencil with the least function value as the new iterate. See [35] for the pseudocode. We provide the pseudocode for implicit filtering in the bound constrained case below in section 4.4.

4.1.4 Quasi-Newton

The quasi-Newton method can replace the steepest descent method to obtain faster convergence [60], [24]. The direction requires the inverse of a quasi-Newton approximation to the exact Hessian: $d = -H^{-1}\nabla_h f(x)$, where $\nabla_h f(x)$ is the finite difference gradient. Kelley [34] mentions that the BFGS and the SR1 quasi-Newton methods have been used to update H. There were certain applications with bound constraints in which SR1 performed better [15], [60], [61], [64], [65].

4.1.5 Difference Gradient

The line search requires gradient information to determine the direction. So, implicit filtering uses the finite difference gradient (denoted by $\nabla_h f(x)$) as an approximation

for the actual gradient, $\nabla f(x)$. The length $h > 0$ is a difference increment (scale or stencil size). The following are definitions of three finite difference gradients.

Definition 4.1 (Centered Difference Gradient)**.** *The ith component of the centered difference gradient is*

$$(\nabla_h f(x))_i = \frac{f(x + he_i) - f(x - he_i)}{2h}.$$

If $x - he_i$ is not in the feasible region, then one can use a forward difference.

Definition 4.2 (Forward Difference Gradient)**.** *The ith component of the forward difference gradient is*

$$(\nabla_h f(x))_i = \frac{f(x + he_i) - f(x)}{h}.$$

Or if $x + he_i$ is not in the feasible region, then one can use a backward difference.

Definition 4.3 (Backward Difference Gradient)**.** *The ith component of the backward difference gradient is*

$$(\nabla_h f(x))_i = \frac{f(x) - f(x - he_i)}{h}.$$

4.1.6 Stencil Gradient

The coordinate search provides the function evaluations of each point on the stencil. This information is reused in finite difference calculations and what is referred to as the stencil gradient. We show that the stencil gradient, defined below, can be used to approximate the actual gradient.

Approximation of gradient

Since we do not know the derivatives of f to form the gradient, we need to determine an approximation. Let's look at a linear model of f centered at x_c:

$$f(x) \approx f(x_c) + \nabla f(x_c)^T (x - x_c).$$

We would like to interpolate f at the points $x_1, \ldots, x_M$. Let $x = x_j$ for $j = 1, \ldots, M$:

$$f(x_j) \approx f(x_c) + \nabla f(x_c)^T (x_j - x_c).$$

Let $v_j = x_j - x_c$:

$$f(x_j) - f(x_c) \approx v_j^T \nabla f(x_c). \tag{4.3}$$

Let $V = [v_1, v_2, \ldots, v_M]$ and define the vector

$$\delta(f, x_c, V) = (f(x_1) - f(x_c), f(x_2) - f(x_c), ..., f(x_M) - f(x_c))^T.$$

We consider equation 4.3 for $j = 1, \ldots, M$ and obtain an approximation for the gradient:

$$\begin{aligned} \delta(f, x_c, V) &\approx V^T \nabla f(x_c) \\ \nabla f(x_c) &\approx (V^T)^\dagger \delta(f, x_c, V). \end{aligned} \tag{4.4}$$

Linear Least Squares Problem

Consider a general stencil containing a base point x_c and points $x_1, x_2, \ldots, x_M$ with M directions v_j and a scale h such that $x_j = x_c + hv_j \in \mathbb{R}^N$ for $j = 1, \ldots, M$. Again, we let V be the matrix of directions:

$$V = [v_1, v_2, \ldots, v_M].$$

We let δ be the vector:

$$\delta(f, x_c, V, h) = \begin{pmatrix} f(x_1) - f(x_c) \\ f(x_2) - f(x_c) \\ \vdots \\ f(x_M) - f(x_c) \end{pmatrix}^T = \begin{pmatrix} f(x_c + hv_1) - f(x_c) \\ f(x_c + hv_2) - f(x_c) \\ \vdots \\ f(x_c + hv_M) - f(x_c) \end{pmatrix}^T$$

Now, let's define the stencil gradient $D(f, x_c, V, h)$ as follows:

Definition 4.4 (Stencil Gradient)**.**

$$\begin{aligned} D(f, x_c, V, h) &= \min_{y \in \mathbb{R}^N} \|hV^T y - \delta(f, x_c, V, h)\| \\ &= (hV^T)^\dagger \delta(f, x_c, V, h) \end{aligned} \tag{4.5}$$

is the stencil gradient and the solution to a linear least squares problem.

This definition allows the stencil gradient to be based on a general V and still exist even if the function cannot be evaluated at some points on the stencil (due to

infeasibility, for example).

Centered Difference Stencil Gradient

Now, let's look at the specific stencil defined earlier (stencil 4.2):

$$\mathcal{S}(x_c, h) = \{z \in \mathbb{R}^N | z = x_c \pm he_i, \quad \text{for } i = 1, .., N\}.$$

Since implicit filtering with a centered difference gradient out-performed that with a forward difference gradient [24], [44], [61], we apply the centered difference gradient. We show that the vector of centered differences is the solution to equation 4.5 for matrix of directions V:

$$V = [e_1, e_2, ..., e_N, -e_1, ..., -e_N] = [I \quad -I]_{N \times 2N}.$$

Define the vector $\delta(f, x_c, V, h)$ as:

$$\delta(f, x_c, V, h) = \begin{pmatrix} f(x_c + he_1) - f(x_c) \\ \vdots \\ f(x_c + he_N) - f(x_c) \\ f(x_c - he_1) - f(x_c) \\ \vdots \\ f(x_c - he_N) - f(x_c) \end{pmatrix}_{2N \times 1}$$

Since V^T has full column rank, compute $(hV^T)^\dagger$ as follows:

$$\begin{aligned}
(hV^T)^\dagger &= (hVhV^T)^{-1}hV \\
&= \left(h^2[I \quad -I] \begin{bmatrix} I \\ -I \end{bmatrix} \right)^{-1} h[I \quad -I] \\
&= \frac{1}{2h^2}[I]h[I \quad -I] \\
&= \frac{1}{2h}[I \quad -I]_{N\times 2N}.
\end{aligned}$$

Now, compute $D(f, x_c, V, h)$ from equation 4.5:

$$
\begin{aligned}
D(f, x_c, V, h) &= (hV^T)^{\dagger}\delta(f, x_c, V, h) \\
&= \frac{1}{2h}[I \ -I] \begin{pmatrix} f(x_c + he_1) - f(x_c) \\ \vdots \\ f(x_c + he_N) - f(x_c) \\ f(x_c - he_1) - f(x_c) \\ \vdots \\ f(x_c - hv_N) - f(x_c) \end{pmatrix}_{2N\times 1} \\
&= \frac{1}{2h} \begin{pmatrix} f(x_c + he_1) - f(x_c) - f(x_c - he_1) + f(x_c) \\ \vdots \\ f(x_c + he_N) - f(x_c) - f(x_c - he_N) + f(x_c) \end{pmatrix}_{N\times 1} \\
&= \begin{pmatrix} \frac{f(x_c+he_1)-f(x_c-he_1)}{2h} \\ \vdots \\ \frac{f(x_c+he_N)-f(x_c-he_N)}{2h} \end{pmatrix}_{N\times 1}
\end{aligned}
$$

Observe that the above stencil gradient consists of centered differences as expected. We define this vector to be the centered difference stencil gradient.

Definition 4.5 (Centered Difference Stencil Gradient)**.**

$$\begin{aligned} D_C(f, x_c) &= (hV^T)^\dagger \delta(f, x_c, V, h) \\ &= \begin{pmatrix} \frac{f(x_c+he_1)-f(x_c-he_1)}{2h} \\ \vdots \\ \frac{f(x_c+he_N)-f(x_c-he_N)}{2h} \end{pmatrix} \end{aligned}$$

For our application, we use the centered difference gradient and let $\nabla_h f(x) = D_C(f, x)$.

4.2 Implicit Filtering in the Bound Constrained Case

In this section, we describe the specifications for the use of implicit filtering in a bound constrained problem.

4.2.1 Feasible Region

We use implicit filtering to solve the bound constrained problem:

$$\min_{x \in \Omega} f(x),$$

where $\Omega = \{x \in \mathbb{R}^N | L_i \leq (x)_i \leq U_i\}$ and $-\infty < L_i \leq U_i < \infty$. The notation $(x)_i$ refers to the ith component of x. Kelley, [35], calls the feasible region Ω a hyper-rectangle in $\mathbb{R}^N$. In $\mathbb{R}^2$, the feasible region is a rectangle.

4.2.2 Stencil

In the bound constrained problem, implicit filtering uses the upper and lower bounds in defining the $2N$ points on the stencil

$$\mathcal{S}(x_c, h) = \{z |\ z = x_c \pm h(L_i - U_i)e_i, \quad 1 \leq i \leq N\}, \tag{4.6}$$

where x_c is the current point at the center, h is the scale (stencil size), L_i is the lower bound, U_i is the upper bound, and e_i is the unit vector in the ith coordinate direction. A change in the bounds to $L_i = 0$ and $U_i = 1$ scales the problem so that the movement for all components of x are of relatively equal size [35]. The scale, h, can be given as a sequence, such as $\{2^{-n}\}_{n=1}^{m}$, for integer $m > 0$. The algorithm reduces h throughout the process.

Notice the stencil is defined so that a coordinate search can be applied. If a point on the stencil lies outside the feasible region, then the function does not evaluate that point.

4.2.3 Termination of Iteration vs. Termination of Algorithm

It is important to distinguish between the outer and inner loops of the implicit filtering algorithm, and define what we mean by an iteration. An iteration starts with the current point and cycles through the inner loop to determine the next point. So, the iteration terminates when the inner loop terminates. The inner loop consists of the coordinate search and line search. There are several instances in which the inner loop terminates and results in a decrease in the scale h. The outer loop keeps track of the number of function evaluations and the value of h. When the outer loop terminates, it means it is the end of the algorithm.

Termination of Iteration

The iteration terminates and the scale h decreases when one of the following occurs:

- line search failure,
- stencil failure, or
- termination criterion met.

A line search failure occurs if the sufficient decrease condition has not been met after the maximum number of steplength reductions:

$$f(x(\lambda)) - f(x) \leq -\alpha \nabla_h f(x)^T (x - x(\lambda)),$$

where $x(\lambda) = \mathcal{P}(x - \lambda \nabla_h f(x))$. In other words, the line search did not find a point in which its functional value was sufficiently smaller than that of the current point. So, the current point wins and the next iteration begins the search on a smaller stencil.

Also, since the negative of the stencil gradient may not be a descent direction, we do not want to waste time trying to meet sufficient decrease that will not happen. So, there is a limit on the number of steplength reductions [35].

A stencil failure occurs when the value of the objective function at the current iterate is less than the function values at all the other points on the stencil:

$$f(x_c) \leq f(x_c \pm he_i), \ \forall \ 1 \leq i \leq N.$$

Again, the current point wins and the stencil size is reduced for the next iteration. There is no reason to implement the line search when a sampling of the stencil gives no indication there is a better point.

The termination criterion involves the norm of the projected gradient:

$$\|x - x(1)\| = \|x - \mathcal{P}(x - \nabla_h f(x))\| \leq \tau h, \text{ for some } \tau > 0.$$

The termination criterion is checked after the coordinate search finds a point on the stencil with a smaller function value than the current point. If the norm of the projected gradient is small enough (on order of the stencil size), then this information may foreshadow that a line search will not be able to meet the sufficient decrease condition and fail. So, the iteration is terminated, h is reduced, and the current point remains the base point.

Termination of Algorithm

The implicit filtering algorithm terminates after a certain number of calls to the function or after h can no longer be reduced. If the process stagnates at a scale h, the algorithm can still terminate after the specified number of function evaluations have been made. The sequence of scales should be selected carefully. Since there is no guarantee the implicit filtering algorithm will find a global or local minimum, it is not necessary to continue searching when h becomes smaller than the noise.

We can tune certain parameters, such as τ or $\{h_k\}_{k=1}^{m}$, to allow for efficient termination of the iteration or algorithm.

4.2.4 Hidden Constraints

It is possible that the function outputs no value (for example, NaN). The function did not meet a constraint hidden within the evaluation process. The implicit filtering algorithm is not aware of these hidden constraints. So, implicit filtering continues the process without the data. Gaps in the optimization landscape indicate violation of the hidden constraints.

4.3 Convergence Theory

Implicit filtering which is designed for noisy optimization problems, samples from a set of points. We have previously referred to this set of points as a stencil. Now, we introduce the term simplex which is used in the convergence theory [7], [34]. Theory requires assumptions of a simplex which is a special case of the stencil. In practice,

though, the code allows for a general stencil since the function may be undefined at some points or a general stencil may provide additional information.

In this section, we define simplex and related terms, provide two lemmas important to convergence, and then provide the convergence theory (for coordinate search and implicit filtering).

Definition 4.6 (Simplex)**.** *A simplex $\mathcal{S} \in \mathbb{R}^N$ is the convex hull of $N+1$ points: $\{x_j\}_{j=1}^{N+1}$, where x_j is the jth vertex of $\mathcal{S}$.*

Definition 4.7 (Matrix of Simplex Directions)**.** *For simplex $\mathcal{S}$, the $N \times N$ matrix of simplex directions, denoted as V, is:*

$$V = [x_2 - x_1, x_3 - x_1, \ldots, x_{N+1} - x_1] = [v_1, \ldots, v_N].$$

Definition 4.8 (Nonsingular Simplex)**.** *A simplex $\mathcal{S}$ is nonsingular if the matrix of simplex directions V is nonsingular.*

Definition 4.9 (Simplex Condition Number)**.** *The simplex condition number $\kappa(V)$ is the 2-norm condition number of matrix of simplex directions V.*

Definition 4.10 (Simplex Gradient)**.** *For nonsingular simplex $\mathcal{S}$, the simplex gradient is:*

$$D(f, \mathcal{S}) = V^{-T}\delta(f, \mathcal{S}),$$

where $\delta(f, \mathcal{S}) = (f(x_2) - f(x_1), f(x_3) - f(x_1), \ldots, f(x_{N+1}) - f(x_1))^T$.

Definition 4.11. *For simplex $\mathcal{S}$,*

$$\sigma_+(\mathcal{S}) = \max_{2 \le j \le N+1} \|x_1 - x_j\|,$$

denotes the maximum distance between point x_1 and another point x_j.

The two lemmas [7], [34] below, require a nonsingularity assumption and have results involving condition numbers. This means the simplex considered here must translate to a matrix that is invertible. Also, the function under consideration is a smooth function with perturbations. We define a measure for the perturbations below.

Definition 4.12. *For any set T,*

$$\|\phi\|_T = \max_{z \in T} |\phi(z)|.$$

The lemma below gives a first order estimate of the gradient, in the case where a smooth function is perturbed [34].

Lemma 4.1. *Let $\mathcal{S}$ be a nonsingular simplex. Let $f(x) = f_s(x) + \phi(x)$ and let ∇f_s be Lipschitz continuous in a neighborhood of $\mathcal{S}$ with Lipschitz constant $2K_s$. Then there is $K > 0$, depending only on K_s, such that*

$$\|\nabla f_s(x_1) - D(f, \mathcal{S})\| \leq K\kappa(V) \left(\sigma_+(\mathcal{S}) + \frac{\|\phi\|_{\mathcal{S}}}{\sigma_+(\mathcal{S})} \right).$$

In the next lemma, Bortz and Kelley [7] show that stencil failure implies $\|\nabla f_s(x)\| = O\left(\sigma_+(\mathcal{S}) + \frac{\|\phi\|_B}{\sigma_+(\mathcal{S})}\right)$, where B is a ball of radius $2\sigma_+(\mathcal{S})$ about x_1. This is important for convergence which we discuss later. They also point out that from this lemma, infinitely many occurrences of stencil failure and $(\sigma_+(\mathcal{S}))_k \to 0$ imply that the simplex gradient converges to zero.

Lemma 4.2. *Let $\mathcal{S}$ be a nonsingular simplex such that for some $\mu_- \in (0,1)$ and $\kappa_+ > 0$,*

$$\kappa(V) \le \kappa_+ \text{ and } x^T V V^T x \ge \mu_- \sigma_+(\mathcal{S})^2 \|x\|^2 \text{ for all } x.$$

Let $f(x) = f_s(x) + \phi(x)$ and ∇f_s be Lipschitz continuously differentiable in a ball B of radius $2\sigma_+(\mathcal{S})$ about x_1. Assume that $f(x_1) < \min_j\{f(x_1 \pm v_j)\}$. Then, if K is the constant from lemma 4.1,

$$\|\nabla f_s(x_1)\| \le 8\mu_-^{-1} K \kappa_+ \left(\sigma_+(\mathcal{S}) + \frac{\|\phi\|_B}{\sigma_+(\mathcal{S})}\right).$$

As mentioned in a previous section, implicit filtering accelerates coordinate search with a quasi-Newton method. If this extension fails and we are left with coordinate search, we still get a convergence result. So we first provide the convergence result for coordinate search [7] (with the notation $\mathcal{S}^k = \mathcal{S}(x, h_k)$ at the kth iteration).

Theorem 4.1. *Let $f(x) = f_s(x) + \phi(x)$. Let coordinate search give the sequence $\{x_k, h_k\}$. If $f(x)$ has bounded level sets and if*

$$\lim_{k\to\infty} \left(h_k + \frac{\|\phi\|_{\mathcal{S}^k}}{h_k}\right) = 0 \tag{4.7}$$

where $\|\phi\|_{\mathcal{S}^k} = \max_{z\in\mathcal{S}^k} |\phi(z)|$,
Then $h_k \to 0$ and any limit point of the sequence $\{x_k\}$ is a critical point of f_s.

The following is a sketch of what we want to show. First, since f has bounded level sets, the decreasing sequence of objective function values is finite and stencil failure occurs for infinitely many k. This means that we reduce h (by one-half for

example) infinitely many times and so $h_k \to 0$. Second, we use the result from Bortz and Kelley [7] that stencil failure implies $\|\nabla f_s(x_k)\| = O\left(h_k + \frac{\|\phi\|_{\mathcal{S}^k}}{h_k}\right)$. Last, we apply assumption 4.8 to obtain the second result, $\|\nabla f_s(x_k)\| \to 0$.

Proof. The nonsingular kth simplex is the set of points: $\mathcal{S}^k(x, h_k) = \{z|\ z = x + h_k e_i, \quad 1 \le i \le N\}$, where e_i is the unit vector in the ith coordinate direction. Coordinate search also evaluates the function at the reflected points: $\mathcal{R}^k(\mathcal{S}^k) = \{z|\ z = x - h_k e_i, \quad 1 \le i \le N\}$. In coordinate search, the scale h of the next iterate is determined as follows:

$$h_{k+1} = \begin{cases} \frac{1}{2}h_k & \text{if } f(x) \le \min\{f(x \pm h_k e_i)\} \quad \text{(stencil failure)} \\ h_k & \text{if } f(x) > \min\{f(x \pm h_k e_i)\}. \end{cases}$$

When the current point, x is the best point, coordinate search reduces h. We choose to reduce h by one-half. And when coordinate search finds a better point, h remains the same. We denote the set of function values of these winning points as $\mathcal{W} = \{f(z_1), f(z_2), \ldots\ |z_1, z_2, \ldots \in \mathcal{S}^k \cup \mathcal{R}^k\}$.

We want to show $\mathcal{W}$ is a finite set and do so by contradiction. Let's assume $\mathcal{W}$ is an infinite set. Since, the elements $\in \mathcal{W}$ form a strictly decreasing sequence, coordinate search must move in a descent direction (and find a point with a smaller function value) for infinitely many k. This happens for f with unbounded level sets. This contradicts our assumption that f has bounded level sets, so $\mathcal{W}$ must be a finite set.

The fact that $\mathcal{W}$ is a finite set means that coordinate search will find a better point

on the stencil only a finite number of times. And so for infinitely many k, stencil failure occurs and h is reduced. This sequence is $\{h_k\} = \{\frac{1}{2^k}h_0\}_{k=1}^{\infty}$ and therefore $h_k \to 0$. We obtain the first result of the theorem.

Next we check the assumptions on the simplex before applying lemma 4.2. The kth simplex $\mathcal{S}^k(x, h_k)$ is nonsingular and $V = [h_k e_1, \ldots, he_n]$ is well-conditioned since $\kappa(V) = 1$ for all h_k. The first requirement for a bounded condition number is met. We check the second requirement next. Note that the maximum distance $\sigma_+(\mathcal{S}) = h$ and

$$x^T V V^T x = h^2\|x\|^2 > \mu_- h^2\|x\|^2 \text{ for all } x.$$

Since we know stencil failure occurs for infinitely many k, we can use the result from lemma 4.2 that stencil failure implies $\|\nabla f_s(x_k)\| = O\left(h_k + \frac{\|\phi\|_{\mathcal{S}^k}}{h_k}\right)$. We apply the assumption that $\lim_{k\to\infty}\left(h_k + \frac{\|\phi\|_{\mathcal{S}^k}}{h_k}\right) = 0$. And we obtain the result we want: $\|\nabla f_s(x_k)\| \to 0$. □

Now, we define a simplex for implicit filtering from [7]. For $x \in \mathbb{R}^N$ and $h > 0$, the simplex is the set of points: x and $x + hv_j$ for $1 \le j \le N$ such that $V = I$. The condition number $\kappa(V) = 1$.

The convergence result for implicit filtering [7]:

Theorem 4.2. *Let $f(x) = f_s(x) + \phi(x)$ and ∇f_s be Lipschitz continuous. Let implicit filtering give the sequence $\{x_k, h_k\}$ and $\mathcal{S}^k = \mathcal{S}(x, h_k)$. Let $h_k \to 0$. Assume that the sufficient decrease condition:*

$$f(x - \lambda\nabla_h f(x)) - f(x) < -\alpha\lambda\|\nabla_h f(x)\|^2$$

holds for all but finitely many k. Then if

$$\lim_{k\to\infty}\left(h_k + \frac{\|\phi\|_{\mathcal{S}^k}}{h_k}\right) = 0 \tag{4.8}$$

then any limit point of the sequence $\{x_k\}$ is a critical point of f_s.

For the convergence of implicit filtering, we must assume the successful termination of the quasi-Newton method. If stencil failure occurs or there is no line search failure for all but finitely many k, then $\|D(f : \mathcal{S}^k)\| \to 0$. Then lemma 4.1 and assumption 4.8 are used to show $\|\nabla f_s(x_c)\| \to 0$ [7].

4.4 Implicit Filtering Algorithm

The MATLAB code, imfil.m written by Kelley [35], implements implicit filtering. Kelley [35] provides an algorithm for the basic implicit filtering in the unconstrained case. The following is an extension of that algorithm to the bound constrained case where $L_i = 0$ and $U_i = 1$.

We provide a description of the algorithm here. The pseudocode follows. Input the initial point x, objective function f, maximum calls to the function *budget*, size of scale h, minimum size of scale h_{min}, maximum number of line searches from current iterate $maxitarm$, and tolerance τ. Let f_{base} be the first function evaluation of the initial point x. Let the matrix of directions V be the positive and negative unit vectors e_i, for $i = 1, \ldots, N$. Let f_{count} be the counter for function evaluations. The algorithm terminates once the budget for function evaluations is exceeded or when a reduction in stencil size causes it to be smaller than the inputted minimum value,

h_{min}.

Until either of these occur, the algorithm proceeds with a coordinate search first. The coordinate search applies only to those stencil points within the bounds. The algorithm compares the function evaluations of the stencil with the function evaluation of the base point x. If stencil failure occurs, meaning the base point has the least function value, then reduce the stencil size by one-half. If there is a point with a smaller function value on the stencil and the projected gradient does not meet the termination criterion, then the algorithm performs a line search to see if a better point, not on the stencil, exists. The line search requires a model of the inverse of the reduced Hessian at the current point, active set information at the new point, the centered difference stencil gradient, and the step length.

The step length parameter λ reduces by a constant factor β until the sufficient decrease condition is met or until the maximum number of step length trials is met. The default in imfil.m is $\beta = 1/2$. The sufficient decrease condition is:

$$f(x(\lambda)) - f(x) \leq \alpha D_C(x, f, V, h)^T (x(\lambda) - x), \tag{4.9}$$

where $x(\lambda) = \mathcal{P}(x - \lambda D_C(x, f, V, h))$ and $\alpha = 10^{-4}$.

So, the line search continues $maxitarm$ number of times or until the sufficient decrease condition is met. If sufficient decrease is met for $m \leq maxitarm$, then the point obtained by the line search becomes the new base point. If the line search fails (sufficient decrease is not met), then the algorithm compares the minimum function value (f_{min}) found by the coordinate search and the function value of the last $x(\lambda)$). If $f(x(\lambda)) \leq f_{min}$, then reduce the stencil size h. In this situation, $f(x(\lambda))$ did not meet

sufficient decrease, so f_{min} does not meet sufficient decrease either. If $f(x(\lambda)) > f_{min}$, then take the stencil point with the minimum function value as the new base point. Here, the coordinate search found the best point.

As long as the number of function evaluations are within the budget and the stencil size is greater than or equal to its minimum value, the algorithm starts another coordinate search centered around the newly determined base point (or the same point if the algorithm reduced the stencil size).

The pseudocode for the basic implicit filtering algorithm is labeled **imfil** below.

4.5 Why Appropriate for Our Problem?

Implicit filtering for bound constrained problems is appropriate for our problem.

- The feasible region has simple bound constraints.
- The stochastics in the objective function show up as low amplitude, high frequency noise in the optimization landscape resulting in many local minima.
- There are gaps in the landscape from violations of hidden constraints concerning reliability and cost variability.
- The derivatives of the objective function are unknown so finite differences can be used as an approximation.

imfil$(x, f, budget, h, h_{min}, maxitarm, \tau)$

Let: $f_{base} = f(x)$, $V = (e_1, e_2, \ldots, e_N, -e_1, \ldots, -e_N)$, $f_{count} = 1$

while $f_{count} \leq budget$ and $h \geq h_{min}$ **do**

Apply a coordinate search only to those stencil points within the bounds:

for $i = 1, ..., N$ **do**

if $0 \leq x + he_i \leq 1$ **then**

Evaluate $f(x + he_i)$

$f_{count} = f_{count} + 1$

end if

if $0 \leq x - he_i \leq 1$ **then**

Evaluate $f(x - he_i)$

$f_{count} = f_{count} + 1$

end if

$i = i + 1$

$f_{min} = \min\{f(x \pm he_i) |\ i = 1, \ldots, N\}$

end for

If stencil failure, reduce h. Otherwise, if projected gradient does not meet termination criterion, then allow the line search to search for a better point. If the line search fails, but a point with a smaller function value exists on the stencil, then take the stencil point as the new iterate:

if $f_{base} \leq f_{min}$ **then**

$h \leftarrow h/2$

else

Compute $D_C(x, f, V, h)$

if $\|x - \mathcal{P}(x - D_C)\| \leq \tau h$ **then**

$h \leftarrow h/2$

else

Compute $R(x, \epsilon, H)^{-1}$

Set $d = -R^{-1}D_C$

Find the least integer $m \geq 0$ such that sufficient decrease condition 4.9 holds for $\lambda = \beta^m$ or $m = maxitarm$.

$f_{count} = f_{count} + m + 1$

if sufficient decrease condition 4.9 does not hold **then**

Compare $f(x(\lambda))$ to f_{min}

if $f(x(\lambda)) \leq f_{min}$ **then**

$h \leftarrow h/2$

else

$x \leftarrow x \pm he_i$ such that $f_{min} = \min\{f(x \pm he_i)\}$

$f_{base} = f(x)$

end if

else

$x \leftarrow x + \lambda d$

$f_{base} = f(x)$

end if

end if

end if

end while

Chapter 5

Optimization Problem without Variance Reduction

The optimization problem, version I, is the optimization problem without variance reduction. We restate the problem and give a brief recap of the methodology that was described fully in chapter 2. The main purpose of this chapter is to provide the results of solving version I of the optimization problem.

5.1 Problem Statement

The objective is to identify the number of permanent rights, leases, and options that minimize the expected annual cost of meeting a city's annual water demand subject to reliability and cost variability constraints.

5.2 Recap of Methodology

In order to evaluate the objective function, a stochastic water market model was built. The model simulates hydrologic and water market conditions by randomly sampling historical data. The model makes a decision every month on whether or not to purchase water and if so, how much. The model computes the annual cost for the 12-month cycle. The model repeats the process 10,000 times, calculates the average of those 10,000 realizations, and uses this average value as the expected annual cost.

In figure 5.1, we plot the cost function against the number of permanent rights N_{R_T} and the number of options N_O to illustrate what the optimization landscape looks like. The gaps indicate where the constraints are violated. The graph also demonstrates the effect of the random variables. The function appears to be relatively smooth but a closer look in figure 5.2 reveals small oscillations in the function values (noise). Note that the landscape in figure 5.2 focuses on the lower range of permanent rights (from 20,000 to 30,000 acre-feet).

To find the least annual cost, the model links to an optimizer that uses implicit filtering. The optimizer starts with an initial point (N_{R_T}, N_O, α_1, α_2, β_1, β_2), calls the model to evaluate the cost function, and then searches for a point with a smaller cost value. The optimizer uses this new point to start another iteration. The process moves along the optimization landscape searching for the least annual cost until some termination criterion is met. Implicit filtering is advantageous here because the random variables cause only low noise in the cost function so it does not get trapped in the many local minima produced by the noise. The noise could be reduced further by increasing the number of realizations but the computational cost would become

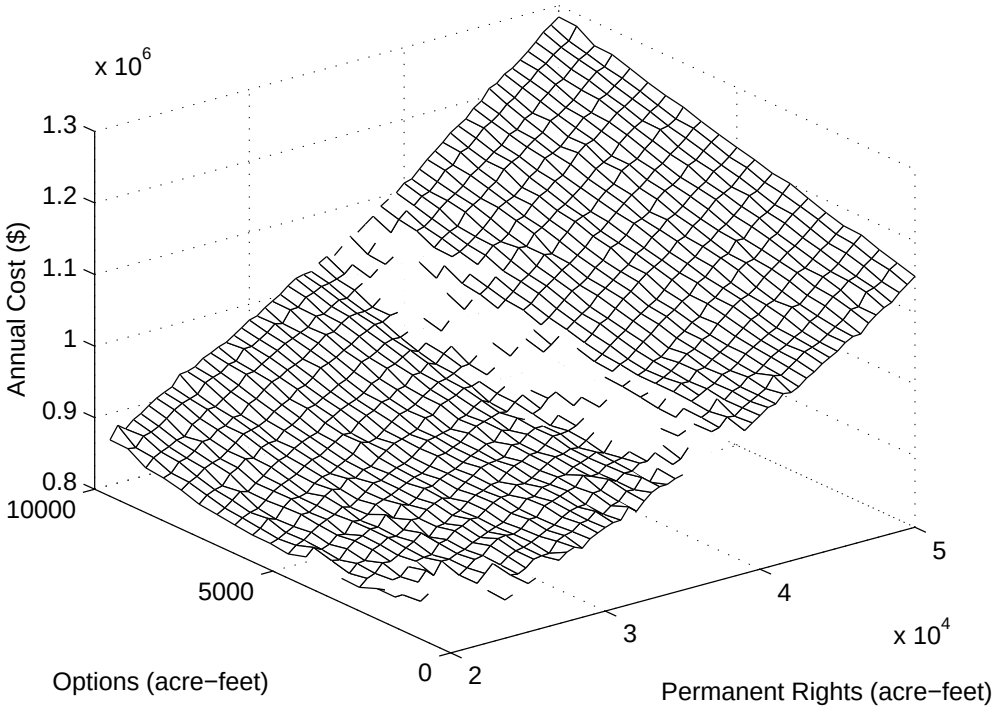

Figure 5.1: Optimization Landscape

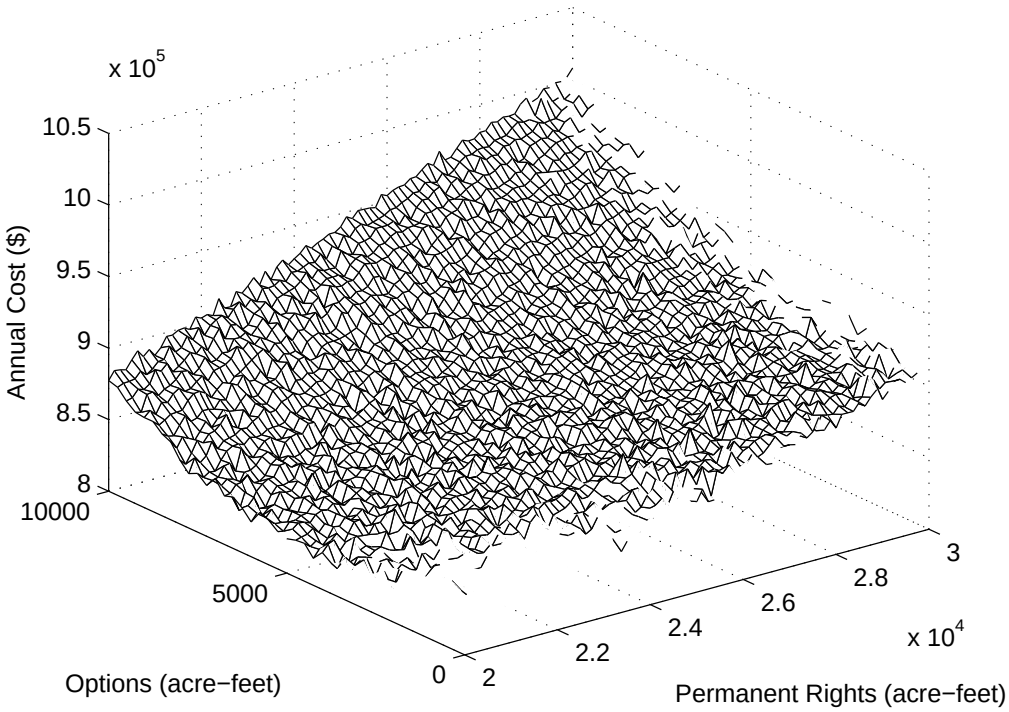

Figure 5.2: Closer Look at Optimization Landscape

too great. We found that using 10,000 realizations produces repeatable results.

5.3 Results

Characklis et al. [13] studied three strategies. Strategy A involves permanent rights only. There is only one decision variable, the total volume of permanent rights (N_{R_T}). Strategy B includes permanent rights and options. When strategy B is studied, there are four decision variables: the total volume of permanent rights (N_{R_T}), volume of options purchased before the start of the year (N_O), and the threshold values (α_2, β_2) after the option exercise month t_X. Strategy C includes all three means of water transfers: permanent rights, options, and leases. The analysis of this alternative includes six decision variables. They include the same four from Strategy B with the addition of two others: the threshold values (α_1, β_1) before the option exercise month t_X.

Each strategy uses the scenario where the city begins the year with the least amount of water available ($f_{R_0} = 0.1$ and $R_0 = 0.8$ million acre-feet (MAF)). Meaning, the city initially receives only 10% of its permanent rights and the reservoir level is at its lowest considered for this problem. Also, within each strategy, portfolios meeting reliabilities of 98%, 99%, and 99.5% were compared. The reliability with respect to critical failures was always set at 99.5%.

5.3.1 Strategy A

Since Strategy A involves permanent rights only, there is no cost variability. The price of permanent rights is a constant, therefore the annual cost is known. Table 5.1

Table 5.1: Comparison of Portfolios for Strategy A ($R_0 = .8$ MAF, $f_{R_0} = 0.1$)

Reliability	Permanent Rights (acre-feet)	Annual Cost (million $)	Year End Supply (acre-feet)
99.5%	70,500	1.59	23,200
99%	66,000	1.49	20,400
98%	62,000	1.40	17,900

compares the permanent rights required to meet the given reliability constraints. For 99.5% reliability, 70,500 acre-feet are required at an annual cost of $1.59 million. The number of acre-feet required and annual cost decreases, as expected, as the reliability decreases. It is also interesting to note that the cost to increase reliability from 99% to 99.5% is greater than the cost to increase reliability from 98% to 99%. This translates to a curve (cost versus reliability) where the slope increases as reliability increases. The slope is referred to as marginal cost of reliability.

5.3.2 Strategy B

Strategy B involves permanent rights and options. Since strategy B only considers permanent rights and options, water demand before the option exercise month ($t = 5$) is met solely from allocations of permanent rights. At $t = 5$, the model can also exercise options. At this point in time, more information is known about the supply. Options provide a means of acquiring water while lowering the annual cost and the average year end supply. See table 5.2. For 99.5% reliability, strategy B requires 52,700 acre-feet of permanent rights and 11,100 acre-feet of options for an expected annual cost of $1.34 million which is 16% less than the annual cost for strategy A.

Table 5.2: Comparison of Portfolios for Strategy B ($R_0 = .8$ MAF, $f_{R_0} = 0.1$)

Reliability	Rights (ac-ft)	Options (ac-ft)	Expected Annual Cost (million $)	CVAR (million $)	α_2	β_2	Year End Supply (ac-ft)
99.5%	52,700	11,100	1.34	1.37	1.67	1.85	17,100
99%	51,800	4,700	1.30	1.31	1.48	2.10	15,300
98%	48,900	4,900	1.23	1.25	1.33	2.15	13,500

And the average year end supply decreased from 23,200 acre-feet to 17,100 acre-feet. This decrease in unused water translates into a lower annual cost for strategy B and more water that could be used by others in the region. The marginal cost of reliability increases for increased reliability just as it did for strategy A.

With the addition of options, comes variability in the cost. Table 5.2 shows the Conditional Value at Risk (CVAR) that meets the cost variability constraint for each level of reliability. In all three cases, the CVAR is still less than the expected annual cost for 98% reliability in strategy A. So, even though there is some cost variability, the expected annual costs are still less than the strategy without options.

Table 5.2 also shows the α_2 and β_2 values that provide the required level of reliability. The model only uses the second set of threshold values here. The values for α_2 and β_2 are relatively high for this strategy because there is only one chance to purchase water. So, in the 99.5% reliability case, the model exercises options whenever supply is less than 1.67 times the demand. Then, enough options are exercised so that the supply becomes 1.85 times the demand.

5.3.3 Strategy C

Strategy C includes all three means to acquire water: permanent rights, options, and leases. Three different types of portfolios were optimized to determine the least expected annual cost:

- C1 - This strategy sets the cost risk threshold to 1.1 which does not consider portfolios where the CVAR exceeds the expected annual cost by more than 10%.

- C2 - This strategy purchases 33,000 acre-feet of permanent rights, allows the purchase of options and leases to augment supply, and does not limit cost variability.

- C3 - This strategy allows the purchase of options and leases only and does not limit cost variability.

The results of Strategy C1 are in table 5.3. For each level of reliability, the portfolios met the cost variability constraint with mostly permanent rights and small amounts of leases. Options are not a part of the optimal portfolio. For 99.5% reliability, the expected annual cost is $1.3 million. The large volume of permanent rights satisfies the demand in the early part of the year. Lease purchases occur later so the model only needs α_2 and β_2. Since lease purchase decisions occur monthly, more risky behavior (than in strategy B) is allowed.

Table 5.3: Comparison of Portfolios for Strategy C1 (R_0 = .8 MAF, $f_{R_0} = 0.1$)

Reliability	Rights (ac-ft)	Expected Leases (ac-ft)	Expected Annual Cost (million $)	CVAR (million $)	α_2	β_2	Year End Supply (ac-ft)
99.5%	56,900	670	1.30	1.41	1.30	1.31	15,600
99%	54,400	900	1.25	1.38	1.20	1.28	14,100
98%	53,000	1000	1.22	1.35	1.20	1.23	13,400

We compare strategy B (permanent rights and options) and C1 (permanent rights and leases) in table 5.4. The expected annual costs for strategy C1 are less than those for the corresponding reliability level of strategy B, while the CVAR and CVAR-to-expected annual cost ratios are higher. This shows that even the purchase of low number of leases result in cost variability. The year end supply decreases with strategy C1. Since strategy C1 has more opportunities to augment the supply, this allows a smaller α_2 indicating more risky behavior. For example, in the 99.5% reliability level, the model purchases water when the supply is less than 1.3 times the demand instead of 1.67 as in strategy B. And the amount of water purchased is less than that in strategy B, with a β_2 of 1.31 instead of 1.85.

Strategy C2 maintains 33,000 acre-feet of permanent rights and augments the supply with leases only. Again, the optimal mix does not include options. See table 5.5. The expected annual costs, CVAR, and year end supply are the lowest of all previous strategies (A, B, C1) discussed, though the CVAR-to-expected annual cost ratio of 1.2 is the highest. For 99.5% reliability, the expected annual cost is $.92 million with a CVAR of $1.1 million and year end supply of 7,100 acre-feet. The model requires both sets of α and β values. The permanent rights alone do not meet

Table 5.4: Comparison of Strategies B and C1 ($R_0 = .8$ MAF, $f_{R_0} = 0.1$)

Reliability	Strategy	Expected Annual Cost (million $)	CVAR (million $)	α_2	β_2	Year End Supply (acre-feet)
99.5%	B	1.34	1.37	1.67	1.85	17,100
	C1	1.30	1.41	1.30	1.31	15,600
99%	B	1.31	1.31	1.48	2.10	15,300
	C1	1.25	1.38	1.20	1.28	14,100
98%	B	1.23	1.25	1.33	2.15	13,500
	C1	1.22	1.35	1.20	1.23	13,400

demand so the model buys leases to augment supply throughout the year. The first set of α and β values are higher than the second set. The α_1 value ensures the model purchases water in the early part of the year because of the low initial reservoir level and initial allocation of water. As long as α_1 is set high enough to trigger purchases, reliability is met. The low supply conditions also require the model to purchase a larger number of leases in order to meet reliability requirements, hence the higher β_1 values. Since the model purchases most of the water early, the model uses the lower α_2 and β_2 values to manage supply later in the year.

The optimal portfolio for strategy C3 relies on leases only. See table 5.6. For 99.5% reliability, the expected annual cost is $.58 million with a CVAR of $1.16 million, and a year end supply of only 2,400 acre-feet. This expected annual cost for strategy C3 is a 55% decrease from the strategy C1 cost and a 37% decrease from the strategy C2 cost. Even though the CVAR is less than the expected values for strategies A, B, and C1, the CVAR-to-expected annual cost ratio is 2. Meaning, there is a risk that the cost can vary to twice the expected value. Since there are no permanent rights,

Table 5.5: Comparison of Portfolios for Strategy C2, where permanent rights are fixed at 33,000 acre-feet ($R_0 = .8$ MAF, $f_{R_0} = 0.1$)

Reliability	Expected Leases (ac-ft)	Expected Annual Cost (million $)	CVAR (million $)	α_1	β_1	α_2	β_2	Year End Supply (ac-ft)
99.5%	6800	.92	1.10	1.56	1.77	.93	1.04	7,100
99%	6000	.91	1.07	1.48	1.74	.90	.93	6,500
98%	5800	.90	1.06	1.62	1.69	.70	.79	6,100

Table 5.6: Comparison of Portfolios for Strategy C3 ($R_0 = .8$ MAF, $f_{R_0} = 0.1$)

Reliability	Expected Leases (acre-feet)	Expected Annual Cost (million $)	CVAR (million $)	β_1	α_2	β_2	Year End Supply (acre-feet)
99.5%	22300	.58	1.16	2.56	.97	1.09	2,400
99%	22000	.57	1.16	2.50	.96	1.04	2,100
98%	21700	.55	1.09	2.32	.75	1.07	1,800

the model purchases water no matter the value of α_1. The β_1 values are greater than 2 indicating that the model purchases most of the water up front in order to meet reliability requirements. The model uses the lower α_2 and β_2 values in a similar manner as in strategy C2.

5.3.4 Comparing Strategies B and C2

Strategy A is the most costly, yet there is no cost variability. When given other alternatives with a CVAR 30% (strategy C2) or 14% (strategy B) less than the annual cost for strategy A, it makes sense to consider those other strategies. Strategy C3

has the lowest expected annual costs but the highest CVAR-to-expected annual cost ratios. This strategy also relies entirely on lease purchases which probably does not make a viable strategy from a political perspective. Strategy C2 has a lower expected annual cost but a higher CVAR-to-expected annual cost ratio than strategy C1. The 29% decrease in expected annual cost for strategy C2 outweighs its higher cost ratio. So, strategies B and C2 seem the most practical and warrant further investigation.

See table 5.7 (strategy B) and table 5.8 (strategy C2) for the portfolios of least expected annual cost given different initial conditions (for 99.5% reliability). In both strategies, the expected annual costs decrease as the initial water allocation (indicated by f_{R_0}) increases. Though, the costs in strategy C2 are not affected as much as in strategy B where the costs may double depending on the initial water allocation. For strategy B, in order to meet the 99.5% reliability, the number of permanent rights needs to be large when the initial water allocation is small. As the initial water allocation increases, fewer permanent rights are required. Since permanent rights are expensive (as seen from strategy A), this affects the expected annual cost directly. On the other hand, strategy C2 has a constraint to maintain 33,000 acre-feet of permanent rights and augments supply with leases. The high and low costs remain within \$.12 million of each other. In this case, the use of leases to augment supply results in expected costs that are not as sensitive to initial water allocation as in strategy B. Note that the average CVAR-to-expected annual cost ratio is higher for strategy C2 at 1.11 instead of 1.03 for strategy B.

The initial reservoir level (R_0) affects the price of options and leases, not the quantity purchased. In both strategies, the higher initial reservoir level results in

Table 5.7: For 99.5% Reliability, Portfolios for Strategy B under different initial conditions (R_0, f_{R_0})

R_0	f_{R_0}	Permanent Rights (acre-feet)	Options (acre-feet)	Expected Exercised Options (acre-feet)	Expected Annual Cost (million $)	CVAR (million $)	Year End Supply (acre-feet)
1.5	0.1	52,900	6,100	3,400	1.32	1.36	16,000
	0.3	34,200	2,500	1,600	0.83	0.84	15,600
	0.5	29,000	0	0	0.66	-	6,200
2.2	0.1	53,000	6,100	3,300	1.26	1.30	15,800
	0.3	27,100	7,700	6,500	0.70	0.72	7,500
	0.5	29,000	0	0	0.66	-	6,200

Table 5.8: For 99.5% Reliability, Portfolios for Strategy C2 under different initial conditions (R_0, f_{R_0})

R_0	f_{R_0}	Permanent Rights (acre-feet)	Options (acre-feet)	Expected Leases (acre-feet)	Expected Annual Cost (million $)	CVAR (million $)	Year End Supply (acre-feet)
1.5	0.1	33,000	0	7,100	0.87	0.98	7,500
	0.3	33,000	0	600	0.76	0.84	7,700
	0.5	33,000	0	0	0.75	-	13,800
2.2	0.1	33,000	0	6,700	0.85	0.94	7,300
	0.3	33,000	0	700	0.76	0.81	7,700
	0.5	33,000	0	0	0.75	-	13,800

lower expected costs. But the effect is small. For strategy B, the expected annual costs decrease at most $.13 million when changing the initial reservoir level from 1.5 to 2.2 million acre-feet. For strategy C2, the decrease is at most $.02 million.

In both strategies, the year end supply is at least 30% of the average annual demand of 21,000 acre-feet. So each portfolio leaves some water to carry over to the next year.

5.3.5 Modified Strategy C2

To look at the impacts of including options in a portfolio with permanent rights and leases, we modify strategy C2. Now, strategy C2 has a constraint of 33,000 acre-feet of permanent rights and an additional constraint on the number of options. See table 5.9 for the 99.5% reliability minimum cost portfolios given several values of options. The expected annual cost increases as the number of options increases. But, the CVAR drops once options enter the portfolio. And the CVAR for each portfolio with options is less than the CVAR for the portfolio without options. Figure 5.3 has the same data as table 5.9 but the graph shows the trend of the expected costs and CVAR values better. Options can lower cost variability for a slight increase in expected cost. The portfolio with 4,000 options and 5,270 leases has an expected cost $.05 million higher than the portfolio with no options and 6,860 leases. But the 4,000 option portfolio has a lower CVAR of $1.095 million rather than $1.12 million. This modified strategy C2 offers some insurance against high lease prices, yet still allows the purchase of leases when it makes sense.

5.4 Conclusions

A portfolio of permanent rights only can reliably meet demand but at a very high cost as seen in strategy A. Strategies B and C show that adding options or leases, respectively, can lower expected costs and still meet reliability constraints. In fact, the portfolio of leases only (strategy C3) has the lowest expected cost of all strategies studied. However, there can still be significant cost savings with less risky portfolios.

Table 5.9: Strategy C2 with Different Option Purchases (99.5% Reliability, $R_0 = .8$ MAF, $f_{R_0} = 0.1$

Permanent Rights (acre-feet)	Options (acre-feet)	Expected Exercised Options (acre-feet)	Expected Leases (acre-feet)	Expected Annual Cost (million $)	CVAR (million $)
33,000	0	0	6,860	.92	1.120
33,000	1,000	630	6,210	.93	1.090
33,000	2,000	1,010	5,820	.94	1.090
33,000	3,000	1,640	5,460	.95	1.090
33,000	4,000	1,820	5,270	.97	1.095

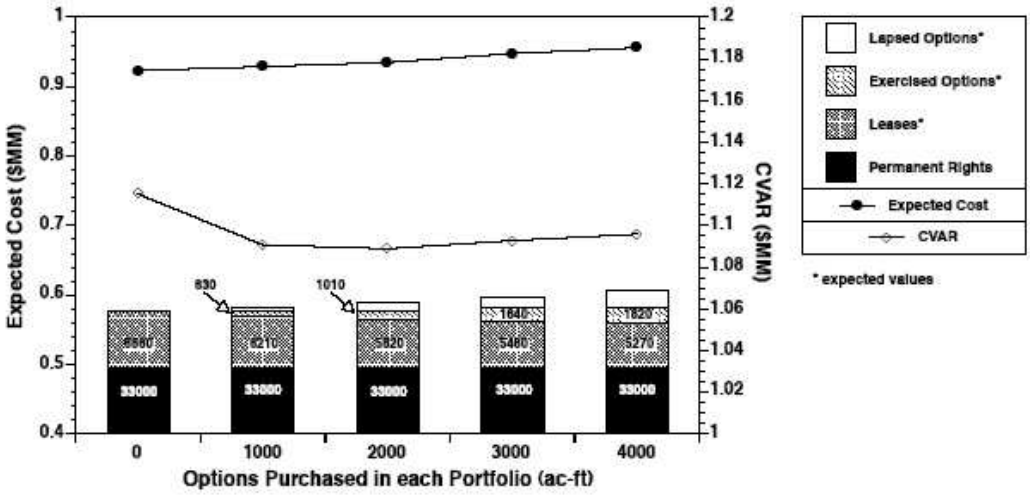

Figure 5.3: Comparison of Expected Cost and CVAR of Portfolios with Different Number of Options

The modified strategy C2 shows how options and leases can both be used to augment supply. This flexibility comes at a cost comparable to strategies without as much flexibility (such as the original strategy C2).

Chapter 6

Optimization Problem with Variance Reduction

The optimization problem, version II, is the optimization problem with variance reduction. In version I, the model output was the average cost value of 10,000 realizations. Variance reduction techniques can be applied to reduce the noise in the simulation. The variance of an estimate is a measure of its accuracy. The smaller the variance, the more accurate the estimate. So, one benefit of using variance reduction is the increased accuracy for the same computational cost (number of realizations). Or one might apply variance reduction in order to decrease computational cost for the same accuracy.

In this chapter, we describe the control variate technique (the variance reduction method we selected). The simplest version involves one control variate which is a random variable denoted as Z. We can easily expand the technique to involve more than one control variate, denoted as Z_i. Then, we describe how we apply the control variate technique to the one-year water market model. We end the chapter with

results and conclusions.

6.1 Control Variate Technique

The following discusses the variance reduction method applied to the stochastic water market model: the control variate technique, as described by Kleijnen [37] and Lavenberg and Welch [38].

6.1.1 Single Control Variate

Throughout this section, we define statistical terms and notation (from [11]) for a general random variable X as needed.

Definition 6.1 (Expected Value)**.** *The expected value of a random variable X is the weighted average of all possible values of X:*

$$E[X] = \mu_x.$$

The output of a Monte Carlo simulation is an expected value, E[Y], where Y is the simulation output of each realization (Y = annual portfolio cost in our stochastic water market model). The control variate technique constructs a different estimator of E[Y], called θ, by using a random variable Z, where E[Z] is known and c is a real number:

$$\theta = Y + c(Z - E[Z]). \tag{6.1}$$

In this variance reduction technique, the goal is to choose a random variable Z and a real number c such that the variance of θ is less than the variance of Y. Before we give a formula for the variance of θ, we need two definitions.

Definition 6.2 (Variance)**.** *The variance of random variable X is:*

$$Var(X) = E[(X - E[X])^2] = E[X^2] - (E[X])^2.$$

The variance gives a measure of the degree of spread of a distribution around its mean. The unit of measurement of variance is the square of the unit of random variable X.

Definition 6.3 (Covariance)**.** *The covariance of random variables X and V is:*

$$Cov(X, V) = E[(X - \mu_x)(V - \mu_v)]$$

where $E[X] = \mu_x$ and $E[V] = \mu_v$.

Covariance measures the strength of a relationship between two random variables X and V.

Now, we give the formula for the variance of θ:

$$Var(\theta) = Var(Y) + c^2 Var(Z) + 2cCov(Y, Z).$$

The value of c can be chosen to minimize the variance of θ (by taking the derivative of Var(θ) with respect to c and setting it equal to zero):

$$\begin{aligned} \frac{dVar(\theta)}{dc} = 2cVar(Z) + 2Cov(Y,Z) &= 0 \\ c^* &= \frac{-Cov(Y,Z)}{Var(Z)} \end{aligned} \tag{6.2}$$

Also,

$$\frac{d^2Var(\theta)}{dc^2} = 2Var(Z) > 0.$$

Since, first and second order conditions for optimality are met, c^* is a minimum.

Variance reduction using the new estimator θ can be achieved:

$$\begin{aligned} Var(\theta) &= Var(Y) + c^2Var(Z) + 2cCov(Y,Z) \\ &= Var(Y) + \left(\frac{-Cov(Y,Z)}{Var(Z)}\right)^2 Var(Z) + 2\frac{-Cov(Y,Z)}{Var(Z)}Cov(Y,Z) \\ &= Var(Y) + \frac{Cov(Y,Z)^2}{Var(Z)} - 2\frac{Cov(Y,Z)^2}{Var(Z)} \\ &= Var(Y) - \frac{Cov(Y,Z)^2}{Var(Z)} \end{aligned}$$

As long as $Cov(Y,Z) \neq 0$, the variance of θ is less than the variance of Y. We refer to Z as the control variate.

The relationship between the original estimate Y and the control variate Z also affects the amount of variance reduction. The correlation coefficient, defined below,

quantifies this relationship. It requires the definition of standard deviation.

Definition 6.4 (Standard Deviation)**.** *Standard Deviation of random variable X:*

$$\sigma_x = \sqrt{Var(X)}.$$

Like variance, the standard deviation also gives a measure of the spread of a distribution around its mean. The unit of measurement for standard deviation is the same as that of the random variable X.

Definition 6.5 (Correlation Coefficient)**.** *The correlation coefficient of random variables X and V is:*

$$\rho_{xv} = \frac{Cov(X,V)}{\sigma_x \sigma_v}.$$

The correlation coefficient standardizes the covariance and is bound by -1 and 1. Values equal to -1 or 1 indicate a perfect linear relationship between X and V.

The variance of θ can also be written in terms of the correlation coefficient between the original estimate Y and control variate Z:

$$Var(\theta) = (1 - \rho_{yz}^2)Var(Y). \tag{6.3}$$

The higher the value of $|\rho_{yz}|$, the better the correlation between Y and Z. This indicates that the more Y and Z are correlated, the greater the variance reduction will be.

6.1.2 Multiple Control Variates

The single control variate technique can be expanded to multiple control variates, Z_i for $i = 1, \ldots, m$ where $E[Z_i]$ is known for each i and $c_i \in \mathbb{R}$:

$$\theta = Y + c_1(Z_1 - E[Z_1]) + \cdots + c_m(Z_m - E[Z_m]). \tag{6.4}$$

The variance of θ is:

$$Var(\theta) = Var(Y) + \sum_{i=1}^{m}\sum_{j=1}^{m} c_i c_j Cov(Z_i, Z_j) + 2\sum_{i=1}^{m} c_i Cov(Y, Z_i).$$

The constants c_i that minimize the variance (also referred to as $c^* \in \mathbb{R}^m$) can be found by finding the least squares solution to the following linear regression:

$$Y = a + b_1 Z_1 + \cdots + b_m Z_m + \epsilon$$

where $c_i = -b_i$ and ϵ is an error term.

6.2 Application of Control Variate Technique to the One-Year Model

6.2.1 Selection of Control Variates

In applying the control variate technique, it is vital to identify the sources of variability within the model. In the stochastic water market model, variability in the expected

annual cost arises from variability in the price of leases and the quantity of transfers. Any combination of lease price and quantity can be used as a control variate as long as the expected value is known (and not estimated). The known expected values come directly from the historical data. First, we identify the control variates. Then, we test them.

We know that some form of the lease price can be a control variate. We observe that most leases are bought at $t = 0$ and $t = 5$ and small quantities of leases are bought throughout the rest of the year. We identify the first control variate as the lease price at $t = 0$ and denote it as $Z_{p_{L,0}}$. Recall from section 2.1.6, the model calculates the quantity of leases to purchase at $t = 0$ based on the initial conditions. Since the initial conditions are fixed for each realization, the amount to purchase will be the same. This means the quantity of leases purchased at $t = 0$ is invariant. So, the only variability at $t = 0$ arises from variation in the lease price. Also $E[Z_{p_{L,0}}]$ is known. The lease prices at $t = 0$ are selected from a discrete set so the expected value is known and is not a sample average.

We consider two other forms of price as potential control variates: the lease price over a span of a few months, for example from $t = 1$ to $t = 4$ and the lease price at $t = 5$. The expected value of the potential control variate is key in selecting an appropriate control variate. Both of these cannot be used as control variates since the expected values are unknown.

We explain that the lease price over several months is not readily defined and so the expected value is unknown. The lease price is randomly selected either from the high-level or low-level reservoir price data set, depending on the current reservoir

level. And the reservoir level can change month to month, depending on the randomly sampled hydrologic data. It is not as simple as calculating the average of the high and low price data sets (from January, February, March, April) to get the expected value. In order to complete the calculation, we need more information. Since the reservoir level changes, we need to know how often the January lease price comes from the low-priced data set and how often it comes from the high-priced data set. And we need this information for February, March, and April as well. We do not have this information so the expected value is not known.

Next, we explain that the expected value of the transfer price at $t = 5$ is unknown. Since $t = 5$ is the month in which options can be exercised, it is possible for the model to exercise all options and then purchase additional leases. Just as in the above scenario, we need more information, such as how often additional leases are purchased. The expected transfer price would depend on a weighted average of the expected option exercise price and the expected lease price at $t = 5$ which is unknown.

We are able to develop control variates using linear combinations of random variables because of the following:

$$\begin{aligned} E[X_1 + X_2 + \ldots + X_n] &= E[X_1] + E[X_2] + \ldots + E[X_n]; \\ \text{For constants a and b, } \; E[aX + b] &= E[aX] + b. \end{aligned}$$

So we define the second potential control variate in this manner: the quantity of allocated water (supply) less the water consumed (demand) in the early part of the year and denote it as Z_{early}. This control variate is an indicator of the quantity of transfers made later in the year. If this difference is small, then more transfers need

Table 6.1: Correlation Coefficient ρ and Var(θ) of each Control Variate, based on the average of 10 Monte Carlo runs of 1000 realizations each ($N_{R_T} = 30000$, $N_O = 5000$, $f_{R_0} = 0.1$)

Control Variate Z_i	ρ	Var(θ)	% Reduction in Variance
Z_{early}	-.2381	$1.72017 \cdot 10^{10}$	2.6%
$Z_{p_{L,0}}$	.9038	$3.1392 \cdot 10^{9}$	82.2%

to be made. It also has a known expected value since both supply and demand are determined from discrete data sets.

The two control variates are:

$$\begin{aligned} Z_{early} &= \text{Supply} - \text{Demand } (t < t_X); \\ Z_{p_{L,0}} &= \text{Lease Price at t=0.} \end{aligned}$$

In applying the control variate technique, no single control variate reduced the variance of portfolio cost by more than 83%. Results of testing the control variates individually (at $N_{R_T} = 30000$, $N_O = 5000$, and $f_{r_0} = 0.1$) are shown in Table 6.1. Additionally, a dominant control variate in one part of the solution surface may be less dominant in other regions of the solution surface. As such, both control variates can be used simultaneously as part of a multiple control variate strategy.

6.2.2 Pilot Simulation

Now that the control variates have been selected, we want to find the c_i for control variate $i = 1, 2$ in equation 6.4 which minimize the variance of θ, denoted as $c^* = (c_1, c_2)^T$. In section 6.1.1, we found that the optimal c^* (equation 6.2) depends

on the covariance between the cost and the control variate i and the variance of control variate i. Since this information is unknown, we use a pilot simulation to estimate c^* as mentioned by Jackel [33]. There would be a bias if the calculation of c^* depended on the same random variables used to calculate θ. And the calculation of θ in equation 6.4 requires c^* to be a known constant. The bias would disappear as the number of iterations approached infinity. However, this would defeat the purpose of applying variance reduction which is supposed to require fewer iterations. So, the model incorporates a pilot simulation with fewer runs than the main simulation to estimate c^* separately from the estimation of θ. Even with the additional runs from the pilot simulation, variance reduction still does significantly reduce the number of runs needed.

6.2.3 Multiple Control Variate Algorithm with Pilot Study

The algorithm **pilot** first generates p realizations of annual cost Y and of the m control variates Z, where $p \leq n$, the number of realizations in algorithm **main**. Then, algorithm **main** uses the values for c_i^* obtained by algorithm **pilot** to calculate θ, the new estimate of annual cost. The notation Y_j refers to the Y value at the jth realization of the model and Z_{i_j} refers to the ith control variate value at the jth realization of the model.

---

pilot(p, x)
  for j = 1 to p **do**
    Generate $Y_j(x), Z_{1_j}, Z_{2_j}, \ldots, Z_{m_j}$
  end for
  Compute c_i^* for $1, \ldots, m$ control variates

---

main(n, c^*, x)
  for j = 1 to n **do**
    Generate $Y_j(x), Z_{1_j}, Z_{2_j}, \ldots, Z_{m_j}$
    Set $\theta_j = Y_j + \sum_{i=1}^{m} c_i^*(Z_{i_j} - E[Z_i])$
  end for
  Set $\overline{\theta} = \sum_{j=1}^{n} \theta_j / n$

6.2.4 Effect of Variance Reduction on Optimization Landscape

Definition 6.6 (Standard Error)**.** *Standard Error describes the variability of the average:*

$$\textit{standard error} = \frac{\sigma}{\sqrt{n}}.$$

(To decrease standard error by a factor of k, the number of realizations n must be increased by k^2.)

The ultimate goal in applying a variance reduction technique in our Monte Carlo simulation is to reduce the standard error in the simulation output of expected annual cost. This can be seen by comparing optimization landscapes with and without variance reduction (figures 6.1 and 6.2). The landscape with variance reduction has reduced noise. In order to show the effect of variance reduction, these landscapes are shown without the constraints.

Figure 6.1: Optimization Landscape without Variance Reduction

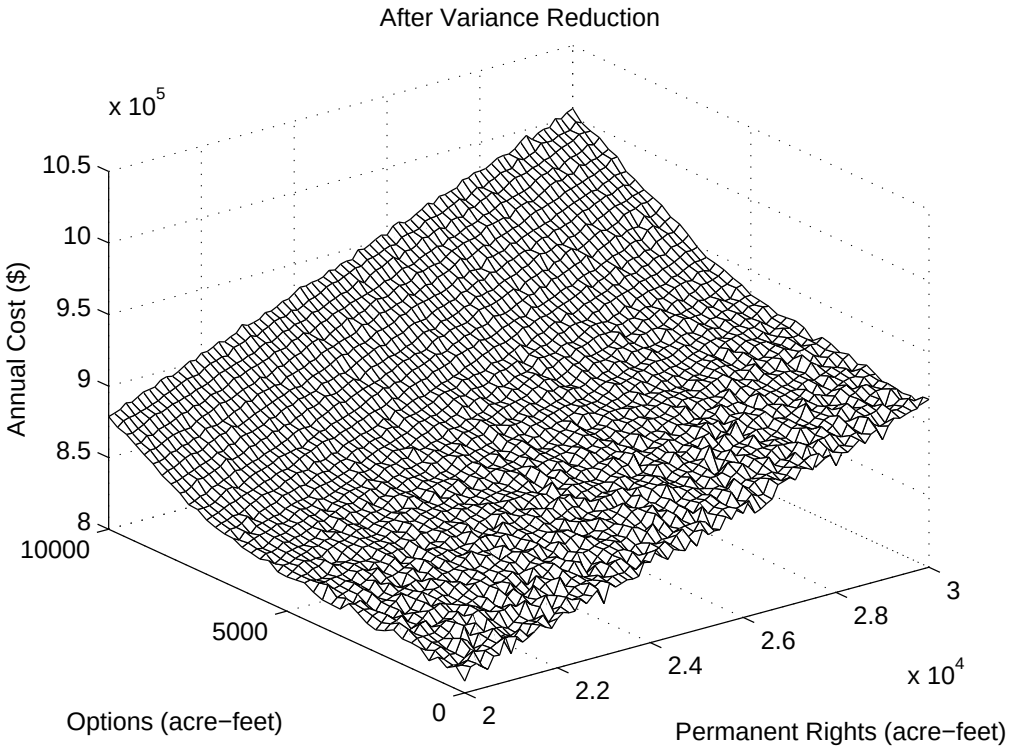

Figure 6.2: Optimization Landscape with Variance Reduction

Chapter 7

Multi-Year Water Market

In this chapter, we expand the one-year model to a multi-year model. We give some benefits of using a multi-year model, describe the differences from the one-year model, and apply the control variate method to the multi-year model (as explained by Kirsch et al [36]). Greg Characklis and Brian Kirsch, Department of Environmental Sciences and Engineering, University of North Carolina at Chapel Hill, modified the one-year model to simulate a multi-year water market.

7.1 Benefits of a Multi-Year Model

Modeling a multi-year water market is more useful to water resource managers. First, the optimal portfolio from the one-year model depends on the initial conditions. We would not expect the managers to re-adjust the portfolio every year based on the starting hydrologic conditions. And since permanent rights are not easily transferrable, cities will not be able to trade permanent rights every year. The multi-year model provides a longer time horizon which is more representative of water supply plans.

Second, it is more realistic since it includes growth in the water demand. Population growth is an issue that managers must consider. Third, the multi-year model allows the investigation of longer term option contracts which may provide another opportunity to reduce cost and/or improve reliability.

7.2 Expansion of One-Year Model to Multi-Year Model

Many details of the one-year model remain the same in the multi-year model. The multi-year model simulates a monthly water market for k years. At $t = 0$ of year 1, the city holds a number of permanent rights (N_{R_T}) and options (N_O). The reservoir storage (R_0) and the amount of water the city has carried over from the previous year (N_{r_0}) are set as initial conditions. To simulate the hydrologic and water market conditions, the model randomly samples from the same historical data. The model applies the same decision rules. Failures and critical failures are considered just as in the one-year model. The constraints of the optimization still involve reliability and cost variability.

There are a few differences. The output of the model is expected cost for the k years, referred to as portfolio cost (PC). The supply calculation is slightly more complicated. Also, the multi-year model includes growth in the water demand.

7.2.1 Portfolio Cost

Since the city pays for water via permanent rights (N_{R_T}), options (N_O), exercised options ($\hat{N}_X$), and leases purchased in month t ($\hat{N}_{L_t}$), the annual cost of water is the sum of all units multiplied by the corresponding price (denoted with the same subscript):

$$\text{Annual Cost} = N_{R_T} p_R + N_O p_O + E[\hat{N}_X] p_X + E\left[\sum_{t=0}^{11} \hat{N}_{L_t} \hat{p}_{L_t}\right].$$

The portfolio cost of k years is:

$$PC = \sum_{j=1}^{k} (\text{Annual Cost})_j.$$

7.2.2 Calculating Supply

The multi-year model is more than just running k one-year simulations and then summing the annual costs. The multi-year model accounts for the amount of water carried over from year to year and expiration dates of leases/exercised options. Both of these were not an issue in the one-year model and affect the calculation of the city's available water supply. The water supply at the start of year 1 is given by the initial conditions. The water supply at the start of years 2 through k is determined by the amount of water carried over from the previous year. Leases/exercised options expire after 12 months and the multi-year model tracks this information. The model applies permanent rights first to meet the monthly demand, then applies transfers as needed. Those transfers not applied to meet the demand after 12 months expire and

are no longer part of the available supply.

We provide the formulas to calculate the available water supply. For months prior to the option exercise month t_X of year k, the city's available water supply for month $t+1$ of year k ($S_{t+1,k}$) is calculated using the city's monthly allocations of water ($\hat{N}_{r_t}$) and purchased leases ($\hat{N}_{L_t}$) less the city's water usage in month t (u_t) and the expired water (N^{expire}) as follows:

$$S_{t+1,k} = \sum_{j=1}^{k} \left[\sum_{i=0}^{t} \hat{N}_{r_{ij}} + \sum_{i=0}^{t-1} \hat{N}_{L_{ij}} - \sum_{i=1}^{t} u_{ij} - \sum_{i=1}^{t} N_{ij}^{expire} \right].$$

For the option exercise month t_X or months after t_X of year k, the calculation accounts for the volume of exercised options ($\hat{N}_X$). In this case, the city's available water supply for month $t+1$ of year k ($S_{t+1,k}$) is:

$$S_{t+1,k} = \sum_{j=1}^{k} \left[\sum_{i=0}^{t} \hat{N}_{r_{ij}} + \sum_{i=0}^{t-1} \hat{N}_{L_{ij}} - \sum_{i=1}^{t} u_{ij} + \hat{N}_{X_j} - \sum_{i=1}^{t} N_{ij}^{expire} \right].$$

Note that the model calculates the monthly water allocations, purchased leases, city's water usage, and exercised options the same as in the one-year model.

7.2.3 Objective Function and Constraints

The expected portfolio cost is determined after n realizations of the simulation:

$$E[\text{PC}] = \frac{1}{n}\sum_{i=1}^{n}(\text{PC})_i.$$

So, for n realizations of the model and k years, we want to minimize the expected portfolio cost:

$$\min_{N_{R_T}, N_O, \alpha_1, \beta_1, \alpha_2, \beta_2} E[\text{PC}]$$

such that for $1 \leq j \leq k$:

$$\begin{aligned}
(E[r_f])_j &\geq \text{monthly reliability threshold, } \in [0,1];\\
(E[r_{cf}])_j &\geq \text{monthly critical reliability threshold, } \in [0,1].\\
\overline{\text{CVAR}/E[\text{Annual Cost}]} &\leq \text{cost risk threshold, } \in [1,\infty).
\end{aligned}$$

The decision variables are the same as in the one-year model: permanent rights, options, and purchase decision threshold values α and β. The following are defined the same: expected monthly reliability against failures ($E[r_f]$), expected monthly reliability against critical failures ($E[r_{cf}]$), and the conditional value at risk (CVAR). See chapter 2.

The reliability (against failures and critical failures) for each year must meet the minimum threshold value. The average ratio of CVAR to expected cost must remain

below a specified value.

7.3 Application of Control Variate Method to Multi-Year Model

When we apply the control variate method to the one-year model, we calculate a reduced-variance cost θ, where the $var(\theta) < var(Y)$ and Y is the original cost. In chapter 6, we explained that variance reduction will occur, as long as the correlation coefficient, ρ, (a number between -1 and 1) does not equal 0 since

$$var(\theta) = (1 - \rho^2)var(Y) \quad [38].$$

We apply this same idea to the multi-year model. We calculate a cost θ_j for each year $j = 1 \ldots k$ such that $var(\theta_j) < var(Y_j)$. We would like to reduce the variance of the overall portfolio cost, meaning: $var\left(\sum_{j=1}^{k} \theta_j\right) < var\left(\sum_{j=1}^{k} Y_j\right)$. Reducing the variance of the overall portfolio cost by reducing the variance of each annual cost is a heuristic that provides good results.

We know:

$$\begin{aligned} var\left(\sum_{j=1}^{k} \theta_j\right) &= var(\theta_1) + \ldots + var(\theta_k) + 2\sum_{i=1}^{k}\sum_{j=1}^{k} cov(\theta_i, \theta_j) \\ &= (1 - \rho_1^2)var(Y_1) + \ldots + (1 - \rho_k^2)var(Y_k) + 2\sum_{i=1}^{k}\sum_{j=1}^{k} cov(\theta_i, \theta_j), \end{aligned}$$

and

$$var\left(\sum_{j=1}^{k} Y_j\right) = var(Y_1) + \ldots + var(Y_k) + 2\sum_{i=1}^{k}\sum_{j=1}^{k} cov(Y_i, Y_j).$$

For the following, we let

$$A = 2\sum_{i=1}^{k}\sum_{j=1}^{k} cov(\theta_i, \theta_j)$$

and

$$B = 2\sum_{j=1}^{k}\sum_{j=1}^{k} cov(Y_i, Y_j).$$

We want to reduce the variance of the overall portfolio cost:

$$\begin{aligned} var\left(\sum_{j=1}^{k} \theta_j\right) &< var\left(\sum_{j=1}^{k} Y_j\right) \\ (1-\rho_1^2)var(Y_1) + \ldots + (1-\rho_k^2)var(Y_k) + A &< var(Y_1) + \ldots + var(Y_k) + B. \end{aligned}$$

If $A < B$, then the variance of the overall cost $\sum_{j=1}^{k} \theta_j$ will be less than the variance of the original overall cost $\sum_{j=1}^{k} Y_j$. We do not know of a relationship between A and B that will prove what we want. But in practice, the heuristic works and we do observe reduced variances.

In applying the control variate technique, it is vital to identify the sources of variability within the model. In the stochastic water market model, variability in the expected cost arises from variability in the price of leases and the quantity of transfers.

Any combination of lease price and quantity can be used as a control variate as long as the expected value is known (and not estimated). The known expected values come directly from the historical data.

Next, we describe the control variates for each year. The control variates for year 1 are the same as those for the one-year model: initial lease price $Z_1^{p_{L,0}}$ and net supply in early part of the year Z_1^{early}. (Early is defined as the period from the start of the year to the option exercise month.) The control variates for year 2 through year k are: net supply in early part of the jth year Z_j^{early} and net supply in later part of the previous year Z_{j-1}^{late}. (The later part of the year is defined to be those months after the option exercise month.) Both quantities are an indicator of the number of transfers needed in year j.

The multi-year model incorporates a pilot study. It has the same purpose as it did in the one-year model. The pilot study estimates the optimal c^* corresponding to each year and sends the information to the main model. The main model uses the c^* to calculate θ_j for each year j:

For the first year,

$$\theta_1 = Y_1 + c_1^{early}(Z_1^{early} - E[Z_1^{early}]) + c_1^{p_{L,0}}(Z_1^{p_{L,0}} - E[Z_1^{p_{L,0}}]).$$

For year $j = 2 \ldots k$,

$$\theta_j = Y_j + c_j^{early}(Z_j^{early} - E[Z_j^{early}]) + c_{j-1}^{late}(Z_{j-1}^{late} - E[Z_{j-1}^{late}]).$$

7.4 Effectiveness of Variance Reduction

The control variate method reduces the variance by 85% on average with the one-year model. We apply the control variate method to the ten-year model and achieve a reduction in the variance by 38% on average. The control variates are the reason for the difference in performance. In particular, the control variate that controls for the variation in the lease price is very effective, as seen in the one-year model. In the multi-year model, we can only use the initial lease price of year 1 as a control variate. We cannot use the lease price as a control variate for the remaining years since we do not know the expected values.

However, we do find that the control variate method is an effective means to reduce the average cost and the number of realizations. In figure 7.1, we observe that the cost is reduced while using variance reduction. Then, in figure 7.2, the standard error is reduced by at most 15% when the control variate method is used. Also, from figure 7.2, we can see that less realizations are required with the control variate method to obtain the same standard error. In fact, we can achieve a 30% reduction in realizations.

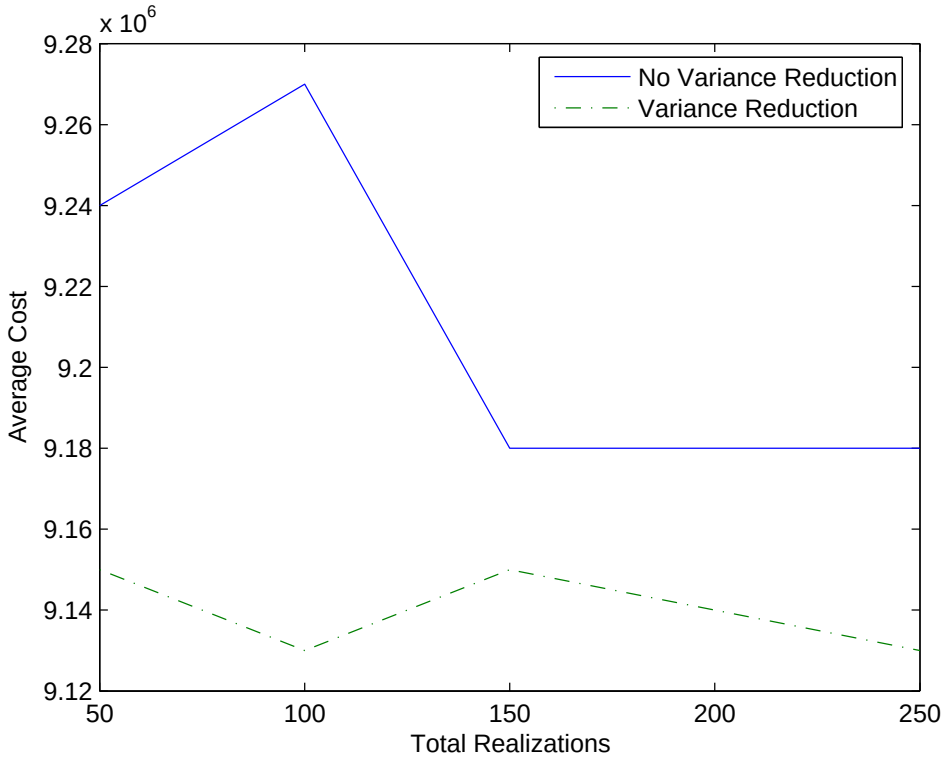

Figure 7.1: Average Cost in the 10 Year Model

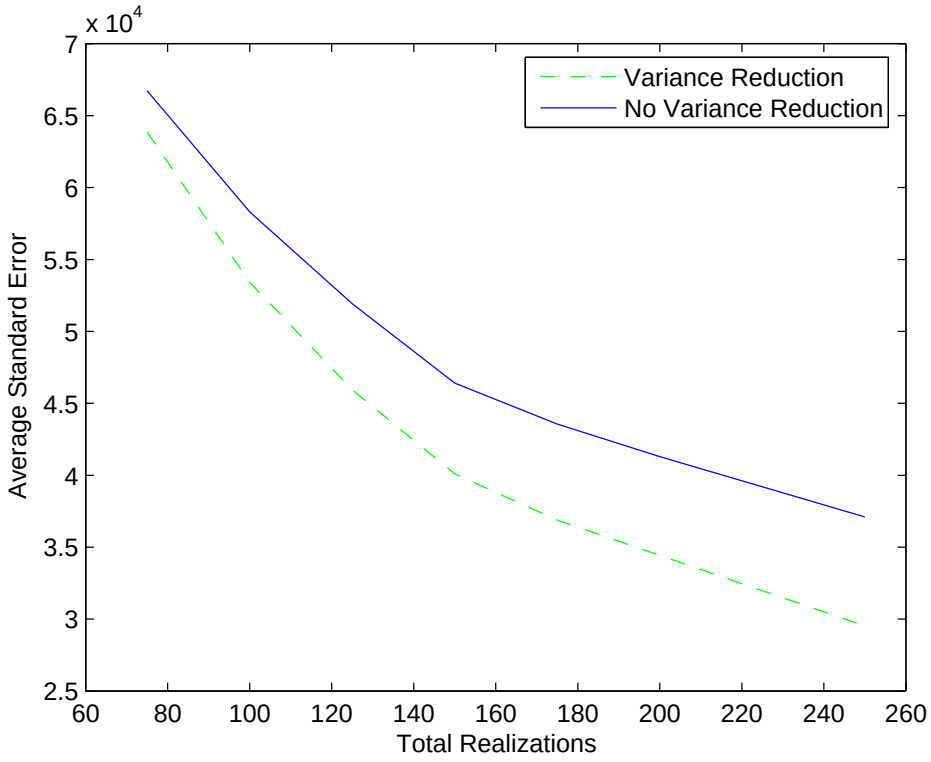

Figure 7.2: Average Standard Error in the 10 Year Model

Chapter 8

Adaptive Model

The third goal is to design a methodology where the model adapts the number of realizations of the main simulation depending on the level of noise. The idea is to increase the number of realizations in areas where the noise is prominent and/or a local minimum is expected. We can use the pilot study to estimate the noise and the amount of variance reduction. The estimated variance reduction is used to determine a lower bound on the number of realizations the main simulation requires.

In this chapter, we define a measure for the noise, develop criteria to determine the number of realizations for the main simulation, and describe the methodology for the adaptive model. We also test the methodology and report results.

8.1 Define a Measure for the Noise

We run n realizations of the model to obtain n values for annual cost and assume these values are independent and identically distributed (iid). The model output is an average of the n values to estimate the expected annual cost. Repeating the same

experiment could result in a different estimate because of the randomness. We would like to quantify a measure for the noise which is the amount the sample mean is perturbed from the true value.

Definition 8.1 (Sample Mean)**.** *For n iid samples* $(X_1, X_2, \ldots, X_n)$*, the sample mean is:* $\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$.

We know there is a potential for error when random sampling is used to estimate a parameter Θ. Maisel and Persell [43] state the statistical quantity that measures this potential error. It is called the root mean error and is defined next.

Definition 8.2 (Root Mean Error)**.** *The root mean error (RME) of an estimator* $\tilde{\Theta}$ *is:*

$$RME(\tilde{\Theta}) = \sqrt{E[(\tilde{\Theta} - \Theta)^2]}$$

for parameter Θ*.*

The root mean error can also be thought of as a total potential error that accounts for sampling error and error due to bias [43]. Sampling error is the variance which was defined previously as, $var(\tilde{\Theta}) = E[(\tilde{\Theta} - E[\tilde{\Theta}])^2] = E[\tilde{\Theta}^2] - (E[\tilde{\Theta}])^2$. The error due to bias is defined next.

Definition 8.3 (Bias of an Estimator)**.** *The bias of an estimator* $\tilde{\Theta}$ *is:*

$$bias(\tilde{\Theta}) = E[\tilde{\Theta}] - \Theta,$$

where Θ *is the true value of the parameter.*

We show from [43] that the root mean error can be calculated from the variance and bias.

$$\begin{aligned} RME(\tilde{\Theta}) &= \sqrt{E[(\tilde{\Theta}-\Theta)^2]} \\ &= \sqrt{E[\tilde{\Theta}^2 - 2\Theta\tilde{\Theta} + \Theta^2]} \\ &= \sqrt{E[\tilde{\Theta}^2] - (E[\tilde{\Theta}])^2 + (E[\tilde{\Theta}])^2 - 2\theta E[\tilde{\Theta}] + \Theta^2} \\ &= \sqrt{var(\tilde{\Theta}) + (bias(\tilde{\Theta}))^2}. \end{aligned} \tag{8.1}$$

In our problem, we use the sample mean to estimate the annual cost. We would like to know the amount the sample mean is perturbed from the true value. We apply equation 8.1 to obtain a formula for the root mean error of the sample mean, $\bar{X}$.

First, we show there is no bias of the sample mean: $bias(\bar{X}) = E[\bar{X}] - \mu = 0$, where μ is the true value for the mean.

$$\begin{aligned} E[\bar{X}] &= E[\frac{1}{n}\sum_{i=1}^{n} X_i] \\ &= \frac{1}{n}E[\sum_{i=1}^{n} X_i] \\ &= \frac{1}{n}nE[X_1] \\ &= \mu. \end{aligned}$$

Second, we find a formula for the variance of the sample mean. We use the following fact about the variance of two independent random variables X and V:

$$var(aX + bV) = a^2 var(X) + b^2 var(V), \tag{8.2}$$

where a, b are constants. In the derivation below, recall from the definition of sample mean that the X_i are iid and so must have the same variance σ^2.

$$\begin{aligned}
\bar{X} &= \frac{X_1 + X_2 + \ldots + X_n}{n} \\
var(\bar{X}) &= var\left(\frac{X_1 + X_2 + \ldots + X_n}{n}\right) \\
&= \frac{1}{n^2} var(X_1 + X_2 + \ldots + X_n) \\
&= \frac{1}{n^2}[var(X_1) + var(X_2) + \ldots + var(X_n)] \\
&= \frac{1}{n^2}[\sigma^2 + \sigma^2 + \ldots + \sigma^2] \\
&= \frac{1}{n^2}[n\sigma^2] \\
&= \frac{\sigma^2}{n}.
\end{aligned}$$

Now, we calculate the root mean error:

$$\begin{aligned}
RME(\bar{X}) &= \sqrt{var(\bar{X}) + (bias(\bar{X}))^2} \\
&= \sqrt{var(\bar{X}) + 0} \\
&= \frac{\sigma}{\sqrt{n}}.
\end{aligned}$$

We will use $RME(\bar{X}) = \frac{\sigma}{\sqrt{n}}$ as the statistical measure to quantify noise. This means that the sample mean has the potential to be perturbed an amount of $\frac{\sigma}{\sqrt{n}}$ from the true value.

Now, we define a measurement for the noise, ϕ, on the kth stencil $\mathcal{S}(x_k, h_k) = \mathcal{S}^k$ to be the root mean error of the sample mean:

$$\|\phi\|_{\mathcal{S}^k} = \frac{\sigma}{\sqrt{n}}.$$

We assume that the random samples $X_1, \ldots, X_n$ are independent and identically distributed.

8.2 Determine the Number of Realizations in Main Simulation

The next step is to determine the number of realizations needed in the main simulation, denoted as n. (Also, we use the notation n_p as the number of realizations in the pilot study and n_θ as the number of realizations in the variance-reduced main simulation.)

The optimization problem is to minimize the objective function which we assume to be a relatively smooth function with some noise $\phi(x)$:

$$f(x) = f_s(x) + \phi(x),$$

where $x \in \mathbb{R}^N$. Next, we develop a formula for n by looking at the error terms of the

gradient when using Taylor's theorem. Let e_i be the ith unit coordinate direction, $h > 0$ be the stencil size, and x_c be the current point. We denote the approximated gradient as $D_h f(x_c) = \left(\frac{f(x_c+he_1)-f(x_c)}{h}, \ldots, \frac{f(x_c+he_N)-f(x_c)}{h}\right)^T$. For all $1 \leq i \leq N$,

$$\begin{aligned}
f_s(x_c + he_i) &= f_s(x_c) + h\nabla f_s(x_c)^T e_i + \mathcal{O}(h^2) \\
\frac{f_s(x_c + he_i) - f_s(x_c)}{h} &= \nabla f_s(x_c)^T e_i + \mathcal{O}(h) \\
\frac{f(x_c + he_i) - f(x_c) + \mathcal{O}\left(\frac{\sigma}{\sqrt{n}}\right)}{h} &= \nabla f_s(x_c)^T e_i + \mathcal{O}(h) \\
\|\nabla f_s(x_c)\| &= \|D_h f(x_c)\| + \mathcal{O}\left(h + \frac{\sigma/\sqrt{n}}{h}\right).
\end{aligned}$$

We do not want the error term to dominate. One reasonable approach is to set the error term to be less than $\|D_h f(x_c)\|$ and solve for n. For $M > 0$,

$$\begin{aligned}
M\left(h + \frac{\sigma/\sqrt{n}}{h}\right) &< \|D_h f(x_c)\| \\
Mh + M\left(\frac{\sigma/\sqrt{n}}{h}\right) &< \|D_h f(x_c)\| \\
M\frac{\sigma}{\sqrt{n}} &< h\|D_h f(x_c)\| \\
n &> \left(\frac{M\sigma}{h\|D_h f(x_c)\|}\right)^2. \qquad (8.3)
\end{aligned}$$

We could simplify this approach and set $\|D_h f(x_c)\| = 1$. Based on observations

in practice, this is reasonable. The number of realizations becomes:

$$n > \left(\frac{M\sigma}{h}\right)^2. \tag{8.4}$$

In the third approach, we want each part of the error term to be less than the norm of the approximated gradient. So, we assume that $h < \|Df\|$ which is reasonable from our observations and $\frac{\sigma/\sqrt{n}}{h} < \|Df\|$. We solve for n to obtain this formula. Notice this approach has a h^4 in the denominator instead of a h^2 as in the second approach.

$$\begin{aligned} M\left(\frac{\sigma/\sqrt{n}}{h}\right) &< \|Df\| \\ M\left(\frac{\sigma/\sqrt{n}}{h}\right) &< h \\ M\frac{\sigma}{\sqrt{n}} &< h^2 \\ n &> \frac{M^2\sigma^2}{h^4}. \end{aligned} \tag{8.5}$$

We compare the three approaches in the results section below.

8.3 Estimate Population Variance

In each of the three approaches, the population variance σ^2 is in the numerator of the formula to determine the number of realizations. In practice, we estimate the

population variance with the sample variance S^2:

$$S^2 = \frac{1}{n_p - 1} \sum_{i=1}^{n_p} (X_i - \bar{X})^2.$$

The sample variance is an appropriate estimate since it is unbiased with minimum variance. See appendix C.

We want to account for the error when estimating σ^2 by S^2. We calculate the root mean error of S^2 by applying equation 8.1: $RME(S^2) = \sqrt{var(S^2) + (bias(S^2))^2}$. We know there is no bias with this estimate since $E[S^2] = \sigma^2$. It is shown in appendix C. There is an upper bound on the variance of S^2, due to Hoeffding [30]:

$$var(S^2) \leq \frac{\mu_4 + (S^2)^2}{n_p},$$

where $\mu_4 = E[(X_i - \bar{X})^4]$ for n_p realizations. See appendix E.

Since we want a worst case estimate of the statistic σ^2, we let

$$\begin{aligned} \sigma^2 &\approx S^2 + RME(S^2) \\ &\approx S^2 + \sqrt{\frac{\mu_4 + (S^2)^2}{n_p}} \end{aligned} \tag{8.6}$$

in the formula to calculate n.

8.4 Methodology

Implicit filtering passes the stencil size to the pilot study. The pilot study estimates σ^2 with 8.6 and then calculates n. Note that this n is the number of realizations the main simulation would accomplish in the non-variance-reduced situation. We would like to determine the number of realizations n_θ that are required to achieve a result with a specified standard error level when variance reduction is applied. From Lavenberg and Welch [38],

$$\begin{aligned} \frac{var(\theta)}{var(Y)} &= 1 - \rho^2 \\ var(\theta) &= var(Y)(1 - \rho^2), \end{aligned}$$

where θ is the variance-reduced estimate, Y is the original estimate, $-1 \leq \rho \leq 1$ is the correlation coefficient. This number indicates how well the expected annual cost and the control variates are correlated. (If $\rho^2 = 1$, there is a perfect linear relationship and if $\rho^2 = 0$, there is no linear relationship.) The pilot study can estimate the ρ^2 and use it in the following manner.

Assuming we want the noise in the variance-reduced case (denoted with subscript θ) to be less than or equal to the noise in the non-variance-reduced case (denoted

with subscript Y), the pilot study can convert n into n_θ as follows:

$$\begin{aligned} \|\phi_Y\| &\geq \|\phi_\theta\| \\ \frac{\sqrt{var(Y)}}{\sqrt{n}} &\geq \frac{\sqrt{var(\theta)}}{\sqrt{n_\theta}} \\ \sqrt{n_\theta} &\geq \frac{\sqrt{var(\theta)}\sqrt{n}}{\sqrt{var(Y)}} \\ n_\theta &\geq \frac{var(\theta)n}{var(Y)} \\ n_\theta &\geq (1-\rho^2)n. \end{aligned} \tag{8.7}$$

So, the main simulation will run n_θ realizations to obtain a variance-reduced result.

8.5 Results with One-Year Model

In this section, we compare the three approaches of the adaptive model to the model with no variance reduction and no adaptation. Recall that the formula to determine n for the first approach is: $n > (\frac{M\sigma}{h\|Df\|})^2$; second approach: $n > (\frac{M\sigma}{h})^2$; and third approach:$n > (\frac{M\sigma}{h^2})^2$. In our experiments, we optimize the same problem 100 times. Then we average the variance of the annual cost and the realizations per function call. We will see that the adaptive model costs less.

After completing the tests, we observe the following. Without the adaptive model, the average number of function calls is 174 in the variance reduction case and 185 in the no variance reduction case. The numbers are the same with the adaptive model. The adaptive model also does not affect the average optimized function value

Table 8.1: Average Optimized Function Value (x10^5)

	No VR	VR
No Adapt	9.18	9.13
1st	9.15	9.09
2nd	9.18	9.10
3rd	9.23	9.13

as shown in table 8.1. The average value with the adaptive model is within 1% of the average value without the adaptive model (with and without variance reduction). While using the adaptive model, the optimizer achieves the same result with the same number of calls to the function.

However, the benefit of applying the adaptive model is the reduction in the average realizations per function call. We compare the adaptive model to the non-adaptive model. The results without variance reduction are in table 8.2. Observe that using exactly 125 realizations per function call results in an average variance of $1.5 * 10^{10}$ in the no variance reduction case. Using the adaptive model can decrease the average realizations per function call by 48%. Next, we apply variance reduction, and as expected, achieve a lower variance of $.2 * 10^{10}$ (see table 8.3). Incorporating the adaptive model in addition to variance reduction results in a 58% decrease in the average realizations per function call (while maintaining the same variance).

Next, we test different values of M. The adaptive model performs the same as the non-adaptive model for $M < 1$ in the first and second approaches and $M < .01$ in the third approach. The M value for the third approach is two magnitudes smaller, in order to achieve a similar number of realizations per function call as the other two approaches. The formula to calculate the number of realizations for the third

Table 8.2: Non-Adaptive vs. Adaptive Model with No Variance Reduction

	Avg Real/Call	Avg Variance (x10^{10})
No Adapt	125	1.49
1st	65	1.50
2nd	84	1.49
3rd	116	1.50

Table 8.3: Non-Adaptive vs. Adaptive Model with Variance Reduction

	Avg Real/Call	Avg Variance (x10^{10})	Variance of 100 Optimized Values (x10^{8})
No Adapt	125	.200	6.10
1st	59	.230	6.43
2nd	53	.210	6.80
3rd	56	.220	7.47

approach is: $n > \frac{M^2\sigma^2}{h^4}$. Notice the formula contains an extra factor of h^2 so an appropriate M^2 is used to compensate.

We select $M = 1$ for the first and second approaches and $M = .01$ for the third approach. The previous results in tables 8.1, 8.2, and 8.3 are based on this choice. These values for M result in the least realizations per function call for the same variance. See tables 8.4, 8.5, 8.6. Also, we see that increasing M, increases the average realizations per function call. We can reduce the variance by 1/2 if we are willing to increase the realizations by at least a factor of 12. We show the results of the variance reduction case.

Since all three approaches are viable, we use the variance of the 100 average optimized values to recommend one. The adaptive model with variance reduction performs the best so we compare the variances of the average optimized value of

Table 8.4: First Approach, with Variance Reduction

	Avg Real/Call	Avg Variance (x10^{10})
M=1	59	.230
M=5	388	.208
M=15	713	.090

Table 8.5: Second Approach, with Variance Reduction

	Avg Real/Call	Avg Variance (x10^{10})
M=1	53	.210
M=5	151	.218
M=20	1178	.132

Table 8.6: Third Approach, with Variance Reduction

	Avg Real/Call	Avg Variance (x10^{10})
M=.01	56	.220
M=.05	184	.181
M=.5	1086	.070

the three approaches in table 8.3. The variances of the mean are: $6.43 * 10^8$ for the first approach, $6.80 * 10^8$ for the second approach, and $7.47 * 10^8$ for the third approach. Therefore, we recommend the formula of the first approach (with $M = 1$) to determine the number of realizations in the one-year model: $n > \left(\frac{\sigma}{h\|D_h f(x_c)\|}\right)^2$.

Chapter 9

Conclusions

My thesis goals:

Goal 1: Simulate a one-year water market for a city and use an optimization technique called implicit filtering to find the scenario of least annual cost. First, solve version I of this optimization problem. Then, apply variance reduction.

Goal 2: Expand the simulation to a multi-year water market and apply variance reduction.

Goal 3: Design a methodology where the simulation adapts the number of runs to the level of noise. So, the number of simulation runs would increase in areas where noise is more prominent.

We have completed the goals. First, we solved the stochastic water resources problem. In the one-year problem, we can reduce the costly permanent rights in a portfolio and augment the water supply with options and leases (which are more risky due to the price volatility). We can significantly lower the expected costs in this manner while still meeting reliability constraints.

We learned that we can apply variance reduction to decrease the computational

cost for the same accuracy or better. In the one-year problem, we achieved 85% variance reduction on average. In the multi-year problem, one challenge was to find appropriate, working control variates. We did see 38% variance reduction on average.

The adaptive model used the pilot study for more than just variance reduction. The pilot study had another important job...to calculate the number of realizations the main simulation should run in order to control the estimated noise. This way, the model would run more realizations in the noisier areas of the landscape. We found that the computational cost could be reduced by 58% in the one-year model.

In this stochastic problem, information is important. The computational cost of the optimization process is reduced when the model has useful information at the right time. The model used information about the control variates. Also, the stencil size and norm of the approximated gradient proved to be useful information.

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APPENDIX

Appendix A

Glossary of Water Resources Terms

Definition A.1 (Conditional Value at Risk)**.** *The expected dollar amount a portfolio will cost if the Value at Risk measure is exceeded. So, given the distribution of annual portfolio costs, it is calculated as the mean of the annual costs falling above the 95th percentile.*

Definition A.2 (Cost variability)**.** *Indicates the risk associated with very high portfolio costs.*

Definition A.3 (Critical failure event)**.** *A month in which the quantity demanded exceeds the available city water supply and the ratio of supply-to-demand for the month is less than or equal to 0.6.*

Definition A.4 (Expected value)**.** *The mean value of a probability distribution. It is the value that is expected to average over the long run of the simulation. This study calculates expected annual cost, expected reliability with respect to failures, and expected reliability with respect to critical failures.*

Definition A.5 (Failure event)**.** *A month in which the quantity demanded exceeds the available city water supply.*

Definition A.6 (Inflows)**.** *Water that is added to the region, by precipitation for example.*

Definition A.7 (Instream loss factor)**.** *Represents the water loss between the two reservoirs, Falcon and Amistad, in the Lower Rio Grande Valley study region. For this region, the factor is equal to 0.175.*

Definition A.8 (Losses)**.** *Events such as evaporation and drainage of water into the ground.*

Definition A.9 (Lower Rio Grande Valley (LRGV))**.** *The United States side of the LRGV is the study region. It is located in the southern tip of Texas.*

Definition A.10 (New water)**.** *Represents the water that is available for allocation (inflows minus losses).*

Definition A.11 (Option contracts)**.** *The contracts the city purchases at the beginning of the year which allows the city to buy water for a set price on a specified date, May 31st in this case.*

Definition A.12 (Options exercised)**.** *The number of acre-feet of water the city purchases on May 31st at the set price.*

Definition A.13 (Outflows)**.** *Water that is released from the region in order to meet demand or released as excess spillage to continue downstream.*

Definition A.14 (Permanent water rights)**.** *The number of acre-feet of water the city has rights to during each year.*

Definition A.15 (Purchase decision threshold value)**.** *The ratio of the expected amount of water available for the remainder of the year to the expected water demand for the remainder of the year. The city chooses this purchase decision factor ahead of time. If this ratio is less than the predetermined factor, the city will buy leases or exercise options. A subscript* 1 *indicates the value is used before the option exercise month* t_X *and a subscript* 2 *indicates the value is used after the option exercise month.*

Definition A.16 (Reliability)**.** *A number between 0 and 1 which indicates the ratio of the number of months that the city's water supply is greater than or equal to its demand to the number of simulated years times 12 months/year. In other words, reliability is an indicator of how often the city will be able to meet its demand.*

Definition A.17 (Reservoir variation)**.** *Variation in reservoir level from one month to the next month (inflows minus outflows and losses).*

Definition A.18 (Rio Grande Watermaster's Office)**.** *The state regulatory office that controls water allocations and transfers in the LRGV. The Rio Grande Watermaster's Office is part of a state environmental agency called the Texas Commission on Environmental Quality.*

Definition A.19 (Spot leases)**.** *The number of acre-feet of water the city can purchase throughout the year at the current market price.*

Definition A.20 (Strategy A)**.** *The alternative that studies permanent rights only.*

Definition A.21 (Strategy B)**.** *The alternative that studies permanent rights and options only.*

Definition A.22 (Strategy C)**.** *The alternative that studies permanent rights, options, and leases.*

Definition A.23 (Value at Risk)**.** *The maximum amount of money a portfolio will cost* 95% *of the time.*

Definition A.24 (Water volume decision threshold value)**.** *The ratio of the expected amount of water available for the remainder of the year plus the amount of water bought or exercised to the expected water demand for the remainder of the year. The city chooses this exercise decision factor ahead of time. Once the decision to buy or exercise has been made, this factor is used to determine the amount of water to buy or exercise. A subscript* 1 *indicates the value is used before the option exercise month* t_X *and a subscript* 2 *indicates the value is used after the option exercise month.*

Appendix B

Glossary of Mathematical Terms

Definition B.1 (δ_{ij})**.**

$$\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j, \\ 1 & \text{if } i = j. \end{cases}$$

Definition B.2 (Gradient of f)**.** *For $x \in \mathbb{R}^n$, $\nabla f(x) \in \mathbb{R}^n$ denotes the gradient of f, where*

$$\nabla f(x) = \left(\frac{\partial f}{\partial x_1}, ..., \frac{\partial f}{\partial x_n}. \right)$$

Definition B.3 (Hessian of f)**.** *The Hessian of f is the Jacobian of ∇f and is denoted by $\nabla^2 f$, where*

$$(\nabla^2 f)_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}.$$

Definition B.4 (Limit Point). *The point $\hat{x} \in \mathbb{R}^n$ is a limit point for the sequence $\{x_k\}$ if there is some infinite subsequence of indices $k_1, k_2, k_3, \ldots$ such that*

$$\lim_{i \to \infty} x_{k_i} = \hat{x}.$$

Definition B.5 (Lipschitz Continuity). *A function f is Lipschitz continuous with Lipschitz constant $L > 0$ if*

$$\|f(x) - f(y)\| \leq L\|x - y\|.$$

Definition B.6 (Positive Definite Matrix). *A matrix $A_{n \times n}$ is positive definite if $x^T Ax > 0$ for every nonzero $x \in \mathbb{R}^n$.*

Definition B.7 (Positive Semidefinite Matrix). *A matrix $A_{n \times n}$ is positive semidefinite if $x^T Ax \geq 0$ for every nonzero $x \in \mathbb{R}^n$.*

Definition B.8 (q-Linear Convergence). *Let $\{x_n\} \subset \mathbb{R}^n$ and local minimizer $x^* \in \mathbb{R}^n$. If*

$$\|x_{n+1} - x^*\| \leq \sigma\|x_n - x^*\| \tag{B.1}$$

for n sufficiently large, then x_n converges to x^* q-linearly with q-factor $\sigma \in (0,1)$.

Definition B.9 (q-Quadratic Convergence)**.** *Let $\{x_n\} \subset \mathbb{R}^N$ and local minimizer $x^* \in \mathbb{R}^N$. If $x_n \to x^*$ and there is a $K > 0$ such that*

$$\|x_{n+1} - x^*\| \leq K\|x_n - x^*\|^2$$

for n sufficiently large, then x_n converges to x^* q-quadratically.

Definition B.10 (q-Superlinear Convergence)**.** *Let $\{x_n\} \subset \mathbb{R}^N$ and local minimizer $x^* \in \mathbb{R}^N$. If $x_n \to x^*$ and there is a $K > 0$ such that*

$$\|x_{n+1} - x^*\| \leq K\|x_n - x^*\|^{\alpha}$$

for n sufficiently large, then x_n converges to x^* q-superlinearly with q-order $\alpha > 1$. Furthermore, $x_n \to x^*$ q-superlinearly if

$$\lim_{n\to\infty} \frac{\|x_{n+1} - x^*\|}{\|x_n - x^*\|} = 0.$$

Theorem B.1 (Sherman-Morrison formula)**.** *If $\boldsymbol{A}_{n\times n}$ is nonsingular and if $\boldsymbol{c}$ and $\boldsymbol{d}$ are $n \times 1$ vectors such that $1 + \boldsymbol{d}^T\boldsymbol{A}^{-1}\boldsymbol{c} \neq 0$, then the sum $\boldsymbol{A} + \boldsymbol{c}\boldsymbol{d}^T$ is nonsingular and*

$$(\boldsymbol{A} + \boldsymbol{c}\boldsymbol{d}^T)^{-1} = \boldsymbol{A}^{-1} - \frac{\boldsymbol{A}^{-1}\boldsymbol{c}\boldsymbol{d}^T\boldsymbol{A}^{-1}}{1 + \boldsymbol{d}^T\boldsymbol{A}^{-1}\boldsymbol{c}}. \tag{B.2}$$

Definition B.11 (Stationary Point for Constrained Optimization)**.** *The point $x^* \in \Omega$ is a stationary point for constrained optimization problems if $\nabla f(x^*)^T(x - x^*) \geq 0$ for all $x \in \Omega$.*

Definition B.12 (Stationary Point for Unconstrained Optimization)**.** *The point x^* is a stationary point for unconstrained optimization problems if $\nabla f(x^*) = 0$.*

Theorem B.2 (Taylor's Theorem)**.** *Suppose that $f : \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable and that $y \in \mathbb{R}^n$. Then,*

$$f(x + y) = f(x) + \nabla f(x + ty)^T y,$$

for some $t \in (0, 1)$. Moreover, if f is twice continuously differentiable, then,

$$\nabla f(x + y) = \nabla f(x) + \int_0^1 \nabla^2 f(x + ty) y dt$$

and

$$f(x + y) = f(x) + \nabla f(x)^T y + \frac{1}{2} y^T \nabla^2 f(x + ty) y,$$

for some $t \in (0, 1)$.

Definition B.13 (2-Norm Condition Number of a Symmetric Positive Definite Matrix)**.** *The 2-norm condition number of symmetric positive definite matrix A is*

$$\kappa_2(A) = \|A\|_2 \|A^{-1}\|_2 = \frac{\lambda_{max}}{\lambda_{min}},$$

where λ_{max} is the largest eigenvalue of A, λ_{min} is the smallest eigenvalue of A, and $\lambda_{max} \geq \lambda_{min} > 0$.

Appendix C

Sample Variance Estimates Population Variance

The purpose of this appendix is to show that for random sample $X_1, \ldots, X_n$, the sample variance $S^2 = \frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{n-1}$, where $\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$, is a uniform minimum-variance unbiased estimator (UMVU) of population variance σ^2.

We begin with the definitions of unbiased estimator and UMVU estimator.

Definition C.1 (Unbiased Estimator)**.** *An estimator* $\tilde{\Theta}(X)$ *of parameter* Θ *is unbiased if*

$$E[\tilde{\Theta}(X)] = \Theta.$$

This means that if on average, the estimate is exact, then the estimator is unbiased.

Definition C.2 (Uniform Minimum Variance Unbiased Estimator)**.** *An unbiased estimator* Θ^* *of parameter* Θ *is a UMVU estimator of* Θ *if* $var[\Theta^*] \leq var[\Theta']$ *where* Θ' *is any other unbiased estimator of* Θ*.*

We estimate the population variance σ^2 with the sample variance S^2. The sample variance is appropriate since it is unbiased with minimum variance, and proving this only requires general assumptions about the sample and cumulative distribution function. In particular, we assume the random samples $X_1, \ldots, X_n$ are independent and identically distributed (iid) with distribution $F(x)$. In order to show the sample variance is a UMVU estimator for the population variance regardless of the distribution, we need to apply such concepts as complete and sufficient statistics, symmetric functions, and order statistics.

C.1 Simplified Version

In this section, we provide a flowchart in figure C.1 to simplify the details in showing S^2 is a UMVU estimator for σ^2 (from Lehmann and Casella [40]). Later in this appendix, we show $E[S^2] = \sigma^2$, and therefore S^2 is an unbiased estimator of σ^2. In appendix D, we define the terms: symmetric function, order statistic, complete statistic, and sufficient statistic. Also, in appendix D, we show S^2 is a symmetric function which means S^2 is a function of the order statistic, and therefore S^2 is a function of a complete and sufficient statistic. To simplify matters in this appendix, we mention these terms without defining them here. Last, once we know S^2 is an unbiased estimator and a function of a complete and sufficient statistic, then S^2 is a UMVU estimator for σ^2.

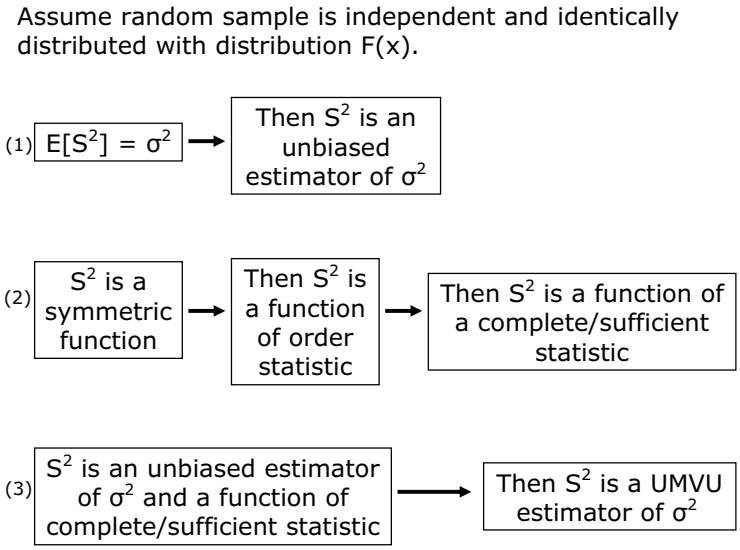

Figure C.1: Flowchart to Show S^2 is UMVU Estimator of σ^2

C.2 Detailed Version

In this section, we provide more details, such as theorems and algebraic manipulations. First, we outline the plan from Lehmann and Casella [40] to show S^2 is a UMVU estimator for σ^2. We use the idea of complete sufficient statistics (defined in appendix D). Given T is a complete sufficient statistic, then there is at most one function of T, call it $\tilde{\Theta}(T)$, which is an unbiased estimator. And any unbiased estimator that is a function of a complete sufficient statistic is a UMVU as well. So, once we find an unbiased estimator $\tilde{\Theta}(T)$, we have found a UMVU as well.

It is easy to show S^2 is an unbiased estimator for σ^2 (see below). The more difficult task is to show S^2 is a function of a complete sufficient statistic. We leave the details of this in appendix D. Let's assume we have a complete sufficient statistic T so we can apply the following two theorems. According to the first theorem, if we find a function $\tilde{\Theta}(T)$ such that $E[\tilde{\Theta}(T)] = \Theta$, then $\tilde{\Theta}(T)$ is unique. In the second theorem, we see that any unbiased estimator of Θ that is a function of T is a UMVU estimator.

Theorem C.1. *Let T be a complete sufficient statistic for parameter Θ. Then, there is at most one function of T which is an unbiased estimator for Θ.*

Theorem C.2. *Let T be a complete sufficient statistic for parameter Θ and $\tilde{\Theta}(T)$ be an unbiased estimator for Θ, then $\tilde{\Theta}(T)$ is a UMVU estimator.*

The plan is to find a function of a complete sufficient statistic for the parameter variance which is unbiased. Using these two theorems, we know that this function must be a UMVU estimator.

Let $X_1, X_2, \ldots, X_n$ be a iid random sample from distribution F with mean μ and

finite variance σ^2. Lehmann and Casella [40] claim, $S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2$ is a function of a complete sufficient statistic for σ^2. (We show this in appendix D.) Next, we show that $E[S^2] = \sigma^2$ and by theorems C.1 and C.2, S^2 is a UMVU estimator.

Let us first set up the various expressions we will need to show S^2 is an unbiased estimator. We will use $\sum_{i=1}^{n}(x_i - \bar{x})^2 = \sum_{i=1}^{n} x_i^2 - n\bar{x}^2$ and verify it here.

$$\begin{aligned}
\sum_{i=1}^{n}(x_i - \bar{x})^2 &= \sum_{i=1}^{n} x_i^2 - 2\bar{x}x_i + \bar{x}^2 \\
&= \sum_{i=1}^{n} x_i^2 + n\bar{x}^2 + \sum_{i=1}^{n}(-2\bar{x}x_i) \\
&= \sum_{i=1}^{n} x_i^2 + n\bar{x}^2 - 2n\bar{x}\sum_{i=1}^{n}\frac{x_i}{n} \\
&= \sum_{i=1}^{n} x_i^2 + n\bar{x}^2 - 2n\bar{x}\bar{x} \\
\sum_{i=1}^{n}(x_i - \bar{x})^2 &= \sum_{i=1}^{n} x_i^2 - n\bar{x}^2. \qquad \text{(C.1)}
\end{aligned}$$

Definition C.3 (Variance)**.** *The variance of random variable X is*

$$var(X) = E[X^2] - (E[X])^2 = \sigma^2,$$

where $E[X]$ = population mean μ.

We apply the definition of variance to our iid random sample X from distribution F with mean μ and finite variance σ^2 in the following manner:

$$
\begin{aligned}
var(X) &= E[X^2] - (E[X])^2 \\
\sigma^2 &= E[X^2] - (E[X])^2 \\
E[X^2] &= \sigma^2 + \mu^2
\end{aligned} \tag{C.2}
$$

We apply the definition of variance to random variable $\bar{X}$ where the iid random sample X_i has the same distribution F and finite variance σ^2 as above. And previously, we showed that $var(\bar{X}) = \frac{\sigma^2}{n}$.

$$
\begin{aligned}
var(\bar{X}) &= E[\bar{X}^2] - (E[\bar{X}])^2 \\
\frac{\sigma^2}{n} &= E[\bar{X}^2] - (E[\bar{X}])^2 \\
E[\bar{X}^2] &= \frac{\sigma^2}{n} + \mu^2
\end{aligned} \tag{C.3}
$$

Now, we are ready to show S^2 is an unbiased estimator of σ^2.

$$
\begin{aligned}
E[S^2] &= E\left[\frac{1}{n-1}\sum_{i=1}^{n}(X_i-\bar{X})^2\right] \\
&= \frac{1}{n-1}E\left[\sum_{i=1}^{n}X_i^2 - n\bar{X}^2\right] \quad \text{from } C.1 \\
&= \frac{1}{n-1}\left(E\left[\sum_{i=1}^{n}X_i^2\right] - nE\left[\bar{X}^2\right]\right) \\
&= \frac{1}{n-1}\left(nE[X^2] - nE[\bar{X}^2]\right) \\
&= \frac{1}{n-1}\left(n(\sigma^2+\mu^2) - n\left(\frac{\sigma^2}{n}+\mu^2\right)\right) \quad \text{from } C.2, C.3 \\
&= \frac{1}{n-1}(n-1)\sigma^2 \\
E[S^2] &= \sigma^2.
\end{aligned}
$$

So, S^2 is an unbiased estimator of σ^2. By theorems C.1 and C.2, we also found a UMVU estimator of σ^2.

Appendix D

Sample Variance and Complete Sufficient Statistics

The purpose of this appendix is to show that for random sample $X_1, \ldots, X_n$, sample variance $S^2 = \frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{n-1}$ where $\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$, is a function of a complete sufficient statistic for population variance σ^2.

Lehmann and Casella [40] show that sample variance is a function of a complete sufficient statistic by using order statistics. Order statistics are complete and sufficient for parameter Θ for independent and identically distributed (iid) random variables, regardless of the distribution [3], [40]. We can find a function of order statistics by finding a symmetric function. A function is a function of order statistics if and only if the function is symmetric [22]. Then, we show S^2 is symmetric. To reiterate, since S^2 is symmetric, it is a function of order statistics which are complete and sufficient.

We begin by defining the order statistic which arranges the values of the random sample from smallest to largest.

Definition D.1 (Order Statistic)**.** *Let $X_1, \ldots, X_n$ be iid random variables with distribution F. The order statistic $T(X_1, \ldots, X_n) = (X_{(1)}, \ldots, X_{(n)})$, where $X_{(1)} \leq X_{(2)} \leq \ldots \leq X_{(n)}$.*

We require the concept of a sufficient statistic and define it here.

Definition D.2 (Sufficient Statistic)**.** *Let $X_1, \ldots, X_n$ be iid random variables with distribution F. A statistic $T = T(X)$ is a sufficient statistic for parameter Θ if the conditional distribution of X given $T = t$ is independent of Θ for all t.*

The idea is that a sufficient statistic $T(X)$ for parameter Θ contains all the information needed from the sample $(X_1, X_2, \ldots, X_n)$ in order to infer something about Θ.

Fraser [22] proved that given an iid random sample with distribution F, the order statistic is a sufficient statistic.

Next, we define a complete statistic.

Definition D.3 (Complete Statistic)**.** *Let $X_1, \ldots, X_n$ be iid random variables with distribution F. Let $\delta(T)$ be a function of T. A complete statistic $T = T(X)$ for parameter Θ satisfies*

$$E[\delta(T)] = 0 \ \forall \Theta \text{ implies } \delta(T) = 0.$$

Meaning, when we have a complete statistic T, the only function of T, called $\delta(T)$, which is an unbiased estimator of zero, is zero itself.

Then, Bell, Blackwell, and Breiman [3] proved that given an iid random sample with distribution F, the order statistic is a complete statistic.

We now have a complete sufficient statistic for parameter Θ, regardless of the distribution, the order statistic. Next, we show that the sample variance is a function of the order statistic by using the following property [22]. An estimator $\delta(x_1, \ldots, x_n)$ is a function of the order statistic if and only if the estimator δ is a symmetric function.

Definition D.4 (Symmetric Function)**.** *A symmetric function of n variables $x_1, \ldots, x_n$ is a function that is unchanged by any permutation of its variables. So, for example, $f(x_1, x_2) = f(x_2, x_1)$.*

Example D.1. *Let $f(x_1, x_2) = x_1 - x_2$. Observe that $f(1, 2) = 1 - 2 = -1$ does not equal $f(2, 1) = 2 - 1 = 1$. This function is not symmetric since the function value does depend on the order of the inputs.*

Example D.2. *Let $g(x_1, x_2) = (x_1 - x_2)^2$. Observe that $g(1, 2) = (1-2)^2 = (-1)^2 = 1$ does equal $g(2, 1) = (2-1)^2 = 1$. This function is symmetric since the function value does not change when the order of the inputs changes.*

Example D.3. *The sample variance*

$$S^2(X_1, \ldots, X_n) = \frac{1}{n-1} \sum_{i=1}^{n} (X_i - \bar{X})^2 = \frac{(X_1 - \bar{X})^2 + \ldots + (X_n - \bar{X})^2}{n-1}.$$

Observe that the function value does not change when the order of the inputs changes.

Since S^2 is a symmetric function, it is a function of the complete sufficient order statistic.

Appendix E

Variance of the Sample Variance S^2

In this appendix, we apply a theorem due to Hoeffding [22], [30], [59] to obtain an explicit formula for the upper bound on the variance of the sample variance. First, we need to define the term U-statistic and then show that sample variance is a U-statistic. We give Hoeffding's theorem which provides bounds for the variance of a U-statistic and use it to calculate the upper bound of the variance of $S^2 = \frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{n-1}$, where $\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i,$.

Definition E.1 (U-Statistic)**.** *Let $X_1, \ldots, X_n$ be independent identically distributed (iid) random variables with distribution F. A U-statistic of order k is of the form:*

$$U_k = \begin{pmatrix} n \\ k \end{pmatrix}^{-1} \sum_{i_1} \cdots \sum_{i_k} \psi_k(X_{i_1}, \ldots, X_{i_k}),$$

where ψ_k is a symmetric function of its k arguments and the summation is extended over all $\begin{pmatrix} n \\ k \end{pmatrix}$ choices of distinct ordered subscripts $1 \leq i_1 < i_2 < \ldots < i_k \leq n$.

Let us show that the sample variance is a U-statistic of order $k = 2$. We start

with the sample variance:

$$
\begin{aligned}
S^2 &= \frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{n-1} \\
&= \frac{\sum_{i=1}^{n} X_i^2 - n\bar{X}^2}{n-1} \\
&= \frac{1}{n-1}\left[\sum_{i=1}^{n} X_i^2 - n\left(\frac{1}{n}\sum_{i=1}^{n} X_i\right)^2\right] \\
&= \frac{1}{n-1}\left[\sum_{i=1}^{n} X_i^2 - n\frac{1}{n^2}\left(\sum_{i=1}^{n} X_i\right)^2\right] \\
&= \frac{1}{n-1}\left[\sum_{i=1}^{n} X_i^2 - \frac{1}{n}\sum_{i=1}^{n} X_i^2 - \frac{2}{n}\sum_{i\neq j} X_i X_j\right] \\
&= \frac{1}{n-1}\left[\frac{n-1}{n}\sum_{i=1}^{n} X_i^2 - \frac{2}{n}\sum_{i\neq j} X_i X_j\right] \\
&= \frac{1}{n(n-1)}\left[(n-1)\sum_{i=1}^{n} X_i^2 - 2\sum_{i\neq j} X_i X_j\right] \qquad \text{(E.1)}
\end{aligned}
$$

We use the symmetric function $\psi_2(x_i, x_j) = \frac{(x_i - x_j)^2}{2}$ and $k = 2$ in the U-statistic definition E.1 to obtain the sample variance. Also, we let $i_1 = i$ and $i_2 = j$.

$$
\begin{aligned}
U_2 &= \frac{2}{n(n-1)} \sum_i \sum_j \frac{(X_i - X_j)^2}{2} \\
&= \frac{2}{n(n-1)} \sum_{1 \le i < j \le n} \frac{(X_i - X_j)^2}{2} \\
&= \frac{1}{n(n-1)} \sum_{1 \le i < j \le n} (X_i^2 - 2X_i X_j + X_j^2) \\
&= \frac{1}{n(n-1)} \left[(n-1) \sum_{i=1}^{n} X_i^2 - 2 \sum_{i \neq j} X_i X_j \right] \\
&= S^2 \quad \text{from} \quad E.1.
\end{aligned}
$$

The sample variance is a U-statistic and we can apply Hoeffding's theorem.

Theorem E.1 (Hoeffding's Theorem)**.** *If $X_1, \ldots, X_n$ are independent identically distributed (iid) random variables with distribution F, then the variance of a U-statistic of order k satisfies:*

$$\frac{k^2}{n}\sigma_1^2 \le var(U) \le \frac{k}{n}\sigma_k^2,$$

where $\sigma_c^2 = var\{E[\psi(X_1, \ldots, X_c, X_{c+1}, \ldots, X_k)|X_1 = x_1, \ldots, X_c = x_c]\}$ for $c = 1, k$ and symmetric function ψ.

Since our interest lies in the worst scenario, we calculate the upper bound of the variance for S^2 (meaning $k = 2$), $\frac{2}{n}\sigma_2^2$. We use the symmetric function $\psi(x_1, x_2) = \frac{(x_1 - x_2)^2}{2}$.

The first step is to find the conditional expectation when $c = 2$ variables are given:

$$E\left[\frac{(X_1 - X_2)^2}{2} | X_1 = x_1, X_2 = x_2\right] = \frac{1}{2}(x_1 - x_2)^2.$$

The next step is to calculate σ_2^2. We verify the result from Lee [39] that $\sigma_2^2 = \frac{1}{2}[\mu_4 + \sigma^4]$, where $\mu_4 = E[(X_1 - \mu)^4]$:

$$\begin{aligned}
\sigma_2^2 &= var\{\frac{1}{2}(X_1 - X_2)^2\} \\
&= \frac{1}{4}var\{(X_1 - X_2)^2\} \\
&= \frac{1}{4}\left[E[(X_1 - X_2)^4] - (E[(X_1 - X_2)^2])^2\right] \quad \text{from definition } C.3 \text{ of variance} \\
&= \frac{1}{4}[2\mu_4 + 6\sigma^4 - (2\sigma^2)^2] \text{ from } E.3, E.2 \text{ below} \\
&= \frac{1}{2}[\mu_4 + \sigma^4],
\end{aligned}$$

where $\mu_4 = E[(X_1 - \mu)^4]$. See the end of this section for details of the above calculation.

Finally, we have the upper bound for the variance of S^2:

$$\begin{aligned} var(S^2) &\leq \frac{2}{n}\sigma_2^2 \\ &\leq \frac{2}{n}\frac{1}{2}[\mu_4 + \sigma^4] \\ &\leq \frac{\mu_4 + \sigma^4}{n}. \end{aligned}$$

The following are calculation details of σ_2^2.

$$\begin{aligned} E[(X_1 - X_2)^2] &= E[X_1^2] - 2E[X_1X_2] + E[X_2^2] \\ &= 2(\sigma^2 + \mu^2) - 2\mu^2 \text{ from equation } C.2 \\ &= 2\sigma^2. \end{aligned} \tag{E.2}$$

We use the formula [57]

$$E[(X_1 - X_2)^m] = \sum_{i=0}^{m} \begin{pmatrix} m \\ i \end{pmatrix} \mu_i \mu_{m-i},$$

where $\mu_i = E[(X_1 - \mu)^i]$ to calculate $E[(X_1 - X_2)^4]$.

$$
\begin{aligned}
E[(X_1 - X_2)^4] &= \sum_{i=0}^{4} \begin{pmatrix} 4 \\ i \end{pmatrix} \mu_i \mu_{4-i} \\
&= \begin{pmatrix} 4 \\ 0 \end{pmatrix} \mu_0 \mu_4 + \begin{pmatrix} 4 \\ 1 \end{pmatrix} \mu_1 \mu_3 + \begin{pmatrix} 4 \\ 2 \end{pmatrix} \mu_2 \mu_2 + \ldots \\
&\quad \ldots + \begin{pmatrix} 4 \\ 3 \end{pmatrix} \mu_3 \mu_1 + \begin{pmatrix} 4 \\ 4 \end{pmatrix} \mu_4 \mu_0 \\
&= \mu_4 + 0 + 6\sigma^4 + 0 + \mu_4 \\
&= 2\mu_4 + 6\sigma^4 \qquad \text{(E.3)}
\end{aligned}
$$

Appendix F

Tips to Run the Water Market Model

F.1 Main Simulation

Input the initial point, $x0$, which is a 6x1 vector. Each component, x_i, is a number in $[0, 1]$. The components are defined as:

$$
\begin{aligned}
x_1 &= \text{permanent rights} \\
x_2 &= \text{options} \\
x_3 &= \alpha_2 \\
x_4 &= \beta_2 \\
x_5 &= \alpha \\
x_6 &= \beta
\end{aligned}
$$

Additional information on $x0$:

- The closer the 1st and 2nd components are to 0, the more variability there is.
- 3rd component must be less than 4th component.
- 5th component must be less than 6th component.
- Works best when 5th and 6th components are greater than 3rd and 4th components.

We can vary the scenario. The following are lines 3-42 of Model.m:

on Options: 0 or 1. Turn on variance reduction: on=1. No variance reduction: on=0.

calcn Options: 1,2,3,4. Set approach for pilot study to calculate n.

1. $n = (M * \sigma)^2/(normgrad * stencilsize)^2$. Eqn 8.3 on p.154. In 1-yr: M=1 best. Need imfil to send normgrad*stencil size.
2. $n = (M * \sigma)^2/stencilsize^2$. Eqn 8.4 on p.155. In 1-yr: M=1 best. Need imfil to send stencil size.
3. $n = (M * \sigma)^2/stencilsize^4$. Eqn 8.5 on p.155. In 1-yr: M=.01 best. Need imfil to send stencil size.
4. No Adapt. Must set mainmin=number realizations you want minus inumber. For example: You want 100 total realizations per function call and inumber=25. So set mainmin=75.

M Set $M > 0$. In one-year, when calcn=1 and calcn=2, best M=1. In one-year, when calcn=3, best M=.01

NumberYears Set number of years > 0. 1 for one-year simulation.

inumber Set number of realizations in pilot study. Recommend 25.

N Set $N > 0$. Set noise multiplicative factor here. Useful when testing noise as termination criterion. $Noise = (N * \sigma)/\sqrt{n}$.

mainmin Set minimum realizations for main simulation. Recommend set equal to inumber.

mainmax Set maximum realizations for main simulation. Useful when testing noise as termination criterion. Can set to be lower, 100 for example.

RelConstraint Set reliability constraint here: a number in [0,1]. Recommend .995. Reliability defined at eqn 2.15 p.26. Reliability constraint defined on p.29.

CostConstraint Set cost variability constraint here: a number >= 1. Set closer to 1, such as 1.1 or 1.2 to limit cost variability. Cost variability described in Sec 2.1.8 p.27. Cost variability constraint defined on p.29.

Pilot Study The model calls the pilot study at line 125.

Also, see lines 52 and 53 to change the initial conditions of the reservoir:

$$
\begin{aligned}
ifri &= .1 \text{ Change the initial fraction of allocated rights.} \\
&= \text{Recommend: .1, .3, .5} \\
iRo &= 800000 \text{ Change the initial reservoir level.} \\
&= \text{Recommend: 800000, 1500000, 2200000}
\end{aligned}
$$

Other required MATLAB files: initialize.m, pilot.m, imfil2.m, imfil3_core, imfil2_optread, imfil2_optset, and simpgrad2.m.

F.2 Pilot Study

In the pilot study, use the correct function value of the initial x (for scaling). Run the model alone to get this value. See line 922 (initialf) for the one-year model. See line 931 (initialf) for the multi-year model.