

Working Paper

The Implementation of the
Stochastic Branch and Bound
Method
for Applications in River Basin
Water Quality Management

Kristoffer Hägglöf

WP-96-89
August 1996



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Abstract

A stochastic branch and bound method is extended and applied to the water quality management problem. The goal is to examine implementation issues, i.e., to look at the research questions which arise when applying a theoretical mathematical method for practical applications. These questions consist of the techniques for bounding and branching and the selection of different stopping criteria. This extended Stochastic Branch and Bound method is then applied to the water quality management problem of meeting specified dissolved oxygen standards in a stream. The problem is to select wastewater treatment facilities at different locations along a stream with the objective of maximizing the likelihood of good management solutions, i.e., maximizing reliability and minimizing vulnerability, given water quality goals and a fixed budget level. The method is demonstrated for the Willamette River in Oregon, USA. Both implementation questions and water quality management issues are analysed. The results show that the method is efficient and accurate in the water quality management case studied here, and may provide computational approaches to many other problems of similar complexity, which appear to be intractable otherwise.

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The Implementation of the Stochastic Branch and Bound Method for Applications in River Basin Water Quality Management*

*Kristoffer Hägglöf***

1 Introduction

Water quality management typically consists of minimizing pollution control costs, maximizing water quality and maximizing equity. The management problem is often formulated as a mathematical programming model that optimizes one of the above objectives subject to limits on one or more of the other goals. This task can however be very difficult, because the behavior of the system is never entirely predictable, due to uncertainties in the inputs to the system. For water quality systems, uncertainty in the pollutant transport model, the reaction rates and the natural variability in the receiving system such as variations in streamflows and temperatures contribute to difficulties in predicting the future behavior of the system as described in Beck [1987]. These input uncertainties then produce uncertainties in the decision outputs. Recently, techniques for maximizing certainty of outcome have been proposed, these include reliability, vulnerability and resiliency. A review of the techniques proposed are presented in Burn and Lence [1992].

In this paper the Stochastic Branch and Bound Method of Norkin, Ermoliev and Ruszczyński [1994] is applied. This method is extended to include reliability, resiliency and vulnerability in Lence and Ruszczyński [1996]. A detailed description of the implementation of the Stochastic Branch and Bound Method, applied for the objectives of maximizing reliability and minimizing vulnerability under cost constraints of a water quality management system, regarding the questions of bounding, branching and stopping is given in this paper. The method is demonstrated for dissolved oxygen management on the Willamette River in Oregon, USA.

The approach used in the Stochastic Branch and Bound Method is to branch the set of possible water quality treatment levels, or management solutions into disjoint subsets such that the union of all subsets equals the set of all possible management solutions, to generate stochastic upper and lower bounds on the objective function for each subset, to delete infeasible subsets and then to branch on the most promising subset further until the stopping criterion is fulfilled. This methodology is implemented and the issues of bounding, branching and stopping are addressed. A heuristic ranking method is introduced for the lower bound calculations and for the issue of how to branch. Upper bound calculations are handled by solving multiple continuous linear programs and different stopping criteria are investigated.

In section 2, the general water quality management model is described. In this model the pollution transport relationship is random due to random flows, temperatures and reaction rates. Then the model is formulated as a probabilistic problem. The decision variables are the discrete design waste water treatment levels of all of the dischargers in the system. In section 3, the Stochastic Branch and Bound Method is described. This method is based on a Branch and Bound algorithm in which branches are subsets of discrete decision variables for waste water treatment levels. The bounds are estimates of the upper and lower limits of the objective functions for reliability and vulnerability for a given branch. Next, the approach for estimating the bounds for a given set of decision variables, the branching technique and the stopping criteria are discussed. In section 5, a study of dissolved oxygen management is described in detail and the technique is applied to the Willamette River in Oregon, USA. Extensive results are presented and analysed in section 6. Finally, the conclusions of the work are presented.

*This work develops the techniques presented by Lence and Ruszczyński [1996], and is a project in Optimization Under Uncertainty, International Institute for Applied Systems Analysis, Laxenburg, Austria.

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2 The water quality model and problem formulations

Consider emission sources $i = 1, \dots, m$, pollutants $l = 1, \dots, L$ and monitoring points $j = 1, \dots, n$. For every source i there is a discrete finite set X_i of available treatment technologies. Each technology $x_i \in X_i$ is characterized by the following functional information

$c_i(x_i)$ - cost

$e_i^l(x_i)$ - emission level of pollutant l , $l = 1, \dots, L$.

Given some emissions e_j^l at the sources, the ambient water quality S_j^l for pollutant l at the monitoring point j can be expressed as

$$S_j^l(x, \omega) = A_j^l(e_1^l(x_1), \dots, e_m^l(x_m), \omega). \quad (2.1)$$

The transfer functions A_j^l describe the effect of reactions involving pollutant l that take place as a consequence of implementing the pollution abatement decisions on the water quality levels along the stream. These pollutant transfer functions are random, e.g., based on random streamflows, temperatures, reaction rates etc. The variability in the system is modelled by ω . If the transfer functions A_j^l are linear, then the coefficients in $S_j^l(x, \omega)$ characterize the water quality improvement along the stream and are called impact coefficients.

Water quality management programs are defined as a selection of technologies $x = (x_1, x_2, \dots, x_m)$ such that $x_i \in X_i, i = 1, 2, \dots, m$ and is characterized by its cost

$$c(x) = \sum_{i=1}^m c_i(x_i) \quad (2.2)$$

and ambient water quality levels at the monitoring points

$$S_j^l(x, \omega) = A_j^l(e_1^l(x_1), \dots, e_m^l(x_m), \omega). \quad (2.3)$$

The following is a common formulation of this problem

$$\begin{aligned} &\text{Minimize} && c(x) && (2.4) \\ &\text{subject to} && S_j^l(x, \omega) \leq \bar{S}_j^l, && j = 1 \dots n, l = 1, \dots, L \\ &&& x \in X \end{aligned}$$

where X is the discrete finite set of available technology combinations and \bar{S}_j^l are the predefined standards for pollutants $l = 1, \dots, L$ at the monitoring points $j = 1 \dots n$. Since the constraint set for this problem is random, the solution that satisfies these constraints for all possible events ω may be extremely conservative, i.e., they may be biased towards extreme system conditions, and could lead to a very expensive worst case design. To arrive at meaningful and practically applicable formulations, water quality management models are typically designed to exploit the probabilistic nature of the problem. Sets of management decisions are selected based on measures of system performance that indicate the extent of environmental damage under critical hydrological and background water quality conditions. In general, the frequency, duration and magnitude of violations of a given environmental standard are indices of pollution control performance that represent the reliability, resiliency and vulnerability, respectively, of the management decisions. The reliability criterion describes how likely compliance to the environmental standards may be achieved. The resiliency and the vulnerability criteria give indications of the degree to which the system will recover from a failure sojourn and the environmental consequences caused by water quality violations, respectively. Reliability, resiliency and vulnerability applied to water resources systems is further discussed by Hashimoto, Stedinger and Loucks [1982].

2.1 Reliability

Given water quality standards, \bar{S}_j^l , for pollutants $l = 1, \dots, L$ at monitoring points $j = 1, \dots, n$, the reliability of the system is defined as the probability that some water quality standards are not violated, i.e., the probability that the satisfactory states are maintained. This definition allows the reliability maximization problem to be stated

$$\begin{aligned} &\text{Maximize} && \mathbb{P}\{S_j^l(x, \omega) \leq \bar{S}_j^l, j = 1 \dots n, l = 1, \dots, L\} && (2.5) \\ &\text{subject to} && c(x) \leq \bar{c} \\ &&& x \in X \end{aligned}$$

where X is the discrete finite set of available technology combinations and \bar{c} is the predefined budget level.

2.2 Vulnerability

The objective described in the previous subsection relies on setting strict standards and design management programs to meet these environmental standards with some level of reliability. This assumes that all water quality levels below these standards are acceptable while those above are unacceptable. This simplifies the management problem but may not be the best approach because it does not describe the severity or likely consequences of a violation. Even when the probability of a violation is small, attention should be paid to the possible consequences of a violation. The severity of a violation can be described by other criteria, therefore, more recently, hierarchies of standards are being used since they are considered to be more appropriate for describing the allowable degree of water quality degradation

$$\bar{S}_j^{l(0)} \leq \bar{S}_j^{l(1)} \leq \dots \leq \bar{S}_j^{l(H)} \quad (2.6)$$

for pollutants $l = 1, \dots, L$ and monitoring points $j = 1, \dots, n$. System vulnerability is then defined as

$$\sum_{h=1}^H c_h \mathbb{P}\{\bar{S}_j^{l(h-1)} \leq S_j^l(x, \omega) \leq \bar{S}_j^{l(h)}, j = 1, \dots, n, l = 1, \dots, L\} \quad (2.7)$$

where the coefficients c_h , $h = 1, \dots, H$, satisfy the inequalities $c_1 \leq c_2 \leq \dots \leq c_H$, measure the severity of the water quality. This definition allows the vulnerability minimization problem to be stated as follows

$$\begin{aligned} \text{Minimize} \quad & \sum_{h=1}^H c_h \mathbb{P}\{\bar{S}_j^{l(h-1)} \leq S_j^l(x, \omega) \leq \bar{S}_j^{l(h)}, j = 1, \dots, n, l = 1, \dots, L\} \\ \text{subject to} \quad & c(x) \leq \bar{c} \\ & x \in X \end{aligned} \quad (2.8)$$

where X is the discrete finite set of available technology combinations and \bar{c} is the predefined budget level.

3 The extended stochastic branch and bound method

The basic approach of this method is to branch the set of all possible strategies X into disjoint subsets X^p , $p \in \mathcal{P}$, such that $\bigcup_{p \in \mathcal{P}} X^p = X$, to generate stochastic lower and upper bounds $\eta(X^p)$ and $\xi(X^p)$ on the objective function for each subset, to delete infeasible subsets and then to branch the most promising subset further until the stopping criterion is fulfilled. The steps in the extended Stochastic Branch and Bound Method are as follows:

Initialization. Form the initial set $\mathcal{P}_0 = \{X\}$, i.e., the finite set of all possible technology combinations available. Calculate the lower and upper bounds, $\eta_0(X)$ and $\xi_0(X)$, respectively, for this set. Set $k = 0$.

Branching. Select the most promising subset Y^k , for reliability $Y^k \in \text{Argmax}\{\xi(X^p) : X^p \in \mathcal{P}_k\}$, i.e., the subset with the largest upper bound $\xi(X^p)$. For vulnerability the subset is $Y^k \in \text{Argmin}\{\eta(X^p) : X^p \in \mathcal{P}_k\}$, i.e., the subset with the smallest lower bound $\eta(X^p)$. An approximate solution x^k is selected, for reliability, $x^k \in X^k \in \text{Argmax}\{\eta_k(X^p) : X^p \in \mathcal{P}_k\}$, i.e., one singleton from the subset with the largest lower bound $\eta(X^p)$. For vulnerability the solution is $x^k \in X^k \in \text{Argmin}\{\xi_k(X^p) : X^p \in \mathcal{P}_k\}$, i.e., one singleton from the subset with the smallest upper bound $\xi(X^p)$. If Y^k is a singleton, stop or set $\mathcal{P}'_k = \mathcal{P}_k$ and go to the Bound Estimation step depending on the stopping criterion used. Such criteria are described in detail in section 4.5. Otherwise, construct a branch of Y^k , $\mathcal{P}''(Y^k) = \{Y_i^k, i = 1, 2, \dots, n_k\}$ where n_k is the number of branches of Y^k . Define the new full branch $\mathcal{P}'_k = (\mathcal{P}_k \setminus Y^k) \cup \mathcal{P}''(Y^k)$. The branching technique used is based upon the proposed ranking method, where the highest ranked emission source is branched. A description of the branching technique is described in detail in section 4.4 and the ranking method used is stated in section 4.6. The elements of \mathcal{P}'_k are also denoted by X^p .

Bound Estimation. For all subsets $X^p \in \mathcal{P}'_k$ select some estimates $\eta_k(X^p)$ and $\xi_k(X^p)$ for the bounds. The applicability and the efficiency of the Stochastic Branch and Bound Method depends on the quality of the random lower and upper bounds, $\eta(X^p)$ and $\xi(X^p)$, respectively. These are described in detail in sections 4.1 - 4.2.

Deletion. Remove all infeasible subsets from branch \mathcal{P}'_k by defining $\mathcal{P}'_{k+1} = \mathcal{P}'_k \setminus \{X^p : \min_{x \in X^p} c(x) > \bar{c}\}$. Set $k = k + 1$ and go to Branching. If the estimates are exact then all sets X^p for which $\eta_k(X^p) > \xi_k(X^p)$ can also be deleted.

4 Problem specific algorithm details

In this section the bound calculations, branching technique and stopping criteria are introduced and a ranking procedure is described.

4.1 Reliability bounds

4.1.1 Lower bounds

For a set X^p choose a point $x^p \in X^p$ such that $c(x^p) \leq \bar{c}$ (if such a point does not exist, the set X^p is deleted at the Deletion Step). However, it is preferable to choose the point $x^p \in X^p$ in such a way that the probability of not violating the water quality standards is as large as possible. Therefore the following linear problem is solved

$$\begin{aligned} & \text{Maximize} && r(x) && (4.1) \\ & \text{subject to} && c(x) \leq \bar{c} \\ & && x \in X^p_R \end{aligned}$$

where the constraints $x \in X^p_R$ are the discrete set of technology combinations $x \in X^p$ which are relaxed and treated as continuous. Coefficients r represent the rank of the emission sources such that the source which improves the probability that the predetermined water quality standards are not exceeded, the most, has the largest rank, and so on. The ranking procedure is described in more detail in section 4.6. Problem (4.1) does not give a discrete point as a solution. Therefore, the solution is rounded down to the nearest feasible discrete point. This solution may not use all of the available budget, that is, the cost constraint may not be binding in such cases. Therefore, the solution may be improved using the remaining budget, starting with the emission source with the largest rank, and so on, if this is possible. Then the stochastic lower bounds for the probability that the water quality standards are not violated, i.e., the stochastic lower bounds for $\mathbb{P}\{S_j^l(x, \omega) \leq \bar{S}_j^l, j = 1 \dots n, l = 1, \dots, L\}$, are defined by calculating

$$\eta^N(X^p) = \frac{1}{N} \sum_{s=1}^N \chi(x^p, \omega^s) \quad (4.2)$$

where $\omega^1, \dots, \omega^N$ are independent observations of ω and the indicator functions are defined as

$$\chi(x^p, \omega) = \begin{cases} 1 & \text{if } S_j^l(x^p, \omega) \leq \bar{S}_j^l \\ 0 & \text{otherwise.} \end{cases} \quad (4.3)$$

These stochastic lower bounds are calculated to get an approximate solution in every step of the algorithm. However, if the algorithm is terminated when the most promising subset consists of a singleton, the stochastic lower bound equals the stochastic upper bound and therefore it is not necessary to calculate these bounds at every iteration. Instead, it is sufficient to check if there exists a feasible point and continue, or otherwise delete the subset in question. This approach has the advantage of the possibility of calculating the lower bound first, and if necessary deleting the subset before the more computationally expensive stochastic upper bound calculation is carried out. This is possible because the ranking used in problem (4.1), which is calculated with the use of the active constraints obtained from the stochastic upper bound calculation, is not needed for checking if a feasible point exists.

4.1.2 Upper bounds

Generating stochastic upper bounds are more complicated, since this task consists of finding a stochastic bound that is larger than the best possible solution available. The key issue is the inequalities

$$\max_{\substack{x \in X^p \\ c(x) \leq \bar{c}}} \mathbb{P}\{S_j^l(x, \omega) \leq \bar{S}_j^l\} \leq \mathbb{P}\{\exists x : S_j^l(x, \omega) \leq \bar{S}_j^l, c(x) \leq \bar{c}, x \in X^p\} \quad (4.4)$$

$$\leq \mathbb{P}\{\exists x : S_j^l(x, \omega) \leq \bar{S}_j^l, c(x) \leq \bar{c}, x \in X_R^p\}$$

where the constraints $x \in X_R^p$ are the discrete set of technology combinations $x \in X^p$ which are relaxed and treated as continuous. Therefore the following linear problem is solved

$$\begin{aligned} & \text{Minimize} && c(x) && (4.5) \\ & \text{subject to} && S_j^l(x, \omega) \leq \bar{S}_j^l \\ & && x \in X_R^p \end{aligned}$$

where ω is a fixed event. The optimal value of this problem is denoted as $\hat{c}(X_R^p, \omega)$. If the problem solution is not feasible, then assign $\hat{c}(X_R^p, \omega) = \infty$. The probability that there exists one singleton in the set of technologies that does not exceed the budget level, or violates the water quality standards, is then less than or equal to the probability that the optimal value of the problem above is less than or equal to the budget level. Then define the stochastic upper bounds for the probability that the water quality standards are not violated, i.e., the stochastic upper bounds for $\mathbb{P}\{S_j^l(x, \omega) \leq \bar{S}_j^l, j = 1 \dots n, l = 1, \dots, L\}$, by calculating

$$\xi^N(X^p) = \frac{1}{N} \sum_{s=1}^N \psi(x^p, \omega^s) \quad (4.6)$$

where $\omega^1, \dots, \omega^N$ are independent observations of ω and the indicator functions are defined as

$$\psi(x^p, \omega) = \begin{cases} 1 & \text{if } \hat{c}(X_R^p, \omega) \leq \bar{c} \\ 0 & \text{otherwise.} \end{cases} \quad (4.7)$$

4.2 Vulnerability bounds

The stochastic reliability bounds can be generalized in a straightforward way to obtain vulnerability bounds. Without loss of generality let $\bar{S}_j^{l(0)} = -\infty$ and $\bar{S}_j^{l(H)} = \infty$.

4.2.1 Lower bounds

To obtain stochastic lower bounds for vulnerability, consider the stochastic upper bound calculation for reliability $\xi^N(X^p)$ described by equation (4.6). Compute this upper bound for the water quality standard $\bar{S}_j^{l(1)}$ for pollutants $l = 1, \dots, L$ at the monitoring points $j = 1, \dots, n$ using the set of independent observations $\omega^1, \dots, \omega^N$ of ω . Then remove all independent observations ω^s for which the indicator function, $\psi(x^p, \omega^s)$, defined in equation (4.7), equals one and calculate the upper bound for the next water quality standard with the remaining independent observations, and so on. Denote those upper bounds $\xi_R^{N(h)}(X^p)$ for $h = 1, \dots, H$. Then define the stochastic lower bounds for the sum of probabilities weighted by the importance of the different degrees of water quality violations,

$$\sum_{h=1}^H c_h \mathbb{P}\{\bar{S}_j^{l(h-1)} \leq S_j^l(x, \omega) \leq \bar{S}_j^{l(h)}, j = 1, \dots, n, l = 1, \dots, L\} \quad (4.8)$$

, as

$$\eta^N(X^p) = \sum_{h=1}^H c_h \xi_R^{N(h)}(X^p). \quad (4.9)$$

These are stochastic lower bounds for the vulnerability case. This follows from the fact that $\eta^N(X^p)$ pushes the probabilities $\xi_R^{N(h)}$ of being between certain standards towards optimistic solutions, i.e., it pushes the probabilities towards better water quality levels. This gives a solution which is smaller than the actual solution since the sum of $\xi_R^{N(h)}$ weighted by the coefficients c_h , which measure the importance of the different degrees of water quality violations, is smaller than or equal to the actual solution,

$$\min_{\substack{x \in X^p \\ c(x) \leq \bar{c}}} \sum_{h=1}^H c_h \mathbb{P}\{\bar{S}_j^{l(h-1)} \leq S_j^l(x, \omega) \leq \bar{S}_j^{l(h)}, j = 1, \dots, n, l = 1, \dots, L\}. \quad (4.10)$$

4.2.2 Upper bounds

To obtain stochastic upper bounds for vulnerability choose a point $x^p \in X^p$ such that $c(x^p) \leq \bar{c}$ (if such a point does not exist, the set X^p is deleted at the Deletion Step). However, it is preferable to choose a point in such a way that the sum of probabilities weighted by the importance of the different degrees of water quality violations, i.e., the stochastic upper bounds for

$$\sum_{h=1}^H c_h \mathbb{P}\{\bar{S}_j^{l(h-1)} \leq S_j^l(x, \omega) \leq \bar{S}_j^{l(h)}\}, \quad (4.11)$$

is as small as possible. To obtain this point x^p , solve the problem (4.1) used for the calculations of the stochastic lower bounds for reliability. Then define for $h = 1, \dots, H$ the indicator functions

$$\chi^{(h)}(x^p, \omega) = \begin{cases} 1 & \text{if } \bar{S}_j^{l(h-1)} \leq S_j^l(x^p, \omega) \leq \bar{S}_j^{l(h)} \\ 0 & \text{otherwise.} \end{cases} \quad (4.12)$$

for the selected $x^p \in X^p$. The stochastic upper bounds for vulnerability are defined by calculating

$$\xi^N(X^p) = \frac{1}{N} \sum_{s=1}^N \sum_{h=1}^H c_h \chi^{(h)}(x^p, \omega^s) \quad (4.13)$$

where $\omega^1, \dots, \omega^N$ are independent observations of ω . These random variables are stochastic upper bounds for the vulnerability case.

4.3 Using multiple scenarios

If the probability of an event of interest is very close to one the estimates of the form (4.6) for the upper bounds on reliability will frequently be equal to one for small N . A large number of observations of the system will be necessary to obtain different estimates for different subsets. One way to overcome this difficulty is to use many observations of the system not only in the averaging formula (4.6) but within the key inequalities (4.4) and therefore also in the linear programs (4.5) used in the upper bound calculation for reliability and in the lower bound calculation for vulnerability. Results showing the efficiency of this approach are presented in section 6.

4.4 Branching technique

Because of the weak deletion rules in the Stochastic Branch and Bound Method it is not wise to branch the most promising subset in a fashion that promotes deletions. Instead, the most promising subset is branched in a way that forces the new most promising subset to converge as fast as possible towards a singleton. One way of doing this is to branch on the emission source with the highest rank, i.e., branch on the emission source which improves the probability that the predetermined water quality standards are not exceeded the most, if an improvement in technology is implemented at that emission source. This gives new subsets of available technology combinations, i.e., new subsets where the technologies for the highest ranked emission source is branched into disjoint subsets of technologies, where a few might be infeasible but where the upper bounds of the feasible subsets can clearly be distinguished from each other. One subset has a very good upper bound and therefore has a very good chance of being the most promising subset in the next iteration and the other subsets have upper bounds in a decreasing order. If the highest ranked emission source is already a single one, i.e., the technology is already decided, branch on the next highest ranked emission source, and so on.

4.5 Stopping criteria

The main result of Norikin et al. [1994] is a convergence theorem. This theorem however is an asymptotic result, i.e., it proves convergence under the assumption that the method is run infinitely long. In practice, of course, the calculation is terminated after some finite time. The experience gained in Norikin et al. [1994] suggests that stopping after achieving the first singleton is a reasonable strategy, since it leads to a good solution, and guarantees finding the best solution if the method is run in a regenerative fashion. The approach used here is slightly different, the algorithm is stopped when the most promising set is a singleton. This algorithm is also tested for the case when the method is run for a ‘‘long time’’. In section 6 results are presented showing the efficiency of the solutions gained from the algorithm with these stopping criteria.

4.6 Ranking method

Given the problem stated above it is necessary to rank the emission sources such that the one which improves the probability that the predetermined pollution levels are not exceeded the most, if an improvement in technology is implemented, is ranked highest, and so on. To find this ranking a heuristic method based on the active constraints from the linear programs used to generate the upper bounds is proposed and implemented. The idea is to use the ratio between the impact coefficients in $S_j^l(x, \omega)$ defined in equation (2.1) for the active constraints and the cost for technology improvement at the given treatment level and rank the emission sources in order of decreasing values of this ratio. However, because many linear problems are solved for each upper bound estimation, the individual rankings have to be weighted and then summed in order to get a good overall ranking. The ranking can be stated as follows for the reliability case

$$r(X^p) = \sum_{s=1}^N \frac{1}{|A_s|} \sum_{i \in A_s} \frac{S_i^l}{c} \quad (4.14)$$

and for the vulnerability case

$$r(X^p) = \sum_{s=1}^N \sum_{h=1}^H c_h \frac{1}{|A_s^{(h)}|} \sum_{i \in A^{(h)}} \frac{S_i^l}{c} \quad (4.15)$$

where A_s and $A_s^{(h)}$ are the set of active constraints for the upper bound calculations for reliability and the set of active constraints for the lower bound calculations for vulnerability, respectively, for the independent observation ω^s .

Another question has to be stressed and that is the issue of whether to use a fixed ranking (i.e., the ranking described above is calculated once for the whole finite set of available technology combinations and then used throughout the algorithm), or whether to use a dynamic ranking (i.e., the ranking is recalculated for each new set obtained in the algorithm). The fixed ranking has the advantage that one can calculate the simpler bound first, i.e., the lower bound for reliability and upper bound for vulnerability, and delete infeasible sets before the more computationally expensive bound, i.e., the upper bound for reliability and lower bound for vulnerability, is calculated. The fixed ranking tends to use fewer iterations while the dynamic ranking tends to give better solutions, i.e., the solutions have better objective values. This is a consequence of calculating the ranking for the whole set which do not have the same active constraints as opposed to the one calculated for more technology constrained subsets as shown in section 6.

5 A case study

The water quality management models described above are applied here for management of biochemical oxygen demanding (BOD) waste discharges, which affect the stream dissolved oxygen (DO) levels, and are demonstrated for the Willamette River basin in Oregon, USA.

5.1 Problem formulations

The general water quality management problem is applied to the discharge of BOD waste in a stream, which affects the stream DO levels.

For each simulation of an event, the generated temperature, flows, velocities and reaeration rates of all reaches are used to produce a steady-state DO response, based on the Camp-Dobbins modification to the Streeter-Phelps equation. This realization of a DO response consists of DO improvements, per unit waste removed by each discharger, i.e., impact coefficients as described in equation (2.1), for each monitoring point, and the minimum required DO improvement at all monitoring points. For more details see Camp [1963] and Dobbins [1964].

This problem requires the stream DO levels to be above certain standards and therefore the problems described in section 2 are reformulated.

5.1.1 Reliability

Given the minimum required DO improvements \bar{S}_j at the monitoring points $j = 1, \dots, n$, define the reliability of the system as the probability that all minimum required DO improvements are exceeded.

This gives the problem

$$\begin{aligned}
& \textbf{Maximize} && \mathbb{P}\{S_j(x, \omega) \geq \bar{S}_j, j = 1 \dots n\} \\
& \textbf{subject to} && c(x) \leq \bar{c} \\
& && x \in X
\end{aligned} \tag{5.1}$$

where X is the discrete finite set of available technology combinations, i.e., the available combinations of BOD removal levels by the dischargers, and \bar{c} is the predefined budget level.

5.1.2 Vulnerability

Introduce a hierarchy of DO improvements

$$\bar{S}_j^{(0)} \geq \bar{S}_j^{(1)} \geq \dots \geq \bar{S}_j^{(H)} \tag{5.2}$$

for the monitoring points $j = 1, \dots, n$ and define the vulnerability of the system as

$$\sum_{h=1}^H c_h \mathbb{P}\{\bar{S}_j^{(h-1)} \geq S_j(x, \omega) \geq \bar{S}_j^{(h)}\} \tag{5.3}$$

where the coefficients c_h measures the severity of violating the level of DO. This gives the problem

$$\begin{aligned}
& \textbf{Minimize} && \sum_{h=1}^H c_h \mathbb{P}\{\bar{S}_j^{(h-1)} \geq S_j(x, \omega) \geq \bar{S}_j^{(h)}\} \\
& \textbf{subject to} && c(x) \leq \bar{c} \\
& && x \in X
\end{aligned} \tag{5.4}$$

where X is the discrete finite set of available technology combinations, i.e., the available combinations of BOD removal levels for the dischargers, and \bar{c} is the predefined budget level.

5.2 The Willamette River

The model, which is described by (5.1) and (5.4), is applied to the 298 km long segment of the Middle Fork of the Willamette River in Oregon, USA. This segment has eight major tributaries and ten BOD waste dischargers.

Cost data (in 1978 dollars) and wasteload characteristics of the dischargers are obtained from Kilgore [1985]. River flow and temperature data are aquired from the United States Geological Survey (USGS). Velocity and reaeration rates are functions of flow and are taken from Worley [1963] and Liebman [1965]. Benthic oxygen demand for the river and its tributaries is assumed to be zero and the background DO concentration (i.e., the DO in the stream in the absence of any emissions) is assumed to be the saturation concentration.

The 7-day average low flow and the highest mean monthly temperature for the months of June through January are used for this analysis. The stretch of the Willamette River modelled is divided into 18 reaches and thirty-five monitoring points are used. All dischargers have as available technologies discrete waste removal levels between 35 % and 95 % and these may be selected in discrete increments of 5 %.

The indicator of water quality is the stream DO, hence, the equations $S_j(x, \omega) \geq \bar{S}_j$ and $\bar{S}_j^{(h-1)} \geq S_j(x, \omega) \geq \bar{S}_j^{(h)}$ used in the objective functions for the problems (5.1) and (5.4), respectively, ensure acceptable DO levels at all monitoring points. All monitoring points use the same water quality standards. The standards used in this study vary between 7.0 mg/l DO and 8.0 mg/l DO for models that maximize reliability, and between 0.0 mg/l DO and 12.0 mg/l DO for models that minimize vulnerability. The function $S_j(x, \omega)$ relates the DO improvement at monitoring point j to the waste removal levels at emission sources. For the Camp-Dobbins modification to the Streeter-Phelps equation used in this work, $S_j(x, \omega)$ is a linear function of x and its coefficients are the impact coefficients obtained from a simulation of the water quality response. \bar{S}_j and $\bar{S}_j^{(h)}$ represent the minimum allowable DO level improvement at monitoring point j .

5.3 Details of the stochastic inputs

The stochastic input information considered is the 7-day averaged low flows, the highest monthly mean temperatures, and the stream velocities and reaction rates for each reach of the river, for the given streamflow conditions.

For each simulation used, a random stream temperature and 7-day averaged low flow are generated based on the two-parameter lognormal distributions for the mean monthly temperature and for the 7-day averaged low flow, respectively. The stream velocity and reaeration rates are subsequently computed based on the generated flows using the functional relationships between flow and stream velocity, and between flow and reaeration rates, respectively, and on normally distributed zero mean noise terms. For a more thorough description of the inputs used see Takyi and Lence [1996].

6 Computational results

As described in the previous section, the Stochastic Branch and Bound Method is applied for maximizing reliability and minimizing vulnerability, for managing DO levels along the Willamette River. The allowable total budget, i.e., capital and operating costs, for the river is varied between 18 and 44 million \$/year. The number of simulations required for each bound calculation depends on the type and complexity of the water quality system and on the number of uncertain input variables and their distributions. In this study, the number of simulations used is 500, which was determined to be adequate by gradually increasing the number of simulations until the statistical properties of the input and output information converged for an experimental trial. The method is implemented in C++ and the callable library Cplex 4.0 is used to solve the linear subproblems.

Figure 6.1a shows the total cost of waste water treatment, above the cost of primary treatment, i.e. 35 % BOD removed, versus reliability of meeting standards between 7.0 mg/l and 8.0 mg/l. This may be used by decision makers in selecting the best choice of management solution given their preferences for the objectives of efficiency and certainty of system outcome. Figure 6.1b illustrates the number of branches needed, i.e., the number of iterations needed for the method to obtain the first singleton. Figure 6.1c shows the number of deleted sets for each reliability level.

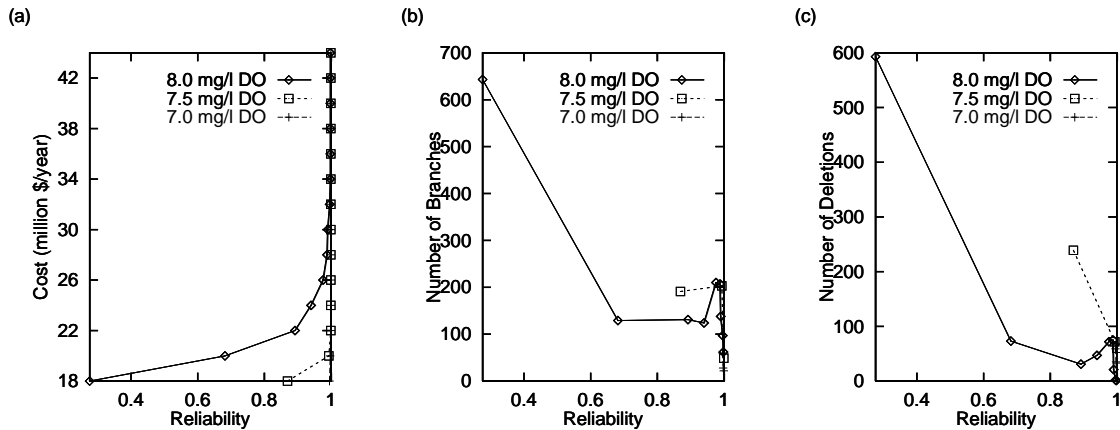


Figure 6.1: (a) Cost versus reliability. (b) Number of iterations for different reliability levels. (c) Number of deletions for different reliability levels.

For reliability levels very close to one less computational effort is required to reach the first singleton, because it is more difficult to differentiate the quality of different subsets on the basis of random simulations. The result of this is that the branched subsets may not be the best ones. For this reason the quality of the singletons obtained in these cases are not good. This can be improved by using the multiple scenarios described in section (4.3). This approach calculates the upper bounds with many scenarios simultaneously which gives slightly lower but still valid upper bounds and therefore improves the possibility that the best subsets are branched. However, the solutions obtained using this approach are also close to or equal to one but this approach suggests that more robust solutions may be obtained. Nevertheless, more research is needed to find a proper approach to the case of a very high reliability. The total single CPU time needed for solving one problem with a specific budget level and one set of standards are in the range of two hours on a SUN Sparc Server 1000 with two CPU's and 128MB memory.

Figure 6.2a shows the reliability values, for the problem of maximizing reliability for the 8.0 mg/l DO standard and a 20 million \$/year budget, as a function of the number of times the method was applied. Figure 6.2b shows the number of reoccurring technology combinations obtained, i.e., each of the lines represents one specific technology combination. Figure 6.2c shows the number of times a certain technology is obtained for a given emission source. In order to generate this figure 200 different runs of the method were made with different seeds for the random number generator used. The algorithm was stopped when the most promising subset was a singleton. The quality of the singletons obtained was then evaluated by a prolonged simulation. Figure 6.2a shows the distribution of the solutions obtained. This graph shows that as the number of method applications increases, the reliability of the system approaches 0.68. It also shows that the best solution found is 0.79. The best solution was only obtained once, but it is interesting to note that all solutions selected in this way have a rather good quality. Another interesting result, illustrated in Figure 6.2b, is that one set of technology combinations reoccurred 14 times, which means that this solution is a very good candidate. Figure 6.2c shows the reoccurrences for certain technologies for the emission sources. This shows that it can be worth while to solve the problem a number of times with fewer simulations and then to resolve the problem with a large number of simulations with the technologies used as the set of available technologies. This means that the set of available technology combinations is reduced substantially for the case with a large number of simulations.

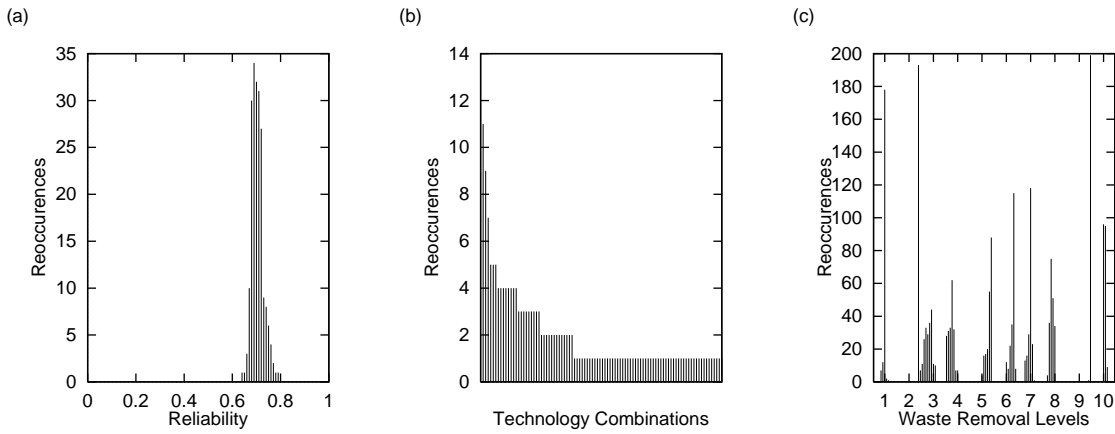


Figure 6.2: (a) Quality distribution of the first singleton. (b) Number of reoccurring technology combinations. (c) Distribution of technologies for the emission sources.

Figure 6.3 shows the singleton solutions obtained for the method when it is run without a stopping criterion.

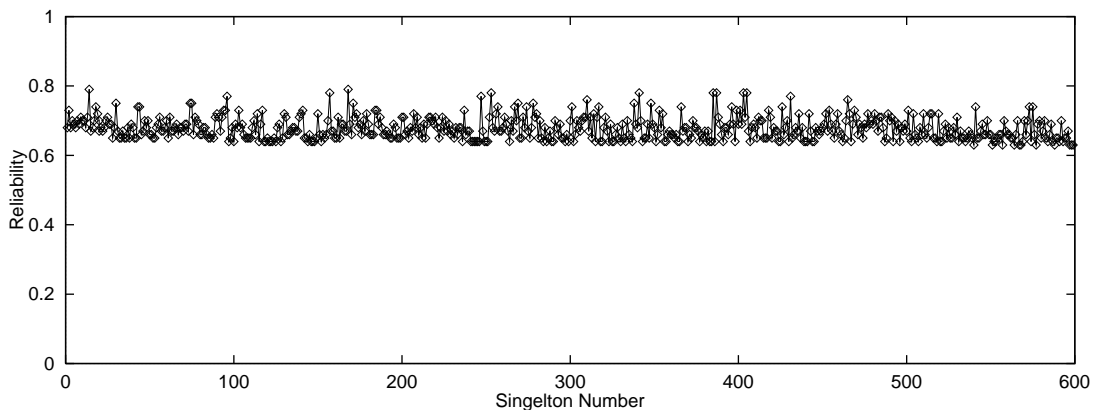


Figure 6.3: Singletons obtained when the method is run without stopping criterion.

The results show that the solutions are slightly better for the first 20 singletons and that the best solution obtained in Figure 6.2a, i.e., a reliability of 0.79, was obtained for the 15th singleton. The singletons obtained later also have a few good solutions but on average they are getting progressively

worse. For the first 100 singeltons no solution below 0.65 was obtained but for the last 100 singeltons several solutions with reliability 0.63 were obtained, which is below the worst solution obtained in Figure 6.2a.

The problem of maximizing reliability for the 8.0 mg/l DO standard and the 20 million \$/year budget is also tested for the fixed rank case and the results show that this approach uses approximately one third of the branches used in the dynamic case but also gives slightly worse solutions. Twenty testruns gave the best result of 0.70 once but also three results of 0.63 and one of 0.61 which is worse than the worst result for the dynamic ranking case.

Figure 6.4 shows the results for the objective of minimizing the vulnerability with a 20 million \$/year budget. The Figure show that if the results are converted to the reliability case described above the solution is worse, but this approach gives a more robust solution because there are no really bad outcomes. In the reliability case this cannot be assured.

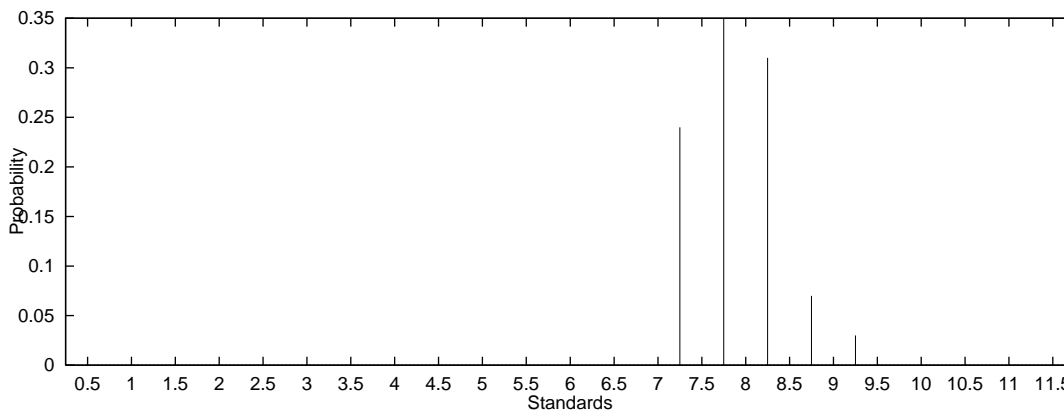


Figure 6.4: Probability of being between certain standars in the vulnerability case.

7 Conclusions

The Stochastic Branch and Bound Method of Norikin et al. [1994] is an attractive approach for solving the problem of maintaining water quality in a stream while maximizing the certainty of system outcome under cost constraints. This method is applied for the performance indicators of reliability and vulnerability in the classical water quality management problem and the questions of bounding, branching and stopping are addressed in this paper. The method is demonstrated for an example stream, and is shown to be efficient and accurate, at least for this application. This suggests that the method may be effective for addressing other problems that require management solutions that are robust to uncertainties in the input information.

There are a number of theoretical, implementational and application-specific issues associated with the Stochastic Branch and Bound Method that are as yet unaddressed. First, since it is unlikely that general approaches exists for identification of bounds and partitioning strategies for all problems, application specific approaches need to be developed. Second, stopping strategies need to be investigated in more detail. The theory guarantees that every recurrent record singleton, i.e., a singleton set which turns out to be the record set infinitely many times, is optimal. Approaches are needed to identify such sets sufficiently early with a reasonable level of reliability. Certainly, stopping at the first singleton is premature. Third, in the case of very high reliability the basic upper bound estimates may frequently lead to upper bounds equal to one, which make it difficult to differentiate the quality of different subsets on the basis of random simulations. This is a highly undesirable outcome, since the subsets branched may not be the best ones. This is a situation when use of multiple realization estimates, as is employed in this paper, may prove useful. The basic idea is to look for decisions which are good for many scenarios simultaneously, so the chance of being successful is lower. However, the solutions obtained using this approach are also close to or equal to one but this approach suggests that more robust solutions may be obtained. More research is needed to find a proper approach to the case of a very high reliability.

In summary, it should be stressed that the Stochastic Branch and Bound Method, having all the advantages of a mathematically sound approach, is a very flexible tool for solving complex decision problems with uncertainty and discrete variables. It has proven to be quite efficient in the water quality

management case and promises to provide computational approaches to many other problems of similar complexity, which appear to be intractable otherwise.

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