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Managing Water Quality Under Uncertainty: Application of a New Stochastic Branch and Bound Method

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Abstract

The problem of water quality management under uncertain emission levels, reaction rates and pollutant transport is considered. Various performance measures: reliability, resiliency and vulnerability are taken into account. A general methodology for finding a cost-effective water quality management program is developed. The approach employs a new idea of the stochastic branch and bound method, which combines random estimates of the performance for subsets of decisions with iterative refinement of the most promising subsets.

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1 Introduction

Devising successful and cost-effective water quality management strategies can be difficult because the inputs to, and the behavior of, the system being managed is never entirely predictable. Decision-makers do not know what conditions will exist in the future nor how these conditions will affect the impact of their decisions on the environment. Vincens et al. [1975] classify uncertainty in modelling hydrologic systems into three categories: uncertainty in the model structure (Type I uncertainty); uncertainty in the model parameters (Type II uncertainty); and uncertainty resulting from natural variability (Type III uncertainty). For water quality systems, uncertainty in the pollutant transport model, the model reaction rates, and the natural variability of emission rates and receiving water conditions, such as streamflow, temperature, and background pollutant loadings from unregulated pollution sources, contribute to difficulties in predicting the future behavior of the system [Beck, 1987]. This paper develops an approach for identifying water quality management solutions under Type II and Type III uncertainty. It is based on an application of the Stochastic Branch and Bound Method of Norkin et al. [1994] to water quality management, which is modified based on the solution characteristics of this problem and extended to account for the performance indicators of reliability, resiliency, and vulnerability. The approach is demonstrated for management of biochemical oxygen demanding wastes (BOD) and dissolved oxygen (DO) impacts for an example river basin based on the Willamette River in Oregon, USA.

With the exceptions of the stochastic linear programming formulation of Sobel [1965], and the dynamic programming formulations of Lohani and Hee [1983] and Cardwell and Ellis [1993], there are three commonly used methods for accommodating input uncertainty in environmental quality management problems, e.g., in surface water, groundwater, or air pollution control. These are: chance constrained optimization, combined simulation and optimization, and, more recently, multiple realization based approaches. Each of these approaches may be used to develop the trade-off between total cost of optimal waste management and system reliability.

Under the chance constrained optimization approach, constraints that ensure acceptable environmental quality are formulated as probabilistic relationships. Each of these probabilistic constraints is assigned an acceptable reliability level that must be achieved. Then, for a given design set of reliability levels, the model is transformed to an equivalent deterministic optimization model. Often, the chance constrained modelling approach requires simplifying assumptions about the input information and its distributions [see, e.g., Lohani and Than, 1978, 1979; Burn and McBean, 1985; Ellis, et al., 1985; 1986; Ellis, 1987; Fujiwara et al., 1986, 1987; Fuessle, 1987; Wagner and Gorelick, 1987; Ponnambalam et al., 1990]. Therefore, the chance constrained optimization approach may be limited in terms of its application to complicated practical problems.

Under the combined simulation and optimization approach for solving environmental quality management programs under uncertainty, Monte Carlo Simulation of system conditions is performed and an environmental optimization model is solved for each realization of such conditions. The objective function values generated, e.g., the system total cost, are then ranked, a cumulative probability distribution of the solutions based on the objective function values and their ranks is developed, and the cumulative distribution is used to evaluate the trade-off between the objective and the probability of environmental quality violation [see, e.g., Fuessle et al., 1987; Burn, 1989]. For typical environmental quality management problems, accurate ranking of the objective function values may be complicated because there is not necessarily a unique correspondence between the optimal value of the objective function and the corresponding vector of decision variables. Therefore, for different sets of model inputs, the same optimal value of the objective function may be obtained, but the optimal vectors of decision variables and the corresponding probabilities of ambient standard violation may be different. For some environmental quality management systems then, this approach may produce inefficient decisions at some reliability levels [see, e.g., Fuessle et al., 1987; Takyi and Lence, 1994].

In a multiple realizations model, a number of possible scenarios of the stochastic input information are generated in a Monte Carlo Simulation and incorporated into a single optimization model. Wagner and Gorelick [1989] introduce this approach but do not indicate how the trade-off relationships between management decisions and reliability may be obtained. Morgan et al. [1993] develop a multiple realizations model that allows a certain proportion of the total number of Monte Carlo Simulations to fail. The proportion of simulations allowed to fail is considered to be an estimate of the risk of not providing adequate environmental protection. This approach results in a large optimization model and exacts a large computational burden. While efforts to reduce the computational burden of a multiple realizations model have been developed [see, e.g., Ranjithan et al., 1993; Ritzel et al., 1994; and Takyi and Lence, 1996], this approach, as well as the chance constrained programming and combined simulation and optimization approaches, cannot be used to estimate the reliability under all types of input uncertainty, e.g., under cases when the emission levels may also vary stochastically, and becomes increasingly difficult to apply as the number and type of random inputs increases.

In general, the frequency, duration, and magnitude of violations of a given environ-

mental quality standard are indices of pollution control performance that represent the reliability, resiliency, and vulnerability, respectively, of the management decision. The reliability criterion describes how likely the environmental standards may be achieved. The resiliency and the vulnerability criteria give indications of the degree to which the system is expected to recover from a failure sojourn and the severity of the consequences of environmental quality violations, respectively. Most studies that account for uncertainty in environmental management modelling include reliability, but not these other important indices. However, each of these are measures of system performance that may offer important insights and information to decision-makers when formulating successful environmental quality programs. The importance of these performance indicators is illustrated for water resources management systems by Glanz [1982]; Hashimoto et al. [1982a, 1982b]; and Fiering [1982a, 1982b, 1982c, and 1982d].

In the following section, the general water quality management model is developed for cases with stochastic input information. In this model emission levels, as well as factors that affect pollution transport and impacts, may be random. Next, the general model is formulated as a probabilistic problem which maximizes reliability and resiliency and minimizes vulnerability under a total cost constraint. The decision variables are the discrete design waste treatment levels of the dischargers in the system. Given a specified set of decision variable values, it is shown that the objective function for this model may be estimated using Monte Carlo Simulation. In Section 4, the Stochastic Branch and Bound Method of Norkin et al. [1994] is described. The method is based on a Branch and Bound algorithm in which branches, or partitions, are subsets of discrete decision variables for waste treatment levels and the bounds are estimates of the upper and lower limits of the reliability, resiliency, and vulnerability, for a given branch. Next, the approach for estimating the bounds for a given set of decision variables is presented. In Section 6 the Stochastic Branch and Bound Method is demonstrated for water quality management using a case study based on the Willamette River in Oregon. Finally, a summary of the work is presented, including insights drawn from the case study, suggestions for future applications, and a description of the research in progress that is examining technical questions related to the implementation of the Stochastic Branch and Bound Method [see, Hägglöf, 1996].

2 The water quality management model

2.1 Stationary model

Consider emission sources $i = 1, \ldots, m$, pollutants $l = 1, \ldots, L$ and monitoring points $j = 1, \ldots, n$. For every source i there is a 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, including the capital and operation and maintenance costs of performing the given technology;

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

Here ω denotes an elementary event in some probability space $(\Omega, \mathcal{F}, \mathbb{P})$. The random emission level accommodates the fact that biological, chemical and physical treatment

technologies face stochastic inflows and operational variability even under the most stable conditions.

The pollutants are transferred from the sources to the monitoring points. 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

$$S_j^l(\omega) = A_j^l(e_1^l, \ldots, e_m^l; \omega). \tag{2.1}$$

Transfer functions A_j^l describe the effect of reactions involving pollutant l that take place between the pollution sources and the monitoring points along the stream. They relate the pollution abatement decisions to the instream water quality levels. These transfer functions are random, depend on ω and the pollutants being emitted, and are developed based on pollutant transport simulation models, pollutant characteristics, streamflow, stream velocity, stream temperature, reaction rates, and background water quality levels. They may be linear or nonlinear with respect to the emission levels, depending on the pollutant simulation model used. For simulation models that are linear with respect to the pollutant emission levels (e.g., the Streeter-Phelps equation or the Camp-Dobbins modification of the Streeter-Phelps BOD-DO model), the transfer functions are represented by a matrix of constants that typically represent the impact obtained by simulating water quality improvement along the river per unit change in the emission levels, for a given set of stream conditions.

When several pollutants are being managed, the transfer function increases in complexity, may be nonlinear, and may be difficult to predict. The environmental effects of several pollutants in combination are classified in Beavis and Walker [1979] as noninteractive and interactive. Noninteractive pollutants exhibit independent effects on stream water quality and interactive pollutants exhibit combined effects on stream water quality. Interactive pollutants are further classified as additive, less-than-additive, more-than-additive, and antagonistic, i.e., pollutants that work against each other to reduce the total impact of their combined emissions [Gaddum, 1968; Sprague, 1970]. The resultant transfer function, in the interactive case, may be difficult to predict, because such functions are dependent on concentrations of more than one pollutant and may vary in form under different emission and background concentration levels.

A *water quality management program* is defined as a selection of technologies $x = (x_1, x_2, \ldots, x_m)$ such that $x_i \in X_i$, $i = 1, 2, \ldots, m$. It is characterized by its cost

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

and ambient quality levels at monitoring points $j = 1, \ldots, n$:

$$S_j^l(x, \omega) = A_j^l(e_1^l(x_1, \omega), \ldots, e_m^l(x_m, \omega); \omega). \tag{2.2}$$

Note that the quality levels associated with a control policy x are random variables, because of the uncertainty of the emissions due to random fluctuations in plant operations, uncertainties in the inputs to the transfer functions, and uncertainty in the form of the transfer functions themselves.

2.2 Nonstationary model

Adding the time dimension provides a more exact description of the relations between emissions and ambient quality levels. In such a model, emissions are stochastic processes $e_i^l(x_i, \omega, t)$ where $t \in \{0, 1, 2, \ldots\}$ denotes discrete time intervals. Then, clearly, the ambient quality levels at monitoring points are stochastic processes, too. Values of their realizations at each time interval t can be written as

$$S_j^l(x, \omega, t) = A_j^l(e_1^l(x_1, \omega), \ldots, e_m^l(x_m, \omega); \omega, t), \tag{2.3}$$

where A_j^l is a causal operator, i.e., such an operator whose values depend on the past emission levels $e_i^l(x_i, \omega, \tau)$ for $\tau \in \{0, 1, \ldots, t\}$, but not on the future ones.

In the next section, a probabilistic form of the water quality management problem is given which has an objective function based on a combination of performance indicators, i.e., reliability, resiliency, and vulnerability, and maintains a limit on total cost, or budget. Although the objective function value cannot be calculated analytically for realistic problems, for a specified set of decision variable values, Monte Carlo Simulation may be used to estimate it. This estimation approach is an integral part of the Stochastic Branch and Bound Method presented in Section 4.

3 Problem formulations

Assume that there are some quality standards $\bar{S}_j^l$ for pollutants l at monitoring points j. Let us define the *state* of the system as the vector $S = (S_j^l)_{\substack{j=1,\ldots,n \\ l=1,\ldots,L}}$ and the set of *satisfactory states*:

$$\mathcal{G} = \{S \in \mathbb{R}^{nL} : 0 \leq S_j^l \leq \bar{S}_j^l,\ j = 1, \ldots, n,\ l = 1, \ldots, L\}. \tag{3.1}$$

One would like to have water quality levels S_j^l below the standards $\bar{S}_j^l$, i.e.,

$$S(x, \omega, t) \in \mathcal{G},\ t = 1, \ldots, T, \tag{3.2}$$

but requiring that this is satisfied for *all* possible events $\omega \in \Omega$ may be extremely conservative and could lead to a very expensive worst-case design. To arrive at meaningful and practically useful formulations typically water quality management programs are 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. Hashimoto et al. [1982a] discuss reliability, resiliency, and vulnerability applied to water resources systems. They derive mathematical expressions for these criteria and utilize the expressions to evaluate the possible performance of water supply conditions for a water supply reservoir. For water quality systems, these measures indicate the acceptable frequency, duration, and magnitude of water quality violation. They may be designed to reflect our knowledge of the damage function for the ecosystem. That is, they may reflect what we know about the acceptable effects of frequent water

quality violations, of different lengths, and at different degrees of contamination, on species in a region.

Reliability

Given the quality standards $\bar{S}$, define the *reliability* of the system as the probability of the event that the state remains in the set of satisfactory states in the planning horizon:

$$R_1(x) = \mathbb{P}\left\{S(x,\omega,t) \in \mathcal{G},\ t = 1,\ldots,T\right\}. \tag{3.3}$$

This allows us to formulate the *reliability maximization* problem:

$$\max_{x \in X} R_1(x) \tag{3.4}$$

subject to

$$c(x) \leq \bar{c}, \tag{3.5}$$

where $\bar{c}$ is a prescribed budget level. By varying $\bar{c}$ one can develop the cost-reliability trade-offs for water quality management.

Reliability under violation length limit

The notion of reliability can be relaxed by allowing violations of a short duration. For example, if violations of only one period in length are allowed, the following performance measure may be introduced:

$$R_2(x) = \mathbb{P}\left\{S(x,\omega,t) \in \mathcal{G} \text{ or } S(x,\omega,t+1) \in \mathcal{G},\ t = 1,\ldots,T-1\right\}. \tag{3.6}$$

In other words, $R_2(x)$ is the probability that a failure sojourn will not last more than one period.

Resiliency

The characteristic of *resiliency* of the system measures the ability of the system to recover from failure states and can be defined as the conditional probability that $S(x,\omega,t+1) \in \mathcal{G}$, if $S(x,\omega,t) \notin \mathcal{G}$. To be more precise, let

$$\mathcal{T}(x,\omega) = \{1 \leq t < T :\ S(x,\omega,t) \notin \mathcal{G}\}$$

and define resiliency as

$$R_3(x) = \mathbb{P}\left\{S(x,\omega,t+1) \in \mathcal{G} \text{ for all } t \in \mathcal{T}(x,\omega) \,|\, \mathcal{T}(x,\omega) \neq \emptyset\right\}. \tag{3.7}$$

Thus the resiliency may be described as the system's average recovery rate and equivalently defined as given in Hashimoto et al. [1982a] as:

$$R_3(x) = \frac{R_2(x)}{1 - R_1(x)}. \tag{3.8}$$

It is clear that in a similar way one can define functions that express the ability of the system to recover from failures within any specified time period.

Vulnerability

Classical water quality management has relied on setting strict standards and designing management programs to meet these standards with some level of reliability. This approach assumes that below some allowable standard the water quality of the system is acceptable, and that above that standard, the system is infinitely damaged. It simplifies the management problem, but may not represent what happens in reality. In some river systems, a hierarchy of water quality standards may be more acceptable for describing the allowable degree of water quality degradation. Furthermore, the frequency and duration of allowable water quality violation may be different for different levels of contamination, e.g., the allowable frequency and duration of water quality violation may decrease with increases in water quality standard levels, as is the case with U.S.E.P.A. chronic and acute ambient standards for ammonia nitrogen levels [U.S.E.P.A., 1992].

Another possibility of defining performance measures is to introduce a hierarchy of quality standards

$$\bar{S} \leq \bar{S}^{(1)} \leq \bar{S}^{(2)} \leq \ldots \leq \bar{S}^{(H)}$$

and the corresponding family of satisfactory states

$$\mathcal{G}^{(1)} \subseteq \mathcal{G}^{(2)} \subseteq \ldots \subseteq \mathcal{G}^{(H)},$$

where

$$\mathcal{G}^{(h)} = \{S \in \mathbb{R}^{nL} : 0 \leq S \leq \bar{S}^{(h)}\}.$$

Let us define the events:

$$\begin{aligned}
\Theta^{(1)}(x) &= \left\{\omega : \ S(x,\omega,t) \in \mathcal{G}^{(1)}, \ t = 1,\ldots,T\right\}, \\
\Theta^{(2)}(x) &= \left\{\omega : \ S(x,\omega,t) \in \mathcal{G}^{(2)}, \ t = 1,\ldots,T\right\} \setminus \Theta^{(1)}(x), \\
&\ldots \\
\Theta^{(H)}(x) &= \left\{\omega : \ S(x,\omega,t) \in \mathcal{G}^{(H)}, \ t = 1,\ldots,T\right\} \setminus \Theta^{(H-1)}(x).
\end{aligned}$$

The performance measure (negatively related to the vulnerability) of the system can be defined as

$$V(x) = \sum_{h=1}^{H} w_h \mathbb{P}\{\Theta^{(h)}(x)\}.$$

If the coefficients w_h, $h = 1,\ldots,H$, satisfy the inequalities: $w_1 \geq w_2 \geq \ldots \geq w_H$, this expression for vulnerability is the opposite of the classical expression for vulnerability given in Hashimoto et al. [1982a], and may be maximized as a performance indicator for certainty of system outcome.

In general, all these performance measures may be included into the the optimization problem (3.4)-(3.5) by formulating a composite objective:

$$\max_{x \in X} \left[F(x) = \gamma_1 R_1(x) + \gamma_2 R_2(x) + \gamma_3 R_3(x) + \gamma_4 V(x)\right] \tag{3.9}$$

subject to

$$c(x) \leq \bar{c}, \tag{3.10}$$

where $\gamma_1, \ldots, \gamma_4$ are some positive weights. However, it is likely that the presence of one objective may eliminate the need for another. For example, if resiliency, R_3 , is considered to be an important objective, the inclusion of R_2 may not be necessary.

The main difficulty associated with the stochastic formulation (3.9)-(3.10) is that it involves functions defined as probabilities of some events. The values of these functions cannot be calculated analytically for realistic models. For example, calculating reliability would require evaluating a multidimensional integral over the set implicitly defined by inequalities (3.2), potentially involving nonlinear models of emissions and transfer. Except for some special cases, e.g., models with one source and one receptor and with linear transfer functions, the only tool available for identifying reliability is *simulation*. In the simulation approach, for selected technologies $x_1, \ldots, x_m$, one can execute the emission and transfer function models with some randomly drawn uncertain parameters $\tilde{\omega}$ and evaluate the function

$$\chi_1(x, \tilde{\omega}) = \begin{cases} 1 & \text{if } S(x, \tilde{\omega}, t) \in \mathcal{G},\ t = 1, \ldots, T \\ 0 & \text{otherwise.} \end{cases} \tag{3.11}$$

Clearly, the reliability is the expected value of this function

$$R_1(x) = \mathbb{E}\{\chi_1(x, \omega)\}. \tag{3.12}$$

Theoretically speaking, the reliability may be estimated by the Monte-Carlo method

$$R_1(x) \approx \frac{1}{N} \sum_{s=1}^{N} \chi_1(x, \omega^s),$$

where $\omega^1, \ldots, \omega^N$ are independent observations (realizations) of ω. However, the number of simulations N necessary to evaluate the reliability at only one management program x with a sufficient accuracy can be very large. The objective of the water quality management problem is to find the best set of waste treatment decisions among all possible options, which requires that the objective be evaluated for many candidate solutions, and makes a straightforward simulation of the combinatorial problem computationally burdensome. In this work, an approach is developed that is capable of determining the best water quality management program without examining all possible programs and without calculating the objective function value (such as, e.g., the reliability) for each of them exactly. The approach adapts the Stochastic Branch and Bound Method of Norkin et al. [1994] to the water quality management problem. At each partition, or branch, the upper and lower bounds of the system reliability may be estimated for subsets of discrete decision variables for waste treatment levels.

Similarly, the values of other performance measures may be estimated using Monte Carlo Simulation. For example, in the case of (3.6), the function χ_1 may be replaced by

$$\chi_2(x, \tilde{\omega}) = \begin{cases} 1 & \text{if } S(x, \omega, t) \in \mathcal{G}, \text{ or } S(x, \omega, t+1) \in \mathcal{G},\ t = 1, \ldots, T-1 \\ 0 & \text{otherwise.} \end{cases}$$

Again,

$$R_2(x) = \mathbb{E}\{\chi_2(x, \omega)\}. \tag{3.13}$$

and we have the Monte-Carlo estimate

$$R_2(x) \approx \frac{1}{N} \sum_{s=1}^{N} \chi_2(x, \omega^s).$$

4 The stochastic branch and bound method

In this section the Stochastic Branch and Bound Method of Norkin et al. [1994] is described. The method is based on the classical integer programming Branch and Bound algorithm in which the partitions, or branches, are based on subsets of discrete decision variables for waste treatment levels. Consistent with the water quality management problem in (3.9)-(3.10), the bounds of the algorithm are estimates of the reliability, resiliency, and vulnerability, under a given budget constraint.

The main idea of the method is to split the set of all possible waste abatement strategies $X = X_1 \times X_2 \times \ldots \times X_m$ into disjoint subsets

$$X^p = X_1^p \times X_2^p \times \ldots \times X_m^p, \; p \in \mathcal{P}$$

such that $\bigcup_{p \in \mathcal{P}} X^p = X$. For each subset X^p, consider the maximization problem resulting from (3.9)-(3.10):

$$\max_{x \in X^p} F(x) \tag{4.1}$$

$$c(x) \leq \bar{c}. \tag{4.2}$$

Let $\hat{F}(X^p)$ denote the maximum objective value attainable within X^p (the optimal value of (4.1)-(4.2)). If, for some X^p and $x^q \in X^q$, $\hat{F}(X^p) < F(x^q)$, then the optimal solution of the original problem cannot lie in X^p. It is sufficient to look for the optimal solution in the subsets other than X^p.

Obviously, problem (4.1)-(4.2) is almost as difficult as the original one (3.9)-(3.10). However, by applying the Stochastic Branch and Bound Method, the subproblems (4.1)-(4.2) need not be solved exactly. It is sufficient to generate for these subproblems (by simulation) some random variables $\xi^N(X^p)$ and $\eta^N(X^p)$ that represent (in some stochastic sense) the bounds for $\hat{F}(X^p)$. Here N is an index by which we can control the accuracy of these estimates (usually the number of simulations involved).

We make the following assumptions.

(A1) For every subset $X^p \subseteq X$

$$\lim_{N \to \infty} \xi^N(X^p) \geq \hat{F}(X^p).$$

(A2) If X^p is a singleton, i.e., it contains only one point x^p, then

$$\lim_{N \to \infty} \xi^N(X^p) = F(x^p).$$

(A3) For every subset $X^p \subseteq X$

$$\lim_{N\to\infty} \eta^N(X^p) \leq \hat{F}(X^p).$$

(A4) If X^p is a singleton, i.e., it contains only one point x^p, then

$$\lim_{N\to\infty} \eta^N(X^p) = F(x^p).$$

In the above assumptions the limits are understood in the sense of almost sure convergence.

The approach by which the stochastic upper bounds $\xi(X^p)$ and lower bounds $\eta(X^p)$ are generated is given in Section 5. The stochastic upper bounds $\xi(X^p)$ are used to select the *record set*: that is the X^p for which the upper bound, $\xi(X^p)$, is the largest. The record set, as the most promising set of possible programs, is partitioned into smaller subsets, and new stochastic bounds are evaluated, etc., until a singleton is achieved. At each stage, an approximate solution $\tilde{x}$ is selected as an element of the set with the largest lower bound $\eta(X^p)$.

Since the bounds are random, the record set is random; consequently, all objects generated by the method are random. For brevity, the argument ω is dropped from the random indices N, random partitions $\mathcal{P}$ and random sets.

The steps in the Stochastic Branch and Bound Method are as follows:

Initialization. Form initial partition $\mathcal{P}_0 = \{X\}$. Calculate the bounds $\xi_0 = \xi^{N_0}(X)$ and $\eta_0 = \eta^{N_0}(X)$. Set $k = 0$.

Partitioning. Select the record subset

$$Y^k \in \operatorname{Arg\,max} \{\xi_k(X^p) : \ X^p \in \mathcal{P}_k\}$$

and an approximate solution

$$x^k \in X^k \in \operatorname{Arg\,max} \{\eta_k(X^p) : \ X^p \in \mathcal{P}_k\}.$$

If the record subset is a singleton, then set $\mathcal{P}'_k = \mathcal{P}_k$ and go to the Bound Estimation step. Otherwise construct a partition of the record set, $\mathcal{P}''_k(Y^k) = \{Y^k_i, \ i = 1, 2, \ldots, n_k\}$, where n_k is the number of partitions of Y^k. Define the new full partition

$$\mathcal{P}'_k = (\mathcal{P}_k \setminus Y^k) \cup \mathcal{P}''_k(Y^k).$$

The elements of $\mathcal{P}'_k$ will also be denoted by X^p.

Bound Estimation. For all subsets $X^p \in \mathcal{P}'_k$ select some estimates $\xi_k(X^p) = \xi^{N_k(X^p)}(X^p)$ and $\eta_k(X^p) = \eta^{N_k(X^p)}(X^p)$ for $\hat{F}(X^p)$.

Deletion. Clean partition $\mathcal{P}'_k$ of infeasible subsets, 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 Partitioning.

If the estimates are exact, i.e., if $\xi_k(X^p) = L(X^p)$ and $\eta_k(X^p) = U(X^p)$, then at the Deletion Step one can also delete all sets X^p for which $\xi_k(X^p) < \eta_k(X^p)$.

Let X^* denote the set of optimal solutions of the original problem. The main result of [Norkin et al., 1994] is the following convergence theorem.

Theorem 4.1. *Assume that the indices $N_k(X^p)$ are chosen in such a way that if a subset $X' \in \mathcal{P}_k$ for infinitely many k, then*

$$\lim_{k\to\infty} N_k(X') = \infty \quad \text{a.s.} \tag{4.3}$$

Then with probability one there exists an iteration number k_0 such that for all $k \geq k_0$

(i) *the record sets Y^k are singletons and $Y^k \subset X^*$;*

(ii) *the approximate solutions $x^k \in X^*$.*

This is an asymptotic result, assuming that the method is run infinitely long. In practice, of course, one has to stop the calculation after some finite time. The experience gained in Norkin et al. [1994] suggests that stopping after achieving the first singleton is a reasonable strategy; it leads to a good solution, and guarantees finding the best solution if the method is run in a regenerative fashion.

Different approaches can be used to determine the most efficient way to partition the initial and subsequent sets of waste abatement strategies. Various partitioning techniques are examined in Hägglöf [1996], but the technique applied here, in a preliminary analysis of the application of the Stochastic Branch and Bound Method for water quality management of BOD waste effluents, is the heuristic ranking method proposed by Hägglöf. This method determines the ranked importance of the emission sources for improving the probability that the water quality goals are met. The rank of an emission source is determined by examining the active constraints from the linear programs used to generate the upper bounds. The rank of the emission source is the rank of its ratio between the transfer function values in the active constraints and the cost for technology improvement, compared to all other emission sources.

5 Stochastic bounds

The applicability and the efficiency of the Stochastic Branch and Bound Method outlined in the previous section depend on the quality of the random upper and lower bounds $\xi^N(X^p)$ and $\eta^N(X^p)$. The purpose of this section is to decribe methods for generating such bounds for our problem.

5.1 Reliability bounds

Beginning with the simpler case of 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). Then define

$$\eta_q^N(X^p) = \frac{1}{N}\sum_{s=1}^{N} \chi_q(x^p, \omega^s), \ q = 1, 2, \tag{5.1}$$

where $\omega^1, \ldots, \omega^N$ are independent observations of ω. These random variables are stochastic lower bounds for the values of the functions $R_q(x)$ in X^p, $q = 1, 2$. Indeed, from (3.12) and (3.13) and the law of large numbers it follows that assumptions (A3) and (A4) are satisfied.

Generating stochastic upper bounds is more involved. The key observation is the inequality:

$$\begin{aligned}\hat{R}_1(X^p) &= \max_{\substack{x \in X^p \\ c(x) \le \bar{c}}} \mathbb{P}\left\{S(x,\omega,t) \in \mathcal{G},\ t = 1, \ldots, T\right\} \\ &\le \mathbb{P}\left\{\exists x \in X^p\ :\ c(x) \le \bar{c},\ S(x,\omega,t) \le \bar{S},\ t = 1, \ldots, T\right\}. \end{aligned} \tag{5.2}$$

Let us generate a random estimate $\xi^N(X^p)$ of the right hand side of the above inequality. Consider the problem with a fixed event ω

$$\min_{x \in X^p} c(x) \tag{5.3}$$

$$S(x,\omega,t) \le \bar{S},\ t = 1, \ldots, T. \tag{5.4}$$

and denote by $\hat{c}_1(X^p, \omega)$ its optimal value. The following equality holds:

$$\mathbb{P}\left\{\exists x \in X^p\ :\ c(x) \le \bar{c},\ S(x,\omega,t) \le \bar{S},\ t = 1, \ldots, T\right\} = \mathbb{P}\{\hat{c}_1(x,\omega) \le \bar{c}\}. \tag{5.5}$$

Define the function

$$\psi_1(X^p, \omega) = \begin{cases} 1 & \text{if } \hat{c}_1(X^p,\omega) \le \bar{c} \\ 0 & \text{otherwise.} \end{cases} \tag{5.6}$$

Combining (5.2) and (5.5) yields

$$\hat{R}_1(X^p) \le \mathbb{E}\{\psi_1(X^p, \omega)\}.$$

Therefore, for independent observations $\omega^1, \ldots, \omega^N$ of ω, the random variables

$$\xi_1^N(X^p) = \frac{1}{N} \sum_{s=1}^{N} \psi_1(X^p, \omega^s) \tag{5.7}$$

satisfy the relations:

$$\mathbb{E}\{\xi_1^N(X^p)\} \ge \hat{R}_1(X^p) \tag{5.8}$$

and, by the law of large numbers,

$$\lim_{N \to \infty} \xi_1^N(X^p) = \mathbb{E}\{\xi_1^N(X^p)\},\ \text{a.s.} \tag{5.9}$$

Thus, (5.7) is a stochastic upper reliability bound satisfying (A1) and (A2).

The bounds (5.7) are relatively easy to calculate. Indeed, for a fixed $\omega = \omega^s$ problem (5.3)-(5.4) is a deterministic cost minimization problem that can be solved by mathematical programming methods.

A stochastic upper bound for the reliability with a violation length limit (3.6) can be calculated in a similar way. The problem (5.3)-(5.4) is replaced by

$$\min_{x \in X^p} c(x) \tag{5.10}$$

$$S(x,\omega,t) \le \bar{S} \quad \text{or} \quad S(x,\omega,t+1) \le \bar{S}, \ t = 1,\dots,T-1, \tag{5.11}$$

its optimal value $\hat{c}_2(X^p,\omega)$ is used to define the indicator function ψ_2 (similarly to (5.6)), and one defines

$$\xi_2^N(X^p) = \frac{1}{N}\sum_{s=1}^{N} \psi_2(X^p,\omega^s). \tag{5.12}$$

Again,

$$\mathbb{E}\{\xi_2^N(X^p)\} \ge \hat{R}_2(X^p) \tag{5.13}$$

and, by the law of large numbers,

$$\lim_{N\to\infty} \xi_2^N(X^p) = \mathbb{E}\{\xi_2^N(X^p)\}, \text{ a.s.} \tag{5.14}$$

so (5.12) is a stochastic upper bound for R_2.

While the estimates of the bounds on reliability are an integral step in the Stochastic Branch and Bound Method, they may also be useful for other general applications, such as for determining the estimated reliability of any management program. This would allow decision-makers to estimate benchmarks for water quality improvement by estimating the reliability of an existing management scheme, or one that is currently being proposed for the system.

5.2 Resiliency bounds

Lower and upper bounds on the reliability measures $\hat{R}_q(X^p)$, $q = 1,2$, together with the expression (3.8) can be used to define stochastic resiliency bounds. Using the bounds (5.1) calculated at the same point $x^p \in X^p$ we can construct the stochastic lower bound

$$\eta_3^N(X^p) = \frac{\eta_2^N(X^p)}{1-\eta_1^N(X^p)}.$$

Indeed,

$$\lim_{N\to\infty} \eta_3^N(X^p) = \frac{R_2(x^p)}{1-R_1(x^p)} = R_3(x^p) \le \hat{R}_3(X^p),$$

so (A3) and (A4) are satisfied.

In a similar way one defines a stochastic upper bound

$$\xi_3^N(X^p) = \frac{\xi_2^N(X^p)}{1-\xi_1^N(X^p)}.$$

Since $\xi_q^N(X^p)$ satisfy (5.9) and (5.14),

$$\lim_{N\to\infty} \xi_3^N(X^p) \ge \frac{\hat{R}_2(X^p)}{1-\hat{R}_1(X^p)} \ge \hat{R}_3(X^p).$$

In fact, if the observations used to generate $\xi_1^N(X^p)$ and $\xi_2^N(X^p)$ are independent, we have a stronger result: for every N

$$\mathbb{E}\{\xi_3^N(X^p)\} \ge \hat{R}_3(X^p).$$

Indeed, by the independence of $\xi_1^N(X^p)$ and $\xi_2^N(X^p)$,

$$\mathbb{E}\{\xi_3^N(X^p)\} = \mathbb{E}\{\xi_2^N(X^p)\} \cdot \mathbb{E}\left\{\frac{1}{1-\xi_1^N(X^p)}\right\}. \tag{5.15}$$

Let us estimate both factors at the right hand side of (5.15). The estimate for the first factor is provided by (5.13). For the second factor, since the function $\varphi(y) = 1/(1-y)$ is convex in (0,1), from Jensen inequality and (5.8) one obtains

$$\mathbb{E}\left\{\frac{1}{1-\xi_1^N(X^p)}\right\} \geq \frac{1}{1-\mathbb{E}\{\xi_1^N(X^p)\}} \geq \frac{1}{1-\hat{R}_1(X^p)}.$$

Therefore

$$\mathbb{E}\{\xi_3^N(X^p)\} \geq \frac{\hat{R}_2(X^p)}{1-\hat{R}_1(X^p)},$$

as required.

5.3 Vulnerability bounds

The stochastic reliability bounds can be generalized in a straightforward way to obtain vulnerability bounds. To obtain a lower bound, define for $h = 1, \ldots, H$ the indicator functions

$$\chi^{(h)}(x,\omega) = \begin{cases} 1 & \text{if } \omega \in \Theta^{(h)}(x) \\ 0 & \text{otherwise.} \end{cases}$$

Then for a selected $x^p \in X^p$ and independent observations $\omega^1, \ldots, \omega^N$ of ω, the random variables

$$\lambda_V^N(X^p) = \frac{1}{N}\sum_{s=1}^{N}\sum_{h=1}^{H} w_h \chi^{(h)}(x^p, \omega^s)$$

are stochastic lower bounds on the vulnerability function. This follows directly from the law of large numbers.

To construct a stochastic upper bound, consider the deterministic problems (with a fixed ω)

$$\min_{x \in X^p} c(x) \tag{5.16}$$

$$S(x,\omega,t) \leq \bar{S}^{(h)}, \ t = 1, \ldots, T, \tag{5.17}$$

for the family of quality standards $h = 1, \ldots, H$. Let $\hat{c}^{(h)}(X^p, \omega)$ denote its optimal value. Define for $h = 1, \ldots, H$ the functions

$$\psi^{(h)}(X^p,\omega) = \begin{cases} 1 & \text{if } \hat{c}^{(h)}(X^p,\omega) \leq \bar{c} \\ 0 & \text{otherwise,} \end{cases}$$

By the ordering of the quality standards, $\psi^{(h)} \leq \psi^{(h+1)}$, $h = 1, \ldots, H-1$. Define

$$\Delta^{(h)}(X^p,\omega) = \psi^{(h)}(X^p,\omega) - \psi^{(h-1)}(X^p,\omega),$$

where we set $\psi^{(0)}(X^p,\omega)=0$. Then, in an identical way as in Section 5.1, one obtains for all $h=1,\ldots,H$ the relations

$$\max_{\substack{x\in X^p\\ c(x)\le\bar c}}\sum_{h=1}^{H} w_h\mathbb{P}\left\{\Theta^{(h)}(x)\right\}\le\sum_{h=1}^{H} w_h\mathbb{E}\left\{\Delta^{(h)}(X^p,\omega)\right\}.$$

Indeed, by selecting x after the event ω is known, one can only improve the quality standard (move to the inner subset), which by the monotonicity of the weights implies the above inequality.

Therefore, for independent observations $\omega^1,\ldots,\omega^N$ of ω, the random variables

$$\xi_V^N(X^p)=\frac{1}{N}\sum_{s=1}^{N}\sum_{h=1}^{H} c_h\Delta^{(h)}(X^p,\omega^s),$$

are stochastic upper bounds on the vulnerability function.

5.4 Using multiple scenarios

If the probability of the event of interest is very close to one the Monte Carlo estimates of the form (5.7) (for the case of reliability) will frequently be equal to one for small N. A large number of observations will be necessary to obtain different estimates for different subsets.

One way to overcome this difficulty is the use of many observations not only in the averaging formula (5.7) (or similar) but within the key inequality of the form (5.2). Let us illustrate this idea on the example of upper bounds for the reliability.

Let ω^ν, $\nu=1,\ldots,M$ be independent identically distributed observations of ω. One has the following extension of (5.2):

$$\begin{aligned}\left[\hat R_1(X^p)\right]^M &= \max_{\substack{x\in X^p\\ c(x)\le\bar c}}\left[\mathbb{P}\left\{S_j(x,\omega,t)\le\bar S_j,\ j=1,\ldots,n,\ t=1,\ldots,T\right\}\right]^M\\ &= \max_{\substack{x\in X^p\\ c(x)\le\bar c}}\prod_{\nu=1}^{M}\left[\mathbb{P}\left\{S_j(x,\omega^\nu,t)\le\bar S_j,\ j=1,\ldots,n,\ t=1,\ldots,T\right\}\right]\\ &\le \mathbb{P}\left\{\exists x\in X^p\ :\ c(x)\le\bar c,\ S_j(x,\omega^\nu,t)\le\bar S_j,\right.\\ &\quad \left. j=1,\ldots,n,\ t=1,\ldots,T,\ \nu=1,\ldots,M\right\}. \qquad (5.18)\end{aligned}$$

For given scenarios ω^ν the verification of the event at the right hand side of (5.18) is equivalent to the verification of whether the optimal value $\hat c_1$ of the problem

$$\min_{x\in X^p} c(x) \qquad (5.19)$$

$$S_j(x,\omega^\nu,t)\le\bar S_j,\ j=1,\ldots,n,\ t=1,\ldots,T,\ \nu=1,\ldots,M, \qquad (5.20)$$

is below $\bar c$. One can then define the characteristic function $\psi_1(X^p,\omega^1,\ldots,\omega^M)$ as in (5.6) and obtain

$$\left[\hat R_1(X^p)\right]^M\le\mathbb{E}\{\psi_1(X^p,\omega^1,\ldots,\omega^M)\}.$$

The resulting Monte-Carlo estimate takes the form

$$\xi_1^{MN}(X^p) = \left[\frac{1}{N}\sum_{s=1}^{N}\psi_1(X^p, \omega^{s,1}, \ldots, \omega^{s,M})\right]^{1/M}, \tag{5.21}$$

where $\omega^{s,\nu}$, $s = 1, \ldots, N$, $\nu = 1, \ldots, M$, are i.i.d. observations of ω.

Similar use of multiple scenarios can be made for estimating R_2, resiliency and vulnerability.

This approach was employed in the preliminary analysis of the application of the Stochastic Branch and Bound Method for management of BOD emissions on the Willamette River which is described in the following section.

6 Application of the Stochastic Branch and Bound Method for Managing BOD Discharges in the Willamette River

The Stochastic Branch and Bound Method is applied here for managing point sources of BOD wastes and their impacts on instream DO for an example river basin based on the Willamette River in Oregon, USA. The 298 km Middle Fork of the river is analyzed and receives waste emissions from eight major tributaries and ten BOD waste dischargers. Cost data (in 1978 $US), waste load characteristics of the dischargers, discharger locations, stream flow and temperature data, and water quality simulation model inputs, such as decay rates, and velocity and reaeration rate versus flow relationships were based on Takyi and Lence [1996]. All emission sources have waste treatment options available that remove BOD at removal levels of between 35% and 95%, and these may be selected in discrete increments of 5%.

The water quality model used to develop the transfer functions is based on the Camp-Dobbins modification of the Streeter-Phelps equation for the coupled reaction of BOD decay and reaeration and its effect on DO. Benthic oxygen demand and the background DO deficit are assumed to be zero. The 7-day average low flow and the highest mean monthly temperature for the months of June through September are used for this analysis. The transfer functions used in the water quality management model are based on the water quality simulation model and describe the unit decrease in DO (usually in mg/l) at monitoring points in the stream as a result of unit increases of BOD effluent (in mg/l or kg/day) at the emission sources. They are linear functions of the waste treatment levels of the emission sources. The river segment is divided into 18 reaches and thirty-five monitoring points are used.

The goal of the simple least cost water quality management model for BOD-DO is to minimize the total cost of waste treatment while meeting lower bounds on the level of allowable DO in the stream. In this case, the quality standards described in Section 3 are lower bounds on water quality. This requires a change in the sign of the inequality in (3.1), but the application of the Stochastic Branch and Bound Method remains the same.

The stochastic inputs to the water quality simulation model are the 7-day averaged low flows at five gauging stations in the river, the highest monthly mean temperatures in the river, based on the Harrisburg gauging station data, and the stream velocities

and reaction rates for each reach of the river under the varying streamflow conditions. For each simulation used in the calculation of the bounds, a random 7-day averaged low flow and stream temperature 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 computed based on the generated flows and functional relationships between velocity and flow and reaeration rate (at 20° C) and flow, respectively, and normally distributed zero mean noise terms, as described in Takyi and Lence [1996].

In this preliminary demonstration, the Stochastic Branch and Bound Method is applied for maximizing reliability, R_1 , for maintaining a DO water quality standard of 8.0 mg/l. The allowable total cost (i.e., capital and operating costs) for the entire river basin is limited to no more than 20 million \$US/year. The adequate number of simulations required for each bound calculation depends on the complexity of the water quality management problem and on the quality of the uncertain input information. For this example, 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.

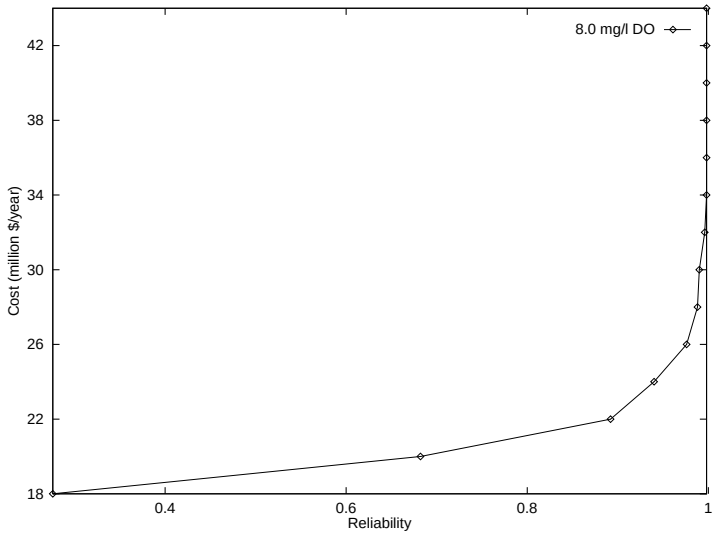

Figure 6.1: Cost vesus reliability of meeting the 8.0 mg/l standard.

Figure 6.1 shows the total cost of waste treatment, above the cost of primary treatment (i.e., 35% BOD removed) versus reliability of meeting the 8.0 mg/l standard. It 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.

The Stochastic Branch and Bound Method results in an efficient use of computational resources. The number of iterations (splittings) needed to obtain the solution (understood here as the first singleton), for one set of simulations and varying budget level, is illustrated in Figure 6.2. We see that 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. For this reason the quality of the singleton obtained is not good in this case. The use of

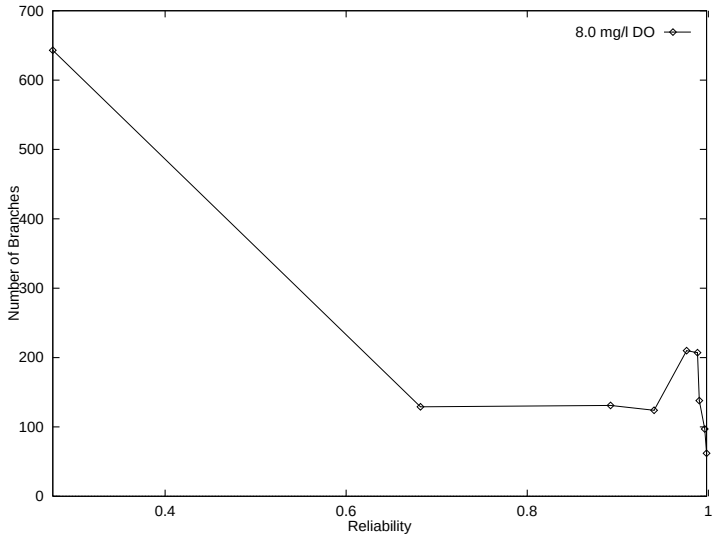

Figure 6.2: The number of iterations of the stochastic branch and bound method for different cost-reliability levels.

the multiple realization approach improves the quality of the singleton (see Hägglöf [1996]), but still more research is needed to find a proper approach to the case of a very high reliability. The total single CPU time needed to solve a problem was in the range of two hours on a SUN Sparc Server 1000 with two CPU's and 128MB memory. Takyi and Lence [1996] present results similar to Figure 6.1 for a two-tiered DO standard of 7.2 and 8.1 mg/l in different reaches of the Willamette River, using the multiple realization based approach of Morgan et al. [1993] with 100 simulations, and their work required 7 days of CPU time on a Sparc2 UNIX station.

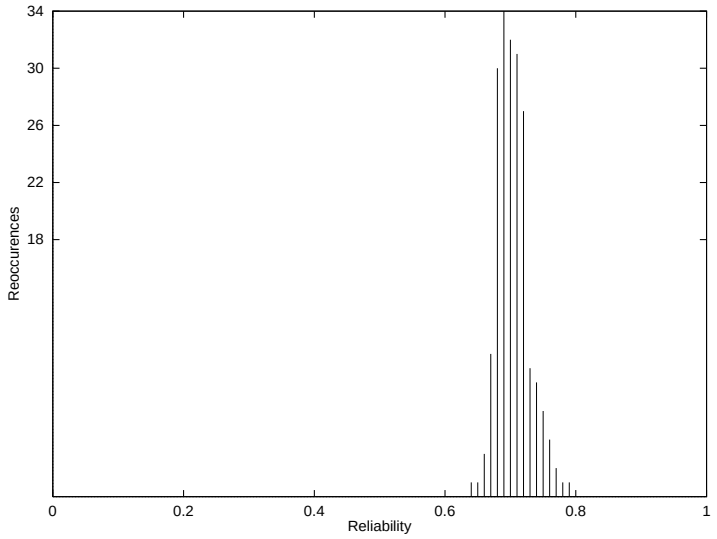

Figure 6.3: Quality distribution of the first singleton.

Finally, Figure 6.3 illustrates the operation of the method run in a regenerative fashion. 200 different runs of the method were made with different seeds for the random

number generator used, and the algorithm was stopped at the first moment at which the record set was a singleton. The quality of the singletons thus obtained was then evaluated by a prolonged simulation. Figure 6.3 illustrates the distribution of the solutions thus obtained. The best singleton (with the reliability level of 0.79) was obtained only once, but it is interesting to note that all the solutions selected in this way have a rather good quality.

7 Conclusions

The Stochastic Branch and Bound Method of Norkin et al. [1994] is an attractive approach for solving the multiobjective problem of maintaining water quality in a river system while minimizing costs and maximizing the certainty of system outcome. This method is extended in this paper for including the performance indicators of reliability, resiliency, and vulnerability in the classical water quality management problem. The method is demonstrated for maximizing reliability in an example river basin, and is shown to be efficient and accurate, at least in this preliminary application. This suggests that the method may be effective for addressing other water quality and water resources 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, research on lower bounds and on partitioning strategies needs to be advanced. Since it is unlikely that general approaches exist for identification of bounds and partitioning strategies for all problems, application-specific approaches need to be developed. The heuristic procedures for determining the lower bound solution and the variables on which to branch should, ideally, exploit the natural ordering of technologies in terms of their cost-benefit properties. The notion of benefit, though, needs to be analyzed in a more precise way in this context. Moreover, it should be stressed that the existing theory of the Stochastic Branch and Bound Method has been developed for the case of deterministic branching, which allows only static (i.e., determined in advance) ordering of the waste abatement strategies. Dynamic ordering strategies (i.e., where the choice is dependent on the outcomes of some experiments at the given node of the branching tree) are stochastic in nature, and require additional theoretical work.

Secondly, 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 record singleton is premature, but this approach should also be investigated in more detail. One might consider such an approach a random selection of a potentially interesting alternative. By running the method in a regenerative fashion (i.e., restarting it with a different random number seeds) one can identify a larger number of record set candidates and then select the best one by performing extensive simulations for each of them.

Thirdly, 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 it does not allow for ranking the sets. This is a situation when the use of multiple realization estimates, as is employed in the example presented here, 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. Research that is currently being conducted in this direction focuses on how to determine the number of observations used to generate upper bounds, whether they should be dependent on the estimated reliability, and whether they should be allowed to change it in the course of computation [see, Hägglöf, 1996].

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