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Working Paper

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Foreword

The optimal use of indivisible resources is often the central issue in the economy and management. One of the main difficulties is the discontinuous nature of the resulting resource allocation problems which may lead to the failure of competitive market allocation mechanisms (unless we agree to "divide" the indivisibles in some indirect way, as discussed in [21]). The problem becomes even more acute when uncertainty of the outcomes of decisions is present.

In this paper we formalize the problem as a stochastic optimization problem involving discrete decision variables and uncertainties. By using some concrete examples, we illustrate how some problems of "dividing indivisibles" under uncertainty can be formalized in such terms. Next, we develop a general methodology to solve such problems based on the concept of the branch and bound method. The main idea of the approach is to process large collections of possible solutions and to devote more attention to the most promising groups. By gathering more information to reduce the uncertainty and by specializing the solution the optimal decision can be found.

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1 Introduction

The aim of this paper is to develop a stochastic version of the branch and bound method for optimization problems involving discrete decision variables and uncertainties. The proposed procedure can be applied in cases when conventional deterministic techniques run into difficulties in calculating exact bounds. Such situations are typical for optimization of discrete stochastic systems with indivisible resources.

An important example which illustrates the difficulties encountered is the following well-known hypothesis testing problem. Suppose that there are two actions $i = 1, 2$ with random outcomes α_i , $i = 1, 2$. The distribution of α_i depends on i , but is unknown. By using results of random observations of α_i , we want to find the action with the smallest expected outcome $\mathbf{E}\alpha_i$. Obviously, this problem is equivalent to the verification of the inequality: $\mathbf{E}\alpha_1 < \mathbf{E}\alpha_2$.

A more general problem which is often referred to as the automaton learning or the multi-armed bandit problem is the following (see [8]). Let $\{1, \dots, N\}$ be the set of possible actions of the automaton and let α_i be the response of the "environment" to action i . Again, the distribution of α_i depends on i but is otherwise unknown. The automaton attempts to improve its behavior (current action) on the basis of the responses to previous actions. In other words, the goal is to find a strategy which generates a sequence of actions i_0, i_1, \dots evolving (in some sense) to the action with the smallest expected outcome (risk)

$$\min_{1 \leq i \leq N} \mathbf{E}\alpha_i.$$

Let us now discuss a seemingly similar, but in fact, a much more difficult example of a discrete stochastic optimization model. The main concern again is the choice among actions with random outcomes, but the set of feasible actions is given implicitly and their number N may be astronomically large. For example, a feasible action may be associated with a vector $x = (x_1, \dots, x_n)$, satisfying the constraint

$$\sum_{j=1}^n b_j x_j \leq d,$$

where components x_j take on values 0 or 1. The parameters d and b_j , $j = 1, \dots, n$, are assumed to be positive. Outcome of a feasible action x is characterized by a random value

$$\sum_{j=1}^n c_j x_j,$$

where the distribution of random coefficients c_j , $j = 1, \dots, n$ is unknown. As in the automaton learning problem, the main question may be the choice of an action leading to the smallest (largest) expected outcome

$$F(x) = \sum_{i=1}^n \mathbf{E}c_i x_i.$$

This is a stochastic version of the well-known knapsack problem which arises in many applications involving allocation of indivisible resources. In section 2 we discuss various other applications and models of discrete stochastic optimization.

An important property of these problems is that the number N of possible solutions (actions) may be very large. Therefore, the use of standard hypotheses testing techniques or techniques developed for automaton learning becomes practically impossible, because they are based on sequential observations of outcomes of *all* feasible actions.

There may be alternative approaches. One of them is to consider the discrete problem as an optimization problem with discontinuous functions and to use the techniques developed in [4]. Another general approach can be based on the estimation of unknown parameters and the use of well-known deterministic procedures to the resulting approximate problem. The convergence of such a procedure follows from the fact that only a finite number of feasible solutions exist.

There are only few works devoted to solving stochastic discrete programming problems, which are usually devoted to special cases, e.g., [22], [2], [19], [11], [12], [16],[20]. Generally, the development of solution techniques for stochastic discrete programming problems is in an embryonic state. The purpose of the present paper is to discuss the capabilities and peculiarities of one of the most popular discrete programming method - the branch and bound method - when applied to stochastic discrete programming. The remarkable feature of the branch and bound method is that it can combine global search and local search (heuristic) procedures (for calculating bounds) in a natural way.

In the stochastic branch and bound method, the whole search area is subdivided into subsets. In the procedure random upper and lower bounds are used. They can be calculated with an accuracy depending on the size of the set and previous values of the estimates. The updating procedure consists of calculating more precise bounds interval for the subsets by using additional observations and subdividing some of the subsets (e.g. the *record set* corresponding to the smallest lower bound). Thus the optimal action (solution) is constructed sequentially without examination of each feasible action. In section 3 the method is described in detail and its convergence is proven. The discussion of section 4 concerns the estimation of stochastic upper and lower bounds. Finally, we have a conclusion section.

2 Models of discrete stochastic optimization

Let us now discuss some stochastic optimization problems which can be approached by using the techniques proposed in the next section.

Suppose that actions or solutions can be characterized by vectors $x = (x_1, \dots, x_n)$ from a finite set $X \subset R^n$. For example, X may be defined as the intersection of some (in particular integer) lattice in R^n with a hypercube in R^n . Often, components of the vector x take on 0–1 values.

We assume that outcomes of an action x can be described by a function $f(x, \theta)$, where $\theta \in \Theta$ and $(\Theta, \Sigma, \mathbf{P})$ is a probability space. The problem is to find the action x that minimizes the expected outcome (sometimes called the risk function)

$$F(x) = \mathbf{E}f(x, \theta) \quad (2.1)$$

among

$$x \in X \cap D, \quad (2.2)$$

where D is a subset in R^n given, for example, by linear or nonlinear constraints

$$D = \{x \in R^n : g_i(x) \leq 0, i = 1, \dots, m\}.$$

Let us now consider some simplified versions of important applied models which can be used later as illustrations for proposed techniques.

Example 1. Pollution control

In the simplest pollution control problem there are emission sources $i = 1, \dots, m$ and reception points $j = 1, \dots, n$. For every source i , a finite set $K(i)$ of treatment technologies is available. Each technology $k_i \in K(i)$ has cost c_{ik_i} and is associated with an emission level e_{ik_i} . The emissions are transferred to receptors to produce depositions

$$y_j(k_1, \dots, k_m, \theta) = \sum_{i=1}^m t_{ij}(\theta) e_{ik_i},$$

where $t_{ij}(\theta)$ are some random transfer coefficients. Finally, there are some target (safe) levels of deposition q_j for the receptors $j = 1, \dots, n$. They can be used to formulate a penalty cost $\varphi_j(y_j)$ associated with each deposition, e. g.,

$$\varphi_j(y_j) = \max(0, y_j - q_j),$$

where q_j are safe levels for receptors j . The problem is to find the technologies k_1, \dots, k_m so as to minimize the pollution penalty

$$F(k_1, \dots, k_m) = \mathbf{E} \left\{ \sum_{j=1}^n \varphi_j \left(\sum_{i=1}^m t_{ij}(\theta) e_{ik_i} - q_j \right) \right\}$$

subject to the budget constraint

$$\sum_{i=1}^m c_{ik_i} \leq R.$$

Example 2. Facility location

We are given a set $\mathcal{N} = \{1, 2, \dots, n\}$ of potential facility locations and a set of clients $I = \{1, 2, \dots, m\}$. A facility placed at location j costs c_j and has capacity u_j . Clients have random demands $d_i(\theta)$, $i = 1, \dots, m$, and the unit cost of satisfying the demand of client i from facility j is q_{ij} . There is also a unit penalty for not satisfying the demand of client i from any of the facilities: q_{i0} . The problem is to choose locations of facilities that minimize the total expected cost. Defining binary variables

$$x_j = \begin{cases} 1 & \text{if facility is placed at } j, \\ 0 & \text{otherwise,} \end{cases}$$

we can formalize the problem as follows

$$\min \left[F(x) = \sum_{j=1}^n c_j x_j + \mathbf{E}\varphi(x, \theta) \right]$$

$$x_j \in \{0, 1\}, \quad j = 1, \dots, n,$$

where $\varphi(x, \theta)$ is defined as the minimum cost of satisfying the demand. Denoting by y_{ij} the amount of the demand of client i served from facility j , we can define $\varphi(x, \theta)$ as the optimal value of the transportation problem

$$\min \sum_{i=1}^m \sum_{j=0}^n q_{ij} y_{ij}$$

$$\sum_{j=0}^n y_{ij} = d_i(\theta), \quad i = 1, \dots, m$$

$$\sum_{i=1}^m y_{ij} \leq x_j u_j, \quad j = 1, \dots, n.$$

$$y_{ij} \geq 0, \quad i = 1, \dots, m, \quad j = 1, \dots, n.$$

Example 3. Project financing

There are n prospective projects that can be implemented. The cost of starting project j is c_j . The projects use resources $i = 1, \dots, m$ available in quantities b_i . The demand of a project j for resource i is a random quantity $d_{ij}(\theta)$. Project j , if successfully completed, may bring a random income $q_j(\theta)$. After the projects are started, the uncertain quantities become known and one has to decide which projects are to be continued. The problem is to find the initial set of projects started so that the expected profit from the whole enterprise is maximized. Using binary variables

$$x_j = \begin{cases} 1 & \text{if project } j \text{ is started,} \\ 0 & \text{otherwise,} \end{cases}$$

we can define the objective (to be minimized) as

$$F(x) = \sum_{j=1}^n c_j x_j - \mathbf{E}\varphi(x, \theta),$$

where $\varphi(x, \theta)$ is the actual income from the projects selected to be continued. It is the optimal value of the multi-knapsack problem:

$$\begin{aligned} \max \sum_{j=1}^n q_j(\theta) y_j \\ \sum_{j=1}^n d_{ij}(\theta) y_j \leq b_i, \quad i = 1, \dots, m, \\ y_j \in \{0, x_j\}, \quad j = 1, \dots, n. \end{aligned}$$

Example 4. *Expansion of arc capacities in a network*

Consider a network with the set of nodes \mathcal{N} , the set of arcs \mathcal{A} and with the node-arc incidence matrix M . The arc capacities x_{ij} , $(i, j) \in \mathcal{A}$, can be chosen from some finite sets X_{ij} with costs $c_{ij}(x_{ij})$. There is a random supply/demand in the network: $d_i(\theta)$, $i \in \mathcal{N}$, and the unit cost of flow on arc (i, j) is q_{ij} . The problem is to invest in arc capacities so as to minimize the objective function

$$F(x) = \sum_{(i,j) \in \mathcal{A}} c_{ij}(x_{ij}) + \mathbf{E}\varphi(x, \theta).$$

The first part of $F(x)$ represents direct investment costs, while $\varphi(x, \theta)$ represents transportation costs defined as the minimum value of the network flow problem:

$$\begin{aligned} \min \sum_{(i,j) \in \mathcal{A}} q_{ij} y_{ij} \\ My = d(\theta), \\ 0 \leq y_{ij} \leq x_{ij}, \quad (i, j) \in \mathcal{A}. \end{aligned}$$

Example 5. *Two-stage network flow problem*

Consider a network with the set of nodes \mathcal{N} , the set of arcs \mathcal{A} and with the node-arc incidence matrix M . Our first-stage decision variables are integer flows (e.g. numbers of flights) x_{ij} for each arc $(i, j) \in \mathcal{A}$. They are non-negative integers and have to satisfy flow conservation conditions

$$Mx = 0$$

and some feasibility conditions, e.g.,

$$\sum_{j \in \delta^+(i)} x_{ij} \leq u_i, \quad i \in \mathcal{N},$$

where $\delta^+(i) = \{j : (i, j) \in \mathcal{A}\}$ and u_i is the capacity of node i .

For each pair of nodes $k, l \in \mathcal{N}$ there is a random amount $b^{kl}(\theta)$ of cargo to be delivered from k to l . The unit cost of moving cargo along arc (i, j) is q_{ij} . The problem is to find a feasible first-stage flow x (schedule) such that the total cost

$$F(x) = \sum_{(i,j) \in \mathcal{A}} c_{ij} x_{ij} + \mathbf{E}\varphi(x, \theta),$$

is minimized. The first part represents direct costs, while $\varphi(x, \theta)$ is the minimum cost for satisfying the demand for cargo shipment once the schedule x is determined. It is the optimal value in the multi-commodity network flow problem defined as follows. For each pair (k, l) , we denote the amount of cargo going from k to l through arc (i, j) by y_{ij}^{kl} and the total flow vector by y^{kl} . Next, we define the supply/demand vector d^{kl} by

$$d_i^{kl}(\theta) = \begin{cases} b^{kl}(\theta) & \text{if } i = k, \\ -b^{kl}(\theta) & \text{if } i = l, \\ 0 & \text{otherwise.} \end{cases}$$

Then our shipment problem can be formalized as

$$\begin{aligned} \min & \sum_{k \in \mathcal{N}} \sum_{l \in \mathcal{N}} \sum_{(i,j) \in \mathcal{A}} q_{ij} y_{ij}^{kl} \\ & My^{kl} = d^{kl}(\theta), \\ & \sum_{k \in \mathcal{N}} \sum_{l \in \mathcal{N}} y_{ij}^{kl} \leq x_{ij} v, \end{aligned}$$

where v denotes the unit capacity of the first-stage flow (maximum payload of an aircraft).

All these examples have common features. There is some indivisible resource to be distributed among many possible activities which makes the number of feasible solutions (actions) very large. Together with that, exact evaluation of the objective function at any of the feasible points is very difficult. For non-trivial distributions of the uncertain parameters, one can only simulate the random data and calculate stochastic estimates of the objective. It is quite clear that we need a method that would be capable of finding a solution or a sufficiently good estimate of it without exhaustive examination of all feasible points. In other words, we need a way to quickly eliminate non-promising solutions from the feasible set. Such a way can frequently be found owing to the convexity of the functions involved, because for convex functions $f(x, \theta)$ we can derive some stochastic bounds on their expected values. Before proceeding to these technical issues let us at first present a general framework in which such bounds can be used.

3 Stochastic branch and bound method

3.1 Outline of the method

Let us consider the discrete stochastic programming problem

$$\min_{x \in X \cap D} [F(x) = \mathbf{E}f(x, \theta)], \quad (3.1)$$

where X is a finite set in some solution space \mathcal{X} , D is some (possibly infinite) subset of the space \mathcal{X} , θ is an elementary event in a probability space $(\Theta, \Sigma, \mathbf{P})$ and \mathbf{E} denotes the mathematical expectation operator.

For example, the n -dimensional Euclidean space R^n may serve as the solution space \mathcal{X} , the set D may be given in R^n by linear or nonlinear inequalities and the set X may be defined as an intersection of some (in particular integer) lattice in R^n with a bounded box.

In the branch and bound method the original set X is sequentially subdivided into subsets X^p generating a partition \mathcal{P} of X (or of its part). Consequently, the original problem is subdivided into subproblems

$$\min_{x \in X^p \cap D} [F(x) = \mathbf{E}f(x, \theta)], \quad X^p \in \mathcal{P}.$$

Let $F^*(X^p)$ denote the optimal value of this subproblem. Clearly, the optimal value of the whole problem equals

$$F^*(X) = \min_{X^p \in \mathcal{P}} F^*(X^p).$$

The main idea of the stochastic branch and bound method is to iteratively execute three operations:

- partitioning into smaller subsets,
- estimation of the objective within the subsets,
- removal of some subsets.

The procedure continues until some stopping criterion is satisfied, e.g., until "interesting" subsets X^p become singletons. Reduction of the exhaustive examination of X is achieved by using statistical estimates of lower and upper bounds of optimal values $F^*(X^p)$.

Let us now describe in detail the concept of stochastic bounds. We make the following assumption.

(A1) There exist functions $L : 2^X \rightarrow R$ and $U : 2^X \rightarrow R$ such that for each $X^p \subset X$

$$L(X^p) \leq F^*(X^p) \leq U(X^p),$$

$$U(X^p) = F(x') \text{ for some } x' \in X^p,$$

and if X^p is degenerated into a singleton then

$$L(X^p) = F^*(X^p) = U(X^p).$$

We also assume that if $X^p \cap D = \emptyset$ then this case can be identified and, by definition, $L(X^p) = U(X^p) = +\infty$.

The functions L and U are usually defined by some auxiliary stochastic optimization problems defined on the subsets X^p . In section 4 we shall discuss some ways of constructing such subproblems.

Obviously, the optimal value $F^*(X)$ cannot be achieved on those sets X^p for which

$$L(X^p) > \min_{X^p \in \mathcal{P}} U(X^p),$$

so such sets (subproblems) could be deleted from the list of subproblems, if we knew the bounds. However, in stochastic problems the bounds $L(X^p)$ and $U(X^p)$ can hardly be computed exactly. Therefore we can only assume that some statistical estimates of $L(X^p)$ and $U(X^p)$ can be obtained.

(A2) In some probability space $(\Omega, \Sigma, \mathbf{P})$, for each subset $X^p \subset X$, there exist sequences of random estimates $\xi^l(X^p, \omega)$, $l = 1, 2, \dots$, and $\eta^m(X^p, \omega)$, $m = 1, 2, \dots$, $\omega \in \Omega$, such that

$$\begin{aligned}\lim_{l \rightarrow \infty} \xi^l(X^p, \omega) &= L(X^p) \text{ a.s.}, \\ \lim_{m \rightarrow \infty} \eta^m(X^p, \omega) &= U(X^p) \text{ a.s.}\end{aligned}$$

Possible structure of the probability space $(\Omega, \Sigma, \mathbf{P})$ will be described in section 3.3. Let us mention here that if the bounds L and U are defined by some auxiliary stochastic problems with continuous variables, a broad collection of methods can be used to generate estimates satisfying (A2) (see [3]).

Let us now describe the stochastic branch and bound algorithm in more detail. For brevity, we skip the argument ω from the random indices l and m , random partitions \mathcal{P} and random sets.

3.2 The algorithm

Initialization. Form initial partition $\mathcal{P}_0 = \mathcal{P}'_0 = \{X\}$. Calculate the bounds $\xi_0 = \xi^{l_0}(X)$ and $\eta_0 = \eta^{m_0}(X)$. Set $k = 1$.

Partitioning. Select the record subset

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

and an approximate solution

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

If the record subset is a singleton, then set $\mathcal{P}_k = \mathcal{P}_{k-1}$ and go to Bound Estimation. Otherwise construct a partition of the record set, $\mathcal{P}''_k(Y^k) = \{Y_i^k, i = 1, 2, \dots\}$, such that $Y^k = \bigcup_i Y_i^k$ and $Y_i^k \cap Y_j^k = \emptyset$ for $Y_i^k, Y_j^k \in \mathcal{P}''_k$, $i \neq j$. Define new full partition

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

Elements of \mathcal{P}_k will be also denoted by X^p .

Bound estimation. For all subsets $X^p \in \mathcal{P}_k$ select some estimates $\xi_k(X^p) = \xi^{l_k(X^p)}(X^p)$ and $\eta_k(X^p) = \eta^{m_k(X^p)}(X^p)$ for $L(X^p)$ and $U(X^p)$, correspondingly.

Deletion. Clean partition \mathcal{P}_k of non-prospective subsets, defining

$$\mathcal{P}'_k = \mathcal{P}_k \setminus \{X^p : X^p \cap D = \emptyset\}.$$

Set $k := k + 1$ and go to Partitioning.

3.3 Convergence

In the deterministic case one need not prove convergence of the branch and bound method, owing to the finite number of possible solutions. On the contrary, convergence in the stochastic case requires some validation, because of the probabilistic character of bound estimates. For example, due to random errors, a subset containing the global solution need not be the record set and may remain unpartitioned. Next, if the algorithm is terminated after a finite number of iterations, the probability of an error and the size of the error have to be estimated.

First of all, let us construct a probabilistic model of the algorithm. Assume that partitioning is done by some deterministic rule \mathcal{P}'' : for every subset $Y \subset X$, $\mathcal{P}''(Y)$ is a collection of disjoint subsets Y_j of Y such that $\bigcup_j Y_j = Y$. We consider a deterministic tree $T(X)$ obtained from the initial set X by sequential application of the rule \mathcal{P}'' to all sets arising in this process, until they become singletons. The set X is the root node. At level 1 there are nodes corresponding to the subsets in $\mathcal{P}''(X)$. Level 2 contains all sets of $\mathcal{P}''(Y)$ for all $Y \in \mathcal{P}''(X)$, etc. For each set $X' \in T(X)$, we denote by $k(X')$ the location depth of X' in $T(X)$.

Suppose that for each set $X' \in T(X)$ there exists a probability space $(\Omega_{X'}, \Sigma_{X'}, P_{X'})$ such that for all subsets $X'' \in \mathcal{P}''(X')$ there are sequences of random estimates

$$\xi^l(X'', \omega'), \omega' \in \Omega_{X'}, l = 1, 2, \dots,$$

for $L(X'')$ and

$$\eta^m(X'', \omega'), \omega' \in \Omega_{X'}, m = 1, 2, \dots,$$

for $U(X'')$. Denote by

$$(\Omega_k, \Sigma_k, \mathbf{P}_k) = \prod_{\{X' \in T(X): k(X')=k\}} (\Omega_{X'}, \Sigma_{X'}, \mathbf{P}_{X'})$$

the product of probability spaces $(\Omega_{X'}, \Sigma_{X'}, \mathbf{P}_{X'})$ over all X' which may arise at iteration k of the algorithm. By construction, the algorithm will perform no more than N partitions, where N is a number of elements of X . Let us consider the product of probability spaces:

$$(\Omega, \Sigma, \mathbf{P}) = (\Omega_0 \times \dots \times \Omega_N, \Sigma_0 \times \dots \times \Sigma_N, \mathbf{P}_0 \times \dots \times \mathbf{P}_N),$$

and denote $\omega = (\omega_0, \dots, \omega_N) \in \Omega$. We shall consider all random objects produced by the algorithm as defined on this general probability space.

We denote by X^* the solution set of (3.1) and by f^* the optimal value of the objective.

Theorem 3.1 *Assume that the indices $l_k(X^p)$ and $m_k(X^p)$ are chosen in such a way that, if a subset $X' \in \mathcal{P}_k$ for infinitely many k , then a. s.*

$$\lim_{k \rightarrow \infty} l_k(X') = \lim_{k \rightarrow \infty} m_k(X') = \infty. \quad (3.2)$$

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 $x^k \in X^*$.*

Proof. Owing to the the finite number of elements in X , there can be only a finite number of iterations with partitioning. Therefore, there exists k_1 such that for al $k \geq k_1$ all record sets are singletons and the partition remains unchanged. We shall denote it \mathcal{P}_∞ . Let us define *recurrent* record sets as those, which are record sets for infinitely many k . Because the number of record sets is finite, there exists k_2 such that for all $k \geq k_2$ all record sets are recurrent. For each recurrent record set Y , at infinitely many k we have

$$\xi^{l_k(Y)}(Y) \leq \xi^{l_k(X^p)}(X^p)$$

for all subsets X^p that remain in the partition \mathcal{P}_∞ , $k \geq k_2$. Passing to the limit in the last inequality, we obtain

$$F(Y) \leq L(X^p),$$

for all subsets $X^p \in \mathcal{P}_\infty$, which completes the proof of assertion (i).

Let us consider now the approximate solutions $x^k \in X^k$. By definition

$$\eta^{m_k(X^k)}(X^k) \leq \eta^{m_k(Y^k)}(Y^k).$$

By assumption, $m_k(Y^k) \rightarrow \infty$, so $\eta^{m_k(Y^k)}(Y^k) \rightarrow F^*$ by the first part of the proof. Thus

$$\limsup_{k \rightarrow \infty} \eta^{m_k(X^k)}(X^k) \leq F^*.$$

Let a set $X' \in \mathcal{P}_\infty$ be the approximate set X^k for infinitely many k , and let the point $x' \in X'$ be chosen infinitely often as the point x^k . By finiteness of the partition \mathcal{P}_∞ and by finiteness of the sets, there exists k_3 such that for all $k \geq k_3$ each X^k and each x^k is recurrent in the above sense. Then

$$F(x') = \lim_{k \rightarrow \infty} \eta^{m_k(X^k)}(X^k) \leq F^*,$$

i.e., $x' \in X^*$. The proof is complete.

Let us now discuss some issues concerning possible implementation of the conceptual method discussed above.

Stochastic lower and upper bounds for the subproblems can be calculated by making some experiments (observations) on the subproblems. In the next section we describe some general rules for calculating the bounds. In any case, however, with no loss of generality one can assume that the numbers l and m in assumption (A2) correspond to the numbers of observations. The assumptions of the theorem can be satisfied by making new observations for each subset at infinitely many iterations (not quitting observations for any of the subsets). This is a major difference between our method and the deterministic branch and bound method: we do not delete subsets X' for which

$$\xi_k(X') > \eta_k(X^k),$$

because of the stochastic nature of the lower and upper bounds. Nevertheless, we have much freedom in specifying the amount of attention devoted to each set, as the following remark shows.

Remark. Let the observations for the subsets be made according to the rules

$$\begin{aligned} l_k(X^p, \omega) &= l_{k-1}(X^p, \omega) + I_k(X^p, \omega), \\ m_k(X^p, \omega) &= m_{k-1}(X^p, \omega) + J_k(X^p, \omega), \end{aligned}$$

with $l_{k-1}(X^p, \omega) = 0$ and $m_{k-1}(X^p, \omega) = 0$ for newly created sets X^p . Assume that for every $X^p \in \mathcal{P}_\infty$ with probability one

$$\sum_{k=k(X^p)}^{\infty} \mathbf{P}\{I_k(X^p) > 0 \mid X^p, l_{k-1}(X^p)\} = \infty$$

and

$$\sum_{k=k(X^p)}^{\infty} \mathbf{P}\{J_k(X^p) > 0 \mid X^p, m_{k-1}(X^p)\} = \infty,$$

where $k(X^p)$ is the iteration number at which X^p was created. Then with probability one, for every $X^p \in \mathcal{P}_\infty$ condition (3.2) is satisfied.

Proof. The result follows immediately from the Borel-Cantelli theorem.

It seems reasonable to make the frequencies of observations dependent on the estimated quality of the subsets. For example, at each iteration we may allocate a fixed number of observations to the record set (or its newly created subsets, if it was partitioned) and another number of observations to all remaining sets. The choice of the particular non-record sets observed at the current iteration can be done at random; for example, with equal probabilities. In this way the assumptions of the theorem will be satisfied, but non-prospective subsets will be observed with a low frequency. Another possibility would be to assign some unequal probabilities $\pi(X^p)$ of observations to the subsets. The probabilities may be functions of the current estimates. In particular, the idea of observing sets with the lowest confidence intervals, introduced for the multi-armed bandit problem in [13], may prove successful here, because it resolves in a natural way the conflict between optimization and exploration.

Another important implementational and theoretical issue is the stopping criterion. Clearly, because of the stochastic nature of the bounds, a solution obtained after a finite number of observations is, in general, an approximation. Only some probabilistic statements can be made about its accuracy. Let us discuss it in more detail.

Remark. Assume that the algorithm stops at iteration s and that we can build for all $X^p \subset \mathcal{P}_s$ confidence intervals $[\underline{\xi}(X^p), \infty)$ for $L(X^p)$ and a confidence interval $(-\infty, \bar{\eta}(x^s)]$ for $F(x^s)$, $x^s \in X^s$, such that

$$\mathbf{P}\left\{ \forall (X^p \subset \mathcal{P}_s) \underline{\xi}(X^p) \leq L(X^p) \text{ and } F(x^s) \leq \bar{\eta}(x^s) \right\} \geq 1 - \delta.$$

Then, with probability at least $1 - \delta$,

$$F(x^s) - F^* \leq \bar{\eta}(x^s) - \min_{x^p \in \mathcal{P}_s} \underline{\xi}(X^p). \quad (3.3)$$

Proof. With probability not smaller than $1 - \delta$, $F^* \geq \min_{X^p \in \mathcal{P}}, L(X^p) \geq \min_{X^p \in \mathcal{P}}, \underline{\xi}(X^p)$ and $F(x^s) \leq \bar{\eta}(x^s)$. Combining these two inequalities we obtain the required result.

It is clear from the error estimate (3.3) that the quality of the approximate solution x^s can be improved by making $\bar{\eta}$ small (that is the motivation for the choice of x^s) and by moving up lower bounds of the confidence intervals for $L(X^p)$. It suggests that more observations should be devoted to non-record subsets which have small $\underline{\xi}(X^p)$.

It should be noted, though, that construction of confidence intervals after the termination of the method cannot be done in a straightforward way. At the iteration s , the numbers of observations devoted to particular subsets of the final partition are random. Indeed, such a number for a set X^p depends on the time $k(X^p)$ when X^p was created. It also may depend, if non-trivial rules for generating numbers of observations are used, on the outcomes of observations, e.g., on the number of times X^p was a record set. We can only have some lower and upper bounds on the number of observations for X^p . Therefore, to guarantee the probability $1 - \delta$ for the error estimates, one needs collections of iteratively computed confidence intervals that hold uniformly for some range of observation numbers. Such collections of intervals can be constructed if we assume some upper bounds on the tails of the distributions of random estimates.

4 Estimation of lower and upper bounds

The main question which remains to be answered is the estimation of the lower and upper bounds. In this section we shall discuss two general ideas:

- interchange of minimization and mathematical expectation operators, and
- dual estimates.

They will be used to construct other discrete or continuous optimization problems which have their optimal values below the optimal value of the original problem. Clearly, some well-known deterministic methods for generating bounds (such as relaxation of the integrality condition) can be used together with the ideas discussed here.

4.1 Interchange of minimization and mathematical expectation operators

Consider a discrete stochastic optimization problem without additional general constraints:

$$\min_{x \in X} \mathbf{E}f(x, \theta).$$

The following estimate is true:

$$F^*(X) = \min_{x \in X} \mathbf{E}f(x, \theta) \geq \mathbf{E} \min_{x \in X} f(x, \theta) = \mathbf{E}f(x^*(\theta), \theta),$$

where

$$x^*(\theta) \in \arg \min_{x \in X} f(x, \theta).$$

Thus the quantity

$$L(X) = \mathbf{E}f(x^*(\theta), \theta)$$

provides a lower estimate for the optimal value $F^*(X)$. In many cases, for a fixed θ , $x^*(\theta)$ can be easily found. Additionally, for the quantity

$$f^*(\theta) = \min_{x \in X} f(x, \theta)$$

itself, simple lower estimates can be constructed using specific properties of the function $f(x, \theta)$. For example, a stochastic estimate of $L(X)$ can be calculated in an acceptable time by means of a Monte Carlo simulation technique:

$$L_n = \frac{1}{n} \sum_{i=1}^n f(x^*(\theta_i), \theta_i),$$

where θ_i , $i = 1, \dots, n$, are i.i.d. random variables with distribution \mathbf{P} .

As an upper bound $U(X)$ for the optimal value $F^*(X)$ the value of the objective function at some feasible point $x' \in X$ can be taken:

$$U(X) = F(x') = \mathbf{E}f(x', \theta).$$

It is important to choose point x' in such a way that $F(x')$ is as small as possible. Such points can be found by any (heuristic) local stochastic discrete optimization method like, for instance, the stochastic approximation (over integer lattice) method [2] or a descent direction method (see [17] for the stochastic version).

The same idea of interchanging minimization and mathematical expectation operators can be applied to two-stage stochastic programming problems. Let us consider a two-stage stochastic programming problem:

$$\min_{x \in X} \left[F(x) = f_1(x) + \mathbf{E} \min_{y \in Y(x, \theta)} f_2(x, y, \theta) \right],$$

where $x \in X$, $\theta \in \Theta$, $y \in Y(x, \theta)$, X and Θ are some sets, $Y(x, \theta)$ is a multi-valued mapping, $(\Theta, \Sigma, \mathbf{P})$ is a probability space, x is a deterministic first stage solution, $y(\cdot)$ is a random second stage solution (correction), and $f_1(x)$ and $f_2(x, y, \theta)$ are performance measures related to the first and the second stage, correspondingly. Let $F^*(X)$ be the optimal value of this problem. Then the following estimate holds:

$$F^*(X) \geq \mathbf{E} \left\{ \min_{x \in X, y \in Y(x, \theta)} [f_1(x) + f_2(x, y, \theta)] \right\} = L(X).$$

We assume here, of course, that the expectation operation is well-defined. Internal minimization problems, under fixed θ , can often be solved quickly, as the following example shows.

Example 6. *Project financing (continued)*

Let us consider the project financing problem of Example 3 and a subproblem

$$\min_{x \in X} F(x)$$

with some $X \subset \{0, 1\}^n$. Denote

$$Y(\theta) = \{y \in X : \sum_{j=1}^n d_{ij}(\theta)y_j \geq b_i, i = 1, \dots, n\}.$$

The optimum value of the subproblem can be estimated from below as follows:

$$\begin{aligned} \min_{x \in X} \mathbf{E} \min_{y \in Y(\theta), y \leq x} \sum_{j=1}^n (c_j x_j - q_j(\theta)y_j) &\geq \mathbf{E} \min_{x \in X} \min_{y \in Y(\theta), y \leq x} \sum_{j=1}^n (c_j x_j - q_j(\theta)y_j) \\ &= \mathbf{E} \min_{y \in Y(\theta)} \min_{x \in X, x \geq y} \sum_{j=1}^n (c_j x_j - q_j(\theta)y_j). \end{aligned}$$

For $c_j \geq 0$ the minimization in x can be carried out analytically, $x_j = y_j$, $j = 1, \dots, n$, and we arrive at the following lower bound:

$$L(X) = \mathbf{E} \min_{y \in Y(\theta)} \sum_{j=1}^n (c_j - q_j(\theta))y_j.$$

Consequently, the lower bound is obtained by postponing the decision of starting the projects until the uncertain data becomes known. Further relaxation of the integrality condition (replacement of X by its convex hull $[0, 1]^n$) allows easy solution of the linear subproblems under the expectation in the expression for $L(X)$.

As the upper bound $U(x)$ we can take the value $F(x')$ at the largest point in X :

$$x' = \max\{x : x \in X\};$$

i.e., all projects are started which can be started in X .

An important matter is the reduction of variance in these kinds of statistical estimates. This is discussed in [1] and [9].

4.2 Dual estimates in one-stage stochastic problems

Dual estimates in combination with nonsmooth optimization methods are widely used in deterministic discrete programming (see for example, Fisher [6], Minoux [14], Shor [18]). Let us discuss peculiarities of dual estimates when they are applied to stochastic discrete programming problems.

Consider a general stochastic programming problem:

$$\min [F(x) = \mathbf{E}f(x, \theta)] \tag{4.1}$$

subject to

$$G_i(x) = \mathbf{E}g_i(x, \theta) \leq 0, i = 1, \dots, m; \tag{4.2}$$

$$x \in X; \tag{4.3}$$

where X is some compact (in particular discrete) set, $\theta \in \Theta$, where $(\Theta, \Sigma, \mathbf{P})$ is a probability space, and \mathbf{E} is a mathematical expectation operator. Some of nonlinear inequality constraints can be deterministic. We denote by F^* the optimal value of the problem.

Let us define the Lagrangian function

$$\begin{aligned}
L(x, \lambda) &= F(x) + \sum_{i=1}^m \lambda_i G_i(x) \\
&= \mathbf{E} \left\{ f(x, \theta) + \sum_{i=1}^m \lambda_i g_i(x, \theta) \right\} \\
&= \mathbf{E} l(x, \theta, \lambda).
\end{aligned} \tag{4.4}$$

The following inequalities hold:

$$\begin{aligned}
F^* &= \min_{x \in X} \max_{\lambda \geq 0} L(x, \lambda) \\
&\geq \max_{\lambda \geq 0} \min_{x \in X} L(x, \lambda) \\
&\geq \max_{\lambda \geq 0} \mathbf{E} \min_{x \in X} l(x, \theta, \lambda) \\
&= \max_{\lambda \geq 0} \mathbf{E} \varphi(\lambda, \theta),
\end{aligned}$$

where the function

$$\varphi(\lambda, \theta) = \min_{x \in X} l(x, \theta, \lambda)$$

is concave in λ (it is supposed to be integrable in θ). Thus, for any $\lambda \geq 0$, the quantity

$$h(\lambda) = \mathbf{E} \varphi(\lambda, \theta),$$

is a dual lower estimate for the optimal value F^* . The quantity

$$h^* = \max_{\lambda \geq 0} \mathbf{E} \varphi(\lambda, \theta)$$

is the optimal dual lower estimate for F^* . The estimates $h(\lambda)$, $\lambda \geq 0$, can be calculated, for example, by a Monte Carlo method and h^* can be found by convex stochastic programming methods (see, for example, [5]). In the last case, one need not solve the estimating stochastic optimization problem until optimality, but we can stop at any feasible approximation.

When calculating dual estimates, one has to solve the following internal minimization problems

$$\min_{x \in X} l(x, \theta, \lambda)$$

under fixed θ and λ . In many cases these problems can be analytically or numerically solved by nonlinear or discrete programming methods. For example, if functions $f(x, \theta)$ and $g_i(x, \theta)$, $i = 1, \dots, m$, are concave in x and X is a convex polyhedron then the minimal value of $l(x, \theta, \lambda)$ is achieved at a vertex of X .

4.3 Dual estimates for two-stage stochastic problems

Let us consider a two-stage stochastic programming problem of the following form:

$$\min_{x \in X} \left[F(x) = \mathbf{E} \left\{ f_1(x, \theta) + \min_{y \in Y(x, \theta)} \sum_{k=1}^K q_k y_k \right\} \right], \tag{4.5}$$

where

$$Y(x, \theta) = \left\{ y \in R^K : g_i(x, \theta) - \sum_{k=1}^K b_{ik} y_k \leq 0, i = 1, \dots, m, \right. \\ \left. y_k \geq 0, k = 1, \dots, K \right\}. \quad (4.6)$$

We assume that the coefficients q_k and b_{ik} are non-negative and do not depend on θ , $\sum_{k=1}^K b_{ik} > 0$, functions $f(x, \theta)$ and $g_i(x, \theta)$ are lower semi-continuous in x , integrable in θ and locally bounded from below by a function integrable in θ . Here, variable x is called the first stage decision, variable y is called the second stage decision (or correction), and random variable θ (environment state) is defined on some probability space $(\Theta, \Sigma, \mathbf{P})$. The second stage solution y is made after first stage solution x has been made and environment state θ has been observed.

Continuous two stage stochastic programming problems were extensively studied (see for example, [5], [10], [3], [7]). Our discussion aims at obtaining lower bounds for discrete two stage stochastic programming problems.

It can easily be shown that the function $F(x)$ is lower semi-continuous; hence, the problem under consideration has optimal solutions. We denote its optimal value by F^* .

Let us define the Lagrangian function:

$$L(x, y, \theta, \lambda) = f_1(x, \theta) + \sum_{k=1}^K q_k y_k + \sum_{i=1}^m \lambda_i \left(g_i(x, \theta) - \sum_{k=1}^K b_{ik} y_k \right) \\ = f_1(x, \theta) + \sum_{i=1}^m \lambda_i g_i(x, \theta) + \sum_{k=1}^K \left(q_k - \sum_{i=1}^m \lambda_i b_{ik} \right) y_k. \quad (4.7)$$

The following inequalities are true:

$$F^* = \min_{x \in X} \mathbf{E} \min_{y \geq 0} \max_{\lambda \geq 0} L(x, y, \theta, \lambda) \\ \geq \min_{x \in X} \mathbf{E} \max_{\lambda \geq 0} \min_{y \geq 0} L(x, y, \theta, \lambda) \\ = \min_{x \in X} \mathbf{E} \max_{\lambda \in \Lambda} \left\{ f_1(x, \theta) + \sum_{i=1}^m \lambda_i g_i(x, \theta) \right\},$$

where

$$\Lambda = \left\{ \lambda \in R^m : \sum_{i=1}^m \lambda_i b_{ik} \leq q_k, \lambda_i \geq 0, i = 1, \dots, m \right\}.$$

Interchanging the operators \mathbf{E} and "max" in the last expression, we arrive to the estimates:

$$F^* \geq \min_{x \in X} \max_{\lambda \in \Lambda} \left\{ \mathbf{E} f_1(x, \theta) + \sum_{i=1}^m \lambda_i \mathbf{E} g_i(x, \theta) \right\} \\ \geq \max_{\lambda \in \Lambda} \min_{x \in X} \left\{ \mathbf{E} f_1(x, \theta) + \sum_{i=1}^m \lambda_i \mathbf{E} g_i(x, \theta) \right\} \\ \geq \max_{\lambda \in \Lambda} \mathbf{E} \min_{x \in X} \left\{ f_1(x, \theta) + \sum_{i=1}^m \lambda_i g_i(x, \theta) \right\}.$$

In this way, we obtained two dual lower bounds:

$$L_1 = \max_{\lambda \in \Lambda} \min_{x \in X} \left\{ \mathbf{E} f_1(x, \theta) + \sum_{i=1}^m \lambda_i \mathbf{E} g_i(x, \theta) \right\}$$

and

$$L_2 = \max_{\lambda \in \Lambda} \mathbf{E} \min_{x \in X} \left\{ f_1(x, \theta) + \sum_{i=1}^m \lambda_i g_i(x, \theta) \right\}.$$

Estimates L_1 and L_2 are obtained as solutions of convex stochastic programming problems. For solution techniques for such problems, see [15] and [5]. Note that one need not solve the estimate problem until optimality and can stop at any feasible approximation.

In many cases, the bounds L_1 or L_2 are easy to calculate. An important class of such problems are linear problems with

$$\begin{aligned} f_1(x, \theta) &= \sum_{j=1}^n c_j(\theta) x_j, \\ g_i(x, \theta) &= d_i(\theta) - \sum_{j=1}^n a_{ij}(\theta) x_j, \quad i = 1, \dots, m \end{aligned}$$

(we already assumed the linearity of the second stage problem in (4.5)-(4.6)). Let us denote mean values by

$$\begin{aligned} \bar{c}_j &= \mathbf{E} c_j(\theta), \quad j = 1, \dots, n, \\ \bar{a}_{ij} &= \mathbf{E} a_{ij}(\theta), \quad i = 1, \dots, m, \quad j = 1, \dots, n, \\ \bar{d}_i &= \mathbf{E} d_i(\theta), \quad i = 1, \dots, m. \end{aligned}$$

Then the estimate L_1 becomes particularly simple:

$$L_1 = \max_{\lambda \in \Lambda} \left\{ \sum_{i=1}^m \bar{d}_i \lambda_i + \min_{x \in X} \sum_{j=1}^n \left(\bar{c}_j - \sum_{i=1}^m \lambda_i \bar{a}_{ij} \right) x_j \right\}. \quad (4.8)$$

If, additionally, X is an intersection of the integer lattice with a hyper-rectangle

$$X = \{x \in R^n : \alpha_j \leq x_j \leq \beta_j, \quad x_j \text{ integer}, \quad j = 1, \dots, n\},$$

then the minimization with respect to $x \in X$ has a closed-form solution

$$x_j^*(\lambda) = \begin{cases} \alpha_j & \text{if } \bar{c}_j - \sum_{i=1}^m \lambda_i \bar{a}_{ij} \geq 0, \\ \beta_j & \text{if } \bar{c}_j - \sum_{i=1}^m \lambda_i \bar{a}_{ij} \leq 0, \end{cases}$$

which can be substituted into (4.8):

$$L_1 = \max_{\lambda \in \Lambda} \left\{ \sum_{i=1}^m \bar{d}_i \lambda_i + \sum_{j=1}^n \min \left[\left(\bar{c}_j - \sum_{i=1}^m \lambda_i \bar{a}_{ij} \right) \alpha_j, \left(\bar{c}_j - \sum_{i=1}^m \lambda_i \bar{a}_{ij} \right) \beta_j \right] \right\}.$$

As an illustration, let us consider the facility location problem of section 2.

Example 7: Facility location (continued)

Let us derive a dual lower bound for the facility location problem from Example 2. There are two groups of constraints in the second stage problem: equality constraints

$$d_i(\theta) - \sum_{j=0}^n y_{ij} = 0, \quad i = 1, \dots, m,$$

and inequalities

$$-u_j x_j + \sum_{i=1}^m y_{ij} \leq 0, \quad j = 1, \dots, n.$$

We shall denote by μ_i , $i = 1, \dots, m$, Lagrange multipliers associated with the equalities and by λ_j , $j = 1, \dots, n$, the multipliers associated with the inequalities.

Elementary calculations lead to the following form of the lower bound (4.8):

$$L_1 = \max_{(\mu, \lambda) \in \Lambda} \left[\sum_{i=1}^m \bar{d}_i \mu_i + \min_{x \in X} \sum_{j=1}^n (c_j - \lambda_j u_j) x_j \right],$$

where

$$\Lambda = \left\{ (\mu, \lambda) \in R^{m \times n} : \mu_i - \lambda_j \leq q_{ij}, \quad i = 1, \dots, m, \quad j = 1, \dots, n, \quad \lambda_j \geq 0, \quad j = 1, \dots, n \right\},$$

and

$$X = \{0, 1\}^n.$$

Minimization in x and maximization in μ (for $\bar{d} \geq 0$) can be carried out analytically:

$$\begin{aligned} x_j^*(\lambda_j) &= \begin{cases} 0 & \text{if } c_j \geq \lambda_j u_j, \\ 1 & \text{if } c_j \leq \lambda_j u_j; \end{cases} \\ \mu_i^*(\lambda) &= \min_{1 \leq j \leq n} (q_{ij} + \lambda_j). \end{aligned}$$

Finally, we obtain the following lower bound:

$$L_1 = \max_{\lambda \geq 0} \left[\sum_{i=1}^m \bar{d}_i \min_{1 \leq j \leq n} (q_{ij} + \lambda_j) + \sum_{j=1}^n \min(0, c_j - \lambda_j u_j) \right],$$

which can be easily calculated by standard linear programming techniques.

If the definition of the set X in (4.5) involves some constraints of form (4.2), we can combine the techniques of the last two sections to derive dual bounds for such a problem. Technically, it means augmenting the Lagrangian function (4.7) with terms associated with direct constraints (4.2), as in (4.4). All the remaining steps remain essentially the same as above.

5 Conclusions

The stochastic branch and bound method presented in this paper combines two basic ideas. The first one is to partition the set of decisions into smaller subsets and to use bounds on the objective within the subsets to guide this process, similarly to deterministic discrete optimization. Exact bounds, however, can hardly be computed, so we use the concept of recursive allocation of observations to the subsets to improve stochastic bounds. This is related to the approaches developed in statistics for the multi-armed bandit problem. As a result, we obtained a rather general and flexible scheme in which partition and observation can be dependent on the outcomes of the previous observations. The method is convergent with probability one under quite general assumptions. We could also develop some constructive methods for calculating stochastic bounds for a broad class of problems.

Some initial computational experiments with the method indicate that it has the potential to solve large stochastic discrete optimization problems. However, there is still a number of theoretical and practical questions that have to be investigated.

There is a need to develop the concept of efficiency of the method in some probabilistic sense. This would allow for introducing more specific partitioning and observation rules into the method. Ideally, one would like to have something similar to the optimal allocation indices of Gittins for the multi-armed bandit problem [8]. Indeed, the approach developed in this paper can be considered as the generalization of the multi-armed bandit problem: observations can be made for collections of actions (arms), not just one. The decision is not only the choice of the next action, but also the partition of the subsets. It is clearly a much more difficult problem, but with a great theoretical and practical importance. Presumably, some more detailed results can be obtained for some specific classes of stochastic discrete problems. Finally, computational experience has to be gained for a sufficiently broad class of application problems to better understand the peculiarities, the advantages and the drawbacks of various possible specifications. We hope to make some progress in these directions in the future.

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