Monte Carlo Sampling-Based Methods for Stochastic Optimization

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Abstract

This paper surveys the use of Monte Carlo sampling-based methods for stochastic optimization problems. Such methods are required when—as it often happens in practice—the model involves quantities such as expectations and probabilities that cannot be evaluated exactly. While estimation procedures via sampling are well studied in statistics, the use of such methods in an optimization context creates new challenges such as ensuring convergence of optimal solutions and optimal values, testing optimality conditions, choosing appropriate sample sizes to balance the effort between optimization and estimation, and many other issues. Much work has been done in the literature to address these questions. The purpose of this paper is to give an overview of some of that work, with the goal of introducing the topic to students and researchers and providing a practical guide for someone who needs to solve a stochastic optimization problem with sampling.

1 Introduction

Uncertainty is present in many aspects of decision making. Critical data, such as future demands for a product or future interest rates, may not be available at the time a decision must be made. Unexpected events such as machine failures or disasters may occur, and a robust planning process must take such possibilities into account. Uncertainty may also arise due to variability in data, as it happens for example in situations involving travel times on highways. Variability also produces uncertainty in physical and engineering systems, in which case the goal becomes, for example, to provide a reliable design. Such problems fall into the realm of *stochastic optimization*, an area that comprises modeling and methodology for optimizing the performance of systems while taking the uncertainty explicitly into account.

A somewhat generic formulation of a stochastic optimization problem has the form

$$\min_{x \in X} \{g_0(x) := \mathbb{E}[G_0(x,\xi)] \mid \mathbb{E}[G_k(x,\xi)] \leq 0,\ k = 1, 2, \ldots, K\}, \tag{SP}$$

where G_k, $k = 0, 1, \ldots, K$ are extended real-valued functions with inputs being the decision vector x and a random vector ξ. We use $K = 0$ to denote (SP) with only deterministic constraints. Typically, there are finitely many stochastic constraints ($K < \infty$) but this does not need to be the case. In fact, there can be uncountably many stochastic constraints (see Section 6.3). The set of deterministic constraints x must satisfy is denoted by $X \subset \mathbb{R}^{d_x}$ and $\Xi \subset \mathbb{R}^{d_\xi}$ denotes the support of ξ, where d_x and d_ξ are the dimensions of the vectors x and ξ, respectively. We assume that ξ has a known distribution, P, that is independent of x, and the expectations in (SP), taken with respect to the distribution of ξ, are well-defined and finite for all $x \in X$.

A wide variety of problems can be cast as (SP) depending on K, X and G_k, $k = 0, 1, 2, \ldots, K$. For example, in a two-stage stochastic linear program with recourse, $K = 0$, $X = \{Ax = b, x \geq 0\}$, and $G_0(x,\xi) = cx + h(x,\xi)$, where $h(x,\xi)$ is the optimal value of the linear program

$$\begin{aligned} h(x,\xi) = \min_{y} \quad & \tilde{q}y \\ \text{s.t.} \quad & \tilde{W}y = \tilde{r} - \tilde{T}x, \quad y \geq 0. \end{aligned}$$

Here, ξ is a random vector that is comprised of random elements of $\tilde{q}$, $\tilde{W}$, $\tilde{R}$ and $\tilde{T}$.

In contrast, in a stochastic program with a single probabilistic constraint (i.e., $P(\tilde{A}'x \geq \tilde{b}') \leq \alpha$), we have $K = 1$, $G_0(x,\xi) = cx$ and

$$G_1(x,\xi) = \mathbb{I}\{\tilde{A}'x \geq \tilde{b}'\} - \alpha,$$

where $\mathbb{I}\{E\}$ denotes the indicator function that takes value 1 if the event E happens and 0 otherwise and $\alpha \in (0,1)$ is a desired probability level. In this case, ξ is comprised of random elements of $\tilde{A}'$ and $\tilde{b}'$. Here, the decision maker requires that the relationship $\tilde{A}'x \geq \tilde{b}$ be satisfied with probability no more than α.

Several other variants of (SP) exist; for example, the objective function may be expressed not as a classical expectation but in a different form, such as a value-at-risk or conditional value-at-risk involving the random variable $G_0(x,\xi)$ or multiple stages can be considered (see e.g., Section 3.2 for multistage stochastic linear programs). There are also cases where the distribution of the underlying random vector ξ depends on the decision variables x even if such dependence is not known explicitly; we shall discuss some of these variations later. For now, we assume that (SP) is the problem of interest, and that $K = 0$ in (SP) so that we only have X, the set of deterministic constraints in (SP)—the case of stochastic constraints is dealt with in Section 6. To simplify notation, we will drop the index 0 from the objective function in (SP). We will refer to (SP) as the "true" optimization problem (as opposed to the approximating problems to be discussed in the sequel).

Benefiting from advances in computational power as well as from new theoretical developments, the area of stochastic optimization has evolved considerably in the past few years, with many recent applications in areas such as energy planning, national security, supply chain management, health care, finance, transportation, revenue management, and many others. New applications bring new challenges, particularly concerning the introduction of more random variables to make the models more realistic. In such situations, it is clearly impossible to enumerate all the possible outcomes, which precludes the computation of the expectations in (SP). As a very simple example, consider a model with d_ξ independent random variables, each with only two possible alternatives; the total number of scenarios is thus 2^{d_ξ}, and so even for moderate values of d_ξ it becomes impractical to take all possible outcomes into account. In such cases, *sampling* techniques are a natural tool to use.

Sampling-based methods have been successfully used in many different applications of stochastic optimization. Examples of such applications can be found in vehicle routing (Kenyon and Morton [128], Verweij et al. [236]), engineering design (Royset and Polak [206]), supply chain network design (Santoso et al. [213]), power generation and transmission (Jirutitijaroen and Singh [122]), and asset liability management (Hilli et al. [104]), among others. More recently, Byrd et al. [34] used these techniques in the context of machine learning. The appeal of sampling-based methods results from the fact that they often approximate well, with a small number of samples, problems that have a very large number of scenarios; see, for instance, Linderoth et al. [152] for numerical reports.

There are multiple ways to use sampling methods in problem (SP). A generic way of describing them is to construct an approximating problem as follows. Consider a family $\{g_N(\cdot)\}$ of random approximations of the function $g(\cdot)$, each $g_N(\cdot)$ being defined as

$$g_N(x) \;:=\; \frac{1}{N}\sum_{j=1}^{N} G(x,\xi^j), \tag{1}$$

where $\{\xi^1,\ldots,\xi^N\}$ is a sample from the distribution[1] of ξ. When $\xi^1,\ldots,\xi^N$ are mutually independent, the quantity $g_N(x)$ is called a *(standard or crude) Monte Carlo* estimator of $g(x)$. Given the family of estimators $\{g_N(\cdot)\}$ defined in (1), one can construct the corresponding approximating program

$$\min_{x\in X} g_N(x). \tag{2}$$

Note that for each $x \in X$ the quantity $g_N(x)$ is random variable, since it depends on the sample $\{\xi^1,\ldots,\xi^N\}$. So, the optimal solution(s) and the optimal value of (2) are random as well. Given a particular realization $\{\hat\xi^1,\ldots,\hat\xi^N\}$ of the sample, we define

$$\hat g_N(x,\hat\xi^1,\ldots,\hat\xi^N) \;:=\; \frac{1}{N}\sum_{j=1}^{N} G(x,\hat\xi^j). \tag{3}$$

[1]Throughout this paper, we will use the terminology "sample [of size N] from the distribution of ξ" to indicate a set of N random variables with the same distribution as ξ. Also, recall that we drop the subscript 0 from g and G as we assume here that $K = 0$.

A remark about the notation is in order. In (3), we write explicitly the dependence on $\hat{\xi}^1, \ldots, \hat{\xi}^N$ to emphasize that, given x, $\hat{g}_N(x, \hat{\xi}^1, \ldots, \hat{\xi}^N)$ is a number that depends on a particular realization of the sample. Such notation also helps, in our view, to understand the convergence results in Section 2. In contrast, in (1) we do not write it in that fashion since $g_N(x)$ is viewed as a random variable. While such a distinction is usually not made in the literature, we adopt it here for explanatory purposes and to emphasize that the problem $\min_{x \in X} \hat{g}_N(x, \hat{\xi}^1, \ldots, \hat{\xi}^N)$ is a deterministic one. Later in the paper we will revert to the classical notation and write simply $g_N(x)$, with its interpretation as a number or a random variable being understood from the context. Also, throughout the majority of the paper we assume that realizations are generated using the standard Monte Carlo method, unless otherwise stated. We discuss alternative sampling methods in Section 7.

Consider now the following algorithm:

ALGORITHM 1

1. Choose an initial solution x^0; let $k := 1$.
2. Obtain a realization $\{\hat{\xi}^{k,1}, \ldots, \hat{\xi}^{k,N_k}\}$ of $\{\xi^1, \ldots, \xi^{N_k}\}$.
3. Perform some optimization steps on the function $\hat{g}_{N_k}(\cdot, \hat{\xi}^{k,1}, \ldots, \hat{\xi}^{k,N_k})$ (perhaps using information from previous iterations) to obtain x^k.
4. Check some stopping criteria; if not satisfied, set $k := k + 1$ and go back to Step 2.

Note that although we call it an "algorithm", Algorithm 1 should be understood as a generic framework that allows for many variations based on what is understood by "perform some optimization steps," "check some stopping criterion," and the choice of the sample size N_k. For example, consider the *Sample Average Approximation* (SAA) approach, which has appeared in the literature under other names as well, as discussed in Section 2. In such an approach, by solving the problem

$$\min_{x \in X} \hat{g}_N(x, \hat{\xi}^1, \ldots, \hat{\xi}^N) \tag{4}$$

—which is now completely deterministic (since the realization is fixed), so it can be solved by standard deterministic optimization methods—we obtain specific estimates of the optimal solution(s) and the optimal value of (SP). The SAA approach can be viewed as a particular case of Algorithm 1 whereby Step 3 fully minimizes the function $\hat{g}_N(\cdot, \hat{\xi}^{1,1}, \ldots, \hat{\xi}^{1,N_1})$, so Algorithm 1 stops after one (outer) iteration. We will discuss the SAA approach and its convergence properties in Section 2.

As another example, consider the classical version of the *Stochastic Approximation* (SA) method, which is defined by the recursive sequence

$$x^{k+1} \ := \ x^k - \alpha_k \eta^k, \quad k \geq 0,$$

where η^k is a random direction—usually an estimator of the gradient $\nabla g(x^k)$, such as $\nabla G(x^k, \xi)$—and α_k is the step-size at iteration k. Clearly, the classical SA method falls into the general

framework of Algorithm 1 where $N_k = 1$ for all k and Step 3 consists of one optimization step ($x^{k+1} := x^k - \alpha_k \eta^k$). We will discuss the SA method and some of its recent variants later.

As the above discussion indicates, many questions arise when implementing some variation of Algorithm 1, such as:

- What sample size N_k to use at each iteration?
- Should a new realization of $\{\xi^1, \ldots, \xi^{N_k}\}$ be drawn in Step 2, or can one extend the realization from the previous iteration?
- How should this sample be generated to begin with? Should one use crude Monte Carlo or can other methods—for instance, aimed to reduce variability—be used?
- How to perform an optimization step in Step 3 and how many steps should be taken?
- How to design the stopping criteria in Step 4 in the presence of sampling-based estimators?
- What can be said about the quality of the solution returned by the algorithm?
- What kind of asymptotic properties does the resulting algorithm have?

Much work has been done in the literature to address these questions. The purpose of this paper is to give an overview of some of that work, with the goal of providing a practical guide for someone who needs to solve a stochastic optimization problem with sampling. In that sense, our mission contrasts starkly with that of the compilations in Shapiro [218] and Shapiro et al. [227, Chapter 5], which provide a comprehensive review of theoretical properties of sampling-based approaches for problem (SP). Our work also complements the recent review by Kim et al. [131], who focus on a comparative study of rates of convergence.

We must emphasize, though, that our goal is *not* to describe in detail specific algorithms proposed in the literature for some classes of stochastic optimization problems. Such a task would require far more space than what is reasonable for a review paper, and even then we probably would not do justice to the subtleties of some of the algorithms. Instead, we refer the reader to the appropriate references where such details can be found.

It is interesting to notice that problem (SP) has been studied somewhat independently by two different communities, who view the problem from different perspectives. On one side is the optimization community, who wants to solve "mathematical programming problems with uncertainty," which means that typically the function $g(\cdot)$ has some structure such as convexity, continuity, differentiability, etc., that can be exploited when deciding on a particular variation of Algorithm 1. On the other side is the simulation community, who focuses on methods that typically do not make any assumptions about the structure of g, and the approximation $\tilde{g}(x)$ is viewed as the response of a "black box" to a given input x. The goal then becomes to cleverly choose the design points x—often via some form of random search—in order to find a solution that has some desirable properties such as asymptotic optimality or probabilistic guarantees of being a good solution.

The resulting algorithms are often called *simulation optimization* methods. Reviews of simulation optimization—sometimes called optimization via simulation—within the past decade can be found in Fu [82], Andradóttir [5] and Chen et al. [43], although much has been done since the publication of those articles.

There are, of course, many common elements between the problems and methods studied by the optimization and the simulation communities, which has been recognized in books that "bridge the gap" such as Rubinstein and Shapiro [210] and Pflug [190]. In fact, the line between simulation optimization and mathematical programs under uncertainty has become increasingly blurry in recent years, as illustrated by the recent book by Powell and Ryzhov [198]. While we acknowledge that the present survey does not fully connect these two areas—it is certainly more focused on the mathematical programming side—we hope that this article will help to bring awareness of some techniques and results to both communities.

We conclude these introductory remarks with a cautionary note. Writing a review of this kind, where the literature is scattered among optimization, simulation, and statistics journals, inevitably leads to omissions despite our best efforts. Our apologies to those authors whose works we have failed to acknowledge in these pages.

The remainder of this paper is organized as follows. In Section 2 we discuss some theoretical properties of the SAA approach and illustrate them by applying the technique to the classical newsvendor problem. Section 3 discusses approaches based on sequential sampling whereby new samples are drawn periodically—as opposed to SAA where a fixed sample is used throughout the algorithm. The practical issue of evaluating the quality of a given solution—which is intrinsically related to testing stopping criteria for the algorithms—is studied in Section 4. Another important topic for practical implementation of sampling-based methods is the choice of appropriate sample sizes; that issue is discussed in Section 5. In Section 6 we study the case of problems with stochastic constraints, which as we will see require special treatment. Monte Carlo methods are often enhanced by the use of variance reduction techniques; the use of such methods in the context of sampling-based stochastic optimization is reviewed in Section 7. There are of course many topics that are relevant to the subject of this survey but which we cannot cover due to time and space limitations; we briefly discuss some of these topics in Section 8. Finally, we present some concluding remarks and directions for future research in Section 9.

2 The SAA approach

We consider initially the SAA approach, which, as discussed earlier, consists of solving problem (4) using a deterministic algorithm. This idea has appeared in the literature under different names: in Robinson [202], Plambeck et al. [195] and Gürkan et al. [95] it is called the *sample-path optimization* method, whereas in Rubinstein and Shapiro [210] it is called the *stochastic counterpart* method. The term "sample average approximation" appears to have been coined by Kleywegt et al. [134]. It is important to note that SAA itself is not an algorithm; the term refers to the approach of replacing

the original problem (SP) with its sampling approximation, which is also sometimes called the *external sampling* approach in the literature.

The analysis of SAA typically assumes that the approximating problem is solved exactly, and studies the convergence of the estimators of optimal solutions and of optimal values obtained from (2) in that context. This type of analysis has appeared in the literature pre-dating the papers mentioned above, without a particular name for the approach—see, for instance, Dupačová and Wets [70], King and Rockafellar [133] and Shapiro [216, 217].

We discuss now the ideas behind the main convergence results. Our goal here is to illustrate the results rather than provide detailed mathematical statements—for that, we refer to the compilations in Shapiro [218] and Shapiro et al. [227, Chapter 5] and papers therein. To illustrate the convergence results to be reviewed in the sequel, we shall study the simple example of the classical newsvendor problem. Of course, such a problem can be solved exactly and hence there is no need to use a sampling method; however, this is precisely the reason why we use that problem in our examples, so we can compare the approximating solutions with the exact ones in order to illustrate convergence results. Moreover, the unidimensionality of that model will allow us to depict some of the results graphically. Let us begin with a definition.

Example 1. *(Newsvendor Problem).* Consider a seller that must choose the amount x of inventory to obtain at the beginning of a selling season. The decision is made only once—there is no opportunity to replenish inventory during the selling season. The demand ξ during the selling season is a nonnegative random variable with cumulative distribution function F. The cost of obtaining inventory is c per unit. The product is sold at a given price r per unit during the selling season, and at the end of the season unsold inventory has a salvage value of v per unit. The seller wants to choose the amount x of inventory that solves

$$\min_x \{g(x) \;=\; \mathbb{E}\left[cx - r\min\{x,\xi\} - v\max\{x-\xi,0\}\right]\}. \tag{5}$$

It is well known that, if $v < c < r$, then any x^* that satisfies

$$F(x) \;\leq\; \frac{r-c}{r-v} \quad \text{for all } x < x^* \qquad \text{and} \qquad F(x) \;\geq\; \frac{r-c}{r-v} \quad \text{for all } x > x^*$$

is an optimal amount of inventory to obtain at the beginning of the selling season. That is, the set of optimal solutions is given by the set of γ-*quantiles* of the distribution of ξ, which can be written as

$$S \;:=\; \{z \in \mathbb{R} \;:\; P(\xi \geq z) \geq 1-\gamma \;\text{ and }\; P(\xi \leq z) \geq \gamma\}, \tag{6}$$

where $\gamma = (r-c)/(r-v)$. Note that S is a nonempty closed interval for all $\gamma \in (0,1)$. □

We will be referring back to the newsvendor problem often throughout the remainder of this section. Let us now apply the SAA approach to this problem.

Example 2. *(Application of the SAA Approach to the Newsvendor Problem).* The approximation

of problem (5) is written as

$$\min_x \left\{ \hat{g}_N(x, \hat{\xi}^1, \ldots, \hat{\xi}^N) \;:=\; \frac{1}{N} \sum_{i=1}^{N} \Big[cx - r \min\{x, \hat{\xi}^i\} - v \max\{x - \hat{\xi}^i, 0\} \Big] \right\}. \tag{7}$$

Any sample γ-quantile is an optimal solution to the above problem. For example, we can take $\hat{x}_N = \hat{\xi}^{(\lceil \gamma N \rceil)}$ as an optimal solution, where $\hat{\xi}^{(1)}, \ldots, \hat{\xi}^{(N)}$ represent an ordering of the realizations (in ascending order) and $\lceil a \rceil$ is the smallest integer larger than or equal to a. □

2.1 Consistency

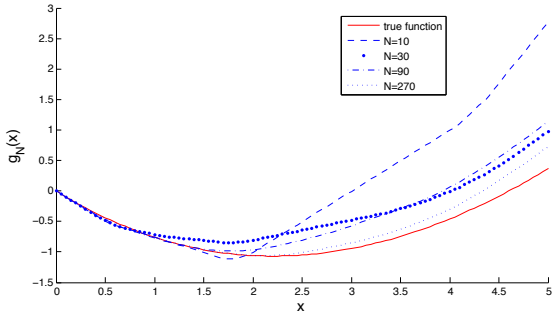
We start by defining some notation. Let x_N and S_N denote respectively an optimal solution and the set of optimal solutions of (2). Moreover, let ν_N denote the optimal value of (2). Then, x_N, S_N and ν_N are statistical estimators of an optimal solution x^*, the set of optimal solutions S^* and the optimal value ν^* of the true problem (SP), respectively.

The first issue to be addressed is whether these estimators are (strongly) *consistent*, i.e. whether they converge to the respective estimated values with probability one. It is important to understand well what such a statement means: given a realization $\{\hat{\xi}^1, \hat{\xi}^2, \ldots, \}$ of $\{\xi^1, \xi^2, \ldots, \}$, let $\hat{x}_N$ be an optimal solution and $\hat{\nu}_N$ the optimal value[2] of problem (4) defined with the first N terms of the sequence $\{\hat{\xi}^1, \hat{\xi}^2, \ldots, \}$. Consistency results make statements about convergence of the sequences $\{\hat{x}_N\}$ and $\{\hat{\nu}_N\}$. If such statements hold regardless of the realization $\{\hat{\xi}^1, \hat{\xi}^2, \ldots, \}$ (except perhaps for some realizations on a set of probability zero), then we have convergence "with probability one" (w.p.1), or "almost surely" (a.s.). When dealing with convergence of solutions, it will be convenient to use the notation $\text{dist}(x, A)$ to denote the distance from a point x to a set A, defined as $\inf_{a \in A} \|x - a\|$.

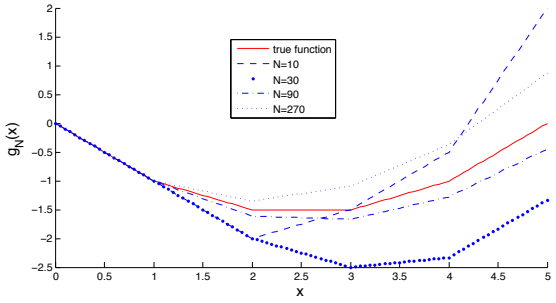
To illustrate the consistency of the SAA estimators, we will next use specific instances of the newsvendor problem. The first newsvendor instance has demand modeled as an exponential random variable and it has a unique optimal solution. Later, we will look at another instance with a discrete uniform demand, which has multiple optimal solutions. The two instances have the same parameters otherwise. The results of the SAA approach to these instances are shown in Table 1 and Figures 1–4.

Example 3. *(Newsvendor Instance with Exponential Demand).* Consider the newsvendor problem defined in Example 1 with model parameters $r = 6$, $c = 5$, $v = 1$ and demand that has Exponential(10) distribution (i.e., the mean is 10). Figure 1a depicts the objective function $g(\cdot)$ for this instance as well as the approximations $\hat{g}_N(\cdot, \hat{\xi}^1, \ldots, \hat{\xi}^N)$ for a particular realization $\{\hat{\xi}^1, \hat{\xi}^2, \ldots, \}$ with various values of $N = 10, 30, 90, 270$. Table 1a shows the optimal solutions and optimal values for the same functions. We see that, for this realization, $N = 270$ approximates the true function very closely and the quality of the other approximations depends on the tolerance allowed. □

[2]To be precise, we should write $\hat{x}_N$ and $\hat{\nu}_N$ as functions of the realization $\{\hat{\xi}^1, \hat{\xi}^2, \ldots, \}$, but we omit that for the sake of brevity of notation.



(a) Exponential demand



(b) Discrete uniform demand

Figure 1: Newsvendor function and corresponding sample average approximations.

N	10	30	90	270	∞
x_N	1.46	1.44	1.54	2.02	2.23
ν_N	-1.11	-0.84	-0.98	-1.06	-1.07

(a) Exponential demand

N	10	30	90	270	∞
x_N	2	3	3	2	[2,3]
ν_N	-2.00	-2.50	-1.67	-1.35	-1.50

(b) Discrete uniform demand

Table 1: Optimal solution and optimal values for the newsvendor function; the column ∞ refers to the true function.

The above example suggests that we have $\hat{\nu}_N \to \nu^*$ and $\hat{x}_N \to x^*$. How general is that conclusion? It is clear that convergence of x_N and ν_N to their estimated values cannot be expected if $g_N(x)$ defined in (2) does not converge to $g(x)$ for some feasible point $x \in X$. However, just having pointwise convergence of $g_N(x)$ to $g(x)$ (w.p.1) for all $x \in X$ is not enough; stronger conditions are required. A sufficient condition that can often be verified in practice is that $g_N(\cdot)$ converge *uniformly* to $g(\cdot)$ on X w.p.1, i.e., for (almost) any realization $\{\hat{\xi}^1, \hat{\xi}^2, \dots, \}$, given $\varepsilon > 0$ there exists N_0 such that

$$|\hat{g}_N(x, \hat{\xi}^1, \dots, \hat{\xi}^N) - g(x)| \; < \; \varepsilon \quad \text{for any } N \geq N_0 \text{ and all } x \in X.$$

Notice that in the above definition the value of N_0 depends on the realization $\{\hat{\xi}^1, \hat{\xi}^2, \dots, \}$. In other words, the accuracy of the approximation for a given N depends on the realization. The uniform convergence condition is satisfied in many cases found in practice—for example, when the function $G(x, \xi)$ is convex and continuous in x for almost all ξ and X is a compact, convex set.

Under the uniform convergence assumption, we have the following results:

1. $\nu_N \to \nu^*$ w.p.1,
2. Under additional assumptions involving boundedness of S^* and continuity of the objective function, $\text{dist}(x_N, S^*) \to 0$ w.p.1.

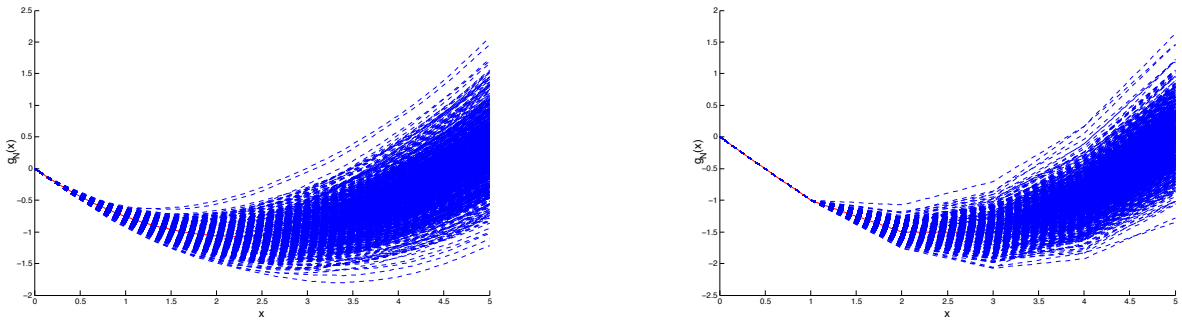
Note that item 2 above does *not* ensure that the estimators x_N converge w.p.1; rather, it says

that x_N gets increasingly closer to the set S^* as N gets large. Of course, in case there is a unique optimal solution x^*—as it was the case in the newsvendor instance with Exponential demand shown in Figure 1a—then x_N converges to x^* w.p.1. To illustrate a situation where $\hat{x}_N$ might not converge, consider another instance of the newsvendor problem.

Example 4. *(Newsvendor Instance with Discrete Uniform Demand).* Consider a newsvendor problem with the same parameters as in Example 3 but with demand having discrete uniform distribution on $\{1, 2, \ldots, 10\}$. Figure 1b depicts the functions $g(\cdot)$ and $\hat{g}_N(\cdot, \hat{\xi}^1, \ldots, \hat{\xi}^N)$ for a particular realization for each of the sample sizes $N = 10, 30, 90, 270$. The corresponding optimal solutions and optimal values are shown in Table 1b. Here the optimal solution set S^* is the interval $[2, 3]$. We see that, while the optimal values $\hat{\nu}_N$ converge to ν^*, the solutions $\hat{x}_N$ alternate between 2 and 3. It is interesting to observe, however, that $\hat{x}_N$ is actually inside the optimal set S^* for all N depicted in the figure even when the approximation is poor (as in the case of $N = 30$). In other words, not only $\text{dist}(\hat{x}_N, S^*) \to 0$ as predicted by the theory but in fact $\text{dist}(\hat{x}_N, S^*) = 0$ for sufficiently large N. This situation is typical of a class of problems with discrete distributions with a finite number of realizations, as we shall see later. □

Figures 1a and 1b have illustrated the behavior of the approximation for a single realization of the random variables for a variety of sample sizes N. But how typical are those realizations?

Example 5. *(1,000 SAAs on the Newsvendor Instances).* Figures 2a and 2b depict the behavior of the approximations for 1,000 realizations for a fixed sample size $N = 270$ for the cases of both exponential and discrete uniform demand studied above. Two observations can be made from the figures. First, as mentioned earlier, the quality of the approximation depends on the realization—as we can see in the figures, some of the approximations are very close to the true function whereas others are far off. Second, many of the approximations lie below the true function, therefore yielding an estimate $\hat{\nu}_N \leq \nu^*$, whereas in other cases $\hat{\nu}_N \geq \nu^*$. □



(a) Exponential demand (b) Discrete uniform demand

Figure 2: 1,000 replications of SAA approach to newsvendor function with $N = 270$.

Given the results of Example 5, it is natural then to consider what happens on the average.

Consider for the moment the case where $N = 1$. Then, we have

$$\mathbb{E}[\nu_1] \;=\; \mathbb{E}\left[\min_{x\in X} G(x,\xi)\right] \;\leq\; \min_{x\in X} \mathbb{E}[G(x,\xi)] \;=\; \min_{x\in X} g(x) \;=\; \nu^*,$$

where the inequality follows from the same principle that dictates that the sum of the minima of two sequences is less than or equal to the the minimum of the sum of the two sequences. It is easy to generalize the above inequality for arbitrary N, from which we conclude that

$$\mathbb{E}[\nu_N] \;\leq\; \nu^*. \tag{8}$$

That is, on the average, the approximating problem yields an optimal value that is below or at most equal to ν^*. In statistical terms, ν_N is a *biased* estimator of ν^*. It is possible to show, however, that the bias $\nu^* - \mathbb{E}[\nu_N]$ decreases monotonically in N and goes to zero as N goes to infinity (Mak et al. [158]).

We conclude this subsection with the observation that in the above discussion about convergence of optimal solutions it is important to emphasize that by "optimal solution" we mean a *global* optimal solution. While this is not an issue in case of convex problems, it becomes critical in case of nonconvex functions. For example, Bastin et al. [15] present a simple example where a local minimizer of the approximating problem converges to a point which is neither a local nor a global minimizer of the original problem. In such cases it is important to look at convergence of second-order conditions. We refer to that paper for a detailed discussion.

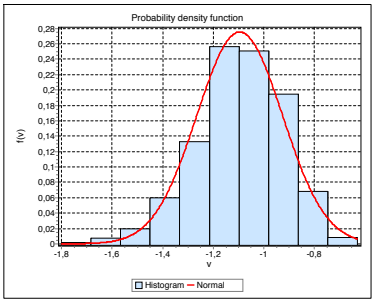
2.2 Rates of convergence

In the discussion above we saw how, under appropriate conditions, we expect the approximating problem (2) to yield estimators x_N and ν_N that approach their true counterparts w.p.1 as N goes to infinity. A natural question that arises is how large N must be in order to yield "good enough" estimates. Such a question can be framed in terms of *rates of convergence*, which we study next.

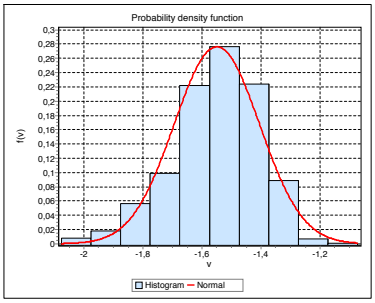
Convergence of optimal values

We first discuss the rate of convergence of the optimal value estimators ν_N. To understand the main results—which we shall describe soon—let us consider again the newsvendor example with the same parameters used earlier, for exponentially distributed demand.

Example 6. *(Newsvendor Instance with Exponential Demand, Continued).* Figure 3a shows a histogram of the optimal values of the functions depicted in Figure 2a, as well as a fitted Normal distribution obtained using distribution-fitting software. The fitted Normal distribution has mean -1.1 and standard deviation 0.169. A goodness-of-fit test—more specifically, the Anderson-Darling (AD) test—indicates that the Normal distribution provides an acceptable fit to the data, as the null hypothesis "the data is normally distributed" is not rejected at a significance level of 0.05. □



(a) Exponential demand



(b) Discrete uniform demand

Figure 3: Histogram of optimal values of SAA approach to newsvendor function with $N = 270$.

To view that result of Example 6 in a more general context, consider a fixed $x \in X$. Then, under mild assumptions ensuring finiteness of variance, the Central Limit Theorem tells us that

$$\sqrt{N}[g_N(x) - g(x)] \xrightarrow{d} Y(x) \sim \text{Normal}(0, \sigma^2(x)), \tag{9}$$

where $\sigma^2(x) := \text{Var}[G(x, \xi)]$, the notation $\xrightarrow{d}$ indicates convergence in distribution to a random variable $Y(x)$ and the symbol $\sim$ indicates that $Y(x)$ has Normal$(0, \sigma^2(x))$ distribution. That is, for large N the random variable $g_N(x)$ is approximately normally distributed with mean $g(x)$ and variance $\sigma^2(x)/N$. As it turns out, such a property still holds when $g_N(x)$ and $g(x)$ in (9) are replaced by their minimum values over X. More precisely, under assumptions of compactness of X and Lipschitz continuity of the function $G(\cdot, \xi)$—which, roughly speaking, means that the derivatives of $G(\cdot, \xi)$ are bounded by a constant, so $G(\cdot, \xi)$ does not vary wildly—we have that

$$\sqrt{N}(\nu_N - \nu^*) \xrightarrow{d} \inf_{x \in S^*} Y(x). \tag{10}$$

Note that the expression on the right-hand side of (10) indicates a random variable defined as the minimum (or infimum) of normally distributed random variables. In general, the resulting distribution is *not* Normal; however, when the original problem has a unique solution x^*, then $S^* = \{x^*\}$ and in that case the right hand side in (10) is indeed normally distributed with mean zero and variance $\sigma^2(x^*)$. Let us take a closer look at Example 6.

Example 7. *(Newsvendor Instance with Exponential Demand, Continued).* As seen earlier, this instance of the newsvendor problem has a unique optimal solution, which explains the nice behavior of ν_N shown in Figure 3a. In fact, recall from Table 1a that the optimal value corresponding to the optimal solution $x^* = 2.23$ is $\nu^* = -1.07$. Moreover, the variance of the expression inside the integral in (5) at the optimal solution $x^* = 2.23$ can be estimated (using a very large sample size) as $\sigma^2(x^*) \simeq 7.44$; therefore, the theory predicts that, for large N, the estimator ν_N has

approximately Normal(ν^*,$\sigma^2(x^*)/N$) =Normal($-1.07, 7.44/N$) distribution. With $N = 270$, the standard deviation is $\sqrt{7.44/270} = 0.166$, so we see that this asymptotic distribution very much agrees with the Normal distribution that fits the histogram in Figure 3a. □

The situation is different in the case of multiple optimal solutions. As mentioned, we do not expect ν_N to be normally distributed, since the limit distribution is given by the infimum of Normal distributions over the set of optimal solutions (recall equation (10)). This is the case in the newsvendor instance with discrete uniform distribution ($S^* = [2, 3]$).

Example 8. *(Newsvendor Instance with Discrete Uniform Demand, Continued).* Figure 3b shows a histogram of the optimal values of the functions depicted in Figure 2b. Although the histogram may seem to be reasonably close to a Normal distribution, that distribution does not pass the AD goodness-of-fit test even at a significance level of 0.01. □

The convergence result (10) leads to some important conclusions about the rate of convergence of the bias $\nu^* - \mathbb{E}[\nu_N]$ to zero. Indeed, suppose for the sake of this argument that convergence in distribution implies convergence of expectations (which holds, for example, when a condition such as uniform integrability is satisfied). Then, it follows from (10) that $\sqrt{N}(\mathbb{E}[\nu_N] - \nu^*) \to \mathbb{E}[\inf_{x\in S^*} Y(x)]$. Recall from (9) that each $Y(x)$ has mean zero. Then, $\mathbb{E}[\inf_{x\in S^*} Y(x)]$ is less than or equal to zero and it is often strictly negative when S^* has more than one element. Thus, when that happens, the bias $\mathbb{E}[\nu_N] - \nu^*$ is exactly of order $N^{-1/2}$, i.e., it cannot go to zero faster than $N^{-1/2}$. On the other hand, when S^* has a unique element, we have $\sqrt{N}(\mathbb{E}[\nu_N] - \nu^*) \to 0$, i.e., the bias goes to zero faster than $N^{-1/2}$. For example, Freimer et al. [79] compute the exact bias for the newsvendor problem when demand has uniform distribution on (0,1)—in which case the optimal solution $x^* = \gamma$ is unique—as

$$\mathbb{E}[\nu_N] - \nu^* \;=\; \frac{\gamma(1-\gamma)}{2(N+1)},$$

so we see that in this case the bias is of order N^{-1}. In general, the rate of convergence of bias for a stochastic program can take a variety of values N^{-p} for $p \in [1/2, \infty)$; see, for instance, Example 5 in Bayraksan and Morton [20].

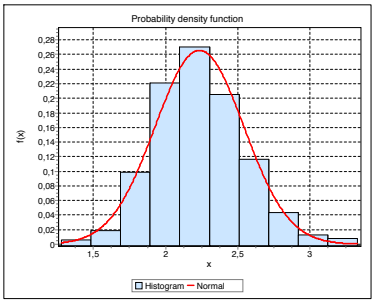
Convergence of optimal solutions

It is possible to study the rate of convergence of optimal solutions as well. The convergence properties of optimal solutions depend on the smoothness of the objective function for a class of problems. Let us take a closer look at the two newsvendor instances to gain an understanding.

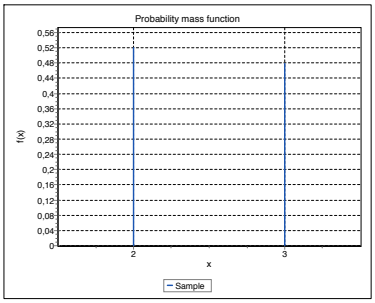
Example 9. *(Optimal Solutions of the SAAs of the Newsvendor Instances).* Notice that the objective function of the exponential demand instance is smooth. We can see in Figure 1a and Table 1a the estimate $\hat{x}_N$ *approaches* the optimal solution x^*. In contrast, the results of the discrete uniform demand instance—which has a nonsmooth objective function—depicted in Figure 1b and Table 1b show that the estimate $\hat{x}_N$ *coincides* with one of the optimal solutions in S^*. Typically this happens once N large enough but $\hat{x}_N$ can be far away if N is small. □

Let us discuss initially the smooth case. As before, we first illustrate the ideas with the newsvendor problem.

Example 10. *(Newsvendor Instance with Exponential Demand, Continued).* Figure 4a shows a histogram of the optimal solutions of the functions depicted in Figure 2a, as well as a fitted Normal distribution, which passes the AD goodness-of-fit test at a significance level of 0.15. The fitted Normal distribution has mean 2.24 (recall that $x^* = 2.23$) and standard deviation 0.308. □



(a) Exponential demand



(b) Discrete uniform demand

Figure 4: Histogram of optimal solutions of SAA approach to newsvendor function with $N = 270$.

Example 10 suggests that the estimator x_N is approximately normally distributed for large N. In a more general context, of course, x_N is a vector, so we can conjecture whether x_N has approximately *multivariate* Normal distribution for large N. Indeed, suppose that there is a unique solution x^* and suppose that the function $g(x)$ is twice differentiable at x_0. Suppose for the moment that the problem is unconstrained, i.e., $X = \mathbb{R}^n$. Then, under mild additional conditions, we have

$$\sqrt{N}(x_N - x^*) \xrightarrow{d} \text{Normal}(0, H^{-1}\Psi H^{-1}), \tag{11}$$

where $H = \nabla^2_{xx} g(x^*)$, and Ψ is the asymptotic covariance matrix of $\sqrt{N}[\nabla g_N(x^*) - \nabla g(x^*)]$. So, we see that when N is sufficiently large the estimator x_N has approximately multivariate Normal distribution. For details on this result, as well as an extension to the constrained case, we refer to King and Rockafellar [133], Shapiro [217], and Rubinstein and Shapiro [210].

A few words about the notation $\nabla g_N(x)$ are in order. This notation represents the random vector defined as the derivative of $g_N(x)$ on each realization of this random variable. It should be noted though that the function $g_N(\cdot)$ may not be differentiable—for example, in the newsvendor case, we can see from (7) that g_N is defined as the average of non-differentiable functions. However, convexity of $G(\cdot, \xi)$ ensures that the set of *subgradients* of $g_N(x)$ converges to $\nabla g(x)$ w.p.1 when g is differentiable. Consequently, for the purpose of asymptotic results, we can define $\nabla g_N(x)$ as any subgradient of $g_N(x)$ at the points where g_N is not differentiable.

Example 11. *(Asymptotic Normality of the SAA Optimal Solutions for the Newsvendor Problem with Continuous Demand Distribution).* To illustrate the use of (11) in the context of the newsvendor problem, note that the newsvendor function $g(x)$ defined in (5) can be written as

$$g(x) \;=\; (r-c)x - (r-v)\mathbb{E}\left[\max\{x-\xi, 0\}\right]. \tag{12}$$

When ξ has continuous distribution with cumulative distribution function F and probability density function f, it is not difficult to show that

$$\begin{aligned} g'(x) &= (r-c) - (r-v)F(x) \\ g''(x) &= -(r-v)f(x). \end{aligned}$$

By writing $g'(x)$ as $g'(x) = \mathbb{E}\left[(r-c) - (r-v)\mathbb{I}\{\xi \le x\}\right]$ we see that, by the Central Limit Theorem, for any given $x \in \mathbb{R}$ we have

$$\sqrt{N}[g'_N(x) - g'(x)] \;\xrightarrow{d}\; \text{Normal}(0, (r-v)^2 P(\xi \le x)[1 - P(\xi \le x)]). \tag{13}$$

Notice that when $x = x^*$ we have $P(\xi \le x^*) = F(x^*) = \gamma = (r-c)/(r-v)$ and hence in this case we have $\Psi = (r-v)^2\gamma(1-\gamma)$. Moreover, since $H = g''(x^*) = -(r-v)f(x^*)$, it follows that (11) is written as

$$\sqrt{N}(x_N - x^*) \xrightarrow{d} \text{Normal}\left(0, \frac{\gamma(1-\gamma)}{[f(x^*)]^2}\right).$$

Of course, asymptotic normality of quantile estimators is a well-known result; the point of the above calculations is just to illustrate the application of the general result (11) in the present context. With the parameters used earlier for the instance with exponential demand (having unique optimum solution), we have $\gamma = 0.2$, $x^* = 2.23$, $f(x^*) = 0.08$ and thus the theory predicts that, for large N, the estimator x_N has approximately Normal$(2.23, 25/N)$ distribution. With $N = 270$, the standard deviation is $\sqrt{25/270} = 0.304$, so by comparing these numbers with the results from the distribution-fitting of the histogram in Figure 4a—which yields mean 2.24 and standard deviation 0.308—we see that the asymptotic distribution of x_N is accurate for the sample size of $N = 270$. In case of multiple optimal solutions, of course, we cannot expect to have asymptotic normality of x_N. □

The convergence result (11) shows that, for large N, x_N is approximately normally distributed with mean x^* and variance equal to K/N for some constant K. As the Normal distribution has exponential decay, we expect $P(\|x_N - x^*\| > \varepsilon)$ to go to zero very fast. Kaniovski et al. [125] make this result more precise and show that there exist constants $C,\ \beta > 0$ such that, asymptotically (and under appropriate conditions), $P(\|x_N - x^*\| > \varepsilon) \le Ce^{-\beta N}$. Dai et al. [51] show a similar result and give a tighter bound in which C is replaced by a function of N.

We discuss now the convergence of optimal solutions in the nonsmooth case.

Example 12. *(Newsvendor Instance with Discrete Uniform Demand, Continued).* Figure 4b shows a histogram of the optimal solutions of the functions depicted in Figure 2b. We see here a very different phenomenon compared to the smooth case—only the solutions $\hat{x}_N = 2$ and $\hat{x}_N = 3$ occur. □

The situation discussed in Example 12 is typical of problems that have three characteristics: (i) the function $G(\cdot, \xi)$ in (SP) is piecewise linear and convex, (ii) the feasibility set X is convex and polyhedral (or the problem is unconstrained), and (iii) the distribution of the random vector ξ has finite support. Two-stage stochastic linear programs with a finite number of scenarios, for example, fit this framework. In such cases, under further boundedness assumptions, it is possible to show that

- The set S^* of optimal solutions of (SP) is polyhedral and the set S_N of optimal solutions of (2) is a face of S^* w.p.1 for N large enough. That is, given an arbitrary realization $\{\hat{\xi}^1, \hat{\xi}^2, \ldots, \}$ of the random vector ξ ("arbitrary" except perhaps for those on a set of measure zero), let $\hat{S}_N$ denote the set of optimal solutions of (4). Then, there exists N_0—whose value depends on the realization—such that $\hat{S}_N \subseteq S^*$ for all $N \geq N_0$.
- The probability that S_N is a face of S^* converges to one *exponentially fast* with N. That is, as N gets large we have

$$P(S_N \text{ is not a face of } S^*) \ \leq \ Ce^{-\beta N} \tag{14}$$

  for some constants $C, \ \beta > 0$.

The above result suggests that, for such problems, the solution of the approximating problem (4) will likely produce an exact solution even for moderate values of N. This is what we see in Figure 4b—the solutions $\hat{x}_N = 2$ and $\hat{x}_N = 3$ are not only optimal for the original problem but they also coincide with the extremities of the optimal set $S^* = [2, 3]$. By fixing the probability on the left side of (14) to a desirable value (call it α) and solving for N, we can then compute the sample size that is sufficiently large to ensure that the probability of *not* obtaining an optimal solution is less than α. When the optimal solution is unique—i.e., $S^* = \{x^*\}$—it can be shown that the resulting value of N depends on two major characteristics of the problem: (i) how flat the objective function $g(x)$ is around the optimal solution x^*, and (ii) how much variability there is. The flatter the objective function (or the higher the variance), the larger the value of N. Precise calculations are given in Shapiro and Homem-de-Mello [223], Shapiro et al. [226], and we review such sample size estimates in Section 5.1 of this paper.

We consider now the case when the feasibility set X is finite—such is the case, for example, of combinatorial problems. As it turns out, the convergence results are very similar to the case seen above of piecewise linear functions, i.e., when the optimal solution x^* is unique we also have $P(S_N \neq \{x^*\}) \ \lessapprox \ e^{-\beta N}$ for some $\beta > 0$. Again, the sample size that is large enough to ensure that $P(S_N \neq \{x^*\})$ is less than some pre-specified value depends on the variability of the problem

and the flatness of the objective function (measured as the difference between the optimal value and the next best value). Details can be found in Kleywegt et al. [134] and an overview is given in Section 5.1.

3 Sequential-sampling solution methods

As mentioned earlier, the SAA approach discussed in Section 2 can be viewed as an "extreme case" of Algorithm 1 in the sense that it fully minimizes the approximation obtained with a single sample. The convergence results seen above give this approach a sound basis. In some cases, however, it may be advantageous to adopt an iterative approach whereby the optimization alternates with the sampling procedure. We will call that a *sequential-sampling approach*.

One situation where a sequential-sampling approach may be needed occurs when one can only draw a few samples at a time. This happens, for example, in data-driven models where samples correspond to data that are collected simultaneously with the algorithm, or when generating samples is very expensive. Another reason could be a matter of computational strategy—it may be desirable to save the sampling effort when the current solution is far from the optimal one, and increase the number of samples as the iterates approach the minimizer. The latter is the principle behind the *Retrospective Approximation* method originally proposed by Chen and Schmeiser [44] and further developed in Pasupathy and Schmeiser [185], although these papers study the method in the context of root-finding problems. Pasupathy [184] provides a detailed study of rates of convergence for the retrospective approximation method. A similar idea to retrospective approximation, in the context of smooth optimization, was studied by Shapiro and Homem-de-Mello [222], where sampling is incorporated into some first- and second-order optimization algorithms. In fact, in principle one could use any deterministic algorithm and replace function values and derivatives with the respective approximations obtained from sampling; in the sequential-sampling approach, a new sample is drawn every iteration, or every few iterations. We see then that the formulation of sequential-sampling methods is closely related to the issues of assessment of solution quality, choice of stopping criteria and sample size selection—these will be discussed in Sections 4 and 5 below.

When a sequential-sampling approach is adopted, it is important to distinguish between two cases: samples could be accumulated—for example, one could use $\{\hat{\xi}^1\}$ in the first iteration, $\{\hat{\xi}^1, \hat{\xi}^2\}$ in the second iteration and so on—or they could be drawn independently, so that the sample used in a certain iteration is statistically independent of the samples in previous iterations. In the latter case, the function being optimized in that iteration is different from the functions in previous iterations, so the optimization algorithm must be able to handle this situation; on the other hand, the use of independent samples reduces the chances of getting trapped in a "bad sample path" as discussed in Homem-de-Mello [108], i.e., a sample path on which the approximation converges only for very large sample sizes—the results in Section 2 ensure that such paths have small probability but nevertheless they may exist. We discuss now some sequential-sampling methods proposed in the literature.

3.1 Stochastic Approximation methods

Perhaps the most well-studied sequential sampling technique for stochastic optimization is the so-called Stochastic Approximation (SA) method. As seen earlier, in its basic form SA is defined by the recursive sequence

$$x^{k+1} \;:=\; x^k - \alpha_k \eta^k, \quad k \geq 0, \tag{15}$$

where $-\eta^k$ is a random direction satisfying some properties—for example, the expectation of such a direction should be a descent direction for the true function g—and α_k is the step-size at iteration k. The condition imposed on the sequence $\{\alpha_k\}$ is that it goes to zero but not too fast, which is usually formalized as $\sum_{k=0}^{\infty} \alpha_k = \infty$, $\sum_{k=0}^{\infty} \alpha_k^2 < \infty$. For constrained problems, x^{k+1} is defined as the projection of $x^k - \alpha_k \eta^k$ onto the feasibility set X.

Since the initial work by Robbins and Monro [200], great effort has been applied to the development of both theoretical and practical aspects of the method. Robbins and Monro's problem was actually to find a zero of a given noisy function; Kiefer and Wolfowitz [129] applied the idea to optimization and used finite-difference estimators of the gradient. The idea of using gradient estimators constructed solely from function evaluations was further developed into a method called *Simultaneous Perturbation Stochastic Approximation*; see Spall [230] for a detailed discussion. A different line of work involves the use of ordinary differential equations to analyze the behavior of SA algorithms; such an approach was introduced by Kushner and Clark [139] and elaborated further in Kushner and Yin [140], see also Borkar and Meyn [31]. Andradóttir [4] proposed a scaled version of SA that aims at circumventing the problem of slow convergence of the original method when the function being minimized is nearly flat at the optimal solution. Some developments in SA have come from the application of this type of method in learning algorithms; see, for instance, the book by Bertsekas and Tsitsiklis [24] and the work of Kunnumkal and Topaloğlu [138] for a more recent account.

Much of the effort in research on SA-type algorithms has focused on strategies that can speed up the algorithm (in terms of improving the convergence) while keeping its adaptive nature. The dilemma here is that, although the basic SA algorithm (15) can be shown to have optimal rate of convergence $O(1/k)$—where k is the number of iterations—such rate is obtained for smooth and/or strongly convex functions and an "optimal" choice of stepsizes, which are typically unknown in practice. When non-optimal stepsizes are used, actual convergence can be very slow (see, e.g., Spall [230]), although Broadie et al. [33] have recently proposed some enhancements to the Kiefer-Wolfowitz algorithm that show promising results in terms of practical performance.

An important development was provided by Polyak and Juditsky [197], who proposed a simple but powerful idea: rather than looking at the iterates $\{x_k\}$ defined in (15), one should analyze the *average* iterates

$$\bar{x}^k \;:=\; \frac{1}{k} \sum_{i=0}^{k-1} x^i.$$

Such a method also achieves the theoretical rate of convergence, but the averaging allows for more

robustness with respect to stepsizes. Earlier, Nemirovski and Yudin [169] had proposed averaging the iterates using the stepsizes as follows:

$$\bar{x}^k \;:=\; \frac{\sum_{i=0}^{k-1} \alpha_i x^i}{\sum_{i=0}^{k-1} \alpha_i}, \tag{16}$$

where the stepsizes α_k are "longer" than those in the classical SA algorithm—for example, α_k can be of order $k^{-1/2}$. The resulting algorithm was shown to be more robust with respect to stepsizes and properties of the function being minimized. The idea of averaging is also present in other variants of SA. For example, Dupuis and Simha [73] proposed a method whereby the stepsize α_k is constant for all k and the estimator η^k is given by a sample average. They used large deviations theory to show convergence of the method and suggested a growth rate for the sample size.

In a different context and for the more structured case in which the integrand function G is *convex* (although possibly nondifferentiable) a closely related method, called Stochastic Quasi-Gradient (SQG), was developed in the seventies. The basic idea is still a recursion like (15), but here the η^k is taken to be a *stochastic quasigradient* of G, that is, a vector satisfying

$$\mathbb{E}\left[\eta^k | x^0, \ldots, x^k\right] \;=\; \nabla g(x^k) + b^k$$

where $\nabla g(x^k)$ denotes a subgradient of g at x^k and $\{b^k\}$ is a sequence such that $\|b^k\| \to 0$. A review of this technique can be found in Ermoliev [75]; discussion on practical aspects such as choice of stepsizes, stopping rules and implementation guidelines are given by Gaivoronski [84] and Pflug [189].

More recently, a new line of SA (or SQG) algorithms for convex problems has been proposed based on the use of proximal-point techniques. Rather than using an iteration of the type (15), these algorithms define the next iterate x^{k+1} as a suitable projection using proximal-type functions. While the idea of using proximal-type functions had been studied earlier (see, e.g., Ruszczyński [211]), the new methods allow for further enhancements. For example, the *Mirror-Descent SA method* introduced by Nemirovski et al. [170] defines

$$x^{k+1} := P_{x^k}(\beta_k \eta^k),$$

where η^k is an unbiased estimator of $\nabla g(x^k)$, $P_x(\cdot)$ is the prox-mapping defined as $P_x(y) = \operatorname{argmin}_{z \in X} y^T(z - x) + V(x, z)$, $\{\beta_k\}$ is a sequence of stepsizes (which need not go to zero), V is the prox-function $V(x, z) = \omega(z) - \omega(x) - \nabla\omega(x)^T(z - x)$, and $\omega(\cdot)$ is a distance-generating function, i.e., a smooth strongly convex function. Notice that this method generalizes the basic SA algorithm, since the choice of $\omega(x) = (1/2)\|x\|_2^2$ (where $\|\cdot\|_2$ denotes Euclidean norm) yields the recursion (15). However, the flexibility in choosing the function $\omega(\cdot)$ allows for exploiting the geometry of the problem. In addition, the iterates are averaged as in (16). As demonstrated in Nemirovski et al. [170], the resulting algorithm allows not only for more robustness with respect to the parameters of the algorithm, but also for excellent performance in the experiments reported

in the paper; indeed, the error obtained with a fixed sample size is similar to that obtained with a standard SAA approach corresponding to the same sample size, but the computational times are much smaller than those with SAA. Lan [141] provided further enhancement to the mirror-descent algorithm by introducing new sequences that aggregate the iterates; the resulting method—called *Accelerated SA*—is shown to achieve optimal rate of convergence both in the smooth and non-smooth cases.

Nesterov [171] proposed a primal-dual method which works in the dual space of the problem, with the goal of preventing the weights of subgradients from going to zero. In the algorithm (called *Stochastic Simple Averages*), the next iterate x^{k+1} is defined as $x^{k+1} := P_{\gamma\beta_k}(\widetilde{\eta}^k)$, where $\widetilde{\eta}^k = \sum_{t=1}^{k} \nabla G(x^t, \xi^t)$, $P_\beta(\cdot)$ is the mapping defined as $P_\beta(s) = \text{argmin}_{z \in X} - s^T z + \beta\omega(z)$, $\{\beta_k\}$ is a sequence of stepsizes (which need not go to zero), γ is a positive constant, and as before $\omega(\cdot)$ is a distance-generating function. The algorithm is shown to have optimal rate in the sense of worst-case complexity bounds.

3.2 Sampling-based algorithms for stochastic linear programs

A number of algorithms have been developed in the literature that exploit the special structures of the specific class of problem they are applied to, and therefore can work well for that class of problems. A set of such algorithms is rooted in the L-shaped method (Van Slyke and Wets [235]), originally devised for two-stage stochastic linear programs. L-shaped method in stochastic programming is commonly known as Benders' decomposition (Benders [22]) in mixed-integer programming and Kelley's cutting plane algorithm in convex programming (Kelley [127], Hiriart-Urruty and Lemaréchal [106]). The L-shaped method achieves efficiency via decomposition by exploiting the block structure of stochastic programs with recourse. The *Stochastic Decomposition* method of Higle and Sen [100] is a sampling-based version the L-shaped method for stochastic linear programs, using sampling-based cutting planes within the L-shaped algorithm. Infanger [120] and Dantzig and Infanger [52] embed *importance sampling* techniques—which aim at reducing variance, see Section 7.4 below—within the L-shaped method.

Specialized sampling-based algorithms have also been developed for the case of *multistage* stochastic linear programs (MSSPs). Such models have been widely used in multiple areas such as transportation, revenue management, finance and energy planning. A general MSSP for a problem with $T + 1$ stages can be written as

$$\begin{aligned} & \min \; c_0 x_0 + \mathbb{E}_{\xi_1}\left[Q_1(x_0, \xi_1)\right] \\ \text{subject to} \quad & \\ & A_0 x_0 = b_0. \\ & x_0 \geq 0 \end{aligned} \tag{MSSP}$$

The function Q_1 is defined recursively as

$$\begin{aligned} Q_t(x_0,\ldots,x_{t-1},\xi_1,\ldots,\xi_t) \;=\; & \min\; c_t x_t + \mathbb{E}_{\xi_{t+1}}\left[Q_{t+1}(x_0,\ldots,x_t,\xi_1,\ldots,\xi_{t+1})\right] \\ & \text{subject to} \\ & A_t x_t = b_t - \sum_{m=0}^{t-1} B_{m+1} x_m, \\ & x_t \geq 0 \end{aligned} \tag{17}$$

$t = 1,\ldots,T-1$. In the above formulation, the random element ξ_t denotes the random components of c_t, A_t, B_t, b_t. Notice that we use the notation $\mathbb{E}_{\xi_{t+1}}\left[Q_{t+1}(x_0,\ldots,x_t,\xi_1,\ldots,\xi_{t+1})\right]$ to indicate the conditional expectation $\mathbb{E}\left[Q_{t+1}(x_0,\ldots,x_t,\xi_1,\ldots,\xi_{t+1}) \,|\, \xi_1,\ldots,\xi_t\right]$. The function Q_T for the final stage T is defined the same way as the general Q_t in (17), except that it does not contain the expectation term in the objective function.

Although the MSSP model fits the framework of (SP), the application of sampling methods to that class of problems is more delicate. As discussed in Shapiro [219], a procedure whereby some samples of the vector $\xi := (\xi_1,\ldots,\xi_T)$ are generated and the corresponding approximating problems are solved exactly will not work well. It is not difficult to see why—the nested structure of MSSP requires that the expectation *at each stage* be approximated by a sample average, which cannot be guaranteed by simply drawing samples of ξ. To circumvent the problem, a conditional sampling scheme, in which samples of ξ_t are generated for each sampled value of ξ_{t-1}, must be used. The resulting structure is called a scenario tree. Of course, this implies that the number of samples required to obtain a good approximation of MSSP grows exponentially with the number of stages. Thus, exact solutions of the approximating problem often cannot be obtained.

To address the problem of large scenario trees, some algorithms have been proposed whereby sampling of scenarios *from the tree* is incorporated into an optimization procedure. Note that the input to these algorithms is a scenario tree, so the sampling that is conducted within the algorithm is independent of any sampling that may have been performed in order to generate a scenario tree. Examples of such algorithms are the Stochastic Dual Dynamic Programming (Pereira and Pinto [188], see also Shapiro [220] for further analysis), CUPPS (Chen and Powell [46]), Abridged Nested Decomposition (Donohue and Birge [64]), and ReSa (Hindsberger and Philpott [105]). A convergence analysis of this class of algorithms is provided by Philpott and Guan [193].

3.3 Sampling-based algorithms for "black-box" problems

Many sampling-based methods have been proposed for problems where little assumption is made on the structure of the function being optimized and the feasibility set X, which can be discrete or continuous. Such algorithms guide the optimization based solely on estimates of function values at different points. This setting is often referred to as *simulation optimization* in the literature. There is vast amount of work in that area, and some excellent surveys have been written; see, for instance Fu [82], Andradóttir [5] and Chen et al. [43], to which we refer for a more comprehensive discussion.

We note that this is a growing area of research; as such, new methods have been investigated since the publication of these reviews. We provide here a brief overview of the sampling-based black-box algorithms.

The challenge in stochastic black-box algorithms is two-fold: on the one hand, the lack of problem structure requires a strategy that balances the effort between visiting different parts of the feasibility set versus gaining more information around the solutions that have shown to be more promising—this is the well-known dilemma of exploration vs. exploitation present in deterministic optimization as well. Often this is accomplished by the use of some random search procedure that makes it more likely to visit the points around the most promising solutions. On the other hand, the fact that the objective function cannot be evaluated exactly creates another layer of difficulty, since one cannot be 100% sure that a certain solution that appears promising is indeed a good solution.

Some of the algorithms proposed in the literature incorporate sampling techniques into global search methods originally developed for deterministic optimization. Examples of such work include algorithms based on simulated annealing (Alrefaei and Andradóttir [3]), genetic algorithms (Boesel et al. [30]), cross-entropy (Rubinstein and Kroese [208]), model reference adaptive search (Hu et al. [116]), nested partitions (Shi and Olafsson [228]), derivative-free nonlinear programming algorithms (Barton and Ivey [12], Kim and Zhang [130]), and branch-and-bound methods (Norkin et al. [174, 175]). Algorithms have also been proposed based on the idea of building a response surface for the function value estimates and using some methodology such a trust-region approach to guide the optimization; examples include Angün et al. [7], Barton and Meckesheimer [13], Bastin et al. [14], Bharadwaj and Kleywegt [26] and Chang et al. [40]. The issues of sample size selection and stopping criteria arise here as well—we will discuss more about that in Sections 4 and 5.

Ranking-and-selection methods aim at guaranteeing that the best solution is found with some pre-specified probability, but such techniques are only practical if the number of feasible alternatives is relatively small. Some recent methods, such as the Industrial Strength COMPASS method proposed by Xu et al. [242], aim at combining features of random search (for exploration), local search (for exploitation) and ranking-and-selection (for probabilistic guarantees).

Another class of algorithms relies on the idea of Bayesian formulations for the optimization problem. Generally speaking, in such methods a prior probability distribution (often a Normal distribution) is placed on the value of the alternatives being evaluated; samples corresponding to one or more alternatives are collected, the parameters of the prior distribution are updated in a Bayesian fashion based on the observed values, and the process is repeated until some stopping criterion is satisfied. A key element in such algorithms is a method to decide which alternative(s) should be sampled in each iteration. Examples of such work—which include methods based on optimization via Gaussian processes, stochastic kriging, and knowledge gradient, among others—are Ankenman et al. [8], Chick and Frazier [47], Chick and Inoue [48], Frazier et al. [77, 78], Huang et al. [118] and Scott et al. [214].

In the context of dynamic discrete problems, stochastic optimization problems are closely related

to Markov decision processes (MDPs). Sampling-based methods have been proposed in that area as well. For example, Chang et al. [39] proposed an adaptive sampling algorithm that approximates the optimal value of a finite-horizon Markov decision process (MDP) with finite state and action spaces. The algorithm adaptively chooses which action to sample as the sampling process proceeds and generates an asymptotically unbiased estimator of the value function.

4 Assessing solution quality

We now turn our attention to how to assess the quality of a solution to a stochastic optimization problem. In this section, we again focus on the class of (SP) with $K = 0$ and will return to problems with stochastic constraints in Section 6. When assessing solution quality, we denote the candidate solution as $\hat{x} \in X$. This candidate solution is *fixed*, and our aim is to figure out if it is optimal or near-optimal. Determining if a solution is optimal or near optimal plays a prominent role in optimization theory, algorithms, computation, and practice. Note that the solution $\hat{x} \in X$ can be obtained by any method. For instance, it can be obtained by the SAA approach by letting $\hat{x} = \hat{x}_N$ for some sample size N. Alternatively, it can be obtained by running a Monte Carlo sampling-based algorithm (e.g., the general Algorithm 1 in Section 1, or any of the methods discussed in Section 3) for k iterations and letting $\hat{x} = x^k$. Other approaches for obtaining the candidate solution are possible. In this section, we first review methods that are independent of the algorithm used to obtain the solution. As such, in Sections 4.1 and 4.2, we assume that if Monte Carlo sampling is used to obtain the candidate solution, this is done independently of the Monte Carlo sampling to assess solution quality. Note that there are also ways to assess solution quality within a specific algorithm, typically using the information (such as subgradients, etc.) obtained throughout the algorithm. We briefly review these in Section 4.3.

4.1 Bounding the optimality gap

One of the classic approaches for assessing solution quality in optimization is to bound the candidate solution's optimality gap. If the bound on the optimality gap is sufficiently small, then the candidate solution is of high quality. In deterministic optimization, because the objective function at candidate solution $\hat{x} \in X$ can typically be calculated, bounding $\hat{x}$'s optimality gap amounts to finding lower bounds on the optimal objective function value. These lower bounds are often obtained through relaxations; for instance, via integrality, Lagrangian or semidefinite programming relaxations. In stochastic optimization, Monte Carlo sampling can be used to obtain (statistical) lower bounds. This approach can also be viewed as a type of relaxation in the sense that instead of considering the whole distribution, we look at a subset dictated by the sample.

Recall that the optimality gap of $\hat{x}$ is $g(\hat{x}) - \nu^*$. The optimal value ν^* is not known but can be bound by the bias result given in (8): $\mathbb{E}[\nu_N] \leq \nu^*$. In essence, instead of using "all" information on ξ, using a subset of observations that are present in the sample leads to, on average, over-optimization. This is in line with optimistic objective function values obtained using "relaxed"

problems in deterministic optimization. Therefore, an upper bound on the optimality gap of $\hat{x}$, $\mathbb{E}\left[G(\hat{x},\xi)\right] - \mathbb{E}\left[\nu_N\right]$, can be estimated via

$$\mathcal{G}_N(\hat{x}) \;:=\; g_N(\hat{x}) - \nu_N. \tag{18}$$

From this point on, we will refer to (18) as a point estimator of the optimality gap of $\hat{x} \in X$ rather than an estimator of its upper bound. When viewed as an estimator of optimality gap, $\mathcal{G}_N(\hat{x})$ is biased; i.e., $\mathbb{E}\left[\mathcal{G}_N(\hat{x})\right] \geq g(\hat{x}) - \nu^*$. While there are different ways to calculate the above optimality gap estimator, a basic version uses the same independent and identically distributed (i.i.d.) observations $\xi^1, \xi^2, \ldots, \xi^N$ from the distribution of ξ for *both* terms in (18). That is, given an arbitrary realization $\{\hat{\xi}^1, \hat{\xi}^2, \ldots, \}$ of the random vector ξ, we compute

$$\hat{\mathcal{G}}_N(\hat{x}) \;:=\; \hat{g}_N(\hat{x}, \hat{\xi}^1, \ldots, \hat{\xi}^N) - \hat{\nu}_N(\hat{\xi}^1, \ldots, \hat{\xi}^N), \tag{19}$$

where the notation $\hat{\nu}_N(\hat{\xi}^1, \ldots, \hat{\xi}^N)$ emphasizes that this quantity corresponds to the optimal value of problem (4) for the particular realization $\{\hat{\xi}^1, \ldots, \hat{\xi}^N\}$.

The use of the same observations in both terms of (19) results in variance reduction via the use of common random variates. As indicated in Section 2.2, ν_N may not be asymptotically normal (see (10)). Therefore, $\mathcal{G}_N(\hat{x})$ is typically not asymptotically normal, complicating statistical inference. This difficulty can be circumvented by employing a "batch-means" approach commonly used in the simulation literature. That is, multiple independent estimators $\mathcal{G}_N^k(\hat{x})$ are generated using $N_{\mathcal{G}}$ "batches" of observations $\xi^{k1}, \xi^{k2}, \ldots, \xi^{kN}$, $k = 1, 2, \ldots, N_{\mathcal{G}}$, and these $\mathcal{G}_N^k(\hat{x})$ are averaged to obtain a point estimator of the optimality gap

$$\bar{\mathcal{G}}(\hat{x}) \;:=\; \frac{1}{N_{\mathcal{G}}} \sum_{k=1}^{N_{\mathcal{G}}} \mathcal{G}_N^k(\hat{x}). \tag{20}$$

The sample variance is calculated in the usual way, $s_{\mathcal{G}}^2 \;:=\; \frac{1}{N_{\mathcal{G}}-1} \sum_{k=1}^{N_{\mathcal{G}}} \left(\mathcal{G}_N^k(\hat{x}) - \bar{\mathcal{G}}(\hat{x})\right)^2$. An approximate $(1-\alpha)$-level confidence interval estimator on the optimality gap of $\hat{x}$ is then obtained by

$$\left[0, \bar{\mathcal{G}}(\hat{x}) + \frac{z_\alpha s_{\mathcal{G}}}{\sqrt{N_{\mathcal{G}}}}\right], \tag{21}$$

where z_α denotes a $1-\alpha$ quantile from a standard Normal distribution. The resulting point estimator (20) and interval estimator (21) are called the *Multiple Replications Procedure* (MRP) estimators. MRP was developed by Mak, Morton, and Wood [158] and the idea of using ν_N to bound ν^* was used by Norkin et al. [175] within a sampling-based branch-and-bound framework. Notice that the confidence interval above is a one-sided (upper) interval. This is in an effort to obtain a more conservative estimate which can help, for instance, when used as a stopping rule (see e.g., (36) in Section 5.3).

The MRP confidence interval (21) for the optimality gap of $\hat{x}$ is asymptotically valid when the batches $\{\xi^{k1}, \xi^{k2}, \ldots, \xi^{kN}\}$, $k = 1, 2, \ldots, N_{\mathcal{G}}$, are i.i.d., coupled with the consistency of the variance

estimator $s_{\mathcal{G}}^2$ of $\sigma_{\mathcal{G}}^2 = \text{Var}[\mathcal{G}_N(\hat{x})]$, through the Central Limit Theorem (CLT)

$$\sqrt{N_{\mathcal{G}}}[\bar{\mathcal{G}}(\hat{x}) - \mathbb{E}\left[\mathcal{G}_N(\hat{x})\right]] \xrightarrow{d} \text{Normal}(0, \sigma_{\mathcal{G}}^2).$$

We assume that $G(x, \xi)$ has finite second moments for all $x \in X$ in order to invoke the CLT. Notice that the CLT holds even when observations *within* each batch are obtained in a non-i.i.d. fashion. Non-i.i.d. sampling schemes that produce *unbiased* estimators for a given solution x, i.e., $\mathbb{E}\left[N^{-1}\sum_{j=1}^{N} G(x, \xi^{kj})\right] = \mathbb{E}\left[G(x, \xi)\right]$, $k = 1, 2, \ldots, N_{\mathcal{G}}$, can be used to generate each batch of observations. This fact can be used to obtain variants of MRP that are aimed to reduce variance and/or bias. See, for instance, Bayraksan and Morton [20] for one such variation that uses randomized quasi-Monte Carlo sampling to generate the batches in an effort to reduce variance.

With an asymptotically valid confidence interval, the output of MRP is a probabilistic statement on the optimality gap of $\hat{x}$ of the form

$$P\left(g(\hat{x}) - \nu^* \leq \bar{\mathcal{G}}(\hat{x}) + \frac{z_\alpha s_{\mathcal{G}}}{\sqrt{N_{\mathcal{G}}}}\right) \approx 1 - \alpha.$$

Notice that the bias of ν_N results in an overestimation of the optimality gap and this can lead to wider confidence levels for small sample sizes. Such conservative coverage has been observed for some problems in the computational results by Bayraksan and Morton [19] and Partani [182].

A major advantage of MRP is its wide applicability. Problem (SP) can contain discrete or continuous decisions and in two-stage stochastic programs with recourse, the discrete and/or continuous decisions can be present at any stage. The problem can have nonlinear terms in the objective or constraints; neither X nor g need to be convex. It is explicitly assumed, however, that the samples of ξ can be generated and the function evaluations $G(x, \xi)$ can be performed. As mentioned above, we also assume finite second moments of $G(x, \xi)$. The most restrictive aspect of MRP is that it requires solution of $N_{\mathcal{G}}$ SAA problems (4) to obtain estimates of ν_N in $\mathcal{G}_N(\hat{x})$. (In implementation, $N_{\mathcal{G}}$ is typically taken to be around 20-30 to induce the CLT.) The ability to solve SAA problems and the computational effort required depends on the class of problem MRP is applied to. Note that the SAA problems can be solved using any specialized algorithm for the problem at hand. We also note that approximate methods that yield lower bounds on ν_N can be used instead but with weakened bounds and more conservative optimality gap estimators. The framework to implement MRP is relatively simple and step by step instructions can be found, for instance, in Bayraksan and Morton [20]. Applications of MRP in the literature include supply chain network design (Santoso et al. [213]), financial portfolio models (Bertocchi et al. [23], Morton et al. [162]), stochastic vehicle routing problems (Kenyon and Morton [128], Verweij et al. [236]), scheduling problems (Morton and Popova [161], Turner et al. [234]), and a stochastic network interdiction model (Janjarassuk and Linderoth [121]).

Typically, MRP can be performed with modest computational effort. In cases where computational effort becomes prohibitive (because we solve $N_{\mathcal{G}}$ SAA problems each of size N), an alternative way to obtain optimality gap point and interval estimators is by using single or two replications

(Bayraksan and Morton [19]). In the *Single Replication Procedure* (SRP), $N_{\mathcal{G}} = 1$ and the point estimator of optimality gap is simply given by (18). A major difference between MRP and SRP is the variance estimator. In MRP, the sample variance of $N_{\mathcal{G}}$ gap estimators $\mathcal{G}_N^k(\hat{x})$, $k = 1, 2, \ldots, N_{\mathcal{G}}$ is calculated. In SRP, with $N_{\mathcal{G}} = 1$, this is not possible. In order to motivate the variance estimator of SRP, let us rewrite (18) as

$$\mathcal{G}_N(\hat{x}) \;=\; \frac{1}{N}\sum_{j=1}^{N}\left(G(\hat{x},\xi^j) - G(x_N,\xi^j)\right),$$

where as before x_N denotes the optimal solution to the sampling problem $\min_{x\in X} g_N(x)$ with optimal value ν_N. Viewing $\mathcal{G}_N(\hat{x})$ as the sample average of the observations $G(\hat{x},\xi^j) - G(x_N,\xi^j)$, $j = 1, 2, \ldots, N$, the sample variance estimator is calculated as

$$s_G^2 \;:=\; \frac{1}{N-1}\sum_{j=1}^{N}\left[\left(G(\hat{x},\xi^j) - G(x_N,\xi^j)\right) - \mathcal{G}_N(\hat{x})\right]^2, \tag{22}$$

where we have omitted the dependence of s_G on N and $\hat{x}$ to simplify the notation. Note that $\hat{x}$ is fixed but x_N is obtained by optimizing a sample mean, i.e., x_N depends on $\xi^1, \ldots, \xi^N$. Therefore, the usual statistical analysis of sample means does not apply. Nevertheless, it is still possible to obtain asymptotically valid $(1-\alpha)$-level confidence intervals

$$\left[0, \mathcal{G}_N(\hat{x}) + \frac{z_\alpha s_G}{\sqrt{N}}\right]. \tag{23}$$

Asymptotic validity of the confidence interval in (23) means that

$$\liminf_{N\to\infty} P\left(g(\hat{x}) - \nu^* \le \mathcal{G}_N(\hat{x}) + \frac{z_\alpha s_G}{\sqrt{N}}\right) \;\ge\; 1-\alpha.$$

To establish the above inequality, a key component is to ensure the consistency of the variance estimator of SRP. Suppose that $\mathbb{E}\left[\sup_{x\in X} G^2(x,\xi)\right] < \infty$, which guarantees the second moments are finite. Consistency of s_G means that asymptotically (as $N \to \infty$) we have that

$$\inf_{x\in S^*} \sigma_{\hat{x}}^2(x) \;\le\; s_G^2 \;\le\; \sup_{x\in S^*} \sigma_{\hat{x}}^2(x) \quad \text{w.p.1}, \tag{24}$$

where $\sigma_{\hat{x}}^2(x) := \mathrm{Var}[G(\hat{x},\xi) - G(x,\xi)]$.

Note that when there is a unique optimum solution, i.e., $S^* = \{x^*\}$, (24) turns into the usual strong consistency result for the variance estimator s_G^2, i.e., $\lim_{N\to\infty} s_G^2 = \sigma_{\hat{x}}^2(x^*)$ w.p.1. When there are multiple optima, however, the variance of $G(\hat{x},\xi) - G(x,\xi)$ might change at each $x \in S^*$ (recall that $\hat{x}$ is fixed). The consistency result in (24) states that the variance estimator is guaranteed to be within a minimum and maximum of variances in the set of optimal solutions. Bayraksan and Morton [19] provide a set of conditions under which (24) is satisfied, including i.i.d. sampling,

Input: $\hat{x} \in X$; a method to generate observations; a method to solve (2)

Output: A point estimator (e.g., $\mathcal{G}_N(\hat{x})$) and a $(1-\alpha)$-level approximate confidence interval estimator of $\mathbb{E}\left[G(\hat{x},\xi)\right] - \nu^*$ (e.g., of the form $[0, \mathcal{G}_N(\hat{x}) + \varepsilon_\alpha]$, where ε_α denotes the sampling error)

	Observations	Point Estimator	Variance Estimator	Sampling Error
MRP	$\xi^{k1}, \xi^{k2}, \ldots, \xi^{kN}$, $k = 1, 2, \ldots, N_{\mathcal{G}}$	$\bar{\mathcal{G}}(\hat{x}) = \frac{\sum_{k=1}^{N_{\mathcal{G}}} \mathcal{G}_N^k(\hat{x})}{N_{\mathcal{G}}}$	$s_{\mathcal{G}}^2 = \frac{\sum_{k=1}^{N_{\mathcal{G}}} \left(\mathcal{G}_N^k(\hat{x}) - \bar{\mathcal{G}}(\hat{x})\right)^2}{N_{\mathcal{G}}-1}$	$\frac{z_\alpha s_{\mathcal{G}}}{\sqrt{N_{\mathcal{G}}}}$
SRP	$\xi^1, \xi^2, \ldots, \xi^N$	$\mathcal{G}_N(\hat{x})$	$s_G^2 = \frac{\sum_{j=1}^{N} \left[\left(G(\hat{x},\xi^j) - G(x_N,\xi^j)\right) - \mathcal{G}_N(\hat{x})\right]^2}{N-1}$	$\frac{z_\alpha s_G}{\sqrt{N}}$
2RP	$\xi^{11}, \xi^{12}, \ldots, \xi^{1N}$, $\xi^{21}, \xi^{22}, \ldots, \xi^{2N}$	$G'(\hat{x}) = \frac{\sum_{k=1}^{2} \mathcal{G}_N^k(\hat{x})}{2}$	$s_G^{2\,\prime} = \frac{\sum_{k=1}^{2} s_{G,k}^2}{2}$	$\frac{z_\alpha s'_G}{\sqrt{2N}}$

Notes: $\mathcal{G}_N(\hat{x})$ is given in (18). 2RP averages two SRP point and variance estimators.
$N_{\mathcal{G}}$ of MRP is typically chosen to be 20-30 in practice.

Table 2: Summary of Procedures for Optimality Gap Estimation

$X \neq \emptyset$ and compact, and $G(\cdot, \xi)$ is continuous, w.p.1. These conditions are satisfied, for instance, by two-stage stochastic linear programs with relatively complete recourse (for each $x \in X$, the second-stage problem is feasible). The i.i.d. assumption is relaxed in Drew [66], who extends the result to the case where the generated vectors are Quasi-Monte Carlo sequences "padded" with Latin Hypercube sampling; see Sections 7.2 and 7.3.

Computational results show that the coverage probability of the SRP confidence interval does not have the same conservative results as MRP. In fact, for some problems, SRP can have undesirably low coverage probability, i.e., the proportion of times in which the interval given by (23) actually contains the true gap $g(\hat{x}) - \nu^*$ is smaller than $1 - \alpha$. In practice, it is better to use two replications instead of one. This is referred to as *2 Replication Procedure* (2RP), or the *Averaged 2 Replication Procedure* (A2RP). In 2RP, $N_{\mathcal{G}} = 2$, and so, two independent estimates of optimality gap $\mathcal{G}_N^k(\hat{x})$ and sample variance $s_{G,k}^2$, $k = 1, 2$ are obtained. Then, these are averaged to obtain

$$G'(\hat{x}) = \frac{1}{2}\sum_{k=1}^{2} \mathcal{G}_N^k(\hat{x}) \quad \text{and} \quad s_G^{2\,\prime} = \frac{1}{2}\sum_{k=1}^{2} s_{G,k}^2.$$

The $(1-\alpha)$-level approximate confidence interval is obtained in a similar way, i.e., $\left[0, G'(\hat{x}) + \frac{z_\alpha s'_G}{\sqrt{2N}}\right]$. The same conditions to ensure asymptotic validity of SRP confidence interval ensure asymptotic validity of 2RP interval estimator. It is also possible to increase the number of replications but computational results suggest that using two replications is typically sufficient in practice (Bayraksan and Morton [19]). Table 2 summarizes the procedures outlined above to obtain optimality gap point and interval estimators for a given solution $\hat{x}$.

Instead of using common random variates as in the above procedures, it is possible to use one sample to estimate $g(\hat{x})$ and another to estimate the lower bound $\mathbb{E}\left[\nu_N\right]$ on ν^*. Let N_U denote

the sample size to estimate $\mathbb{E}[G(\hat{x},\xi)]$ via the sample mean $\bar{U} = N_U^{-1}\sum_{j=1}^{N_U} G(\hat{x},\xi^j)$. Similarly, let N_L be the number of batches to estimate $\mathbb{E}[\nu_N]$ via $\bar{L} = N_L^{-1}\sum_{j=1}^{N_L}\nu_N^j$. These two estimators subtracted from one another, $\bar{U}-\bar{L}$, gives a point estimator of optimality gap. Due to variation, this estimate can be negative, so, $\max\{\bar{U}-\bar{L},0\}$ can be used instead. To form an asymptotically valid interval estimator, the sampling errors of $\bar{U}$ and $\bar{L}$ are calculated separately, invoking the CLT, and are combined using the Boole-Bonferroni inequality (for details, we refer the reader to Section 3.1 of Mak et al. [158]). Because estimation of $\mathbb{E}[G(\hat{x},\xi)]$ is computationally cheaper, N_U can be chosen to be very large. The computational bottleneck is again the solution of N_L SAA problems and N_L is taken to be $20-30$ to induce the CLT. When the correlation between $G(\hat{x},\xi)$ and ν_N is low, using a very large value of N_U can result in an overall sampling error less than the one using common random variates. However, when there is a strong positive correlation between $G(\hat{x},\xi)$ and ν_N, we may expect significant variance reduction when using the common random variates version of MRP in Table 2. For computational results on these versions, see, for instance Mak et al. [158], Kenyon and Morton [128] and Verweij et al. [236].

When the point or interval estimator of the optimality gap of a candidate solution turns out to be large, this could be due to (i) the candidate solution being far from optimal, (ii) variability is large, or (iii) bias is large. Suppose the candidate solution is indeed a high-quality solution. We can still have large estimators due to variance and/or bias and this can hinder our ability to validate that it is in fact a high-quality solution. For variance reduction, above, we mentioned using alternative sampling techniques to reduce variability in MRP, SRP, and 2RP estimators. The issue of bias in optimality gap estimation, on the other hand, is analogous to weak bounds in deterministic optimization. For instance, in integer programming, sometimes when an optimal solution is found, it takes significant computational effort to prove its optimality due to weak bounds. Similarly, bias results in a weak lower bound, on average, on ν. Because bias decreases as N increases, one way to decrease bias is to simply increase N when calculating ν_N. However, this can be computationally burdensome and the decrease in bias can be slow—of order $O(N^{-1/2})$ as discussed in Section 2.2. For bias reduction, Partani [182] and Partani et al. [183] present an adaptive version of MRP, which is motivated by the generalized jacknife estimators in statistics (Gray and Schucany [94]). Stockbridge and Bayraksan [232] use stability results in stochastic programming to reduce bias in 2RP estimators by partitioning the $2N$ observations into two groups of N by minimizing the distance between the resulting empirical distributions. We end by noting that some sampling methods aimed to reduce variance, like Latin Hypercube sampling, have been observed to reduce bias as well, see, e.g., the computational results in Freimer et al. [79]. These sampling methods spread the observations more evenly than random sampling. Consequently, it can be less likely to over-optimize, resulting in a reduction in bias (recall the discussion in the paragraph preceding equation (18)).

4.2 Testing optimality conditions

Another classic approach to assessing solution quality in optimization is determining whether a solution satisfies conditions that ensure optimality. For instance, Karush-Kuhn-Tucker (KKT) conditions provide necessary and sufficient conditions for optimality for a class of problems. Because we are dealing with a stochastic optimization problem, the function values and (sub)gradients needed for evaluation of optimality conditions are typically not readily available and need to be estimated via Monte Carlo sampling. For example, a class of two-stage stochastic linear programs with recourse can be viewed as (sub)differentiable convex optimization problems and assessment of solution quality via statistical evaluation of KKT conditions have been studied for this class of problems. Of course, the problem class is larger than a subset of two-stage stochastic linear programs with recourse. We note that evaluation of KKT conditions based on Monte Carlo sampling-based estimates, compared to a procedure like MRP, is more restrictive in terms of the problem class it applies to. Below, we sketch out one way to evaluate KKT conditions in the presence of Monte Carlo sampling-based estimators of function values and gradients and the difficulties that arise in this statistical evaluation of KKT conditions.

Suppose $g(\cdot)$ is differentiable at the candidate solution $\hat{x} \in X$ and also $G(\cdot, \xi)$ is differentiable at $\hat{x}$, w.p.1, and that it is possible to interchange expectation and differentiation; i.e., $\nabla g(\hat{x}) = \mathbb{E}\left[\nabla_x G(\hat{x}, \xi)\right]$. In two-stage stochastic linear programs with recourse, for instance, these assumptions can hold when the distribution of ξ is continuous. Given an i.i.d. sample $\xi^1, \xi^2, \ldots, \xi^N$ from the distribution of ξ, a Monte Carlo sampling-based estimator of $\nabla g(\hat{x})$ can be formed by

$$\nabla g_N(\hat{x}) = \frac{1}{N} \sum_{j=1}^{N} \nabla_x G(\hat{x}, \xi^j). \tag{25}$$

If $\nabla_x G(\hat{x}, \xi)$ has finite second moments, then, by the CLT, $\sqrt{N}[\nabla g_N(\hat{x}) - \nabla g(\hat{x})] \xrightarrow{d} \text{Normal}(\mathbf{0}, \mathbf{\Sigma})$, where $\mathbf{\Sigma}$ is the covariance matrix of $\nabla_x G(\hat{x}, \xi)$, assumed to be nonsingular. Let $[\cdot]'$ denote the transpose of its argument. The sample covariance matrix

$$\mathbf{\Sigma}_N = \frac{1}{N-1} \sum_{j=1}^{N} \left[\nabla_x G(\hat{x}, \xi^j) - \nabla g_N(\hat{x}))\right] \left[\nabla_x G(\hat{x}, \xi^j) - \nabla g_N(\hat{x}))\right]' \tag{26}$$

provides an unbiased and consistent estimator of $\mathbf{\Sigma}$. Given Monte Carlo sampling-based estimators $\nabla g_N(\hat{x})$ and $\mathbf{\Sigma}_N$ of $\nabla g(\hat{x})$ and $\mathbf{\Sigma}$, respectively, our aim is to evaluate statistically if $\hat{x}$ satisfies the KKT conditions. Let us now review the KKT conditions.

Suppose X is composed of m_1 equality and $m - m_1$ inequality constraints

$$X = \{x : \ h_i(x) = 0, \ i = 1, 2, \ldots, m_1; \ h_i(x) \leq 0, \ i = m_1 + 1, \ldots, m\}.$$

Suppose further that $h_i(\cdot)$, $i = 1, \ldots, m$ are continuously differentiable and $g(\cdot)$ is differentiable at optimal solution $x^* \in X$. Let $\mathcal{I}(x) = \{i : h_i(x) = 0, \ i = m_1 + 1, \ldots, m\}$ denote the index set of

inequality constraints that are active at x. We assume that any necessary constraint qualification conditions are satisfied. One way to write the KKT conditions is

$$-\nabla g(x^*) \in N_X(x^*), \tag{27}$$

where $N_X(x^*)$ denotes the normal cone of X at x^*, written as

$$N_X(x^*) = \left\{ z \in \mathbb{R}^n \colon z = \sum_{i=1}^{m_1} \alpha_i \nabla h_i(x^*) + \sum_{i \in \mathcal{I}(x^*)} \alpha_i \nabla h_i(x^*), \text{ where } \alpha_i \geq 0 \text{ for } i \in \mathcal{I}(x^*) \right\}.$$

The aim is to test whether $\hat{x}$ satisfies KKT conditions; i.e., if $-\nabla g(\hat{x}) \in N_X(\hat{x})$ (null hypothesis H_0) or not (alternative H_1). Assume that all conditions satisfied at x^* such as differentiability are satisfied at $\hat{x}$. One way to do this is to determine the distance between the point $-\nabla g(\hat{x})$ and the set $N_X(\hat{x})$. Because $\nabla g(\hat{x})$ is not known, we replace it by its Monte Carlo sampling-based estimator in (25). Then, the test statistic can be defined as

$$T_N(\hat{x}) = \text{dist}(-\nabla g_N(\hat{x}), N_X(\hat{x})), \tag{28}$$

where $\text{dist}(a, B)$ denotes the distance between point a and set B. The test statistic can be obtained in different ways. For instance, one can use

$$T_N(\hat{x}) = N \min_{z \in N_X(\hat{x})} [\nabla g_N(\hat{x}) - z]' \boldsymbol{\Sigma}_N^{-1} [\nabla g_N(\hat{x}) - z]. \tag{29}$$

With nonsingular $\boldsymbol{\Sigma}_N$, (29) is a quadratic programming problem. Suppose strict complementarity condition holds ($\alpha_i > 0$ for $i \in \mathcal{I}(\hat{x})$). Under the null hypothesis, (29) converges in distribution to a chi-squared random variable with $d_x - (m_1 + |\mathcal{I}(\hat{x})|)$ degrees of freedom. Then, a large p-value, close to 1, suggests a high quality solution whereas a small p-value indicates that either $\hat{x}$ is far from optimal or there is a large error in the estimation. Recall that p-value can be calculated by $P(Y \geq T_N(\hat{x}))$, where Y is distributed chi-squared with $d_x - (m_1 + |\mathcal{I}(\hat{x})|)$ degrees of freedom.

The above discussion is based on Shapiro and Homem-de-Mello [222], to which we refer for a more detailed description of the statistical methods used to test the hypotheses. There are also other papers that study approaches to test KKT conditions under uncertainty. For example, Higle and Sen [101] use KKT conditions within the framework of the stochastic decomposition algorithm for a class of two-stage stochastic linear programs and use bootstrapping to assess the variability in their estimates; see also Higle and Sen [102]. Note that in many cases—both in two-stage stochastic programs and in simulation—$g(\cdot)$ is not differentiable but only subdifferentiable. Similar ideas to the statistical tests described above can be used in the subdifferentiable case, as discussed by Linderoth et al. [152] who also present extensive computational results. We refer the readers to Shapiro [218] for convergence of Monte Carlo sampling-based estimators of subdifferentials and for alternative test statistics of type (28).

We end this section by noting that above methods assume deterministic constraints. In the case with stochastic constraints, Bettonvil et al. [25] develop a series of hypotheses tests for verification of KKT conditions. Royset [204] uses the so-called optimality function, which has two parts, one that is related to feasibility of the candidate solution with respect to the stochastic constraints and the other testing the more general Fritz-John conditions (similar to KKT conditions) for optimality.

4.3 Assessing solution quality for specific sampling-based algorithms

Above, we discussed how to assess the quality of a given solution which may be obtained in any way. In many cases, solutions are produced sequentially as part of an algorithm and assessment of quality must be made throughout the algorithm to determine a stopping time, or sometimes to aid the next iteration. In this section, we briefly mention some of these methods. Note that for a given $\hat{x} \in X$, typically, estimation of $\mathbb{E}[G(\hat{x}, \xi)]$ is relatively easier compared to estimating a lower bound on ν^* (for a minimization problem). Many sampling-based algorithms produce such bounds throughout the algorithm, so, an estimator of a lower bound on ν^* can be obtained more efficiently within a specific algorithm. Lan et al. [142] develop a lower bound for the mirror descent SA algorithm using the gradient estimates obtained throughout the algorithm. This lower bound solves a lower-approximating linear program for a convex problem, hence is computationally cheaper than solving an SAA problem, but it can be looser than ν_N on average. Similar ideas using duality have been proposed earlier to obtain a statistical lower bound within the stochastic decomposition method by Higle and Sen [101, 102] and improved via quadratic programming duality for "in-sample" tests in Higle and Sen [103]. We also point to other work that uses Monte Carlo sampling-based versions of lower bounds obtained in sampling-based adaptations of deterministic cutting plane algorithms: Higle and Sen [101] use bootstrapping to check verification of generalized KKT conditions in stochastic decomposition; Glynn and Infanger [89] provide an asymptotic analysis of the bounds used in the sampling-based cutting plane algorithm for two-stage stochastic linear programs described in Dantzig and Glynn [53], Dantzig and Infanger [54] and Infanger [120]; and Homem-de-Mello et al. [111] discuss statistical stopping criteria in the context of the SDDP algorithm for multistage stochastic linear programs. When $|X|$ is finite and moderate, the estimator in Ensor and Glynn [74] for a grid-search algorithm can be viewed as a lower bound on ν^*.

5 Choice of sample sizes

An important question when using Monte Carlo sampling-based algorithms is what sample size is required to obtain a high-quality solution. For instance, one might be interested in determining a sample size such that the solution obtained via an SAA approach, x_N, is optimal with a high probability. Estimates of sample sizes for this purpose have been obtained using large deviations theory for a class of problems. In Section 5.1, we briefly review these. A related question concerns the stopping rules for sampling-based algorithms. When should these algorithms stop in order to have a high-quality solution? This also determines—in an indirect way—the sample sizes needed

to obtain a high-quality solution. Choice of sample sizes may also affect the performance of a specific sampling-based algorithm. Is there a way to allocate the sample sizes within iterations of an algorithm to obtain high-quality solutions quickly? In the remainder of this section, we discuss answers to these questions. In Section 5.2 we review sample size selection strategies and in Section 5.3, we review stopping rules for sampling-based algorithms to have a priori control on the quality of solutions obtained.

5.1 Theoretical sample size estimates

The rates of convergence discussed in Section 2.2 provide ways to estimate sample sizes to solve a stochastic optimization problem with a given accuracy via an SAA approach. These estimates have been derived using large deviations theory (Stroock [233]) in a series of papers by Shapiro and Homem-de-Mello [223], Shapiro et al. [226] and Kleywegt et al. [134], see also Ahmed and Shapiro [1]. We briefly review these here; for a more detailed summary we refer the readers to Shapiro et al. [227].

Let S^ϵ and S_N^ϵ denote the set of ϵ-optimal solutions to the original problem (SP) and its SAA (4). For a class of problems, under assumptions such as the existence of appropriate moment generating functions, given $0 \leq \delta < \epsilon$,

$$1 - P(S_N^\delta \subset S^\epsilon) \leq Ce^{-N\beta} \tag{30}$$

for two constants $C, \beta > 0$; see also (14). These constants depend on the problem characteristics and the values of δ and ϵ (we suppress any dependence for notational simplicity). The expression in (30) states that the probability that a δ-optimal solution to SAA is an ϵ-optimal solution to the original problem goes to 1 exponentially fast. Setting the right-hand side of (30) to be less than or equal to a desired value of α and solving for N, the sample sizes

$$N \geq \beta^{-1} \ln\left(\frac{C}{\alpha}\right) \tag{31}$$

guarantee that the probability of obtaining ϵ-optimal solutions via solving an SAA problem with δ precision is at least $1 - \alpha$. Even with exponential convergence, if β is small, convergence can be slow and the sample size estimate may be large.

Suppose X is finite. This is the case when the decisions to be made are discrete. In simulation, for instance, one might like to determine an optimal number of servers or buffer size, for which decisions are discrete. In this case, $C = |X|$ and β is obtained as a minimal large deviations exponential decay rate. By using a bound on β, the sample size estimate in (31) turns to

$$N \geq \frac{3\sigma_{\max}^2}{(\epsilon - \delta)^2} \ln\left(\frac{|X|}{\alpha}\right), \tag{32}$$

where $\sigma_{\max}^2 = \max_{x \in X \setminus S^\epsilon} \mathrm{Var}[G(x^*, \xi) - G(x, \xi)]$ for an optimal solution $x^* \in S^*$. Let us now

examine the above sample size estimate. When the sampling problems are solved to optimality, i.e. $\delta = 0$, the sample size estimate (32) grows proportional to $1/\epsilon^2$ as higher-quality solutions are demanded. On the other hand, as δ approaches ϵ, the sample sizes grow. As can be expected, the higher the variability in the problem, the higher the sample sizes need to be. The estimate (32) also indicates that the sample sizes grow logarithmically in $|X|$ and α. For example, with d_x binary decisions, the size of solution set $|X| = 2^{d_x}$ may be very large, but the sample size only grows proportional to d_x. The estimate (32) is typically too conservative for practical purposes and may be hard to estimate; for instance, estimating $\sigma^2_{\max}$ can be difficult.

When X is bounded but not finite, by reducing X to an "appropriate" finite subset X_ν we can obtain similar sample size estimates to solve the original problem to an ϵ accuracy. Here, "appropriate" means that for any $x \in X$ there exists an $x_\nu \in X_\nu$ such that $\|x - x_\nu\|_\infty \leq \nu$. Note that the set X has finite diameter $D := \sup_{x,y \in X} \|x - y\|_\infty$, so we can choose X_ν such that it has at most $(D/\nu)^{d_x}$ elements. If, further, the expectation $g(x)$ is Lipschitz continuous on X with Lipschitz constant L, then it is possible to show that the sample size estimate analogous to that in (32) is

$$N \geq \frac{12\sigma^2_{\max}}{(\epsilon - \delta)^2} \left(d_x \ln \frac{2DL}{\epsilon - \delta} - \ln \alpha \right).$$

For piecewise linear convex stochastic programs with finite Ξ and sharp, unique optimum Shapiro et al. [226] introduce a *condition number* to explain the sample size needed for SAA to find an optimal solution, by using exponential rates of convergence and characteristics of this class of problems. When the condition number is low, the problems can be considered well-conditioned for solving via SAA and when the condition number is high, one may expect larger sample sizes to obtain high-quality solutions. Their analysis suggests that problems that have high variability and flat objective functions around the optimal solution are ill-conditioned.

5.2 Allocation of sample sizes

The theoretical sample size estimates presented in Section 5.1 aim to determine a minimal sample size for solving a single SAA problem to obtain high-quality solutions with a desired probability. Now we shift focus to Monte Carlo sampling-based methods. Ideally, we would like to have a procedure to automatically choose appropriate sample sizes in each iteration of a sampling-based algorithm.

The main idea behind sample size allocation schemes is to allocate a minimal number of samples while maintaining high accuracy of the approximations. The larger the sample sizes, the better the approximation but the higher the computational cost. We already know that, at a minimum, the sample sizes must tend to infinity for asymptotic properties such as consistency of the optimal values to hold. By strategically allocating a sequence of samples, could we maximize, or at least increase, the rate of convergence? Is there a way to allocate the sample sizes in order to minimize the computational effort within a specific sampling-based algorithm?

Before looking at a strategic allocation of sample sizes, we can study the rate at which sample

sizes must grow. As we mentioned above, the sample sizes must grow in order to have consistent estimators but at *what (minimal) rate* must they grow to ensure this? Homem-de-Mello [108] investigates this question to ensure consistency of the objective function estimator in variable-sample methods, and derives associated error statements in the spirit of the law of the iterated logarithm. Under appropriate conditions, linear and superlinear growth of sample sizes with respect to the iteration number k (e.g., the sample size N_k at iteration k satisfy $N_k \geq ck$ for some $c > 0$) as well as a subset of sublinear sample sizes (e.g., N_k grows of $O(\sqrt{k})$) ensure consistency. However, a sublinear growth of $O(\log k)$ requires more stringent conditions to ensure consistency. Next, we turn our attention to strategic sample size allocation.

The sample size allocation schemes often use one of two main computational objectives and/or constraints: (a) to minimize *expected* total computational cost or total computational cost per run, or (b) assume a fixed computational budget B and try to do the best within this budget, although in the second case, B is often taken to infinity to provide asymptotically optimal sampling schemes. On the convergence of desired quantities, we see that most research focuses on (i) efficient/fast convergence of limit points of solutions $\{x_n^*\}$ to an optimal solution and some on (ii) convergence of certain quantities (e.g., ν_N or the true objective function evaluated at x_N) to optimal value ν^* by judicious sample size allocations. These two broad categorizations of computational cost and consistency properties are often mixed and studied from both theoretical and practical points of view for different classes of sampling-based algorithms. Other similar goals are possible.

On the computational objective (a)—minimizing expected total computational cost—we point to, for instance, the works of Byrd et al. [35], Polak and Royset [196], and Royset [205] for different sampling-based methods. Byrd, Chin, Nocedal, and Wu [35] present ways to dynamically allocate sample sizes within a stochastic gradient method (both pure gradient and a Hessian-free Newton's method with conjugate gradients). Their method increases the sample size when the variance estimate of the gradient is sufficiently large. When this condition is triggered, a larger sample size is obtained in an effort to satisfy an estimated descent condition. Byrd et al. [35] also provide theoretical analysis on an idealized version of their practical dynamic pure stochastic gradient method. They show that if the sample sizes grow geometrically with iteration number k, that is, $N_k = \lceil a^k \rceil$ for some $a > 1$, then the expected total work to obtain an ϵ-optimal solution is $O(1/\epsilon)$ for uniformly convex objective functions. Another approach to computational objective (a) is to formulate a discrete-time optimal control problem to minimize the expected computational cost of obtaining a solution to a sequence of SAA problems. For stochastic nonlinear programs, Polak and Royset [196] propose a control problem that aims to minimize the computational effort required to reduce an initial optimality gap by a prespecified fraction in the context of so-called diagonalization schemes. Recent work by Royset [205] extends on this approach to characterize sample size selection policies when solving smooth stochastic programs. A dynamic program is solved to determine the sample sizes to use for each SAA problem as well as the computational effort that should be expended to solve each SAA problem.

For the computational budget constraint approach (b), we point to, for instance, the recent work

of Royset and Szechtman [207] and the selection procedures from the simulation literature like the optimal computing budget allocation (OCBA) (see, e.g., Chen and Lee [42]). Royset and Szechtman [207] focus on a single SAA problem of sample size N and execute k iterations of a numerical procedure to obtain an approximate solution. They also consider convergence rates in the spirit of convergence goal (ii). The computational effort to obtain an approximate solution can be viewed proportional to $N \times k$. For a given computational budget $B = N \times k$, they study the relationship between N—the sample size selection—vs. k—how much effort should be expended to solve the SAA problem—as $B \to \infty$ to obtain the fastest rate of convergence to ν^* of the true and the SAA objective function values evaluated at the (approximate) solution obtained. When there is a modest number of alternatives to optimize, sample sizes can be wisely allocated to each alternative. This is especially prominent in the simulation literature. OCBA (Chen and Lee [42]) aims to maximize probability of correct selection (PCS) subject to a budget constraint of $N_1 + N_2 + \ldots + N_k = B$, where B is the total computing budget and N_i is the sample size, or computational cost, allocated to each alternative $i = 1, 2, \ldots, k$. Instead of maximizing the PCS, an approximation of PCS is found under an approximate normality assumption. This approximate normality assumption is justified by the CLT, as the estimators used are sample averages and B is large enough. Glynn and Juneja [90], instead, use large deviation results to determine asymptotically optimal sample size allocations to maximize the decay rate of $1-$PCS. Chick and Inoue [48], on the other hand, maximize the expected value of information. We refer the readers to Branke et al. [32] for other ways to dynamically allocate samples, including the indifference zone procedures (see, e.g.,, Kim and Nelson [132]) to select a best system among a discrete set of alternatives evaluated via simulation.

Several papers focus on convergence goal (i)—limit points of $\{x_n^*\}$ belong to the set of optimal solutions—by judicious sample size allocations. Pasupathy [184] presents guidelines on choosing the parameters of a *retrospective approximation* algorithm by looking at the product of computational work and squared normed difference between approximate solutions and optimal solutions. In retrospective approximation, a stochastic root finding method, a sequence of SAA problems with sample sizes $\{N_k\}$ at iteration k is solved to error tolerances $\{\varepsilon_k\}$. The sample sizes $\{N_k\}$ need to tend to infinity and the error tolerances $\{\varepsilon_k\}$ need to converge to 0 in order to ensure consistency of the solutions. The results of this paper indicate that the sample sizes and error tolerances should be in balance with each other and with the numerical procedure used the solve the SAA problems. For instance, if the numerical procedure exhibits linear convergence, then the sample sizes should grow linearly and $\varepsilon_k = C/\sqrt{N_k}$ for some constant $C > 0$. Note that, here, the linear growth of the sample sizes is characterized as $\limsup_{k\to\infty} N_k/N_{k-1} < \infty$. For instance, this can include $N_k = \lceil ck \rceil$ or $N_k = \lceil cN_{k-1} \rceil$, $k = 1, 2, 3, \ldots$ for some constant $c > 1$ so that in the latter case, sample sizes can be increased by $100(c-1)\%$ at each iteration. If, on the other hand, the numerical procedure exhibits polynomial convergence, then the sample sizes can grow polynomially as well (e.g., $N_k = \lceil N_{k-1}^c \rceil$ for some $c > 1$) and ε_k needs to shrink of order $O(1/\sqrt{N_k})$. Another work that focuses on increases in sample sizes to ensure the set of solutions to the approximate problems have limit points in the set of optimal solutions is by Deng and Ferris [57]. For unconstrained

stochastic optimization ($X = \mathbb{R}^{d_x}$) solved via a variable-number sample-path quadratic sampling approximation scheme, they compute increasingly stringent probabilities of sufficient reduction of the estimated objective function values. If this probability is not satisfied at a desired level, the sample size is increased. Bastin et al. [14] propose a trust-region algorithm with varying sample sizes to solve unconstrained mixed logit models and examine consistency of solutions. Their system of sample size updates adapts trust region methods to the sampled case.

5.3 Stopping rules

Stopping rules aim to determine solutions to Monte Carlo sampling-based algorithms such that the obtained solution is of high-quality with a desired probability. We note that the use of the word "algorithm" here is more general than the sampling-based algorithms discussed in Section 3. For instance, an algorithm in the context of stopping rules might be simply solving a sequence of SAA problems with increasing sample size. The important thing to note here is that the stopping rules theory attempts to determine high-quality solutions with *a priori* control.

Recall Algorithm 1. Here, we are interested in Step 4, which in turn will determine—in an algorithmic way—at what sample size to stop. The stopping rules theory that we discuss here uses the procedures for solution quality assessment presented in Section 4. The main difference between assessing solution quality for a given solution $\hat{x}$ and using it to design stopping rules is that the candidate solution $\hat{x}$ and the sample size N are no longer fixed. They change during the course of an algorithm and are therefore random variables themselves. Because of the iterative statistical testing of the stopping criteria in Step 4, their analysis differs from the static solution quality assessment; see, e.g., similar sequential analysis in statistics (Chow and Robbins [49], Nadas [164], Ghosh et al. [85]), and in simulation of stochastic systems (Glynn and Whitt [91], Law and Kelton [144], Law et al. [143]).

The stopping rules presented below can work in conjunction with a range of algorithms using a variety of optimality gap estimators—including the ones presented in Sections 4.1 and 4.3—provided certain conditions are met. These conditions are as follows: (i) when no stopping criterion is applied, the algorithm eventually generates at least one optimal solution w.p.1; (ii) the statistical estimator of the optimality gap converges in probability to the true optimality gap uniformly in X, and if it is biased, it has the correct direction of bias (overestimation is preferred to minimize error); (iii) the sample variance of the optimality gap also satisfies desired convergence properties; (iv) sampling is done in a way that a form of CLT holds (e.g., i.i.d. sampling, antithetic, bootstrapping, etc.).

At iteration k of Algorithm 1, we have candidate solution x^k. Suppose using n_k samples, we obtain its optimality gap estimator $\mathcal{G}_k$ and its associated variance estimator s_k^2. For instance, these could be (18) and (22). Note that n_k may be different than N_k in Algorithm 1. The N_k observations are used to obtain the candidate solution x^k; in contrast, n_k observations are used to obtain the optimality gap statistical estimators. We assume that these two samples are independent from one another. Let $h' > 0$ and $\epsilon' > 0$ be two scalars. The following stopping criterion terminates the

algorithm at iteration

$$T = \inf_{k \geq 1} \{k : \mathcal{G}_k \leq h' s_k + \epsilon'\}. \tag{33}$$

In words, the algorithm terminates the first iteration when $\mathcal{G}_k$'s width relative to s_k falls below h' plus a small positive number ϵ'. Let $h > h'$ and $\epsilon > \epsilon'$ (both epsilon terms are small; see the below discussion on parameter settings). When the algorithm stops at iteration T with candidate solution x^T, a confidence interval on its optimality gap is given by

$$[0,\ hs_T + \epsilon]. \tag{34}$$

Note that the width of the confidence interval (34) is larger than the bound $h's_T + \epsilon'$ used for stopping.

Under a finite moment generating function assumption, when the sample sizes used for solution quality assessment are chosen according to

$$n_k \geq \left(\frac{1}{h - h'}\right)^2 \left(c_q + 2q \ln^2 k\right), \tag{35}$$

the confidence interval in (34) is asymptotically valid. That is,

$$\liminf_{h \downarrow h'} P\left(g(x^T) - \nu^* \leq hs_T + \epsilon\right) \geq 1 - \alpha$$

(note that the random elements in the above expression are T, x^T and s_T). Therefore, when h is close to h', or when n_k is large enough, we may expect the optimality gap of x^T to be within $[0,\ hs_T + \epsilon]$ with at least the desired probability of $1 - \alpha$. For fixed values of the parameters, it can be shown that the algorithm stops in a finite number of iterations w.p.1. The minimal sample size (35) grows as $O(\ln^2 k)$ with the iteration number k. When the moment generating function assumption is relaxed, larger growth in the sample sizes is required. For instance, when only finite second moments are assumed—which is a minimal assumption as we are using consistent sample variances—the growth in sample sizes needs to be essentially linear, $O(k)$.

The above stopping rule has some parameters to be selected. First, in implementation, the ϵ and ϵ' terms are not critical. They can be set to very small numbers, e.g., around 10^{-7}. They are needed to ensure finite stopping in theory and in practice they can serve as numerical tolerances. The more critical parameters are h and h'. How to select these parameters? Notice first that the minimal sample size growth formula for solution quality assessment given in (35) has an intercept term c_q. Here, $q > 0$ (hence $c_q > 0$) can be chosen to minimize computational effort. In order to minimize the number of parameters to select, simply a value from Table 1 of Bayraksan and Morton [18] can be used. Even if this parameter is not chosen correctly, the difference in the sample sizes used is not that dramatic. Next, an initial sample size n_1 is chosen depending on the problem at hand and the computational resources. The value of n_1 automatically dictates (via (35)) a value for $\Delta h = h - h'$. Choosing a value of h' requires more care. For this, a preliminary run with moderate

sample sizes can be conducted to examine the values of $\mathcal{G}_k/s_k$ and h' can be set to a value slightly lower than this. The value of h is then set such that $h = h' + \Delta h$.

The stopping rule in (33) can be viewed as a *relative*-width stopping rule; it is relative to the variability in the problem as measured by s_k. If there is a larger variance, the algorithm can stop with a larger value of $\mathcal{G}_T$ and a larger confidence interval on the quality of the obtained solution is made. Similarly, when the variability is low, the quality statement (34) will be tighter. Recent work looks at solving SAA with increasing sample sizes and stopping when the confidence interval on the candidate solution's optimality gap plus an inflation factor falls below a *fixed*-width (Bayraksan and Pierre-Louis [21]). This stopping rule using, for instance, the Single Replication Procedure (SRP) discussed in Section 4.1 is

$$T = \inf_{k \geq 1} \left\{ k : \mathcal{G}_k + \frac{z_\alpha s_k}{\sqrt{n_k}} + h(n_k) \leq \epsilon \right\} \tag{36}$$

where $h(n)$ is an inflation factor, which can be set to $1/\sqrt{n}$. This stopping rule aims to obtain ϵ-optimal solutions. It has fewer parameters (inflation factor, which can be simply set to $1/\sqrt{n}$, and ϵ, which can be based on knowledge on the problem or determined by a preliminary computational analysis); however, it is restricted to a class of problems that exhibit the exponential rate of convergence (see e.g., (30)).

6 Problems with stochastic constraints

We return now to formulation (SP), and consider the case where there are stochastic constraints, i.e., $K > 0$. Such problems arise naturally in applications where the decision x must satisfy inequalities but the functions defining the inequalities depend on a random parameter such as demand or future prices. For example, Atlason et al. [9] study a call staffing problems where the constraints ensure that the expected number of answered calls must be at least a certain percentage of the expected total number of received calls. The expected number of calls is approximated by sampling. Krokhmal et al. [137] study a portfolio optimization problem where the constraints are defined by the conditional value-at-risk (CVaR) of the random returns. CVaR constraints can also be used to provide convex approximations to chance constrained problems, as discussed in Nemirovski and Shapiro [168]. There are however some classes of problems where stochastic constraints play a fundamental modeling role, as we shall see below in Sections 6.1–6.3. Since specialized methods have been developed for these classes of problems, we will study them separately.

6.1 Problems with general expected-value constraints

We first discuss some general results that do not exploit any particular structure of the constraints. Bastin et al. [15], King and Rockafellar [133], Shapiro [217] and Wang and Ahmed [238] provide detailed analyses of the SAA approach to problems with expected-value constraints. In that case

the approximating problem is

$$\min_{x \in X} \left\{ \frac{1}{N} \sum_{j=1}^{N} G_0(x, \xi^j) \;\middle|\; \frac{1}{N} \sum_{j=1}^{N} G_k(x, \xi^j) \leq 0, \; k = 1, 2, \ldots, K \right\}. \tag{37}$$

The focus in Bastin et al. [15], King and Rockafellar [133] and Shapiro [217] is on the asymptotic convergence of optimal values and optimal solutions, which is accomplished under assumptions of continuity and/or convexity of the underlying functions and a study of the corresponding KKT conditions. In contrast, Wang and Ahmed [238] provide some results for finite sample sizes.

The main issue that arises when using sampling approximations within the constraints is that of *feasibility*. For example, consider a single constraint of the form $\mathbb{E}[G_1(x, \xi)] \leq 0$, and let $\bar{x}$ be a point on the boundary of the feasibility set so that $\mathbb{E}[G_1(\bar{x}, \xi)] = 0$. Moreover, suppose that $G_1(\bar{x}, \xi)$ is normally distributed. Consider the sampling approximation $\frac{1}{N} \sum_{j=1}^{N} G_1(\bar{x}, \xi^j)$. Clearly, by the strong law of large numbers, this quantity converges to zero w.p.1, so $\bar{x}$ is asymptotically feasible to the approximating problem. However, no matter how large N is, there is always a 50% chance that $\frac{1}{N} \sum_{j=1}^{N} G_1(\bar{x}, \xi^j) > 0$—in which case $\bar{x}$ is infeasible to the approximating problem. To circumvent this issue, we can replace the constraint $\mathbb{E}[G_1(x, \xi)] \leq 0$ with

$$\mathbb{E}[G_1(x, \xi)] \;\leq\; \epsilon, \tag{38}$$

where $\epsilon \in \mathbb{R}$. A positive value of ϵ provides a relaxation of the problem, whereas a negative value tightens the problem. Let U^ϵ denote the set defined by the set of $x \in X$ satisfying (38), and let U_N^ϵ be the corresponding set defined by the sampling approximation. Then, it is possible show that, under proper assumptions—which include compactness of X along with other conditions on $G_1(x, \xi)$ such as Lipschitz continuity—one has that, for any $\epsilon > 0$,

$$P\left(U^{-\epsilon} \subseteq U_N^0 \subseteq U^\epsilon\right) \;\geq\; 1 - Me^{-\beta \epsilon^2 N} \tag{39}$$

for some constants $M > 0$, $\beta > 0$. In other words, the probability that the feasibility set of the approximating problem is "sandwiched" between $U^{-\epsilon}$ and U^ϵ goes to one exponentially fast. The rate of convergence, of course, depends on the value of ϵ. Again, we refer to Wang and Ahmed [238] for details.

Under the SAA approach, given a realization $\{\hat{\xi}^1, \hat{\xi}^2, \ldots, \}$ of $\{\xi^1, \xi^2, \ldots, \}$, one then solves (37) for that realization. As before, any appropriate deterministic algorithm can be used to solve the corresponding problem, depending on the underlying structure (discrete, convex, etc.). In particular, one can use a penalization technique to bring the constraints into the objective function; see, for instance, Liu et al. [153] for a discussion. We are not aware of other approaches—for example, based on sequential-sampling methods such as those discussed in Section 3—designed specifically for general problems with expected-value constraints in mathematical programming. In contrast to mathematical programming, in the simulation community, often no assumptions on the

structure of G_k are made. The approximations are obtained through simulations of the system for a given decision x. There is a growing literature in the recent years that extend the simulation optimization methods to problems with expected-value constraints; see, e.g., Andradóttir and Kim [6], Batur and Kim [17], Lee et al. [148], Hunter and Pasupathy [119].

As in the case of problems with deterministic constraints, it is important to have a method that allows us to calculate statistical lower and upper bounds for the optimal value of problem (SP). The methods discussed in Section 4 can be extended to this setting, with some adjustments. Wang and Ahmed [238] suggest the following approach to derive a lower bound. Notice that the optimal value of $\min_{x\in X}\{\mathbb{E}[G_0(x,\xi)]\,|\,\mathbb{E}[G_1(x,\xi)]\leq 0\}$ is bounded from below by the optimal value of $\min_{x\in X}\{\mathbb{E}[G_0(x,\xi)]+\lambda\mathbb{E}[G_1(x,\xi)]\}$ for any $\lambda\geq 0$. Since the latter problem does not have stochastic constraints, the methods described in Section 4.1 can be used to obtain a lower bound for its optimal value. For example, by solving M independent approximations of the form

$$\nu_N(\lambda) \;:=\; \min_{x\in X}\left\{\frac{1}{N}\sum_{j=1}^{N}\left[G_0(x,\xi^j)+\lambda G_1(x,\xi^j)\right]\right\}$$

one can construct confidence intervals for $\mathbb{E}[\nu_N(\lambda)]$, which in turn is a lower bound for $\min\{\mathbb{E}[G_0(x,\xi)]+\lambda\mathbb{E}[G_1(x,\xi)]\}$. Of course, the quality of the overall bound will depend on the value of λ. One possible choice is to take λ as the optimal dual multiplier of the problem

$$\min_{x\in X}\left\{\frac{1}{N}\sum_{j=1}^{N}G_0(x,\hat{\xi}^j)\;\middle|\;\frac{1}{N}\sum_{j=1}^{N}G_1(x,\hat{\xi}^j)\leq 0\right\},$$

where the sample is independent of the samples drawn in each of the M replications. Note however that when the original problem is not convex (e.g., when the feasibility set is finite) such a lower bound can be loose even if N is large.

As in the case of problems with deterministic constraints, an upper bound for the optimal value of (SP) can be obtained simply by evaluating the objective function at any feasible solution. However, as we saw above, in case of stochastic constraints feasibility cannot be guaranteed since the functions defining the constraints cannot be evaluated exactly. One way (suggested by Shapiro et al. [227]) to ensure feasibility of a given $x\in X$ with a given confidence is to fix $0<\beta<1$ and construct a one-sided $100(1-\beta)\%$ confidence interval for $\mathbb{E}[G_1(x,\xi)]$ as

$$\frac{1}{N}\sum_{j=1}^{N}G_1(x,\xi^j)+z_\beta\sqrt{\frac{s_N^2(x)}{N}},$$

where $s_N^2(x)$ is the sample variance of the sample $\{G_1(x,\xi^1),\ldots,G_1(x,\xi^N)\}$. If the above quantity is less than or equal to zero, then we are $100(1-\beta)\%$ confident that x is feasible and consequently the objective value at x yields upper bound for the optimal value of (SP).

6.2 Problems with probabilistic constraints

This class of problems can be written as

$$\min_{x \in X} \{ \mathbb{E}\left[G_0(x,\xi)\right] \mid P\left(H(x,\xi) \leq 0\right) \geq 1-\alpha \}. \tag{40}$$

Clearly, such a problem falls into the framework of (SP) since we can write $P(H(x,\xi) \leq 0) \geq 1-\alpha$ as $\mathbb{E}[(1-\alpha) - \mathbb{I}\{H(x,\xi) \leq 0\}] \leq 0$, where as before $\mathbb{I}\{E\}$ denotes the indicator function of the event E. The constraints in (40) are used in situations where violation of the constraint inside the probability has a qualitative instead of a quantitative nature—that is, it matters whether the constraints are violated or not; the amount of violation is less important. Such constraints often used to model service level or reliability restrictions, such as "demand must be satisfied in at least 95% of the cases." Note that problems with joint constraints of the form $P(H_1(x,\xi) \leq 0, \ldots, H_K(x,\xi) \leq 0) \geq 1-\alpha$ can be represented as $P(H(x,\xi) \leq 0) \geq 1-\alpha$ by defining $H(x,\xi) := \max\{H_1(x,\xi), \ldots, H_K(x,\xi)\}$, although some properties such as differentiability may be lost in such representation. Still, using this representation, we can again assume that $K = 1$. Problems with probabilistic constraints (also called *chance constraints*) have been studied for decades, starting with the work of Charnes and Cooper [41]. As pointed out by Ahmed and Shapiro [2], the two major difficulties with such problems are that (i) evaluating $P(H(x,\xi) \leq 0)$ can be difficult (e.g., it may involve multidimensional integrals), and (ii) the set $\{x : P(H(x,\xi) \leq 0) \geq 1-\alpha\}$ may be nonconvex. This subject is very rich; we refer to Prékopa [199] for a thorough discussion, and to Ahmed and Shapiro [2] for a more recent view. For the purposes of this survey, we will review work that uses Monte Carlo methods to approximate the chance constraints.

We start by discussing a direct SAA approach for this class for problems. That is, we consider the problem

$$\min_{x \in X} \left\{ \frac{1}{N} \sum_{j=1}^{N} G_0(x,\xi^j) \;\middle|\; \frac{1}{N} \sum_{j=1}^{N} \mathbb{I}\{H(x,\xi^j) \leq 0\} \geq 1-\gamma \right\} \tag{41}$$

and as before consider the behavior of the optimal value and optimal solutions of (41) as function of N. Note that we have replaced the term $1-\alpha$ on the right hand side with $1-\gamma$, where γ is a parameter—as before, by allowing γ to be different from α we obtain a problem that is either more relaxed or more tight than the original one, which is important when considering feasibility issues. It is important to point out that the convergence analysis discussed in Section 6.1 cannot be used here since the function $\mathbb{I}\{H(\cdot,\xi^j) \leq 0\}$ is not continuous. Nevertheless, similar results to those seen in Section 2 can be derived in this setting. For example, Pagnoncelli et al. [180] show that, if (i) both G_0 and H are continuous in x, (ii) the set X is compact and (iii) there exists an optimal solution x^* such that, given any neighborhood of x^*, there exists some x in that neighborhood such that $P(H(x,\xi) \leq 0) > 1-\alpha$, then—using the same notation as in Section 2—$\nu_N \to \nu^*$ and $\text{dist}(x_N, S^*) \to 0$ w.p.1. Luedtke and Ahmed [156] show that, under similar assumptions to those discussed earlier—such as compactness of X and Lipschitz continuity of H with respect to x, or finiteness of X—an exponential convergence of the type (39) holds in this setting as well.

A natural question that arises is, how to solve the approximating problem (41)? To keep consistency with the notation used throughout the paper, let $\{\hat{\xi}^1, \hat{\xi}^2, \ldots, \}$ be a realization of $\{\xi^1, \xi^2, \ldots, \}$, and consider problem (41) defined for that specific realization. Here we need to distinguish between the two cases $\gamma = 0$ and $\gamma > 0$. When $\gamma = 0$, problem (41) can be equivalently written as

$$\min_{x \in X} \left\{ \frac{1}{N} \sum_{j=1}^{N} G_0(x, \hat{\xi}^j) \ : \ H(x, \hat{\xi}^j) \leq 0, \ j = 1, \ldots, N \right\}. \tag{42}$$

Depending on the structure of H—for example, when H is linear or convex in x—this can be a very tractable problem. The downside, of course, is that the replacement of $\alpha > 0$ with $\gamma = 0$ yields a more conservative model. Still, Campi et al. [38] improve upon an original result by Calafiore and Campi [36] and show that, given $0 < \delta \leq 1$, by choosing

$$N \ \geq \ \frac{2}{\alpha} \left(\log \frac{1}{\delta} + d_x \right)$$

(recall that d_x is the dimension of x in (SP)), the optimal solution to (42) is feasible to the original problem (40) with probability at least $1 - \delta$, regardless of the distribution of ξ when $H(\cdot, \xi)$ is convex. Nemirovski and Shapiro [167] show that a better value for N, which grows as $\log(1/\alpha)$ instead of $1/\alpha$, can be obtained under further assumptions on H and the distribution of ξ. Campi and Garatti [37] and Pagnoncelli et al. [181] discuss approaches to remove some of the sampled constraints in order to obtain a less conservative problem.

The situation is rather different when $\gamma > 0$ in (41). It is easy to see that convexity is lost because of the presence of the indicator functions even if H has nice properties. Note however that (41) is still a chance-constrained problem, where the underlying distribution is the empirical distribution defined by $\{\hat{\xi}^1, \ldots, \hat{\xi}^N\}$. Thus, any method proposed for chance-constrained problems with finite number of scenarios can be used to solve (41). For example, Dentcheva et al. [61] aim to find the so-called *p-efficient points* corresponding to the constraints, whereas Luedtke et al. [157] provide a strengthened integer programming formulation for the problem when $H(x, \xi)$ is of the form $\max_i\{\xi_i - h_i(x)\}$, i.e., one can separate the random component from the function.

A different sampling-based approach for chance constrained problems is proposed by Hong et al. [113] for the situation where, given $x \in X$, the function $H(x, \xi)$ is differentiable at x with probability one. Note that when H represents joint chance constraints such an assumption typically will not hold when ξ has discrete distribution, because of the "kinks" of the max function. When this assumption (and some others) do hold, Hong et al. [113] show that the constraint $P(H(x, \xi) \leq 0) \geq 1 - \alpha$ can be written as a difference of convex (DC) functions. As a result, the original problem can be approximated (by successive linearization of one of the functions in the DC formulation) by a sequence of convex problems, and in the limit one obtains a KKT point for the original problem. Because the functions in the DC formulation cannot be evaluated exactly, a sampling-based approach is proposed to solve each of these convex problems. Recently, problems with probabilistic constraints have also been studied from the perspective of ranking and selection

procedures; see Hong and Nelson [112].

It is possible to derive statistical lower and upper bounds for the optimal value of (40), ν^*. For a given $x \in X$ consider the estimator

$$\hat{p}(x) \ := \ \frac{1}{N} \sum_{j=1}^{N} \mathbb{I}\{H(x, \xi^j) > 0\}$$

of $p(x) := P(H(x, \xi) > 0)$. As discussed before, any feasible x yields an upper bound for the optimal value of the problem. A given $x \in X$ is feasible for (40) if $p(x) \leq \alpha$. In our context, computing $p(x)$ is impractical so we would like to use the estimator $\hat{p}(x)$. One way of doing this is to construct a one-sided $100(1-\beta)\%$ confidence interval for $p(x)$ similarly to the idea described for general expected-value constrained problems, i.e., given a realization $\{\hat{\xi}^1, \hat{\xi}^2, \ldots, \}$ of $\{\xi^1, \xi^2, \ldots, \}$, compute the value of $\hat{p}(x)$ corresponding that sample and check whether

$$\hat{p}(x) + z_\beta \sqrt{\frac{\hat{p}(x)(1-\hat{p}(x))}{N}} \ \leq \ \alpha, \tag{43}$$

where we used the fact that $\sum_{j=1}^{N} \mathbb{I}\{H(x, \xi^j) > 0\}$ has binomial distribution with parameters N and $p(x)$ and assumed that N is sufficiently large to ensure that the binomial distribution can be well approximated by a normal distribution with mean $Np(x)$ and variance $Np(x)(1-p(x))$. If (43) is satisfied, we are $100(1-\beta)\%$ confident that x is feasible.

More efficient techniques have been developed by exploiting the structure of the probabilistic constraints. Following Nemirovski and Shapiro [168], let $B(k; p, n)$ denote the cumulative distribution function of the binomial distribution with parameters n and p. Given $0 < \beta < 1$, define the quantity $U(x) := \sup\{\rho \in [0,1] \,|\, B(N\hat{p}(x); \rho, N) \geq \beta\}$ (note that $U(x)$ is random). Then, it is possible to show that $P(p(x) < U(x)) \geq 1 - \beta$. This suggests the following procedure: given a realization $\{\hat{\xi}^1, \hat{\xi}^2, \ldots, \}$ of $\{\xi^1, \xi^2, \ldots, \}$, compute the values of $\hat{p}(x)$ and $U(x)$ corresponding to that sample; if $U(x) \leq \alpha$, then we are $100(1-\beta)\%$ confident that x is feasible.

The calculation of lower bounds for the optimal value of (40) can in principle follow the method described in Section 6.1, but again the lack of convexity implies that Lagrangian-based bounds are not useful due to the existence of an optimality gap. The following alternative approach is suggested in Nemirovski and Shapiro [168] and Pagnoncelli et al. [180]. Consider problem (40), and suppose the objective function is deterministic (call it g_0). Consider M independent estimators of the optimal value ν^* of (40), defined by the optimal value of (41) with M independent samples of size N each. Let ν_N^j be the optimal value of the jth replication, and let $\nu_N^{(1)} \leq \ldots \leq \nu_N^{(M)}$ denote the corresponding order statistics. The procedure calls for using $\nu_N^{(L)}$ as a statistical lower bound for the optimal value of (40), as it can be shown that

$$P\left(\nu_N^{(L)} \leq \nu^*\right) \ \geq \ 1 - B(L-1; \theta_N, M),$$

where θ_N is defined as $B(\lceil \gamma N \rceil; \alpha, N)$ and as before $B(k; p, n)$ denotes the cumulative distribution

function of the binomial distribution with parameters n and p. This suggests the following procedure: given M independent realizations of $\{\xi^1, \xi^2, \ldots, \}$, let $\nu_N^{(j)}$ be the jth smallest value among the corresponding optimal values of the approximating problems. Choose L, M and N in a such a way that $B(L-1; \theta_N, M) \leq \beta$; then, we obtain that $\nu_N^{(L)}$ is a lower bound for ν^* with confidence of at least $100(1-\beta)\%$. Of course, there are many such possible choices for L, M and N, and an appropriate choice must take into account computational considerations; we refer to Pagnoncelli et al. [180] for a comprehensive discussion.

6.3 Problems with stochastic dominance constraints

We turn now to the class of optimization problems with *stochastic dominance* constraints. Stochastic dominance is used to compare the distributions of two random variables (e.g., see Müller and Stoyan [163]), thus providing a way to measure risk. Dentcheva and Ruszczyński [58, 59] first introduced optimization problems with stochastic dominance constraints as an attractive approach for managing risks in an optimization setting. While pursuing expected profits, one avoids high risks by choosing options that are preferable to a random benchmark. Recently, optimization models using stochastic dominance have increasingly been the subject of theoretical considerations and practical applications in areas such as finance, energy, and transportation (Karoui and Meziou [126], Roman et al. [203], Dentcheva and Ruszczyński [60], Dentcheva et al. [62], Drapkin and Schultz [65], Gollmer et al. [93], Luedtke [155], Nie et al. [172]). In the context of simulation, Batur and Choobineh [16] have used stochastic dominance to compare the performance metrics of multiple simulated systems, a task that requires appropriate statistical tests.

For completeness, we briefly review the main concepts of stochastic dominance. Given a real-valued random variable Z, we write the cumulative distribution function of Z as $F_1(Z; \eta) := P(Z \leq \eta)$. Furthermore, for $n \geq 2$, define recursively the functions

$$F_n(Z; \eta) := \int_{-\infty}^{\eta} F_{n-1}(Z; t)\, dt,$$

assuming that the first $n-1$ moments of Z are finite. We then say that Z stochastically dominates another random variable Y in nth order (denoted $Z \succeq_{(n)} Y$) if

$$F_n(Z; \eta) \;\leq\; F_n(Y; \eta) \quad \text{for all } \eta \in \mathbb{R}.$$

Let $(a)_+ = \max\{a, 0\}$. It is useful to note the equivalence given in Ogryczak and Ruszczyński [176] for $n \geq 2$

$$F_j(Z; \eta) \;=\; \frac{1}{(j-1)!}\mathbb{E}\left[((\eta - Z)_+)^{j-1}\right], \quad j = 2, \ldots, n, \tag{44}$$

which implies that the condition that the first $n-1$ moments of Z are finite suffices to ensure that $F_n(Z; \eta) < \infty$ for all η.

The concept of stochastic dominance is also related to utility theory (von Neumann and Morgenstern [237]), which hypothesizes that for each rational decision maker there exists a utility function

u such that the (random) outcome Z is preferred to the (random) outcome Y if $\mathbb{E}[u(Z)] \geq \mathbb{E}[u(Y)]$. Often the decision maker's exact utility function is not known; in such cases one would say that Z is preferred to Y if $\mathbb{E}[u(Z)] \geq \mathbb{E}[u(Y)]$ for all u belonging to a certain set of functions. This set of functions is determined by the risk attitude—for example, a *risk-averse* decision maker's utility function is nondecreasing and concave. To see the connection with the notions of stochastic dominance defined above (for $n = 1, 2$), let $\mathcal{U}_1$ be the set of all nondecreasing functions $u : \mathbb{R} \mapsto \mathbb{R}$ and let $\mathcal{U}_2$ be the set of all nondecreasing concave functions $u : \mathbb{R} \mapsto \mathbb{R}$. Then, it is well known that

$$Z \succeq_{(n)} Y \iff \mathbb{E}[u(Z)] \geq \mathbb{E}[u(Y)], \quad \forall u \in \mathcal{U}_n, \tag{45}$$

whenever the expectations exist. Stochastic dominance is also closely related to concepts of stochastic ordering; for example, the condition $\mathbb{E}[u(Z)] \geq \mathbb{E}[u(Y)]$ for all $u \in \mathcal{U}_2$ is called stochastic increasing concave order (see, e.g. Shaked and Shanthikumar [215]).

Using the above concepts, an optimization model with stochastic dominance constraints can then be formulated as follows (Dentcheva and Ruszczyński [58, 59]):

$$\begin{aligned} &\min g_0(x) \\ &\text{s.t. } H(x, \xi) \succeq_{(n)} Y \\ &\quad x \in X. \end{aligned} \tag{46}$$

The cases that have received most attention in the literature are $n = 1$ and $n = 2$. The difficulties with the $n = 1$ case are similar to those arising with probabilistic constraints, notable nonconvexity. The case $n = 2$, on the other hand, is a convex problem so long as $g_0(\cdot)$ is convex, $H(\cdot, \xi)$ is concave and the set X is convex—indeed, the equivalence (44) allows us to write the problem with expected value constraints, yielding

$$\begin{aligned} &\min g_0(x) \\ &\text{s.t. } \mathbb{E}\left[(\eta - H(x, \xi))_+\right] \leq \mathbb{E}\left[(\eta - Y)_+\right] \quad \forall \eta \in \mathbb{R} \\ &\quad x \in X, \end{aligned} \tag{47}$$

which is a convex program.

In principle, problem (47) falls into the general framework of Section 6.1, as it contains expected-value constraints. A major difference, however, is the fact that (47) has one constraint for each $\eta \in \mathbb{R}$—that is, it has uncountably many constraints. This issue is circumvented when the random variable Y has finitely many outcomes $y_1, \ldots, y_r$; in that case, Dentcheva and Ruszczyński [58] show that it suffices to write the constraints in (47) only for $\eta = y_j$, $j = 1, \ldots, r$, thus yielding a problem with finitely many expected-value constraints. When the distribution of ξ also has finite support, the expectations in (47) can be written as sums, so the problem becomes deterministic. When Y has infinitely many outcomes, it is natural to resort to sampling methods; note however that the analysis is more delicate than that described in Section 6.1 since it involves not only approximating

the expectations but also sampling over the set of (uncountably many) constraints. We will discuss that issue further shortly.

It is also useful to consider the case when the function H in (46) is vector-valued, which we write as $(H_1(x,\xi),\ldots,H_m(x,\xi))$. This situation occurs in many practical settings—for example, when $H(x,\xi)$ is a linear function of the form $A(\xi)x$, where $A(\xi)$ indicates a random matrix. Of course, in this case, Y is also an m-dimensional random vector. We have then two alternatives: one is to write the problem with m one-dimensional stochastic dominance constraints, i.e., $H_j(x,\xi) \succeq_{(n)} Y_j$, $j = 1,\ldots,m$. Even though such a formulation provides a direct extension of the unidimensional case seen above, it disregards the dependence among the components H_j of H. Alternatively, we can use concepts of multivariate stochastic dominance. One such concept is that of *convex dominance* introduced by Hu et al. [117]. Given m-dimensional random vectors Z and Y and a convex set $\mathcal{C} \subset \mathbb{R}^m$, we say that Z dominates Y in nth order linearly with respect to $\mathcal{C}$ if

$$v^T Z \ \succeq_{(n)} \ v^T Y \quad \text{for all } v \in \mathcal{C}. \tag{48}$$

Note that the notion of convex dominance includes as a particular case the concept of positive linear dominance (see, e.g., Müller and Stoyan [163]), which corresponds to $\mathcal{C} = \mathbb{R}^m_+$. Under convex dominance problem (47) is then written as

$$\begin{array}{l} \min g_0(x) \\ \text{s.t. } \mathbb{E}\left[\left(\eta - v^T H(x,\xi)\right)_+\right] \ \le \ \mathbb{E}\left[\left(\eta - v^T Y\right)_+\right] \quad \forall \eta \in \mathbb{R},\ \forall v \in \mathcal{C} \\ \qquad x \in X. \end{array} \tag{49}$$

Homem-de-Mello and Mehrotra [110] extend the aforementioned results of Dentcheva and Ruszczyński [58] and show that, when Y has finitely many outcomes $y_1,\ldots,y_r$ and the set $\mathcal{C}$ is polyhedral, the dominance relationship (48) for $n = 2$ can be written as

$$\mathbb{E}\left[\left(v_k^T y_j - v_k^T H(x,\xi)\right)_+\right] \ \le \ \mathbb{E}\left[\left(v_k^T y_j - v_k^T Y\right)_+\right] \quad j = 1,\ldots,r,\ k = 1,\ldots,K,$$

where $v_1,\ldots,v_K$ are certain vectors in the set $\mathcal{C}$. Thus, in that case the problem still has finitely many expected-value constraints.

Hu et al. [117] provide an analysis of sampling approximations to problem (49) (which includes (47) as a particular case). The corresponding sample average approximation is written as

$$\begin{array}{l} \min g_0(x) \\ \text{s.t. } \dfrac{1}{N}\displaystyle\sum_{j=1}^N \left((v_k^i)^T Y^i - (v_k^i)^T H(x,\xi^j)\right)_+ \ \le \ \dfrac{1}{N}\displaystyle\sum_{j=1}^N \left((v_k^i)^T Y^i - (v_k^i)^T Y^j\right)_+ \\ \qquad i = 1,\ldots,N,\ k = 1,\ldots,K \\ x \in X. \end{array} \tag{50}$$

In the above formulation, $\{(\xi^j,\ Y^j)\}$, $j = 1, \ldots, N$ are samples from $(\xi,\ Y)$, and the $\{v_k^i\}$, $i = 1, \ldots, N$ are certain vectors in $\mathcal{C}$. Typically, the v_k^i vectors are unknown in advance; to remedy the problem, a cutting-surface algorithm based on the ideas in Homem-de-Mello and Mehrotra [110] is proposed. Hu et al. [117] show that the algorithm converges in finitely many iterations to an optimal solution of (50). Moreover, the feasibility set U_N of (50) satisfies

$$P\left(U^{-\epsilon} \subseteq U_N \subseteq U^{\epsilon}\right) \ \geq \ 1 - Me^{-\beta\epsilon^2 N}$$

where U^{ϵ} is the feasibility set corresponding to the dominance constraint in (47) perturbed by ε on the right hand side.

Statistical lower and upper bounds (e.g., to assess solution quality) can also be derived for the approximation (50). Hu et al. [117] propose procedures which are based on similar ideas to those discussed in Section 6.1—more specifically, a Lagrangian-based relaxation for the lower bound, and the objective value of a feasible solution for the upper bound—but with the necessary adaptation to the setting of (49). Zhang and Homem-de-Mello [243] discuss an alternative procedure for the case where H is real-valued (rather than vector-valued) but the set X is nonconvex (for example, discrete). The basic idea is to formulate a hypothesis test to check feasibility of a given solution, and then use a multiple-replication procedure similar to that described in Section 4.1—but modified to discard certain replications—to calculate an optimality gap. We refer to that paper for details.

7 Variance reduction techniques

Monte Carlo sampling-based approximations and algorithms can be significantly improved by reducing the variability of the estimates they generate. Variance reduction techniques have a long history in the simulation and statistics literature. The main goal of such methods is to provide estimators of values associated with a random variable—for example, its mean—that have better properties than the standard Monte Carlo estimators. Consider for example the quantity $g_0(x)$ defined in (SP) for a fixed $x \in X$ and its sample average estimator defined in (1). When the sample $\{\xi^1, \ldots, \xi^N\}$ is independent and identically distributed, its variance is given by

$$\mathrm{Var}[g_N(x)] \ = \ \frac{\mathrm{Var}[G_0(x,\xi)]}{N}.$$

Although $\mathrm{Var}[G_0(x,\xi)]$ is typically unknown, it can be estimated by a sample variance as follows:

$$S_N^2(x) \ := \ \frac{\sum_{i=1}^N [G_0(x,\xi^i) - g_N(x)]^2}{N-1}.$$

The above estimator is unbiased, i.e., $\mathbb{E}[S_N^2(x)] = \mathrm{Var}[G_0(x,\xi)]$.

Of course, it is desirable to have estimators with as small variance as possible. While this is the case in the context of pointwise estimation, it is even more so in the case of optimization, since poor estimates of the objective (or of its derivatives) may lead to slow convergence of an algorithm.

Clearly, if $\text{Var}[G_0(x,\xi)]$ is large then $\text{Var}[g_N(x)]$ will be large as well, unless the sample size can be chosen to counterbalance that effect. In many cases, however, choosing a large sample size is not practical, as the evaluation of $G_0(x,\hat{\xi})$ for a given $\hat{\xi}$ can be costly.

The goal of variance reduction techniques is to derive estimators $g_N(x)$, ν_N, etc. with smaller variance than those obtained with standard Monte Carlo. While in some cases this is accomplished by exploiting the structure of the problem, some general techniques do exist. We discuss next some variance reduction methods and their use in the stochastic optimization context.

In our presentation below, we revert to the case where there are no stochastic constraints (K in (SP) is 0) and we drop the subscript 0 from the objective function in (SP). To further ease exposition, we present the ideas in terms of estimating $\mathbb{E}[G(x,\xi)]$ for a given $x \in X$ and point to references where there is also optimization of $\mathbb{E}[G(x,\xi)]$ over $x \in X$. Also, for some of the methods discussed below we assume that the vector ξ has independent components. When such an assumption does not hold one can often write the components of ξ as functions of some independent uniform random variables; see, for instance, Biller and Ghosh [27].

7.1 Antithetic Variates

Antithetic Variates (AV) aims to reduce variance by inducing correlations. Suppose N is even and components of ξ are independent. Instead of using N i.i.d. random variates, the AV estimator aims to use $N/2$ negatively correlated pairs $(\underline{\xi}^j,\ \overline{\xi}^j)$, $j = 1,\ldots,N/2$. This is typically achieved by generating $N/2$ i.i.d. random vectors $U^1,\ldots,U^{N/2}$ of dimension d_ξ distributed uniformly over $[0,1]^{d_\xi}$, and their corresponding antithetic variates from the opposite end of the distribution (taken component-wise), $1-U^1,\ldots,1-U^{N/2}$, which are also i.i.d. distributed uniformly over $[0,1]^{d_\xi}$ but $(U^j, 1-U^j)$, $j = 1,\ldots,N/2$ are negatively correlated. Then, regular variate generation techniques are utilized to generate the pairs $(\underline{\xi}^j, \overline{\xi}^j)$ using $(U^j, 1-U^j)$. For the case with dependent components of ξ, we refer to Rubinstein et al. [209].

In contrast to the standard Monte Carlo estimator of $\mathbb{E}[G(x,\xi)]$ with variance $N^{-1}\sigma^2(x) := N^{-1}\text{Var}[G(x,\xi)]$, the antithetic variates estimator

$$g_{N,\text{AV}}(x) = \frac{1}{N/2}\sum_{j=1}^{N/2}\frac{G(x,\underline{\xi}^j) + G(x,\overline{\xi}^j)}{2}$$

has variance $N^{-1}\sigma^2(x)+N^{-1}\text{Cov}(G(x,\underline{\xi}^j), G(x,\overline{\xi}^j))$. Therefore, as long as $\text{Cov}(G(x,\underline{\xi}^j), G(x,\overline{\xi}^j)) < 0$, the antithetic estimator has a smaller variance than its crude Monte Carlo counterpart and they both produce unbiased estimators of the expectation.

The degree of variance reduction depends on the extent to which the negative correlation between the pair $(\underline{\xi}^j,\ \overline{\xi}^j)$ is preserved after $G(x,\cdot)$ is applied to this pair. Higle [99] argues that the negative correlation can be preserved for a class of two-stage stochastic linear programs with stochasticity only on the right-hand side and presents computational results. This is because $G(x,\cdot)$ is a monotone function of the right-hand side of the second stage problem for this class of prob-

lems. In general, if $G(x, \cdot)$ is a bounded and monotone function in each of its arguments that is not constant in the interior of its domain, variance reduction can be achieved using AV (Lemieux [150]). Koivu [135] and Freimer et al. [79] expand the work of Higle [99] by also considering ν_N, the optimized sample means. Freimer et al. [79] analytically show the extent of variance reduction using AV on a newsvendor problem and present computational results on two-stage stochastic linear programs. The computations in Koivu [135] indicate that when the monotonicity in the objective function is lost, AV can increase (e.g., double) the variance. However, when AV is effective, combination of AV with other variance reduction techniques such as randomized quasi-Monte Carlo is found to be very effective. These papers indicate that antithetic variates can result in modest variance reduction with minimal computational effort for a class of stochastic optimization problems.

7.2 Latin Hypercube Sampling

A fairly general way of obtaining estimators with smaller variance is based on the concept of stratified sampling (see, for instance, Fishman [76] and references therein). Generally speaking, the idea is to partition the sample space and fix the number of samples on each component of the partition, which should be proportional to the probability of that component. This way we ensure that the number of sampled points on each region will be approximately equal to the *expected* number of points to fall in that region. It is intuitive that such a procedure yields smaller variance than crude Monte Carlo; for proofs see Fishman [76]. Notice however that, though theoretically appealing, implementing such a procedure is far from trivial, since the difficulty is to determine the partition as well as to compute the corresponding probabilities.

There are many variants of this basic method; a classical one is the so-called *Latin Hypercube Sampling* (LHS) approach, introduced in McKay et al. [159]. The LHS method operates as follows. Suppose we want to draw N samples from a random vector ξ with d_ξ independent components, each of which has a Uniform(0,1) distribution. The algorithm consists repeating the two steps below for each dimension $j = 1, \ldots, d_\xi$:

1. Generate
$$Y^1 \sim U\left(0, \frac{1}{N}\right),\ Y^2 \sim U\left(\frac{1}{N}, \frac{2}{N}\right), \ldots, Y^N \sim U\left(\frac{N-1}{N}, 1\right);$$
2. Let $\xi_j^i := Y^{\pi(i)}$, where π is a random permutation of $1, \ldots, N$.

Figure 5 illustrates a Latin hypercube sample of size $N = 4$ for a two-dimensional vector.

In McKay et al. [159], it is shown that each sample ξ_j^i (viewed as a random variable) has *the same distribution* as ξ_j, which in turn implies the estimators generated by the LHS method are unbiased. In case of arbitrary distributions, the above procedure is easily modified by drawing the sample as before and applying an inversion method.

It is also shown in McKay et al. [159] that, under some conditions, the LHS method does indeed reduce the variance compared to standard Monte Carlo. Stein [231] and Owen [178] show

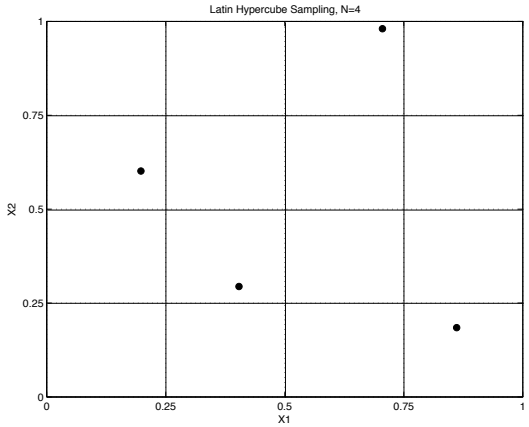


Figure 5: Latin Hypercube sample of $N = 4$ points in two dimensions.

that, asymptotically (i.e., as the sample size N goes to infinity), LHS is never worse than standard Monte Carlo, even without the assumptions of McKay et al. [159]. More specifically, $V_{LHS} \leq N/(N-1)V_{MC}$, where V_{LHS} and V_{MC} are respectively the variances under LHS and standard Monte Carlo. Thanks to such properties (and to the simplicity of the method), the LHS technique has been widely used in simulation, showing up even in off-the-shelf spreadsheet-based software.

One drawback of using the LHS method is that, by construction, the generated samples are *not* independent—indeed, variance is reduced precisely because of the correlation introduced by the method. Lack of independence implies that classical statistical results such as the Central Limit Theorem do not apply directly to the resulting estimator; consequently, confidence intervals cannot be built in the standard way. It is worthwhile mentioning that Owen [177] proves a version of the CLT for LHS estimators, which is useful from the perspective of rates of convergence but not necessarily for the construction of confidence intervals as the result involves some quantities that are difficult to estimate. In practice, in order to derive confidence intervals one typically performs multiple independent replications (for example, m replications, each with a sample of size N) and applies the classical theory to the data set consisting of the LHS average estimator from each replication.

The use of LHS in stochastic optimization, while not as widespread as in simulation, has demonstrated the benefits of that approach, as reported in papers such as Bailey et al. [10], Shapiro et al. [226], Linderoth et al. [152], Homem-de-Mello et al. [111]. Freimer et al. [79] study in detail the effect of using LHS in the context of the newsvendor model, and draw some general conclusions about the effectiveness of that approach for stochastic optimization. Homem-de-Mello [109] studies the rates of convergence of estimators of optimal values and optimal solutions, very much along the lines of the discussion in Section 2.2. Again, the difficulty in the latter paper lies in the lack of independence of the samples generated with LHS; by building upon the works of Owen [177] and Drew and Homem-de-Mello [68], it is shown that the rates obtained with LHS are not worse than those obtained with standard Monte Carlo and typically are better.

7.3 Quasi-Monte Carlo

Quasi-Monte Carlo (QMC) methods have a long history as tools to approximate integrals, and as such have been widely used in many areas. Describing all the nuances and the properties of such methods would fall out of the scope of this paper; thus, we only provide a brief discussion. We refer to Niederreiter [173], Lemieux [150] and Dick and Pillichshammer [63] for comprehensive treatments of QMC concepts. To set the stage, consider again the function $G(x, \xi)$ and assume that ξ is a random vector with independent components, each with uniform distribution on $[0, 1]^{d_\xi}$. Consider the problem of estimating $g(x) := \mathbb{E}[G(x, \xi)]$ for a fixed x.

The basic idea of QMC is to calculate a sample average estimate as in the standard Monte Carlo but, instead of drawing a random sample from the uniform distribution on $[0, 1]^{d_\xi}$, a certain set of points $\hat{\xi}^1, \ldots, \hat{\xi}^N$ on space $[0, 1]^{d_\xi}$ is carefully chosen. The deterministic estimate

$$g_{N,\mathrm{QMC}}(x) := \frac{1}{N} \sum_{i=1}^{N} G(x, \hat{\xi}^i) \tag{51}$$

is constructed. A key result is the so-called Koksma-Hlawka inequality which, roughly speaking, states that the quality of the approximation given by $g_{N,\mathrm{QMC}}(x)$ depends on the quality of the chosen points (measured by the difference between the corresponding empirical measure and the uniform distribution, which is quantified by the so-called *star-discrepancy*) as well as on the nature of the function $G(x, \cdot)$ (measured by its total variation). A great deal of the research on QMC methods aims at determining ways to construct *low-discrepancy sequences*, i.e., sequences of points $\hat{\xi}^1, \hat{\xi}^2, \ldots$ for which the star-discrepancy is small for all N. Particular types of sequences that have proven valuable are the so-called *digital nets* and also *lattice rules*. For example, some types of digital nets can be shown to yield approximations such that the error $|g_{N,\mathrm{QMC}}(x) - g(x)|$ is of order $(\log N)^{d_\xi}/N$. Figure 6 illustrates a particular type of QMC sequence of $N = 27$ points for a two-dimensional vector. In the figure, we see nine major boxes, each one divided into nine smaller boxes. We can see that each major box contains exactly three points and, moreover, those three points are placed in such a way that each row and each column of every major box contains exactly one point.

Despite the theoretical attractiveness of QMC methods with respect to error rates, an issue that arises when using such techniques in practice is the fact that the bounds provided by the Koksma-Hlawka inequality involve difficult-to-compute quantities such as the total variation of $G(x, \cdot)$, i.e., they yield qualitative (rather than quantitative) results; hence, obtaining a good estimate of the error may be difficult. A common way to overcome this issue is to incorporate some randomness into the choice of QMC points. By doing so, errors can be estimated using standard methods, e.g., via multiple independent replications. Some choices for randomizing the points of the QMC sequence include the so-called Cranley-Patterson procedure—where every number in the sequence is perturbed (modulo 1) by a single number generated from a Uniform(0,1) distribution—and scrambling the digits of each number in the sequence in a particular way; we refer to L'Ecuyer and

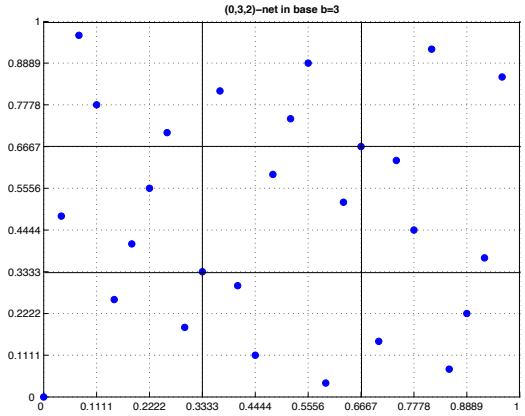


Figure 6: Quasi-Monte Carlo sample of $N = 27$ points in two dimensions.

Lemieux [146] for details.

Even with the randomization, one should be cautious when using QMC methods since oftentimes these techniques "backfire" in problems with moderate or large dimensionality if not used properly. This can be explained by the fact that the error rates depend on the dimensionality—for example, the $(\log N)^{d_\xi}/N$ rate seen above. In such cases, one may try to determine the *effective dimension* of the problem, i.e., the number of variables that account for most of the variability, and then apply a QMC strategy only for those variables. Such notion can be made precise, see for instance Owen [178, 179]. Moreover, the theoretical rates derived for QMC often rely on smoothness of the integrand, which may not always be present. Still, when used properly such techniques can be highly valuable, resulting in estimators that are orders of magnitude better than standard Monte Carlo.

Similarly to what happens with standard random numbers, generating a good QMC sequence may not be simple. Some sequences are easy to generate but the more powerful ones require sophisticated methods. Fortunately, public software is available—here we mention Friedel and Keller [80], Lemieux et al. [151], L'Ecuyer [145], L'Ecuyer and Munger [147] where libraries can be found.

A few papers study the application of QMC methods to stochastic optimization problems. In Kalagnanam and Diwekar [123], empirical results are provided for the use of Hammersley sequences (one form of QMC). Drew and Homem-de-Mello [67] use the aforementioned concept of effective dimension to develop an algorithm for two-stage stochastic programs that attempts to determine the "important variables" in the problem based on dual information. The remaining variables are "padded" with either Monte Carlo or Latin Hypercube sampling; a rigorous analysis of such strategy can be found in Drew [66]. As in the case of LHS discussed in Section 7.2, theoretical results on convergence—along the lines of those described in Sections 2.1 and 2.2—are harder to obtain than in the Monte Carlo case due to the loss of the i.i.d. property. In Pennanen [186] and Pennanen and Koivu [187], the authors show that, under mild assumptions, the estimator function g_N constructed with QMC points *epiconverges* to the true function g, which guarantees convergence of optimal values and optimal solutions under appropriate further conditions; in Koivu [135] those

results are applied to the case where the QMC sequence is randomized with the Cranley-Patterson procedure. The numerical results in those papers also suggest considerable gains in terms of rates of convergence when using QMC methods. Homem-de-Mello [109] studies the rates of convergence of estimators of optimal values under randomized QMC. Results are provided for a specific QMC method for which a Central Limit Theorem exists. One particular difficulty that arises when using QMC methods for stochastic programming problems lies in the fact that such problems do not have smooth integrands, although recent work by Heitsch et al. [98] sheds new light on the issue.

7.4 Importance Sampling

Importance Sampling (IS) aims to reduce variance by concentrating the sampling to the most important regions. Suppose again the aim is to estimate $\mathbb{E}[G(x,\xi)]$ for a given $x \in X$ and suppose ξ has density f. Then, $g(x) = \mathbb{E}[G(x,\xi)] = \int_\Xi G(x,\xi) f(\xi) d\xi$. Now consider another density q over Ξ such that $q(E) = 0$ for every set E for which $f(E) = 0$ and rewrite $\mathbb{E}[G(x,\xi)] = \int_\Xi G(x,\xi)\mathcal{L}(\xi) q(\xi) d\xi$. Here, $\mathcal{L}(\xi) = \frac{f(\xi)}{q(\xi)}$ is the *likelihood ratio*, which we assume is well-defined (for this, we may set $\mathcal{L}$ to zero whenever both f and q are zero). Instead of the usual Monte Carlo estimator $g_N(x) = \frac{1}{N}\sum_{j=1}^N G(x,\xi^j)$ that uses an i.i.d. sample $\xi^1, \xi^2, \ldots, \xi^N$ from the density f, the importance sampling estimator

$$g_{N,\mathrm{IS}}(x) = \frac{1}{N}\sum_{j=1}^N G(x,\tilde{\xi}^j)\mathcal{L}(\tilde{\xi}^j)$$

uses an i.i.d. sample $\tilde{\xi}^1, \tilde{\xi}^2, \ldots, \tilde{\xi}^N$ from the new density q. Note that both estimators are unbiased. However, not all choices of density q will lead to a reduction in variance. In fact, if q is not chosen appropriately, it might lead to an increase in variance. Therefore, finding an appropriate density q is critical to IS and much of the research in this area is directed to this issue.

To understand how to find q, consider the following facts. First, $\mathbb{E}[G(x,\tilde{\xi})\mathcal{L}(\tilde{\xi})] = \mathbb{E}[G(x,\xi)]$ and $\mathbb{E}[G^2(x,\tilde{\xi})\mathcal{L}^2(\tilde{\xi})] = \mathbb{E}[G^2(x,\xi)\mathcal{L}(\xi)]$. Therefore, the variance of the IS estimator is given by

$$\mathrm{Var}[g_{N,\mathrm{IS}}(x)] = \frac{1}{N}\left[\mathbb{E}[G^2(x,\xi)\mathcal{L}(\xi)] - (\mathbb{E}[G(x,\xi)])^2\right], \tag{52}$$

and the variance is reduced if and only if $\mathbb{E}[G^2(x,\xi)\mathcal{L}(\xi)] < \mathbb{E}[G^2(x,\xi)]$. If we want to minimize the variance—i.e., have zero variance—in (52), we need to have q such that $\mathbb{E}[G^2(x,\xi)\mathcal{L}(\xi)] = (\mathbb{E}[G(x,\xi)])^2$. When $G(x,\cdot)$ is nonnegative, this results in the optimal zero-variance density $q^*(\xi) = \frac{f(\xi)G(x,\xi)}{\mathbb{E}[G(x,\xi)]}$. This optimal density, however, requires the knowledge of an unknown quantity, $\mathbb{E}[G(x,\xi)]$, and is therefore unattainable. Nevertheless, this gives the intuition that q should be approximately proportional to $f(\xi)G(x,\xi)$ in order to achieve variance reduction even though the proportionality constant may not be known.

Importance sampling is one of the earliest variance reduction methods applied to two- and multistage stochastic linear programs (Dantzig and Glynn [53], Infanger [120], Dantzig and Infanger [52]). Dantzig and Glynn [53] suggest using an additive approximation of $G(x,\xi)$ given by $G(x,\overline{\xi}) + \sum_{i=1}^{d_\xi}\Delta_i G(x,\xi)$, where $\overline{\xi}$ is a base case and each $\Delta_i G(x,\xi)$ gives the marginal effect of the ith

element of ξ. They suggest finding the marginal effects by $\Delta_i G(x,\xi) = G(x,\overline{\xi}_i) - G(x,\overline{\xi})$, where $\overline{\xi}_i$ agrees with the base case $\overline{\xi}$ in all elements except for the ith element, which agrees with ξ. This results in solving $d_\xi + 1$ linear programs to determine q, one for each marginal and one for the base case. The authors argue that in the context of power generation, IS can capture rare events such as power supply down and high demands better than crude Monte Carlo, which are supported by the computations in Infanger [120]. Higle [99] applies this method to a wider range of problems and the computations here indicate that the method can be effective in reducing variance of $\mathbb{E}[G(x,\xi)]$ estimates for some problems but it can also lead to complications in defining the sampling distribution whenever $\Delta_i G(x,\xi)$ turns out to be zero and can actually increase variance for some other problems.

There is significant work on how to determine the IS distribution in the literature as this is critical to the success of IS. We briefly mention these without getting into much detail. In exponential tilting, the IS distribution is restricted to belong to an exponential family of distributions (Glasserman [87], Siegmund [229]). Similarly, a method of Rubinstein and Shapiro [210] parameterizes the IS distribution and solves a stochastic optimization problem to determine the parameters of this distribution in order to minimize variance. This optimization can be done via a sampling-based method and perturbation analysis; see, e.g., Fu [81]. Other approaches in the literature to obtain the IS distribution include large deviations theory (Glasserman et al. [88]), nonparametric methods (Neddermeyer [165], Zhang [244]), and minimization of the Kullback-Leibler distance to the optimal distribution (de Boer et al. [55]).

In the context of stochastic optimization, changes in x throughout an optimization routine can result in different IS distributions for different x. Shapiro and Homem-de-Mello [222] discuss the idea of using *trust regions* on which the same IS distribution can be used, but the results are inconclusive. Barrera et al. [11] employ IS techniques for a chance-constrained problem in which the violation probabilities α_k in (40) are very small, so the methods for choice of sample sizes discussed in Section 6.2 are not practical. They show that, for the application they study, there exist IS distributions that are good for all $x \in X$. Recent work of Kozmík and Morton [136] apply IS within the stochastic dual dynamic programming algorithm for multistage stochastic programs with nested mean-CVaR objectives and show promising results. As only relatively few scenarios under random sampling contribute to estimating CVaR, an IS scheme provides better estimators by concentrating the sampling to the important regions. A thorough study of sequential IS methods remains an open research area (Birge [29]).

7.5 Control Variates

Like antithetic variates, Control Variates (CV) aim to reduce variance by inducing correlations. In the case of control variates, though, this is achieved by introducing a *control variable* that can either be negatively or positively correlated with $G(x,\xi)$. Let C denote the control variable and λ be a scalar. Suppose $\mathbb{E}[C] = 0$. Note that if the mean of the control variable is known, which is often the case, then it can be subtracted from it to obtain a variable with zero mean. The control

variate estimator of $\mathbb{E}[G(x,\xi)]$ is given by

$$g_{N,\mathrm{CV}}(x) = \frac{1}{N}\sum_{j=1}^{N}\left(G(x,\xi^j) + \lambda C^j\right).$$

For any given λ, $g_{N,\mathrm{CV}}(x)$ is an unbiased estimator with variance

$$\frac{1}{N}\left(\sigma^2(x) + \lambda^2 \mathrm{Var}[C] + 2\lambda \mathrm{Cov}[G(x,\xi), C]\right). \tag{53}$$

We can minimize this variance by setting λ to $\lambda^* = \frac{-\mathrm{Cov}[G(x,\xi),C]}{\mathrm{Var}[C]}$. Plugging λ^* back in (53), we see that as long as C and $G(x,\xi)$ are correlated, the variance of the CV estimator

$$\mathrm{Var}[g_{N,\mathrm{CV}}(x), \lambda^*] = \frac{1}{N}\left(\sigma^2(x) - \frac{\mathrm{Cov}^2[G(x,\xi),C]}{\mathrm{Var}[C]}\right)$$

is less than the variance of the crude MC estimator, $N^{-1}\sigma^2(x)$. Notice that even though $\mathrm{Var}[C]$ may be known, $\mathrm{Cov}[G(x,\xi),C]$ is unknown but can be estimated, resulting in an estimator of λ^*. Unfortunately, when an estimator of λ^* is used, $g_{N,\mathrm{CV}}(x)$ is no longer unbiased. However, this can still yield significant variance reduction and the resulting CV estimator obeys a CLT of the form

$$\sqrt{N}\left(g_{N,\mathrm{CV}}(x) - \mathbb{E}[G(x,\xi)]\right) \xrightarrow{d} \mathrm{Normal}(0, \mathrm{Var}[g_{N,\mathrm{CV}}(x), \lambda^*])$$

due to a result of Nelson [166].

Higle [99] presents a number of control variates to estimate $\mathbb{E}[G(x,\xi)]$ that are cheap to compute and are quite effective across a number of test problems. Shapiro and Homem-de-Mello [222] use linear control variates to obtain more accurate estimators of the gradient, Hessian, and the value of $\mathbb{E}[G(x,\xi)]$ at a current solution point x in each iteration of a Monte Carlo sampling-based method to solve two-stage stochastic linear programs. Similarly, Pierre-Louis et al. [194] use a subgradient-inequality-based linear control variate within stratified sampling to estimate $\mathbb{E}[G(x,\xi)]$ at each iteration's solution x of an algorithm for a class of two-stage stochastic convex programs. Both papers show that control variates significantly reduce variance (up to more than 1,000 times in some cases) and allow these Monte Carlo sampling-based solution procedures to be numerically more viable.

8 Other topics

There are several topics related to Monte Carlo methods for stochastic optimization that we have not covered in this survey, as that would make this paper much longer than what it already is. In this final section we briefly discuss some of these topics.

One area that has received considerable attention in recent literature is that of *scenario generation methods*. The idea of such methods is to select particular scenarios to approximate the original

problem, rather than picking them randomly as in the Monte Carlo approach. Quasi-Monte Carlo methods can be viewed in this category, but other approaches exist where not only are the scenarios chosen but also the weight of each scenario—recall that in QMC all scenarios have weight $1/N$. This is the case, for example, of sparse grid methods, where scenarios can even have negative weights; see Chen et al. [45] for a study of such methods in stochastic optimization. Another class of methods, based on probability metrics, aims at finding a distribution Q with relatively few scenarios in such a way that Q minimizes a distance $d(P, Q)$ between Q and the original distribution P. Typically, these approaches rely on stability results that ensure that the difference between the optimal values of the original and approximating problems is bound by a constant times $d(P, Q)$. Several distances for distributions can be used for that purpose, such as the Wasserstein distance and the Fortet-Mourier metric. This type of approach has gained attention especially for the case of multistage problems, where the goal is to derive a scenario tree that properly approximates the original problem, though more sophisticated distances are required in that case. We refer to Pflug [191], Dupačová et al. [72], Heitsch and Römisch [96, 97], Pflug and Pichler [192] and references therein for further discussions on this type of methods. Other existing approaches for scenario generation include clustering (e.g., Dupačová et al. [71]) and moment-matching techniques, see for instance Høyland and Wallace [114], Høyland et al. [115] and Mehrotra and Papp [160].

An important class of stochastic optimization problems that does not fall directly into the framework of SP is that of problems with *stochastic equilibrium constraints*. Such constraints are often expressed as variational inequalities of the form

$$G(x, y, \xi)^T(y' - y) \;\geq\; 0 \quad \text{w.p.1} \quad \forall y' \in \mathcal{C}, \tag{54}$$

where $\mathcal{C}$ is a non-empty closed convex subset of $\mathbb{R}^m$. Several variations of (54) are possible—for example, y may be allowed to depend on ξ or may have to be chosen before ξ is known; another variation is to impose that (54) hold with $\mathbb{E}[G(x, y, \xi)]$ in place of $G(x, y, \xi)$. The case with $\mathcal{C} = \mathbb{R}^m_+$ corresponds to problems with linear complementarity constraints. SAA approaches have been developed for such problems, and many convergence results (including rates of convergence) are available; see for instance Gürkan et al. [95], Birbil et al. [28], Shapiro and Xu [225], Xu [240] and Liu et al. [153].

Another prominent issue that arise in the optimization of stochastic problems of the form (SP) is the *estimation of derivatives*. In the discussion presented above (see Algorithm 1), it was assumed that one can take "optimization steps" from the current iterate. In some cases that task can be accomplished by computing the gradient—or a subgradient—of the function $g_N(\cdot)$ in (1), which in turn is given by the average of the gradients of the summands. Such a procedure can shown to be unbiased and consistent, in the sense that $\mathbb{E}[\nabla g_N(x)] = \nabla g(x)$ and $\nabla g_N(x) \to \nabla g(x)$ w.p.1; typical conditions for that are some kind of uniform convergence (w.p.1) of $g_N(\cdot)$ to $g(\cdot)$, which in particular is the case of convex problems. In other cases, however, the gradient $\nabla G(x, \xi)$ cannot be computed; such problems often appear in simulation, for example. Gradient estimators still can be computed in such cases through more involved procedures such as perturbation analysis, likelihood

ratios, and conditional Monte Carlo, to name a few. Classical treatment of such problems can be found in Glasserman [86], Rubinstein and Shapiro [210], Pflug [190] and Fu and Hu [83], see also Robinson [201] and Homem-de-Mello [107] for the case where the function $g(\cdot)$ is non-differentiable.

One important feature of the problems studied in this paper is the assumption that the distribution of the underlying random vector ξ is known, so samples can be drawn from that distribution. In many problems, however, the distribution is actually unknown. Typically, there are two ways to approach this issue. One is to assume that the distribution belongs to a certain set, and then optimize over the worst-case distribution in that set. In other words, problem (SP) is replaced by a min-max problem of the form $\min_x \max_P \mathbb{E}_P[G_0(x,\xi)]$. Such an approach has a long history; see for instance Dupačová [69]. Shapiro and Kleywegt [224] study the application of Monte Carlo sampling—more specifically, the SAA approach—for this type of problem. More recently, the min-max approach has become known as *distributionally robust optimization*, and a great deal of attention has been given into finding tractable approximation for such problems. We refer the reader to Goh and Sim [92] for some recent work in this area. Another way to deal with the problem of unknown distributions is to use a data-driven approach that optimizes directly from the data—for example, this is typical in the area of machine learning. Liyanage and Shanthikumar [154] discuss a technique for that purpose which they call operational statistics. As it turns out, the distributionally robust and the data-driven approaches are not exclusive; in fact, for the case of i.i.d. data one can derive robustness sets of distributions based on the data, as done in Delage and Ye [56] and Xu et al. [241].

The issue of learning from the data gets more complicated when the data points are not i.i.d. observations from a (unknown) distribution. For example, Lee et al. [149] discuss a simple variant of the newsvendor model where the observed demand depends on the current order quantity. A more general way to view the problem is to think that one cannot observe the random vector ξ but only the function value $G(x,\xi)$ for each given value of x. This situation is akin to that of multi-armed bandit problems, though considerably more complicated in this case given the multi-dimensionality of the decision vector x. It is worthwhile noticing that, while such setting has some overlap with the framework of simulation optimization discussed in Section 3.3, there is a major difference—namely, one cannot generate samples but rather can only observe the function values. Learning algorithms for such a problem have been recently developed, we refer to Ryzhov et al. [212] and references therein.

9 Conclusions and Future Directions

In this paper, we have surveyed the current landscape of theory and methodology of Monte Carlo sampling for stochastic optimization. Our goal was to provide an overview of this rich area for students, practitioners, and researchers, with the aim of stimulating further research in this field. In particular, we have discussed stochastic optimization problems with deterministic and stochastic constraints, reviewing the theoretical results and algorithms, including aspects such as solution

quality assessment, stopping criteria, and choice of sample sizes under standard Monte Carlo sampling. We have also discussed alternative sampling techniques for variance reduction and pointed the readers to other topics in the literature. For future research, in addition to improvements to the methods described in the paper, we list below some topics that are of interest.

One of the open areas of research is the use of *Monte Carlo sampling in optimization of risk measures*. Managing risk is critically important in many applications and there is a growing literature of risk models developed by our community. While some recent work started to appear in this area (see, e.g., Shapiro [221]), the theory and efficient methodology of using Monte Carlo sampling for these models still need to be investigated.

Data-driven methods: In practice, many applications are data-rich. While Monte Carlo sampling-based methods are amenable to rich data use, direct links between real-world data and stochastic optimization still remain to be established. Data-driven methods that incorporate data into optimization problems need to be further developed. Additionally, in many real-world systems, the underlying stochastic process is non-stationary and methods to handle these non-stationary systems need to be investigated. Of interest are the machine learning, Bayesian, and other statistical methods to handle data-rich applications from a practical and theoretical point of view.

Connections between simulation-optimization methods and Monte Carlo methods for more structured stochastic optimization methods such as those for stochastic programming need to be explored. Many real-world applications contain uncertain portions that can only be handled by expensive simulations. As stochastic optimization problems become more complex (multistage, nonlinear mixed integer, etc.), the theoretical and algorithmic advances in optimization can help model and solve simulation-based approximations. While different communities work on this problem either mainly from a simulation perspective or from an optimization perspective, the two approaches can complement one another, enabling solution of problems that are currently beyond our capabilities.

Software: Finally, for the success of Monte Carlo simulation-based methods in practice, software to accompany these methods needs to be developed. Practitioners need to seamlessly connect data to models to solution algorithms and then need reliable ways to determine the quality of their obtained solutions that are embedded in these software. While there is a growing collection of software aimed in this direction, there is still much to do. As examples, on the simulation side, we point to Arena® commercial simulation software's Process Analyzer and OptQuest and the industrial strength COMPASS of Xu et al. [242] for optimizing a performance measure or selecting a best among alternatives generated by a stochastic simulation. @RISK® spreadsheet software combines Monte Carlo simulation with OptQuest. On the optimization side, examples of software with Monte Carlo sampling capabilities include SLP-IOR of Kall and Mayer [124], the SUTIL C++ Library of Czyzyk, Linderoth, and Shen [50] that allow Monte Carlo sampling for two- and multistage stochastic linear programs, FrontlineSolvers® simulation optimization suite, and open source software PySP of Watson et al. [239]. We note that the aforementioned software is in no way an exhaustive list and only provides some examples that involve an aspect of simulation-based optimization.

We end by noting that Monte Carlo sampling-based methods for stochastic optimization is an exciting and growing area of research. Aside from the classes of problems discussed in this survey, there are other classes of stochastic optimization models that are being developed or will be developed in the future by our community, and Monte Carlo methods for these models will need to be investigated.

We hope that the survey will provide a base for practitioners to apply Monte Carlo sampling-based methods to solve their problems, which will invariably result in new research directions, and that students and researchers will be able to use this survey to start working on many questions that still await answers.

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