

SAMPLE AVERAGE APPROXIMATION FOR FUNCTIONAL DECISIONS UNDER SHAPE CONSTRAINTS

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ABSTRACT

Sample average approximation methods are most often applied when the set of decision variables is finite. This research develops a method of finding optimal solutions to infinite-dimensional simulation optimization problems when the decision variable is a monotone function on a random variable used to model the uncertainty itself. This problem is motivated from approximately solving the principal-agent problem in economics, but also has close connection to nonparametric statistical estimation. We demonstrate how to approximate the infinite-dimensional problem with a discrete formulation that allows the use of standard sample average approximation methods. We also demonstrate how to utilize related bounding techniques on the optimal value, and show convergence results for the estimated optimal values and solutions.

1 INTRODUCTION

We present an approach for using sample average approximation (SAA) to solve problems with decision variables that are defined as functions. We focus on situations where the decision variable (function) to be optimized is monotone, defined over a random variable that itself models the uncertainty in the objective. When the random variable is continuous, this problem is in a sense infinite-dimensional. SAA is used to approximately solve a variety of optimization problems with expected value objective, by replacing the expectation with a sample average. It is most useful when this expectation is difficult to evaluate in closed form or when only data or Monte Carlo samples are available. In our considered context, since the decision variable relates to the underlying random variable through a functional relation, our sampling equivalent to the expectation, in its implementable form, would involve an increasing number of real-valued decision variables as the sample size increases, which renders our setting different from the conventional one in SAA.

This paper was originally motivated by attempts to solve the principal-agent problem, which is a classical model in economics whereby a seller (principal) attempts to optimize her expected profit by selling a product to a heterogeneous population of buyers (agents). One form of the problem involves the

principal incentivizing agents with differing valuations of a product to purchase it when there are infinite types of agents following a continuous distribution for their hidden true valuation of the product. There exists *information asymmetry* because only the agent knows his true valuation, though the principal knows the distribution of the valuations across the population of agents. The principal offers a menu of options to an agent listing different quantity and price combinations, and the agent picks the option that maximizes his value function. It is optimal for the principal to design an option for each type of agent, so if the types of agents follow a continuous distribution, the menu of options will be continuous functions. Thus, the problem is to derive the optimal price and quantity functions to offer the agents. For background on continuous principal-agent models, see Chapter 3 of Laffont and Martimort (2002).

Traditionally, these continuous principal-agent problems were solved using simplified functions such that calculus could be used to find analytical solutions. More commonly, the agent types are assumed discrete, often taking only two possible values. Singham and Cai (2017) was the first attempt to use an SAA-type method to numerically approximate continuous principal-agent problems when these continuous settings failed to be analytically tractable. That method was further developed in Singham (2019), which used a bootstrap method to obtain approximate bounds on the optimal objective value. This paper generalizes the approach from the specifics of the principal-agent problem, and provides stronger bounds and new convergence results.

We describe more related literature. Shapiro, Dentcheva, and Ruszczyński (2014) provide a comprehensive survey on SAA. Most of the results apply to formulations with finite-dimensional decision variables which, intuitively speaking, can be separately modeled from the randomness in the objective. In addition to convergence results on the solution or the objective value, including central limit theorems and concentration inequalities (e.g., Kleywegt, Shapiro, and Homem-de Mello (2002)), data-driven bounding techniques have been derived to quantify the optimality gap or the quality of solutions. Mak, Morton, and Wood (1999) use a batching approach to estimate optimality gaps under minimal assumptions, a technique that we would later utilize. Bayraksan and Morton (2006) provide a single-replication approach that reduces the computational load of Mak, Morton, and Wood (1999). In the simulation literature, recent work along these lines include Jaiswal, Honnappa, and Pasupathy (2018) who derive an optimal linear sample allocation rule when evaluating a sample average function over a grid of finite decision points, Lam and Qian (2018) who employ a bagging approach to obtain optimality gap bounds, Phelps, Royset, and Gong (2016) who use SAA to obtain consistent solutions for an uncertain optimal control problem where the objective functional depends on stochastic parameters.

Regarding the problem of interest, our formulation can be viewed as a functional optimization. An example of related classical problems is variational problems where the goal is to find an extremal function with certain smoothness conditions. For these types of problems, calculus of variations can be used to determine the optimal functionals (see Gelfand, Fomin, and Silverman (2000) for a reference). These problems, however, typically do not involve randomness as in stochastic optimization. Our problem is closer to statistical problems where the goal is to minimize the expected loss of a statistical procedure. These problems have a similar structure as ours, in that they typically use an empirical optimization as an approximation to obtain estimated parameters (such as in M -estimation). More relatedly, in the nonparametric setting, the decision variable, or the estimation or training target, can be an entire function. Examples include density estimation and nonparametric regression (Tsybakov 2008). Furthermore, the line of literature on shape-restricted inference considers estimating functions that satisfy certain monotonicity or convexity properties (Royset and Wets (2015), Groeneboom and Jongbloed (2014) and Guntuboyina and Sen (2018)). Compared to using kernels, these approaches have the advantages of not relying on bandwidth selection that could be challenging to well-tune in high dimension. Moreover, these approaches can also provably speed up estimation convergence, as exemplified by results in adaptive risk bounds (Guntuboyina and Sen 2018). For example, Royset and Wets (2017) derive a unified framework for constrained M -estimation that considers many types of soft information to improve convergence. Lastly, our work is also related to Blanchet, He, and Lam (2017) who, motivated from applications in optimal transport and robust

estimation, sought to find the worst-case joint distribution between two random variables. They apply an SAA approach and similarly face a growing dimension of decision variables as sample size increases.

In the following, we will describe our procedure to obtain nearly optimal solutions to optimization problem over the space of monotone functions. We also provide procedures to estimate the optimal objective value, and present consistency and convergence rate properties. These results add rigor to past work in Singham (2019) which was specific to the principal-agent problem, and relied on bootstrapping to calculate approximate bounds on the true objective. While Singham (2019) suggested consistency might be possible through numerical results, this paper formally derives consistency. Section 2 describes the continuous problem. Section 3 presents the corresponding SAA formulation. Section 4 describes the details of the computational algorithm to deliver solution estimates to the continuous problem. Section 5 derives bounds on the optimal values and convergence results, and Section 6 concludes.

2 PROBLEM FORMULATION

This section describes our main formulation. The decision variable is a continuous univariate function $x : \Theta \rightarrow \mathbb{R}$ defined over a single-dimensional random variable θ , the latter itself describing the uncertainty in the objective function. We assume θ lies in a bounded range $\Theta = [\underline{\theta}, \bar{\theta}]$, with density $f(\theta)$.

Our objective function is the expectation of the cost $c(x(\theta))$, which is a function of the function $x(\theta)$ evaluated at θ . We want to solve:

$$\Phi = \min_{x(\cdot)} E[c(x(\theta))] = \int_{\underline{\theta}}^{\bar{\theta}} c(x(\theta))f(\theta)d\theta \quad (1)$$

$$\text{subject to } x(\cdot) \in \Omega. \quad (2)$$

We refer to this formulation as the ‘‘continuous formulation’’. Here, the feasible region Ω contains requirement on the geometry of the considered functions. In particular, we consider:

Assumption 1 Assume that Ω is the space of non-decreasing functions $x : \Theta \rightarrow \mathbb{R}$, and $c(\cdot)$ is Lipschitz continuous.

The continuous principal-agent problem is an example of a common problem meeting these assumptions.

We note that our continuous formulation does not fall immediately into the typical SAA framework, as our decision variable is infinite-dimensional and, as sample size grows, the number of real-valued decision variables would correspondingly grow when we approximate the objective function of (1). Next, we present an algorithm for estimating Φ and then provide some bounding techniques and convergence guarantees in our SAA estimates.

3 DISCRETE SAA FORMULATION

We suppose that $f(\cdot)$ is unknown but samples of θ are available, or that the expectation cannot be obtained in closed form easily. We now formulate the corresponding SAA for Φ :

$$\hat{\Phi}_N = \min_{x(\cdot)} \frac{1}{N} \sum_{n=1}^N c(x(\theta_n)) \quad (3)$$

$$\text{subject to } x(\cdot) \in \Omega. \quad (4)$$

Here, $\theta_1, \dots, \theta_N$ are N samples of θ drawn from density $f(\theta)$. The SAA formulation replaces the expectation with a sample average. Note that this is still an optimization problem with an infinite-dimensional decision variable $x(\cdot)$.

Next, we construct an equivalent formulation that has only a finite set of real-valued decision variables. Note that the objective function in (3) only depends on x through $x(\theta_n), n = 1, \dots, N$. Thus, let us consider

a new set of decision variables x_1, \dots, x_N , each corresponding to each sample of $\theta_n, n = 1, \dots, N$ in that $x_n = x(\theta_n)$ is the function value at θ_n . We consider

$$\Phi_N = \min_{\{x_n\}_{n=1, \dots, N}} \frac{1}{N} \sum_{n=1}^N c(x_n) \quad (5)$$

$$\text{subject to } \{(\theta_n, x_n)\}_{n=1, \dots, N} \in \Omega_N, \quad (6)$$

Here Ω_N is the constraint space for the pairs $\{(\theta_n, x_n)\}$. The constraint on $x(\cdot)$ imposed by Ω must be carried over to constraining the relations among $\{(\theta_n, x_n)\}$, such that an appropriate interpolation of $\{(\theta_n, x_n)\}$ falls in Ω . Intuitively, Ω_N is a relaxation of the space of Ω , whereby the constraints defining Ω_N need only hold at points $\{(\theta_n, x_n)\}$ as opposed to all $\{(\theta, x(\theta))\}$ values. Below show some examples of constraints that we can handle using this framework:

Nonnegativity: If Ω is the set of all nonnegative functions, then $\Omega_N = \{x_n \geq 0, n = 1, \dots, N\}$.

Monotonicity: If Ω is the set of all non-decreasing functions, then for θ_n ordered so that $\theta_n \leq \theta_{n+1}$ for $n = 1, \dots, N-1$, we have $\Omega_N = \{x_n \leq x_{n+1}, n = 1, \dots, N-1\}$.

Boundedness: If Ω is the set of functions bounded between $[l, u]$, then $\Omega_N = \{l \leq x_n \leq u, n = 1, \dots, N\}$.

When Ω is any intersection of the above constraints, Ω_N would consist of the intersection of the corresponding discretized versions. Moreover, there are other constraints that can be handled, such as unimodality and convexity, but we only consider the above (especially monotonicity) as they are relevant to our problem.

We claim that $\hat{\Phi}_N = \Phi_N$. It is easy to see that any solution for $\hat{\Phi}_N$ can be converted into one for Φ_N via a projection $x_n = x(\theta_n)$ on the points $\theta_n, n = 1, \dots, N$. To see the other direction, we would need to show that, for any set of pairs $\{(\theta_n, x_n)\}$ in Ω_N , there exists an interpolation such that $x(\theta)$ lies in Ω . To facilitate discussion, define a function I as an interpolation rule such that $\tilde{x}(\cdot) = I(\{(\theta_n, x_n)\})(\cdot)$. That is, I applied to $\{(\theta_n, x_n)\}$ results in a function on a continuous range. We need $I(\{(\theta_n, x_n)\}) \in \Omega$ whenever $\{(\theta_n, x_n)\} \in \Omega_N$.

To this end, consider two examples of interpolation rules I : 1) linear interpolation and 2) piecewise constant, right-continuous. We can see which interpolations will maintain certain types of generic function constraints in Table 1. For example, if $\{(\theta_n, x_n)\}$ meets the nonnegativity constraint (i.e., all x_n are nonnegative), then both types of interpolations will also be nonnegative. For any specific constraint, we need to do a specific but straightforward check to see that the interpolation is feasible for the continuous problem.

Table 1: Feasibility of constraints maintained after interpolation from Ω_N to Ω .

Constraint	Linear Interp	Piecewise Constant Interp
Nonnegativity	✓	✓
Unimodal	✓	
Monotonicity	✓	✓
Continuity	✓	
Bounded	✓	✓
Convexity	✓	

From Table 1, we see that, using either linear or piecewise constant interpolation, we can convert a feasible solution in Ω_N into a corresponding feasible solution in Ω . Thus $\hat{\Phi}_N = \Phi_N$. We call Φ_N the discrete SAA formulation.

4 ALGORITHM

The discussion in Section 3 suggests to solve formulation Φ_N to obtain a set of pairs $\{(\theta_n, x_n)\}$, on which we interpolate to get a continuous function $\tilde{x}(\cdot)$ from $I(\{(\theta_n, x_n)\})$. This is summarized by the simple algorithm as follows:

1. Sample N values of θ from density $f(\theta)$ to obtain $\theta_1, \dots, \theta_N$.
2. Solve the discrete formulation in (5)-(6) using these samples to obtain optimal $x_n^*, n = 1, \dots, N$.
3. Interpolate the solution $\{(\theta_n, x_n^*)\}$ to obtain a feasible solution $\tilde{x}(\cdot) = I(\{(\theta_n, x_n^*)\})$, i.e., $\tilde{x}(\theta) \in \Omega$ for (1)-(2). I here can represent either linear or piecewise constant interpolation.
4. Evaluate the continuous objective function using $\tilde{x}(\theta)$, by way of numerical integration if the objective can be directly calculated:

$$\tilde{\Phi}_N = \int_{\underline{\theta}}^{\bar{\theta}} c(\tilde{x}(\theta))f(\theta)d\theta \quad (7)$$

or using J new samples $\theta_1, \dots, \theta_J$ drawn from density $f(\theta)$ applied to $\tilde{x}(\theta)$ to estimate the continuous objective

$$\tilde{\Phi}_N^J = \frac{1}{J} \sum_{j=1}^J c(\tilde{x}(\theta_j)). \quad (8)$$

The first two steps involve sampling θ and solving the corresponding discrete problem. The third step interpolates the discrete solution to obtain a feasible solution to the continuous problem. The fourth step is needed only if we need to evaluate the objective value at the attained feasible solution. We note that the solution of the discrete problem and the estimation of the objective function in (8) are standard calculations as part of SAA problems. Thus, this algorithm is as easy to implement as any SAA problem, though it becomes harder to solve as N increases due to the increasing number of decision variables and constraints.

5 BOUNDS AND CONVERGENCE

Next we establish bounds on Φ using our capability to solve Φ_N , using the results in Mak, Morton, and Wood (1999). Such type of bounds are used commonly in the SAA literature and readily apply to our setting, as they do not require any assumptions on the form of decision variables and are very general. Thus, once we have seen that Φ_N is equivalent to $\hat{\Phi}_N$, we can use Mak, Morton, and Wood (1999) directly. This gives the following proposition. For completeness, we provide a proof that pinpoints exactly where we use $\hat{\Phi}_N = \Phi_N$:

Proposition 1 $E[\Phi_N] \leq \Phi \leq E[\tilde{\Phi}_N^J]$, and $E[\Phi_N]$ monotonically increases as N increases.

Proof: To show the upper bound, note that since $\tilde{x}(\theta)$ is a feasible solution for the continuous problem, plugging it into (7) will yield an upper bound $\Phi \leq \tilde{\Phi}_N$. As the estimator used in (8) is unbiased, we have $E[\tilde{\Phi}_N^J] = \tilde{\Phi}_N$.

To show the lower bound, we consider

$$E[\Phi_N] = E[\hat{\Phi}_N] = E \left[\min_{x(\cdot) \in \Omega} \frac{1}{N} \sum_{n=1}^N c(x(\theta_n)) \right] \leq \min_{x(\cdot) \in \Omega} E \left[\frac{1}{N} \sum_{n=1}^N c(x(\theta_n)) \right] = \min_{x(\cdot) \in \Omega} E[c(x(\theta))].$$

Additionally, to show $E[\Phi_N] \leq E[\Phi_{N+1}]$, we consider

$$\begin{aligned} E[\Phi_{N+1}] &= E[\hat{\Phi}_{N+1}] = E \left[\min_{x(\cdot) \in \Omega} \frac{1}{N+1} \sum_{n=1}^{N+1} c(x(\theta_n)) \right] = E \left[\min_{x(\cdot) \in \Omega} \frac{1}{N+1} \sum_{n=1}^{N+1} Z_N^{(n)} \right] \\ &\geq \frac{1}{N+1} \sum_{n=1}^{N+1} E \left[\min_{\{x(\cdot) \in \Omega\}} Z_N^{(n)} \right] = E[\hat{\Phi}_{N+1}] = E[\Phi_{N+1}] \end{aligned}$$

where $Z_N^{(n)}$ is the leave-one-out sample average that removes the n -th sample, i.e., $Z_N^{(n)} = (1/N) \sum_{m \neq n} c(x(\theta_m))$. \square

Thus the simple algorithm presented in Section 4 can be used to provide bounds in expectation on the true optimal objective value. Singham (2019) derives bounds using a bootstrap method that develops an approximation to the objective Φ using a fixed number of samples N' . Then an SAA method using a bootstrap with smaller samples $N < N'$ provides a lower bound to the problem with size N' . The method employed in Proposition 1 is not only generalizable beyond the principal-agent problem, but is more direct in that it does not rely on the bootstrap approximation. The numerical examples in Singham and Cai (2017) and Singham (2019) show the bounds shrinking around the true optimal objective value as N increases using the bootstrap method.

Next we show convergence from Φ_N to Φ . Note that the standard SAA convergence results (Shapiro, Dentcheva, and Ruszczyński 2014) do not directly apply due to the dimensionality of the decision variables. However, we can use the underpinning empirical process to handle the problem. We derive two convergence results. First is the convergence of the estimated optimal value in the discrete SAA formulation, Φ_N , to the optimal value of the original problem, Φ . Second is the convergence of the obtained solution $\tilde{x}(\cdot)$ in the algorithm in Section 4, to the optimal in terms of the true objective function evaluation in the continuous formulation.

For these convergences to hold, we need a stronger assumption that $x(\cdot)$ is bounded. Thus, from now on, we strengthen Assumption 1 as:

Assumption 2 Assume that Ω is the space of non-decreasing functions $x : \Theta \rightarrow \mathbb{R}$, bounded in say $[l, u]$, and $c(\cdot)$ is Lipschitz continuous.

Note that by our discussion in converting Ω_N to Ω in the case of boundedness constraints in Section 3, all our previous results do not change by using the Ω in Assumption 2 instead of Assumption 1. We are ready to state our theorem:

Theorem 1 Under Assumption 2, we have

$$\Phi_N - \Phi = O_p \left(\frac{1}{\sqrt{N}} \right)$$

Proof: The class of bounded monotone functions is Donsker (Theorem 2.7.5 of Van Der Vaart and Wellner (1996)). Since x is bounded, we have a finite envelope, i.e., $E[\sup_x |c(x(\theta))|] < \infty$, and since $c(\cdot)$ is Lipschitz, $c(x(\cdot))$ is Donsker (Theorem 2.10.6 of Van Der Vaart and Wellner (1996)). Thus we have

$$\sqrt{N} \left(\frac{1}{N} \sum_{n=1}^N c(x(\theta_n)) - E[c(x(\theta))] \right) \Rightarrow v(x) \text{ in } \ell^\infty(\Omega) \quad (9)$$

where $v(\cdot)$ denotes a mean-zero Gaussian process parametrized by $x \in \Omega$, with covariance

$$\text{cov}(v(x_1), v(x_2)) = \text{cov}(c(x_1(\theta)), c(x_2(\theta))),$$

and $\ell^\infty(\Omega)$ denotes the space of uniformly bounded functions from Ω to \mathbb{R} .

Now, consider $\Phi_N - \Phi = \hat{\Phi}_N - \Phi$. Suppose there is an optimal solution to the true continuous formulation given by $x^*(\cdot)$. We have

$$\hat{\Phi}_N - \Phi \leq \frac{1}{N} \sum_{n=1}^N c(x^*(\theta_n)) - \Phi$$

by the definition of $\hat{\Phi}_N$ as the optimal value for the discrete SAA, and the right hand side above satisfies

$$\sqrt{N} \left(\frac{1}{N} \sum_{n=1}^N c(x^*(\theta_n)) - \Phi \right) \Rightarrow N(0, \text{var}(c(x^*(\theta)))) \quad (10)$$

On the other hand,

$$\hat{\Phi}_N - \Phi \geq \hat{\Phi}_N - E[c(\tilde{x}(\theta_n))]$$

by the definition of Φ as the optimal value for the continuous formulation. By (9), we have that the right hand side above satisfies

$$\hat{\Phi}_N - E[c(\tilde{x}(\theta_n))] \geq -\sup_x \left| \frac{1}{N} \sum_{n=1}^N c(x(\theta_n)) - E[c(x(\theta_n))] \right| = O_p \left(\frac{1}{\sqrt{N}} \right) \quad (11)$$

Putting these together, we thus have that

$$\hat{\Phi}_N - \Phi = O_p \left(\frac{1}{\sqrt{N}} \right)$$

Note that this above assumes $x^*(\cdot)$ exists. If this is not the case, we find an ε -near optimal solution and the arguments apply analogously. This concludes the theorem. \square

Besides the convergence of the estimated optimal value of the discrete SAA formulation to the continuous optimal, we can also show the convergence of the solution in terms of its continuous objective value. This is presented in the next theorem:

Theorem 2 Under Assumption 2, we have

$$E[c(\tilde{x}(\theta))] - \Phi = O_p \left(\frac{1}{\sqrt{N}} \right)$$

Proof: Suppose there is an optimal solution to the true continuous formulation given by $x^*(\cdot)$. We consider $E[c(\tilde{x}(\theta))] - \Phi$, which is always non-negative by the definition of Φ . We write

$$\begin{aligned} & E[c(\tilde{x}(\theta))] - \Phi \\ &= \left(E[c(\tilde{x}(\theta))] - \frac{1}{N} \sum_{n=1}^N c(\tilde{x}(\theta_n)) \right) + \left(\frac{1}{N} \sum_{n=1}^N c(\tilde{x}(\theta_n)) - \frac{1}{N} \sum_{n=1}^N c(x^*(\theta_n)) \right) + \left(\frac{1}{N} \sum_{n=1}^N c(x^*(\theta_n)) - \Phi \right) \end{aligned}$$

The second term is non-positive by the optimality of \tilde{x} for $\hat{\Phi}_N$. The third term satisfies (10). Analogous to (11), the first term satisfies

$$\left| E[c(\tilde{x}(\theta))] - \frac{1}{N} \sum_{n=1}^N c(\tilde{x}(\theta_n)) \right| \leq \sup_x \left| \frac{1}{N} \sum_{n=1}^N c(x(\theta_n)) - E[c(x(\theta_n))] \right| = O_p \left(\frac{1}{\sqrt{N}} \right)$$

Thus, putting together, we have

$$E[c(\tilde{x}(\theta))] - \Phi = O_p \left(\frac{1}{\sqrt{N}} \right)$$

Like the proof of Theorem 1, note that this above assumes $x^*(\cdot)$ exists. If this is not the case, we find an ε -near optimal solution and the arguments apply analogously. This concludes the theorem. \square

6 CONCLUSIONS

We present a straightforward SAA algorithm to obtain approximate solutions to infinite-dimensional stochastic optimization problems when the decision variable is a monotone function over the random variable that defines the uncertainty in the objective. Our algorithm comprises an optimization with a finite number of real-valued decision variables that consistently represent the functional constraint in the original problem. We demonstrate how we can utilize bounding techniques in the SAA literature in this setting. We also show the canonical rate of the estimated optimal value using our algorithm in converging to the true optimal value, and our estimated solution in converging to optimal in terms of the objective value. The former also explains the observed convergence in the optimal values observed in past bootstrap experiments. An application of this problem is the classical example of the continuous principal-agent problem, and future work will explore other applications such as distributionally robust estimation.

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