

SIMULATION BASED OPTIMIZATION

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ABSTRACT

In this talk we consider a problem of optimizing an expected value function by Monte Carlo simulation methods. We discuss, somewhat in details, the stochastic counterpart (sample path) method where a relatively large sample is generated and the expected value function is approximated by the corresponding average function. Consequently the obtained approximation problem is solved by deterministic methods of nonlinear programming. One of advantages of this approach, compared with the classical stochastic approximation method, is that a statistical inference can be incorporated into optimization algorithms. This allows to develop a validation analysis, stopping rules and variance reduction techniques which in some cases considerably enhance numerical performance of the stochastic counterpart method.

1 INTRODUCTION

Consider the optimization problem

$$\min_{x \in S} f(x) \quad (1)$$

of minimization of a function $f(x)$ over a set $S \subset \mathbb{R}^m$. Suppose that the objective function $f(x)$ is given as an expected value $f(x) := \mathbb{E}_P\{g(x, \omega)\}$ with respect to a probability measure (distribution) P defined on a sample space (Ω, \mathcal{F}) . One can try then to solve the optimization problem (1) by a Monte Carlo simulation. A classical approach to such an optimization is the stochastic approximation (SA) method (e.g., Kushner and Clark, 1978). In case for every $\omega \in \Omega$ the function $g(\cdot, \omega)$ is convex, not necessarily differentiable, one can use a closely related stochastic subgradient (stochastic quasigradient) method (Ermoliev, 1988). In order to apply these methods only calculation of the gradient (in the convex case calculation of a subgradient) of the functions $g(\cdot, \hat{\omega})$ at iteration

points for generated realizations (sample paths) $\hat{\omega}$ is required.

Drawbacks of the SA method are well known - slow convergence, absence of a good stopping rule, difficulty in handling constraints. In this talk we discuss an alternative approach to the above optimization problem which became known as the stochastic counterpart (or sample path) method. In the stochastic counterpart method a (large) sample $\omega_1, \dots, \omega_n$ is generated and the function $f(\cdot)$ is approximated by the corresponding average function

$$\hat{f}_n(\cdot) = n^{-1} \sum_{i=1}^n g(\cdot, \omega_i).$$

This leads to the (stochastic counterpart) approximating problem

$$\min_{x \in S} \hat{f}_n(x), \quad (2)$$

which is solved by (deterministic) techniques of nonlinear programming. For such an approach to be applicable one needs a mechanism to evaluate the approximating functions $\hat{f}_n(x)$, and their derivatives, for all x in a given region in \mathbb{R}^m . There are basically two types of techniques which are available for that purpose, namely the likelihood ratios (LR) (also called the score function) method and the sample path generation.

Let us observe at this point that the SA and stochastic counterpart (SC) methods are asymptotically equivalent provided the expected value function $f(x)$ is smooth (differentiable), the "true" optimal solution x_0 is an interior point of the feasible region S and the SA method is implemented with the optimal choice of the corresponding step sizes (Shapiro, 1996). This should be not surprising in view of asymptotic optimality (efficiency) properties of SA estimators (Nevl'son and Has'minskii, 1978). It was discovered recently that by choosing relatively large step sizes and by averaging the obtained SA iterates

it is possible (in the smooth case) to achieve asymptotic efficiency in an automatic way (Polyak, 1990). Therefore, for smooth problems, from the asymptotic point of view both methods are comparable.

There is, however, a number of advantages in the SC method which (when applicable) make this method computationally attractive. The involved constraints can be treated quite efficiently by (deterministic) optimization algorithms. A statistical inference for the SC method is available (e.g., Shapiro, 1996). This statistical inference allows to develop (statistically based) stopping rules, validation techniques and to construct confidence intervals and, in some cases, confidence regions for the optimal value and optimal solutions, respectively (cf. Shapiro and Homem-de-Mello, 1996). Furthermore, the SC method can be used together with variance reduction techniques which in some cases lead to significant improvements in the computational efficiency.

2 AN EXAMPLE OF GI/G/1 QUEUE

In this section we discuss an example of GI/G/1 queue whose service times depend on a parameter vector \mathbf{x} . Although relatively simple this example demonstrates various aspects of the method. Let Y_i be the time between arrivals of the $(i-1)^{\text{th}}$ and i^{th} customers, and for a fixed value of \mathbf{x} , let $Z_i(\mathbf{x})$ be the service time of the i^{th} customer, $i = 1, 2, \dots$, and let $G_i(\mathbf{x})$ denote the i^{th} sojourn time (i.e. the total time spent by the i^{th} customer in the queue). We assume that the first customer arrives at an empty queue and that for every $\mathbf{x} \in S$ the queue is regenerative with the expected number of customers served in one busy period (regenerative cycle) being finite. Note that a recursion relation between the sojourn times is given by the Lindley's equation

$$G_i(\mathbf{x}) = Z_i(\mathbf{x}) + [G_{i-1}(\mathbf{x}) - Y_i]_+. \quad (3)$$

Under standard regularity conditions, the long-run average functions

$$\hat{f}_n(\mathbf{x}) = n^{-1} \sum_{i=1}^n G_i(\mathbf{x})$$

converge (pointwise) w.p.1, as $n \rightarrow \infty$, to the expected value (mean) steady state sojourn time $f(\mathbf{x})$. Consider the optimization problem

$$\min_{\mathbf{x} \in S} f(\mathbf{x}) + \psi(\mathbf{x}), \quad (4)$$

where $\psi(\mathbf{x})$ is a (deterministic) cost function. By using Lindley's equation (3) a recursive relation between the gradients of the sojourn time functions

can be derived and consequently the optimization problem (4) can be numerically solved by SA type algorithms (see, e.g., Chong and Ramadge (1993), L'Ecuyer and Glynn (1994), and references therein).

An alternative approach is to generate a large sample of interarrival and service times and then to solve a constructed approximation of (4) by deterministic methods of nonlinear programming. Suppose that the service times can be generated in the form $Z_i = \eta(U_i, \mathbf{x})$, where U_1, \dots , is a sequence of iid random numbers and $\eta(u, \mathbf{x})$ is a known function. For example, if the service times have an exponential distribution with mean \mathbf{x} , then one can take $\eta(u, \mathbf{x}) = -\mathbf{x} \ln u$ with U_i having the uniform (0,1) distribution. After a sample of Y_1, \dots, Y_n , and U_1, \dots, U_n , is generated the long-run average functions $\hat{f}_n(\mathbf{x})$ and their gradients can be calculated, at any given point \mathbf{x} , by using Lindley's equation (3), separately for every busy period, and consequently the corresponding sample path approximation of the program (4) can be constructed. It is worth noting that constructed in that way, the approximating functions $\hat{f}_n(\mathbf{x})$ are typically *nondifferentiable*, piecewise smooth functions. Moreover, in some cases when the interarrival and service times distributions contain atoms, these nondifferentiability are carried over to the steady state, and hence the mean steady state function $f(\mathbf{x})$ is not everywhere differentiable (Shapiro and Wardi, 1994).

A somewhat different approach to construction of a stochastic approximation of $f(\mathbf{x})$ is based on a LR transformation. Denote by $\tau(\mathbf{x})$ the number of customers served in one busy period. It is well known in the renewal theory of regenerative processes that, for a given \mathbf{x} and $\tau = \tau(\mathbf{x})$, $G_i = G_i(\mathbf{x})$, the mean steady state sojourn time $f(\mathbf{x})$ can be written in the form

$$f(\mathbf{x}) = \frac{\mathbb{E}\{\sum_{i=1}^{\tau} G_i\}}{\mathbb{E}\{\tau\}}, \quad (5)$$

provided both expectations in the right hand side of (5) exist.

Suppose now that the service times Z_1, \dots , are iid and have a (common) pdf $p(z, \mathbf{x})$ depending on the parameter vector \mathbf{x} . Then it is possible to show (Asmussen and Rubinstein, 1992, Rubinstein and Shapiro, 1993) that $f(\mathbf{x})$ can be represented in the form

$$f(\mathbf{x}) = \frac{\mathbb{E}_{p_0}\{\sum_{i=1}^{\tau^*} G_i^* L_i(\mathbf{x})\}}{\mathbb{E}_{p_0}\{\sum_{i=1}^{\tau^*} L_i(\mathbf{x})\}}, \quad (6)$$

where Z_1^*, \dots , is an iid random sample of service times generated from a (fixed) pdf $p_0(z)$, G_i^* and τ^* are the sojourn times and the number of customers served in one busy period, respectively, corresponding to the service times Z_i^* , and $L_i(\mathbf{x})$ is the likelihood ratio

process

$$L_t(\mathbf{x}) = \prod_{i=1}^t \frac{p(Z_i^*, \mathbf{x})}{p_0(Z_i^*)}.$$

Typically one takes the dominating pdf in the form $p_0(\mathbf{z}) = p(\mathbf{z}, \mathbf{x}_0)$ for a chosen value \mathbf{x}_0 of the parameter vector.

By generating n busy periods (regenerative cycles) and replacing the expectations in (6) by their sample averages, one obtains a (regenerative) LR estimator $\hat{f}_n(\mathbf{x})$ of $f(\mathbf{x})$. Note that once a sample of the service and interarrival times is generated and the corresponding sojourn times G_1^*, \dots , are calculated, the function $\hat{f}_n(\cdot)$ is given explicitly through the corresponding LR process $L_t(\cdot)$.

It should be noted that the above LR construction depends on two crucial assumptions, namely on identifiability of the regenerative cycles and a possibility of moving the parameter vector \mathbf{x} into the corresponding pdf $p(\mathbf{z}, \mathbf{x})$. In more complex situations it may happen that the regenerative cycles are too long or cannot be easily identified (the system is never empty). Note also that in order to keep the variance of the obtained LR estimators under control the reference value \mathbf{x}_0 of the parameter vector, used in the dominating pdf $p_0(\mathbf{z}) = p(\mathbf{z}, \mathbf{x}_0)$, should be carefully selected (see Rubinstein and Shapiro, 1993, for a discussion of this problem).

3 OPTIMIZATION ALGORITHMS

An important issue in an implementation of the SC method is the choice of a deterministic optimization algorithm. In case the considered problem is convex, it is suggested in Plambeck, Fu, Robinson and Suri (1996) to use a bundle type optimization procedure. An alternative approach is to apply a steepest descent method with an approximate line search, say by using Armijo step sizes (cf. Wardi, 1990). In this respect let us make the following observations.

Usually calculations of the average-function $\hat{f}_n(\mathbf{x})$ value, and its gradient $\nabla \hat{f}_n(\mathbf{x})$, at an iteration point $\mathbf{x} = \mathbf{x}_k$, are expensive with the time effort is proportional to the used sample size n . By the Central Limit Theorem, the involved stochastic error is inversely proportional to \sqrt{n} . Therefore, typically, in simulation based optimization one cannot hope to achieve an accuracy often attainable in deterministic optimization. Increasing the sample size does not help much since in order to improve the accuracy, say by one digit (10 times), one would need to increase the sample size 100 times.

Often the average-functions $\hat{f}_n(\mathbf{x})$ are piecewise smooth nondifferentiable functions. Consequently

reliable estimates of the second order derivatives $\nabla^2 f(\mathbf{x})$, of the expected value function $f(\mathbf{x})$, are either unavailable or are too expensive to calculate. Therefore applicable algorithms are usually first-order optimization routines. In any case it does not make sense to try to solve the constructed stochastic counterpart problem (2) with high accuracy. Especially at first iterations, when the iterates are far away from the optimal solution, the sample size can be relatively small and can be increased gradually as the algorithm proceeds. In this respect steepest descent type algorithms offer more flexibility in updating the sample sizes than bundle type methods. It is shown in Shapiro and Wardi (1996) that, under mild regularity conditions, such steepest descent type algorithms produce iterates which converge with probability one to the set of "true" optimal solutions as the sample sizes are increasing to infinity.

4 VALIDATION ANALYSIS AND STOPPING RULES

Suppose that we are given a point \mathbf{x}^* which is suggested as an approximation of an optimal solution \mathbf{x}_0 of the program (1). Can we evaluate a quality of this approximation? Closely related to this question is a choice of stopping criteria for a considered algorithm. In this section we discuss some statistical tests for validation of optimality of the solution \mathbf{x}^* .

Suppose that the expected value function $f(\mathbf{x})$ is *differentiable* at the point \mathbf{x}^* . Also, assume that the feasible set S is defined by constraints as follows

$$S = \left\{ \mathbf{x} \in \mathbb{R}^m : \begin{array}{l} c_i(\mathbf{x}) = 0, \quad i = 1, \dots, k, \\ c_i(\mathbf{x}) \geq 0, \quad i = k + 1, \dots, l \end{array} \right\},$$

where $c_i(\mathbf{x})$ are (deterministic) continuously differentiable functions. By the first-order optimality conditions we have that if \mathbf{x}_0 is an optimal solution of the problem (1), then (under a constraint qualification) there exist Lagrange multipliers λ_i such that $\lambda_i \geq 0$, $i \in J(\mathbf{x}_0)$, and

$$\nabla f(\mathbf{x}_0) - \sum_{i \in J(\mathbf{x}_0)} \lambda_i \nabla c_i(\mathbf{x}_0) = 0, \quad (7)$$

where $J(\mathbf{x}) = \{i : c_i(\mathbf{x}) = 0, i = k + 1, \dots, l\}$ denotes the index set of inequality constraints active at \mathbf{x} and $I(\mathbf{x}) = \{1, \dots, k\} \cup J(\mathbf{x})$. Consider the polyhedral cone

$$C(\mathbf{x}) = \left\{ \mathbf{z} \in \mathbb{R}^m : \begin{array}{l} \mathbf{z} = \sum_{i \in J(\mathbf{x})} \alpha_i \nabla c_i(\mathbf{x}), \\ \alpha_i \geq 0, \quad i \in J(\mathbf{x}) \end{array} \right\}.$$

Then the optimality conditions (7) can be written in the form $\nabla f(\mathbf{x}_0) \in C(\mathbf{x}_0)$.

Suppose now that the gradient $\nabla f(x^*)$ can be estimated by a (random) vector $\gamma_n(x^*)$ such that $\gamma_n(x^*) \rightarrow \nabla f(x^*)$ w.p.1 as $n \rightarrow \infty$ and $\gamma_n(x^*)$ has (approximately) a multivariate normal distribution with mean vector $\mu = \nabla f(x^*)$ and a covariance matrix Ω_n . For example, if the gradient of $f(x)$ is estimated by the gradient $\gamma_n(x^*) = \nabla \hat{f}_n(x^*)$ of the corresponding average function, then asymptotic normality of $\gamma_n(x^*)$ follows by the Central Limit Theorem. Note that in this case the covariance matrix Ω_n can be consistently estimated from the same sample.

By using the estimator $\gamma_n(x^*)$, we can test the hypothesis:

$$H_0 : \nabla f(x^*) \in C(x^*)$$

against the alternative

$$H_1 : \nabla f(x^*) \notin C(x^*).$$

In order to test the (optimality-conditions) hypothesis H_0 one can use the following procedure (cf. Shapiro and Homem-de-Mello, 1996). Suppose that the covariance matrix Ω_n is nonsingular, and hence is positive definite, and that a consistent estimator $\hat{\Omega}_n$ of Ω_n is available. Then

$$T = \min_{z \in C(x^*)} (\gamma_n(x^*) - z)^T \hat{\Omega}_n^{-1} (\gamma_n(x^*) - z)$$

is an asymptotic analogue of the Hotelling's test statistic which is used in multivariate analysis. It is possible to show that if all Lagrange multipliers corresponding to the inequality constraints active at x^* are positive (*strict complementarity condition*), then the test statistic T has approximately (asymptotically) a noncentral chi-square distribution with $m - s$ degrees of freedom, where

$$s = \text{card}(I(x^*)) = k + \text{card}(J(x^*)),$$

("card(I)" denotes cardinality of the set I) and the noncentrality parameter

$$\kappa = \min_{z \in C(x^*)} (\nabla f(x^*) - z)^T \Omega_n^{-1} (\nabla f(x^*) - z).$$

In particular, under H_0 we have that $\kappa = 0$ and hence the null distribution of T is (asymptotically) central chi-square with $m - s$ degrees of freedom. Therefore for a calculated value T of the test statistic we can calculate the corresponding p -value, that is $p = \text{Prob}\{\chi_{m-s}^2 \geq T\}$. This p -value gives an indication of the quality of the suggested solution x^* with respect to the stochastic precision. A large (close to one) p -value means that such precision was reached, so the algorithm cannot proceed further, whereas a small (close to zero) p -value indicates that either the

current solution is far from the optimal or the deterministic error starts to dominate.

The test statistic T can be calculated at each (at some) iteration points and can be used in developing stopping criteria for considered algorithms. Numerical experience reported in Shapiro and Homem-de-Mello (1996) suggests that this test statistic is useful although alone does not give a good stopping rule and should be combined with other criteria. It may happen that the covariance matrix $\hat{\Omega}_n$ of $\nabla \hat{f}_n(x)$, at a current iteration point $x = x_k$, is large and consequently the corresponding T -value is small although, in fact, x_k is far away from x_0 . In that case the algorithm reached its stochastic precision and either the sample size should be increased or some variance reduction procedure should be implemented.

On the other hand a reason for large T -value can be a small value of the covariance matrix $\hat{\Omega}_n$. In that case the deterministic error of the implemented optimization algorithm dominates the corresponding stochastic error and the algorithm can be stopped by a deterministic criterion.

It is also possible to construct a confidence region for $\nabla f(x_k) - P(\nabla f(x_k))$, where $P(\nabla f(x_k))$ denotes a point of the cone $C(x_k)$ closest to $\nabla f(x_k)$, with respect to the metric induced by the inverse of the covariance matrix. This can give an indication of the order of the stochastic error and hence to help in the choice of the generated sample size.

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