



Constrained Optimization via Stochastic Approximation with a Simultaneous Perturbation Gradient Approximation*

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Key Words—Optimization; stochastic approximation; SPSA; constraints; Kuhn–Tucker point.

Abstract—This paper deals with a projection algorithm for stochastic approximation using simultaneous perturbation gradient approximation for optimization under inequality constraints where no direct gradient of the loss function is available and the inequality constraints are given as explicit functions of the optimization parameters. It is shown that, under application of the projection algorithm, the parameter iterate converges almost surely to a Kuhn–Tucker point. The procedure is illustrated by a numerical example. © 1997 Elsevier Science Ltd.

1. Introduction

The simultaneous perturbation stochastic approximation (SPSA) algorithm has recently attracted considerable attention for multivariate optimization problems where only noisy measurements of the loss function are available (i.e. no gradient information is directly available); see e.g. Cauwenberghs (1994), Chin (1994), Parisini & Alessandri (1995), Maeda *et al.* (1995), and Rezayat (1995).

SPSA was introduced in Spall (1987) and more thoroughly analyzed in Spall (1992). The algorithm is a variant of the stochastic approximation (SA) in a Kiefer–Wolfowitz setting (Kushner and Clark, 1978) where only noisy measurements of the loss function are available (used for gradient approximations). The essential feature of SPSA is its highly efficient gradient approximation that requires only *two* loss-function measurements regardless of the number of optimization parameters. The gradient approximation is generated by simultaneous (random) perturbation relative to the current estimate of the parameter θ . Note the contrast of two function measurements with the $2p$ measurements required in the classical finite-difference-based Kiefer–Wolfowitz SA algorithm, where p is the number of parameters. Under reasonably general conditions, it was shown in Spall (1992) that the p -fold saving in function measurements per gradient approximation translates directly into a p -fold saving in the total number of measurements needed to achieve a given level of accuracy in the optimization process.

The original SPSA algorithm as presented in Spall (1992) is an unconstrained algorithm. Constraints, on the other hand, are essential parts of almost all real-world optimization applications. The present work may be regarded as the extension of the convergence result of Spall (1992) to constrained optimization problems. This paper presents a projection SPSA algorithm that can handle *inequality* constraints. A similar approach is pursued in L'Ecuyer and

Glynn (1994) for optimization of queuing systems using stochastic approximation. Here we focus on SPSA and treat more general constraints. However, we restrict attention to constraints that are given as explicit functions of the optimization parameter. In the Kiefer–Wolfowitz stochastic approximations, function evaluations often mean *real measurements* on the system. We are interested in situations where the constraints are determined by the feasible operating conditions of the system. Hence we assume that function evaluations at the points where the constraints are violated are not feasible. This is stronger than the requirement of restricting the solution to the feasible domain (as in constrained versions of Robbins–Monro-type SA algorithms; see Kushner and Clark, 1978). In this regard, the projection algorithm is advantageous relative to other constrained SA optimization techniques such as the Lagrangian method (Kushner and Clark, 1978) where the parameter iterate only asymptotically lies in the feasible set. We establish the almost-sure convergence of the parameter iterate to a Kuhn–Tucker point under application of the projection algorithm.

The organization of the rest of the paper is as follows. Section 2 studies the projection SPSA algorithm and the convergence result. Section 3 presents a numerical example where the procedure is illustrated and tested using (finite-sample) numerical experimentations. Finally, Section 4 offers concluding remarks.

2. Projection SPSA algorithm and strong convergence

In this section, we treat a projection SPSA algorithm for minimization under constraints, i.e. the problem of

$$\min_{\theta \in G} L(\theta),$$

where, similarly to the regularity conditions for the unconstrained case (Spall, 1992), the loss function $L(\theta)$ is continuously differentiable on an open set containing G . The reader is referred to Spall (1992) for a detailed treatment of the (unconstrained) SPSA algorithm. We deal with *inequality* constraints and introduce the following assumption.

Assumption 1. The set $G = \{\theta: q_i(\theta) \leq 0, i = 1, \dots, s\}$ is non-empty and bounded, and the functions $q_i(\theta)$, $i = 1, \dots, s$, are continuously differentiable. At each $\theta \in \partial G$, where ∂ denotes the boundary, the gradients of the active constraints are linearly independent. Furthermore, there exists an $\epsilon < 0$ such that the set $G^- = \{\theta: q_i(\theta) \leq \epsilon, i = 1, \dots, s\}$ is non-empty for $\epsilon \leq r < 0$ (i.e. the set G has a non-empty interior).

The proof of convergence to a Kuhn–Tucker point that follows later is based on Theorem 5.3.1 of Kushner and Clark (1978), where the assumption on G (Kushner and Clark, 1978, p. 190, A5.3.1) states that G is the closure of its interior rather than the non-emptiness of G^- in Assumption 1. It is easy to see that because of the continuity of the $q_i(\theta)$, the set

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$\{\theta: q_i(\theta) < 0, i = 1, \dots, s\}$ is open and indeed equal to $\text{int } G$ (where int denotes interior). This, together with the non-emptiness of G^- , yields $G = \text{int } G$. Assumption 1 is formulated with the goal of easing later presentation.

Another type of constrained problems involves constraint functions that can only be observed in the presence of noise (see e.g. Ljung *et al.*, 1992). Such constraints will not be examined here.

Let $\hat{\theta}_k$ denote the estimate for θ at the k th iteration, and for all $\theta \in \mathbb{R}^p$, let $P(\theta)$ be the nearest point to θ on G , where the norm is defined as the usual Euclidean norm. The projection algorithm has the general form

$$\hat{\theta}_{k+1} = P(\hat{\theta}_k - a_k \hat{g}_k(\hat{\theta}_k)), \quad (1)$$

where the gain sequence $\{a_k\}$ must satisfy certain conditions (see below) and $\hat{g}_k(\hat{\theta}_k)$ is an approximation to the gradient at $\hat{\theta}_k$. The simultaneous perturbation estimate for the gradient at θ , $g(\theta)$, is defined as follows. Let $\Delta_k \in \mathbb{R}^p$ be a vector of p mutually independent zero-mean random variables $\{\Delta_{k1}, \Delta_{k2}, \dots, \Delta_{kp}\}$ satisfying certain conditions (Spall, 1992). A condition on random perturbations is norm-boundedness, i.e. $\|\Delta_k\| \leq \alpha_0$ for some $\alpha_0 > 0$. In Spall (1992), the boundedness condition is $\|\Delta_k\| \leq \alpha_0$ a.s. Noting that the user has full control over random perturbations, for simplicity we follow the strict boundedness assumption. Consistent with the usual framework of stochastic approximations, we have noisy measurements of the loss function. In particular, at the k th iteration,

$$y_k^{(+)} = L(\theta + c_k \Delta_k) + \epsilon_k^{(+)},$$

$$y_k^{(-)} = L(\theta - c_k \Delta_k) + \epsilon_k^{(-)},$$

where $\{c_k\}$ is a gain sequence and $\epsilon_k^{(+)}$ and $\epsilon_k^{(-)}$ represent measurement noise terms that satisfy $E\{\epsilon_k^{(+)} - \epsilon_k^{(-)} \mid \theta, \Delta_k\} = 0$. The gain sequences $\{a_k\}$ and $\{c_k\}$ are positive for all k and tend to zero as $k \rightarrow \infty$. Moreover, $\sum_{k=0}^{\infty} a_k = \infty$, and $\sum_{k=0}^{\infty} (a_k/c_k)^2 < \infty$. For convenience, we take $c_k = c/k^\gamma$, $\gamma \geq 0$.

The basic simultaneous perturbation (SP) form for the estimate of $g(\theta)$ at iteration k is defined by

$$g_k^{\text{SP}}(\theta) = \begin{bmatrix} \frac{y_k^{(+)} - y_k^{(-)}}{2c_k \Delta_{k1}} \\ \vdots \\ \frac{y_k^{(+)} - y_k^{(-)}}{2c_k \Delta_{kp}} \end{bmatrix}.$$

Note that at each iteration, only two measurements are needed to form the estimate. The main features of our proposed solution compared with the unconstrained SPSA algorithm are as follows. Firstly, the projection $P(\cdot)$ always restricts the iterates $\hat{\theta}_k$ to remain within G , which is obviously not needed for the unconstrained case. The projection is indeed an essential feature of the constrained algorithm; eliminating $P(\cdot)$, the iterates may vary anywhere in \mathbb{R}^p as a result of noisy observations, no matter how the gain or random perturbation sequences of the algorithm are selected. Secondly, in the unconstrained algorithm, we have $\hat{g}_k(\hat{\theta}_k) = g_k^{\text{SP}}(\hat{\theta}_k)$. Such an approximation cannot be directly used here, since it may happen that $\hat{\theta}_k \in G$ but $\hat{\theta}_k \pm c_k \Delta_k \notin G$. Especially, in the case $\hat{\theta}_k \in \partial G$, there is always a (random) direction Δ_k such that $\hat{\theta}_k \pm c_k \Delta_k \notin G$, no matter how small the gain c_k is selected. Note that the case $\hat{\theta}_k \in \partial G$ is expected to occur frequently in the very relevant situation where the true optimum belongs to the boundary of the feasible domain. Except for simulation-based optimization cases, function evaluations involve real measurements on the system, and it is usually not allowed to take measurements outside the feasible domain. To overcome this problem, we further project $\hat{\theta}_k$ onto a (closed) set G_k contained within G to obtain $P_k(\hat{\theta}_k)$, which will (only) be used for computing an SP gradient approximation at the k th

iteration. If the distance d_k between the nearest points on ∂G and ∂G_k is equal to or larger than $c_k \alpha_0$ then $P_k(\hat{\theta}_k) \pm c_k \Delta_k \in G$, ensuring that the SP approximation to the gradient at $P_k(\hat{\theta}_k)$ (instead of $\hat{\theta}_k$) requires no function measurement outside G . The SP gradient approximation at $P_k(\hat{\theta}_k)$ obviously introduces an (extra) error term relative to the SP gradient approximation at $\hat{\theta}_k$. However, if $G_k \rightarrow G$ as $k \rightarrow \infty$ then continuous differentiability of $L(\theta)$ yields that the extra error term tends to zero. This line of argument will be used in the proof of convergence later. But first, we describe a procedure for selecting the G_k (a simple case of this is given in the illustrative example). Define $G_k \subset G$ by $G_k = \{\theta: q_i(\theta) \leq r_k < 0, i = 1, \dots, s\}$, where $r_k \rightarrow 0$ as $k \rightarrow \infty$. Assumption 1 states that there exists an $\epsilon < 0$ such that G_k is non-empty for $\epsilon \leq r_k < 0$, $k = 1, 2, \dots$. Hence select $\epsilon \leq r_1 < 0$ and select c such that $d_1 \geq c_1 \alpha_0$. Once c is selected, choose $r_k \rightarrow 0$ such that $d_k \geq c_k \alpha_0$ (note that $c_k \rightarrow 0$ as $k \rightarrow \infty$).

Remark 1. It follows from the above that the bottom line in computing an SP gradient approximation at $P_k(\hat{\theta}_k)$ is to ensure the feasibility of function evaluations. There may therefore exist different methods to obtain a point $\theta'_k \in G$ for the SP gradient approximation at iteration k such that $\theta'_k \pm c_k \Delta_k \in G$, and, in some sense, the magnitude of $\theta'_k - \hat{\theta}_k$ is small for all k (to avoid large error terms on the gradient approximations) and becomes infinitesimally small as $k \rightarrow \infty$. The proposed solution of the paper provides a suitable technique that can be generically applied to all types of constrained problems where Assumption 1 holds.

Finally, it should be noted that projections in general are unfortunately not very easy to compute unless linear approximations to $q_i(\theta)$ at the current iterate are obtained first. Such approximations can often be justified in practice, since $a_k \rightarrow 0$.

Proposition 1. Let Assumption 1 above and Assumptions A1–A5 and the conditions of Lemma 1 (for simplicity, replace the a.s. boundedness of Δ_k by strict boundedness) of Spall (1992) hold where all the regularity conditions on $L(\cdot)$ hold on an open set containing G . Then, under the projection algorithm (see 1)), where $\hat{g}_k(\hat{\theta}_k) = g_k^{\text{SP}}(P_k(\hat{\theta}_k))$, as $k \rightarrow \infty$

$$\hat{\theta}_k \rightarrow KT \quad \text{a.s.,}$$

where KT is the set of Kuhn–Tucker points (i.e. the set of points θ where there are $\lambda_i \geq 0$ such that $g(\theta) + \sum_{i: q_i(\theta)=0} \lambda_i dq_i(\theta)/d\theta = 0$).

Proof. Decompose the error $\hat{g}_k(\hat{\theta}_k) - g(\hat{\theta}_k) = g_k^{\text{SP}}(P_k(\hat{\theta}_k)) - g(\hat{\theta}_k)$ into a sum of $b_k^I = E(g_k^{\text{SP}}(P_k(\hat{\theta}_k)) \mid \hat{\theta}_k) - g(P_k(\hat{\theta}_k))$, $e_k = g_k^{\text{SP}}(P_k(\hat{\theta}_k)) - E(g_k^{\text{SP}}(P_k(\hat{\theta}_k)) \mid \hat{\theta}_k)$ and $b_k^{II} = g(P_k(\hat{\theta}_k)) - g(\hat{\theta}_k)$. Identically to the proof of Lemma 1 and Proposition 1 of Spall (1992), it can be shown that

- (i) $\sup_k |b_k^I| < \infty$ and $b_k^I \rightarrow 0$ a.s. as $k \rightarrow \infty$;
- (ii) $\lim_{k \rightarrow \infty} \Pr \left(\sup_{m \geq k} \left| \sum_{i=k}^m a_i e_i \right| \geq \eta \right) = 0$ for any $\eta > 0$,
where $\Pr(\cdot)$ denotes probability; moreover, since G is bounded, $G_k \rightarrow G$, and $L(\theta)$ is continuously differentiable at all $\theta \in G$;
- (iii) $\sup_k |b_k^{II}| < \infty$ and $b_k^{II} \rightarrow 0$ as $k \rightarrow \infty$.

Then the assumptions of Theorem 5.3.1 of Kushner and Clark (1978) are satisfied, and the proposition follows. \square

Remark 2. In the above proof, we have used (ii) rather than A5.3.2 of Kushner and Clark (1978, p. 191), which states that, for some $T_0 > 0$ and any $\eta > 0$,

$$\lim_{n \rightarrow \infty} \Pr \left(\sup_{i \geq n} \max_{t \leq T_0} \left| \sum_{i=m(t; T_0)}^{m(i; T_0)+1} a_i e_i \right| \geq \eta \right) = 0, \quad (2)$$

where $m(t) = \max \{n: \sum_{i=0}^{n-1} a_i \leq t\}$ for $t \geq 0$ and $m(t) = 0$ otherwise. Equation (2) is indeed the assumption used to prove Theorem 5.3.1 of Kushner and Clark (1978). However,

(ii) is a stronger condition and implies (2); see Kushner and Clark (1978, p. 28–29).

Remark 3. Referring to Kushner and Clark (1978, p. 51), conditions (i) and (ii) of Proposition 1 also hold for the basic (two-sided) finite-difference stochastic approximation (FDSA). Adjusting the G_k to the component-wise perturbation of parameters for gradient approximations, it then follows that the same convergence proof holds for the projection FDSA.

3. Illustrative example

We study a simple numerical example of finding the optimal temperature profile in a tubular reactor for two first-order irreversible consecutive reactions. See Fan (1966) for details. The first-order reactions $A \rightarrow B \rightarrow C$ take place in the reactor. The reaction $A \rightarrow B$ has the specific rate $k_1(t)$ and $B \rightarrow C$ has the rate $k_2(t)$ at time t . Denoting the concentration of A by $x_1(t)$ and the concentration of B by $x_2(t)$, we arrive at the following state-space equation describing the dynamics of the reactions (Fan, 1966):

$$\begin{aligned} \dot{x}_1(t) &= -k_1(t)x_1(t), \\ \dot{x}_2(t) &= k_1(t)x_1(t) - k_2(t)x_2(t). \end{aligned} \quad (3)$$

The specific rates are given by $k_1(t) = k_{10}e^{-E_1/RT(t)}$ and $k_2(t) = k_{20}e^{-E_2/RT(t)}$, where $T(t)$ is the temperature profile (the control variable), and k_{10} , k_{20} , E_1 , E_2 and R are constants.

We wish to find the temperature profile that (starting from time $t_0 = 0$) maximizes $x_2(t_f)$, i.e. the concentration of the product B at $t = t_f$. By selecting a sampling time, the problem becomes a multivariate optimization problem where the temperature values at discrete time points should be determined such that the final concentration of B is maximized. We present solutions both under no constraints and under the situation that the applied profiles should satisfy $335 \leq T(t) \leq 342$. Unlike the (unconstrained) solution given in Fan (1966), our solution is in principle based on trials and experimentations on the system. The trials consist of applying temperature profiles to the system and performing measurements on $x_2(t_f)$ for each applied profile. We shall not require any model in order to find the optimum. Nor do we require knowledge of the values of the constants. In this example, we use the presented model for (and only for) simulation, data generation and testing our procedure.

Let us assume the following numerical values (Fan, 1966): $k_{10} = 5.34 \times 10^{10} \text{ min}^{-1}$, $k_{20} = 0.461 \times 10^{18} \text{ min}^{-1}$, $E_1 = 18\,000 \text{ cal mol}^{-1}$, $E_2 = 30\,000 \text{ cal mol}^{-1}$, $R = 2 \text{ cal mol}^{-1} \text{ K}^{-1}$, $t_f = 8 \text{ min}$, $x_1(0) = 0.8160 \text{ mol l}^{-1}$, $x_2(0) = 0.2260 \text{ mol l}^{-1}$.

Let us further assume that the temperature $T(t)$ is constant for $i-1 \leq t < i$, $i = 1, 2, \dots, 8$ (i.e. a piecewise-constant input). The i th element of the eight-dimensional optimization parameter θ is equal to $T(t)$ for $i-1 \leq t < i$.

The following constants are used throughout the example unless otherwise specified. The number of iterations for the SPSA algorithm is 250, the random perturbations are Bernoulli-distributed with magnitude one, i.e. $\Pr(\Delta_{k_i} = \pm 1) = 0.5$ for $i = 1, \dots, 8$, and all $k = 1, 2, \dots$, and the gain sequences are selected as $a_k = 1000/k^{0.602}$, $c_k = 1/k^{0.101}$. These decay rates for a_k and c_k are empirically found to yield optimal performance for the unconstrained SPSA algorithm in finite sample cases (see Spall, 1996). It should, however, be noted that the optimal sequences for the constrained case may be quite different, and finding good gain sequences may in general be difficult. It is moreover assumed throughout the example that the measured values of $x_2(t_f)$ are corrupted with additive i.i.d. Gaussian noise with standard deviation 0.0005, and, finally, the initial temperature profile $T_{in}(t)$ for the optimizations is chosen to be 342 K at $t = 0$ and to drop by 1 K min^{-1} .

In order to determine the true optimal profiles, we use standard techniques that, unlike SPSA, make use of the model given by (3) and assume noise-free data. Equation (3) can be written as $\dot{x}(t) = A(t)x(t)$, where $x(t)$ is the state vector and $A(t)$ is a piecewise-constant matrix ($A(t)$ is constant in the interval $i-1 \leq t < i$, $i = 1, \dots, 8$). The

explicit relation between the objective function and the control variable is obtained using $x(t_f = 8) = \exp[\sum_{j=0}^{t_f-1} A(j)]x(0)$, and standard optimization algorithms can be applied to find the optimal profiles. We use the MATLAB® optimization toolbox functions CONSTR and FMINS (Grace, 1994) for the constrained and unconstrained cases respectively.

Now, let us try both the constrained and unconstrained SPSA algorithms to estimate the optimal profiles. We define $G_k = \{\theta : 335 + c_k \leq \theta \leq 342 - c_k, i = 1, \dots, 8\}$ for the constrained case. For each of the constrained and unconstrained cases, we estimate the optimal profile 500 times (i.e. 500 cross-sections for each algorithm). The obtained estimates are denoted by $\hat{T}_c(t)$ and $\hat{T}_u(t)$ respectively (note the randomness in the iterates due to measurement noise for SPSA). As expected, all the 500 realizations of $\hat{T}_c(t)$ are restricted to lie within $[335, 342]$ (for all $0 \leq t < 8$), while the largest value (among 500 realizations) of $\hat{T}_u(t)$ is 345.5. For each realization of $\hat{T}_c(t)$ and $\hat{T}_u(t)$, we compute (i) the relative error defined by

$$\left\{ \frac{\int_0^{t_f} [T^*(t) - T_r(t)]^2 dt}{\int_0^{t_f} [T^*(t) - T_{in}(t)]^2 dt} \right\}^{1/2},$$

where $T_r(t)$ and $T^*(t)$ are the relevant realization and true optimal profile (as computed previously), and (ii) the noise-free value of $x_2(t_f)$ corresponding to the realization (hence randomness in this computed value is only due to randomness in $\hat{T}_c(t)$ and $\hat{T}_u(t)$). By averaging over these computed values, we obtain an average relative error (ARE) and an average final-product value (AFP) for both the constrained and unconstrained cases. The results are summarized in Table 1, where OFP denotes the relevant optimal final product value as given by the true optimal profiles.

In order to investigate the effect of the extra error on the gradient approximation (introduced to make the measurements feasible), we estimate the constrained optimal profile 500 times using the projection SPSA algorithm, but we use $\hat{g}_k(\hat{\theta}_k) = g_k^{SP}(\hat{\theta}_k)$. The corresponding ARE and AFP values for this case are 0.1561 and 0.6988 respectively. Comparing the obtained ARE with 0.1819 (see Table 1) indicates improvement, but at the expense of infeasibility of the measurements.

It is also of interest to assess the convergence rate of the constrained algorithm. We estimate the optimal profile 500 times using constrained SPSA with 1000 iterations (and with the same algorithm constants as before) for each cross-section, which yields an ARE value of 0.1139. We then use $-\log(0.1819/0.1139)/\log(250/1000) = 0.338$ as an assessment of the convergence rate. Using Proposition 2 of Spall (1992), the (asymptotic) convergence rate of the unconstrained algorithm for the gain sequences of this example is equal to 0.2, which is considerably less than the computed rate 0.338.

Finally, we apply the constrained two-sided FDSA algorithm 500 times with the same algorithm constants as for the constrained SPSA, but 32 iterations for each cross-section. Note that the total number of measurements for the FDSA algorithm with 32 iterations is equal to $32 \times 2 \times 8 = 512$, which is slightly larger than the total number of measurements for the SPSA algorithm with 250 iterations ($250 \times 2 = 500$). The ARE and AFP values become 0.2117 and 0.6988. The ARE value for the constrained FDSA is noticeably larger than 0.1819 obtained for the constrained SPSA algorithm for (almost) the same number of measurements.

Table 1. Constrained and unconstrained optimization using 500 cross-sections of SPSA. All the final product values are based on noise-free evaluations of $x_2(t_f)$

Constrained		Unconstrained			
ARE	AFP	OFP	ARE	AFP	OFP
0.1819	0.6988	0.6989	0.3291	0.6996	0.6999

It should be noted that a formal treatment of the convergence rate and accuracy of the estimate of the constrained SPSA algorithm is required before one is able to draw any definitive conclusion about the behavior of the algorithm.

4. Concluding remarks

This paper has presented a projection algorithm for constrained optimization via stochastic approximation with a simultaneous perturbation gradient approximation where no gradient information is directly available. The algorithm can handle inequality constraints given as explicit functions of the parameter. The constraints should define a set with a non-empty interior. We have considered the case where measurements outside the constraint set are not feasible, which is stronger than restricting the solution to the feasible domain. We have established almost-sure convergence of the iterate to a Kuhn–Tucker point.

Possible directions for future study are the performance of the algorithm, distribution or convergence rate of the iterate, possible error bounds on the estimate, and optimal tuning of the algorithm constants, i.e. optimal selection of gain sequences. Finally, an identical proof of convergence can be applied to a projection FDSA algorithm (see Remark 3). It will be of interest to compare the number of measurements that constrained SPSA and constrained FDSA need to reach a certain level of accuracy (see Section 1 and Spall (1992) for a similar comparison in the unconstrained case).

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