STOCHASTIC APPROXIMATION[1, 2]

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1. Introduction. In certain applications, as in bioassay, sensitivity testing, or fatigue trials, the statistician is often interested in estimating a given quantile of a distribution function on the basis of data which is of the zero-one type. For example, suppose $F(x)$ denotes the probability that a metallic test specimen will fracture if subjected to x cycles in a fatigue trial. Then a specimen, when tested in such a way, represents an observation which takes on the value one or zero depending on whether or not it fractures. It is of interest to estimate that number of cycles x such that, for a given α, $F(x) = \alpha$. The techniques of possible use in this connection, such as probit analysis [8] and the "up and down" method of Dixon and Mood [6], depend to a great extent on parametric assumptions concerning the distribution function $F(x)$. Robbins and Monro [13] considered a problem of which the above problem, with or without parametric assumptions, is a special case. Suppose for every real value x, the random variable $Y(x)$, denoting the value of a response to an experiment carried out at a controlled level x, has the unknown distribution function $H(y \mid x)$ and regression function $M(x) = \int_{-\infty}^{\infty} y \, dH(y \mid x)$. Let α be any given real number. Robbins and Monro considered the problem of estimating the root of the equation $M(x) = \alpha$, assuming the existence of a unique root. If $Y(x) = 1$ or 0 with probabilities $F(x)$ and $1 - F(x)$ respectively, where $F(x)$ is a distribution function and $0 \leqq \alpha \leqq 1$, then $M(x) = F(x)$, and we have the above special case.

The problem of estimating a root of a given regression function has its counterpart in the literature of the more classical mathematics. Newton's method of approximation is, perhaps, the best-known iterative procedure used for such a problem when no random element is present. However, even if $Y(x) = M(x)$ with probability one—i.e., if no randomness exists—Newton's method is not applicable; for Newton's method and other classical procedures depend on knowing the functional form of $M(x)$, whereas, here, such knowledge is not assumed.

Because of the nonparametric nature of the problem, a method of approach not based on the usual curve-fitting techniques, is clearly necessary. As a solution, Robbins and Monro put forward the following iterative scheme. Let $\{a_n\}$ $(n \geqq 1)$ be a fixed sequence of positive constants such that

$$(1.1) \qquad \sum_{n=1}^{\infty} a_n = \infty, \qquad \sum_{n=1}^{\infty} a_n^2 < \infty.$$

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The sequence $a_n = 1/n$, for example, satisfies (1.1). Let x_1, the level of the first experiment, be arbitrary. Succeeding levels are defined recursively by

$$x_{n+1} = x_n + a_n(\alpha - y_n), \tag{1.2}$$

where y_n denotes the response at level x_n—a random variable dependent only on x_n and having the distribution function $H(y \mid x_n)$. Thus at each stage of experimentation, a new level is chosen, based upon the deviation of the previous response from α and on the number of experiments already performed.

Since the proposal of their scheme, considerable attention has been focused in this direction. Some of this attention has been directed towards establishing conditions under which the Robbins-Monro procedure is reasonable; some has been directed towards treating similar problems with different but analogous schemes; and some has been directed towards providing a more general theory of stochastic approximation. This paper is an exposition of work done along these lines.

2. The Robbins-Monro Process. Let θ be the root of the equation $M(x) = \alpha$. Robbins and Monro [13] proved that x_n defined by (1.2) converges in the mean to θ, i.e., $\lim_{n\to\infty} E(X_n - \theta)^2 = 0$, in two separate cases. In one case the function $M(x)$ is discontinuous at θ with $| M(x) - \alpha |$ being bounded away from zero for all $x \neq \theta$. (In fact, $M(\theta)$ need not equal α.) In the other case, $M(x)$ is nondecreasing, $M(\theta) = \alpha$, and $M'(\theta) > 0$. In both cases the rather strong condition that $Y(x)$ be bounded with probability one for all x was imposed. However, it should be remarked that for the purpose of estimating a quantile with zero-one data, the condition is not restrictive.

Wolfowitz [16] was the next to take up the problem. He showed that x_n converges to θ in probability under weaker conditions. His most significant improvement was to replace the boundedness condition of Robbins and Monro with the condition that $M(x)$ and $\sigma_x^2 = \int_{\infty}^{\infty} (y - M(x))^2 \, dH(y \mid x)$ be bounded functions of x.

The following conditions, which are weaker than both the Robbins-Monro and Wolfowitz conditions, were assumed by Blum [1].

$$| M(x) | \leqq c + d\,| x | \qquad \text{for some } c, d \geqq 0, \tag{2.1}$$

$$\sigma_x^2 \leqq \sigma^2 < \infty \qquad \text{for all } x, \tag{2.2}$$

$$M(x) < \alpha \ (x < \theta), \qquad M(x) > \alpha \ (x > \theta), \tag{2.3}$$

$$\inf_{\delta_1 \leqq |x-\theta| \leqq \delta_2} | M(x) - \alpha | \qquad \text{for every } \delta_1, \delta_2 > 0. \tag{2.4}$$

Under these assumptions Blum was able to show that $P(\lim_{n\to\infty} x_n = \theta) = 1$. That this is true, with no stronger assumption than (2.4), is somewhat surprising. For (2.4) allows the possibility that $M(x) \to \alpha$ as $| x | \to \infty$, and in such a case one would expect that there might be positive probability of $| x_n |$ converging to ∞.

While the proofs of Robbins and Monro and of Wolfowitz used arguments rather special to the process under consideration, Blum's method related to other known results. More specifically, it can be shown using Martingale theory or, more directly, Kolmogorov's inequality that because of (1.1) and (2.2), $\sum_{j=1}^{\infty} a_j(y_j - M(x_j))$ converges with probability one. (See Loève [12], p. 387.) Consequently

$$x_{n+1} - \sum_{j=1}^{n} a_j(\alpha - M(x_j)) = x_1 - \sum_{j=1}^{n} a_j(y_j - M(x_j))$$

converges with probability one. Imposing the conditions of (2.1) and (2.3), Blum was able to show that x_n converges with probability one to a random variable W which is finite with probability one. Then (2.4) was enough of a further assumption to allow him to prove that $W = \theta$ with probability one.

Recently, Dvoretzky [7] has shown that under Blum's conditions, x_n also converges in the mean to θ. Dvoretzky's work will be discussed below.

While the results of Blum and Dvoretzky show that under wide conditions the Robbins-Monro process converges to θ both in mean square and with probability one, it is of interest, particularly for statistical purposes, to obtain sharper convergence theorems. To this end, Chung [4] considered two cases. In his first (bounded) case he assumed that

$$M(x) = \alpha + \alpha_1(x - \theta) + o(|x - \theta|) \qquad (0 < \alpha_1 < \infty), \tag{2.5}$$

$$\inf_{|x-\theta|>\delta} |M(x) - \alpha| = K_0(\delta) > 0 \qquad \text{for every } \delta > 0, \tag{2.6}$$

$$P(|Y(x) - \alpha| \leqq K_1 < \infty) = 1 \qquad \text{for all } x, \tag{2.7}$$

$$\lim_{x\to\theta} \sigma_x^2 = \sigma_\theta^2 > 0. \tag{2.8}$$

Under the conditions of (2.5), (2.6), (2.7), and (2.8), Chung showed that if $a_n = 1/(n^{1-\epsilon})$, where $1/[2(1 + K_4)] < \epsilon < \frac{1}{2}$ (K_4 being a constant arising in his analysis), then $n^{(1-\epsilon)/2}(x_n - \theta)$ tends in distribution to the normal distribution with mean 0 and variance $\sigma_\theta^2/(2\alpha_1)$. In his second (quasi-linear) case, he replaced (2.7) with

$$K|x - \theta| \leqq |M(x) - \alpha| \leqq K'|x - \theta| \quad K > 0, K' > \infty, \tag{2.9}$$

and

$$\int_{-\infty}^{\infty} |y - M(x)|^p \, dH(y \mid x) \leqq K(p) < \infty \qquad p = 1, 2, \cdots, \tag{2.10}$$

and showed that if $a_n = c/n$, $c > 1/(2K)$, then $n^{\frac{1}{2}}(x_n - \theta)$ tends in distribution to the normal distribution with mean 0 and variance $(\sigma_\theta^2 c^2)/(2\alpha_1 c^2 - 1)$. Both results were proved by showing the proper convergence of moments. In earlier papers, Kallianpur [10] and Schmetterer [14] and [15] obtained certain bounds for $E(x_n - \theta)^2$. For the most part, however, their results are contained in those of Chung.

The question arises as to whether other limiting distributions might exist.

Chung also showed that all stable laws are possible limiting distributions; and furthermore, no limiting distribution need necessarily exist.

For purposes of application, Chung's results still left something to be desired. Kiefer, who contributed largely to the last section of [4], remarked that, for the quasi-linear case, if $a_n = c/n$, with $c = 1/\alpha_1$, the Robbins-Monro estimate of θ is, under certain regularity conditions, asymptotically minimax if the loss function of an estimate d is $|\theta - d|^r$, $r \geqq 0$. That this is true follows with slight modification from results obtained by Wolfowitz [17] on minimax estimation of the mean of a normal distribution with known variance. However, the conditions of the quasi-linear case are not satisfied if $M(x)$ is a distribution function—as is the case in the quantal response problem. Here the bounded case is applicable, but the estimate based on $a_n = 1/n^{1-\epsilon}$ has asymptotic efficiency zero. Hodges and Lehman [9], using an idea attributed to Stein, bridged the gap between the quasilinear case and the bounded case, proving that, in the bounded case, $n^{\frac{1}{2}}(x_n - \theta)$ also converges in distribution to the normal distribution with mean 0 and variance $(\sigma_\theta^2 c^2)/(2\alpha_1 c^2 - 1)$ if $a_n = c/n$, $c > 1/(2K'')$, where $K'' = \inf_{|x-\theta|<A} |M(x) - \alpha| / |x - \theta|$ (A being any positive number such that $K'' > 0$). It is not known whether the moments of $n^{\frac{1}{2}}(x_n - \theta)$ converge to the moments of the limiting distribution. Their method was to show, using Blum's probability one convergence theorem, that the asymptotic distribution of x_n depends only on those values of $M(x)$ defined in the neighborhood of $x = \theta$. Within any finite interval, a function $M(x)$ satisfying the conditions of the bounded case will also satisfy the conditions of the quasi-linear case, so that as far as the asymptotic distributions are concerned, the two cases are the same.

Coming back to the quasi-linear case, it has been remarked that for $a_n = 1/(\alpha_1 n)$ and loss function $|\theta - d|^r$, the Robbins-Monro procedure is asymptotically minimax over all possible procedures. Dvoretzky [7] has shown that if it is known that $|x_1 - \theta| \leqq C \leqq [(2\sigma^2)/K(K' - K)]^{\frac{1}{2}}$, where σ^2 is defined by (2.2), then the choice of $a_n = (KC^2)/(\sigma^2 + nK^2C^2)$ yields estimates such that

$$E(x_n - \theta)^2 \leqq \frac{\sigma^2 C^2}{\sigma^2 + (n-1)K^2C^2} \qquad n \geqq 1, \tag{2.11}$$

and if any other coefficients are used, there exists an x_1 and a function $M(x)$ satisfying the quasi-linear conditions such that (2.11) does not hold. Except for the case $K = \alpha_1$, Dvoretzky's coefficients lead to estimates having asymptotic variance larger than that obtained by letting $a_n = 1/(\alpha_1 n)$. This loss in asymptotic efficiency is, of course, the price paid for small-sample optimality.

Lehmann and Hodges raised the questions as to how much agreement exists between asymptotic and small-sample theory and how c, if one uses the coefficients $a_n = c/n$, is to be chosen if $\alpha_1 = M'(\theta)$ is unknown. Since the behavior of the variance of the estimate is unknown for $c < 1/(2K)$, they remarked that one would be tempted, if an a priori guess is to be made, to overestimate c. They would also overestimate c on the grounds that $(\sigma_\theta^2 c^2)/(2\alpha_1 c - 1)$, the asymptotic variance of $n^{\frac{1}{2}}(x_n - \theta)$, increases more slowly for increasing $c >$

$1/\alpha_1$ than for decreasing $c < 1/\alpha_1$. In order to gain more insight concerning the proper choice of n and c, they considered the special case of a linear $M(x)$ and constant σ_x^2. Here it is possible to compute exact variances for all n and to study the effect of varying c on the exact variance. They found, for this special case, rather close agreement between asymptotic and small-sample theory for $n = 20$ and $c > 1/\alpha_1$. However, for $c < 1/\alpha_1$, it appears that the rate of approach of the small-sample variance to the asymptotic variance is much slower, and thus the danger due to underestimating c is, perhaps, not as great as the asymptotic theory suggests.

3. The Kiefer-Wolfowitz Process. Kiefer and Wolfowitz [11] considered the problem of estimating the value of $x = \theta$ such that $M(x)$ is maximum, assuming the existence of a unique maximum. They suggested the following scheme. Let $\{a_n\}$ and $\{c_n\}$ be sequences of positive numbers such that

$$(3.1) \qquad c_n \to 0, \qquad \sum_{n=1}^{\infty} a_n = \infty, \qquad \sum_{n=1}^{\infty} a_n c_n < \infty, \qquad \sum a_n^2 c_n^{-2} < \infty.$$

For example, $a_n = 1/n$, $c_n = 1/n^{\frac{1}{4}}$ are such sequences. Let x_1 be arbitrary. Then define recursively

$$(3.2) \qquad x_{n+1} = x_n + a_n c_n^{-1}(y_{2n} - y_{2n-1}),$$

where y_{2n-1} and y_{2n} are independent random variables with respective distributions $H(y \mid x_n - c_n)$ and $H(y \mid x_n + c_n)$. They proved under certain regularity conditions that x_n converges in probability to θ. Using the same method as with the Robbins-Monro process, Blum [1], under weaker conditions, showed that the process converges with probability one. It also turns out that the condition $\sum a_n c_n < \infty$ is unnecessary. The conditions of Blum and of Kiefer and Wolfowitz are of such a nature that functions like $M(x) = e^{-x^2}$, $-x^2$ are ruled out. Derman [5] considered functions which might be called "quasi-parabolic," analogous to Chung's quasi-linear functions—i.e., functions whose difference quotients lie between two straight lines with positive slopes. Functions like $-x^2$ satisfy these conditions. It was shown in such cases that x_n converges in the mean to θ and in more restrictive cases, where $M(x)$ is locally parabolic at θ, there is, with proper normalization, convergence to the normal distribution. Burkholder [3] also obtained results pertaining to asymptotic normality.

The weakest set of conditions for convergence of the Kiefer-Wolfowitz process which allow both e^{-x^2} and $-x^2$ were given by both Burkholder and Dvoretzky. Burkholder proved probability one convergence and Dvoretzky proved both convergence with probability one and in the mean square. These conditions in Dvoretzky's form are as follows:

$$(3.3) \qquad | M(x + 1) - M(x) | < A \,| x | + B < \infty \quad \text{for all } x \text{ and some A, B,}$$

$$(3.4) \qquad \sup_{1/k<x-\theta<k} \bar{D}M(x) < 0, \qquad \inf_{1/k<\theta-x<k} \underline{D}M(x) > 0 \qquad \text{for } k = 1, 2, \cdots,$$

$$(3.5) \qquad \sigma_x^2 < \sigma^2 < \infty,$$

where $\bar{D}M(x)$ and $\underline{D}(x)$ denote the upper and lower derivates of $M(x)$ at x and σ_x^2 is as in (2.2).

An undesirable feature of the Kiefer-Wolfowitz process is that two observations must be taken at each stage of experimentation. This of course raises the question of whether there exists a procedure having desirable convergence properties which requires only one observation at each stage.[3] No such procedure has yet been suggested. However, the approach taken by Dvoretzky appears as if it might allow results in this direction. In the cases that Derman considered, it also turns out that the Kiefer-Wolfowitz procedure yields estimates which have zero asymptotic efficiency—i.e., if x_n is any estimate based on one set of coefficients $\{a_n\}$ and $\{c_n\}$, there exists another estimate x_n' based on coefficients $\{a_n'\}$ and $\{c_n'\}$ such that $\lim_{n\to\infty} E(x_n' - \theta)^2/E(x_n - \theta)^2 = 0$. Thus a better procedure seems desirable from this point of view. It is of some interest to note that for cases where $M(x)$ is symmetric about θ, the Robbins-Monro procedure may be used. More explicitly, let ϵ be a small positive number and let $\bar{M}(x) = M(x + \epsilon) - M(x - \epsilon)$ and $y_n' = y_{2n} - y_{2n-1}$, where y_{2n} and y_{2n-1} are observations at $(x + \epsilon)$ and $(x - \epsilon)$ respectively. Then, since $\bar{M}(x)$ is a monotone function of x, and θ is the value of x such that $\bar{M}(x) = \alpha = 0$, the Robbins-Monro procedure $x_{n+1} = x_n - a_n y_n'$ is applicable. Burkholder has pursued this idea further into cases where $M(x)$ is not necessarily symmetric. In such cases, if x_n converges, it converges to a constant which will, in general, differ from θ.

4. Other Procedures. Blum [2] has considered multidimensional analogues to the above problems. Let $Y(x)$ be a k-dimensional random vector with joint distribution function $H(y \mid x)$, where x is also a k-dimensional vector, and let $M(x)$ denote the expectation of $Y(x)$, where by this we mean that the ith component of $M(x)$ is the expectation of the ith component of $Y(x)$. Conditions were found to ensure that, for a given vector α, a multidimensional version of the Robbins-Monro procedure converges with probability 1 to a vector $x = \theta$, where $M(\theta) = \alpha$. Suppose $Y(x)$ is a random variable which is dependent on x, a k-dimensional vector, and has expectation $M(x)$, a function of x assumed to have a unique maximum. Conditions were also found such that a generalization of the Kiefer-Wolfowitz procedure ($k + 1$ observations at each stage) would yield estimates converging to the vector $x = \theta$, where $M(\theta)$ is maximum. Martingale theory was employed in the convergence proofs.

Returning to one dimension, Burkholder [3] investigated a process slightly more general than either the Robbins-Monro or the Kiefer-Wolfowitz process. Burkholder's process is of the form

$$x_{n+1} = x_n + a_n z_n, \tag{4.1}$$

where $\{a_n\}$ is a sequence of positive numbers and z_n is a random variable with distribution function $H_n(z \mid x_n)$—i.e. the distribution functions and therefore the regression functions depend on n. For example, $M_n(x) = (1/c_n)(M(x + c_n) - M(x - c_n))$ in the Kiefer-Wolfowitz procedure is a function of n. Using methods

[3] As a matter of fact, this was the original problem concerning the maximum of a regression function posed by H. Robbins.

of Blum, Chung, and Lehmann and Hodges, Burkholder was able to prove various convergence theorems concerning his process. His results carry over to situations where x_n converges to a nonconstant random variable—this occurring when there is no uniqueness of, say, the root of $M(x) = \alpha$ or the maximum of $M(x)$. As a special case of his process, he exhibited a procedure which converges to the point of inflection of a function; e.g., estimating the maximum of a density function with zero-one data is a particular application of such a procedure. Another application permitted by his more general procedure is that of estimating, by taking additional observations at each stage, unknown constants of interest such as α_1 and σ_θ^2, arising in Section 2.

5. A more general approach to stochastic approximation. A more general approach taken by Dvoretzky [7], viewing a stochastic approximation procedure as a convergent deterministic procedure with a superimposed random element, has proved to be enlightening. For example, suppose $T_n(x_1, \cdots, x_n)$ is any transformation of an n-dimensional Euclidean space $\mathcal{E}_n$ into the real numbers such that for some $x = \theta$,

$$(5.1) \quad | T_n(x_1, \cdots, x_n) - \theta | \leqq F_n | x_n - \theta | \quad \text{for all } (x_1, \cdots, x_n) \in \mathcal{E}_n,$$

where F_n is a sequence of positive numbers satisfying

$$(5.2) \quad \prod_{n=1}^{\infty} F_n = 0.$$

Suppose

$$(5.3) \quad x_{n+1} = T_n(x_1, \cdots, x_n) + Y_n,$$

where Y_n $(n = 1, \cdots)$ are random variables such that $E(Y_n \mid x_1, \cdots, x_n) = 0$ and $\sum_{n=1}^{\infty} \sigma_n^2 = \sum_{n=1}^{\infty} EY_n^2 < \infty$. Then, putting $V_n^2 = E(x_n - \theta)^2$ and using (5.1), we have

$$(5.4) \quad V_{n+1}^2 \leqq F_n^2 V_n^2 + \sigma_n^2.$$

Let $b_{n-v} = \prod_{i=v+1}^{n} F_i^2$. On iterating (5.4) we get

$$(5.5) \quad V_{n+1}^2 \leqq \sum_{i=1}^{n-1} \sigma_i^2 b_{n-i} + \sigma_n^2 + V_1^2 b_{n-1}.$$

For every fixed v, $b_{n-v} \to 0$ as $n \to \infty$ by (5.2); and since $\sum_{n=1}^{\infty} \sigma_n^2 < \infty$, it follows, assuming $V_1^2 < \infty$, that the right side of (5.5), and consequently the left, tends to 0 as $n \to \infty$. Thus any stochastic approximation procedure given by (5.3), with T_n satisfying (5.1) and (5.2) and x_1 chosen such that $V_1^2 < \infty$, yields an estimate which converges in the mean to θ. For the Robbins-Monro scheme, $T_n = x_n + a_n(\alpha - M(x_n))$ and $Y_n = a_n(M(x_n) - y_n)$. Under certain restrictive conditions, (5.1) and (5.2) hold. However, in order that this approach be more generally applicable, it is necessary to weaken condition (5.1). For example, such a weakening is that for sequences of non-negative real numbers α_n, β_n, and γ_n, satisfying $\lim_{n\to\infty} \alpha_n = 0$, $\sum_{n=1}^{\infty} \beta_n < \infty$, $\sum_{n=1}^{\infty} \gamma_n = \infty$,

$$(5.6) \quad | T_n(x, \cdots, x_n) - \theta | \leqq \max(\alpha_n, (1 + \beta_n) | x_n - \theta | - \gamma_n).$$

A further weakening permits α_n, β_n, γ_n to depend on $x_1, \cdots, x_n$. Under such conditions Dvoretzky was able to prove that the process (5.3) converges to θ in the mean and with probability one. These conditions are weak enough to apply to the Robbins-Monro and Kiefer-Wolfowitz processes, yielding results mentioned above.

One might expect, then, that whenever a convergent deterministic iteration procedure converges, its stochastic counterpart given by (5.3) will also converge. Dvoretzky constructed a counterexample to show that this is not the case. Thus the conditions $E(Y_n \mid x_1, \cdots, x_n) = 0$ and $\sum_{n=1}^{\infty} EY_n^2 < \infty$ are not strong enough to allow conditions like (5.6) to be removed.

A further advantage of this general approach is that the convergence theorems hold, with appropriate changes, if x is an element of a normed linear space. Such generality is useful since, in many applications, x will not be a one-dimensional variable. For example, the multidimensional cases treated by Blum can be considered from this point of view.

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