MULTIDIMENSIONAL STOCHASTIC APPROXIMATION METHODS[1]

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1. Summary. Multidimensional stochastic approximation schemes are presented, and conditions are given for these schemes to converge a.s. (almost surely) to the solutions of k stochastic equations in k unknowns and to the point where a regression function in k variables achieves its maximum.

2. Introduction. Let $H(y \mid x)$ be a family of distribution functions depending upon a real parameter x and let $M(x) = \int_{-\infty}^{\infty} y \, dH(y \mid x)$ be the regression function corresponding to the family $H(y \mid x)$. Robbins and Monro [1] define a stochastic approximation method to solve the equation $M(x) = \alpha$, where α is a specified constant. Their method is such that the approximating random variables converge in probability to θ, where θ is a root of the equation $M(x) = \alpha$. These results are generalized by Wolfowitz [2]. Kiefer and Wolfowitz [3] define a stochastic approximation scheme which converges in probability to θ, where θ is the point at which $M(x)$ achieves a maximum. Finally, it is shown [4] that in fact, in both of the situations mentioned above, the approximating sequence of random variables converges a.s. to θ.

The object of this paper is to extend these results to several dimensions. More precisely we consider the following two problems.

(A) Let $\{Y^{(1)}_{x_1, \cdots, x_k}\}, \cdots, \{Y^{(k)}_{x_1, \cdots, x_k}\}$ be k families of random variables with corresponding families of distribution functions $\{F^{(1)}_{x_1, \cdots, x_k}\}, \cdots, \{F^{(k)}_{x_1, \cdots, x_k}\}$, each depending on k real variables $(x_1, \cdots, x_k)$. Let $M^{(i)}(x_1, \cdots, x_k) = \int_{-\infty}^{\infty} y \, dF^{(i)}_{x_1, \cdots, x_k}$, for $i = 1, \cdots, k$, be the corresponding regression functions. Then, if $\alpha_1, \cdots, \alpha_k$ are k specified numbers, it is desired to find a stochastic approximation method such that the sequence of approximating random vectors converges a.s. to a solution of the equation

$$M^{(i)}(x_1, \cdots, x_k) = \alpha_i, \qquad i = 1, \cdots, k.$$

Here it is assumed that the distributions $F^{(i)}$ and the regression functions $M^{(i)}$ are unknown; however, it is possible to make an observation on the random variable $Y^{(i)}_{x_1, \cdots, x_k}$ for $i = 1, \cdots, k$, and any choice of real numbers $(x_1, \cdots, x_k)$.

(B) Let $\{Y_{x_1, \cdots, x_k}\}$ be a family of random variables, $F_{x_1, \cdots, x_k}$ be the corresponding distribution functions, and $M(x_1, \cdots, x_k)$ the corresponding regres-

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sion function. Subject to the assumptions of (A), it is desired to estimate that set of numbers $(\theta_1, \cdots, \theta_k)$ for which the function M achieves its maximum.

The approximating sequences defined in this paper are straightforward generalizations of the sequences defined in [1] and [3]. The methods of proof used here were strongly motivated by the methods used in [2] and [3].

3. A theorem on almost sure convergence. The following theorem is an immediate consequence of the martingale convergence theorem of Doob [5].

THEOREM. *Let X_n be a sequence of random variables satisfying*

(i) $\sup_n E\{|X_n|\} < \infty$,
(ii) $\sum_{n=1}^{\infty} E\{[E\{X_{n+1} - X_n \mid X_1, \cdots, X_n\}^+]\} < \infty$.

Then X_n converges a.s. *to a random variable.*

As usual, we define X^+ by $X^+ = \frac{1}{2}[X + |X|]$. We immediately obtain the following

COROLLARY. *Let X_n be a sequence of integrable random variables which satisfy condition* (ii) *of the theorem and are bounded below uniformly in n. Then X_n converges* a.s. *to a random variable.*

PROOF. Let $Y_n = X_n - a$, where a is chosen so that $Y_n \geqq 0$ for all n. Then

$$E\{|Y_n|\} = E\{Y_n\} = E\{Y_1\} + \sum_{j=1}^{n-1} E\{Y_{j+1} - Y_j\} \leqq E\{Y_1\} + \sum_{j=1}^{n-1} E\{[E\{X_{j+1} - X_j \mid X_1, \cdots, X_j\}^+]\}.$$

Hence the theorem applies to the sequence Y_n and consequently to the sequence X_n.

4. Convergent sequences of random vectors. Let E_k be a real k-dimensional vector space spanned by the orthogonal unit vectors $u_1, \cdots, u_k$. If x and y are two vectors in E_k, we denote their inner product by $\langle x, y\rangle$ and their norms by $\|x\|$ and $\|y\|$, respectively. Suppose that to each $x \varepsilon E_k$ corresponds a random vector $Y_x \varepsilon E_k$. Denote by $M(x)$ the vector representing the conditional expectation of Y_x when x is fixed.

Let now $f(x)$ be a real-valued function defined on E_k and possessing continuous partial derivatives of the first and second order. The vector of first partial derivatives will be denoted by $D(x)$ and the matrix of second partial derivatives by $A(x)$. That is

$$D(x) = \left(\frac{\partial f}{\partial x_i}\right) \mid x, \qquad A(x) = \left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right) \mid x.$$

Then, for any real number a, we have by Taylor's theorem

$$f(x + aY_x) = f(x) + a\langle D(x), Y_x\rangle + \tfrac{1}{2}a^2\langle Y_x, A(x + \theta a Y_x)Y_x\rangle,$$

where θ is a real number with $0 \leqq \theta \leqq 1$. Consequently we may take expectations on both sides to obtain

$$E\{f(x + aY_x)\} = f(x) + a\langle D(x), M(x)\rangle + \tfrac{1}{2}a^2 E\{\langle Y_x, A(x + \theta a Y_x)Y_x\rangle\}. \tag{4.1}$$

Let now $\{a_n\}$ be a sequence of positive numbers and consider the following sequence of recursively defined random vectors

$$X_{n+1} = X_n + a_n Y_n, \tag{4.2}$$

where X_1 is chosen arbitrarily and where Y_n has the distribution of Y_x when X_n yields the observation x. The object of this section is to set down conditions under which X_n converges a.s. to zero.

To simplify writing we shall employ the following notation throughout:

$$Z_x = f(x), \qquad U(x) = \langle D(x), M(x)\rangle, \qquad V_a(x) = E\{\langle Y_x, A(x + \theta a Y_x)Y_x\rangle\}.$$

When we substitute the random variables X_n for x and the numbers a_n for a, the corresponding random variables will be denoted by Z_n, U_n, and V_n. We shall assume throughout that $M(0) = 0$.

Consider now the following set A of conditions:

A_1: $\sum_{n=1}^{\infty} a_n = \infty, \quad \sum_{n=1}^{\infty} a_n^2 < \infty;$

A_2: $Z_x \geqq 0;$

A_3: $\sup_{\epsilon \leqq ||x||} U(x) < 0$ for every $\epsilon > 0$;

A_4: $\inf_{\epsilon \leqq ||x||} |Z_x - Z_0| > 0$ for every $\epsilon > 0$;

A_5: $V_a(x) \leqq V < \infty$ for every number a.

Then we have

THEOREM 1. *If the sequence a_n satisfies A_1 and if there exists a real-valued function $f(x)$ with continuous first and second partial derivatives satisfying $A_2 \cdots A_5$, then the sequence $\{x_n\}$ defined by* (4.2) *converges* a.s. *to zero.*

PROOF. From (4.1) we obtain

$$E\{Z_{n+1} \mid Z_1, \cdots, Z_n\} = Z_n + a_n E\{U_n \mid Z_1, \cdots, Z_n\} + \frac{a_n^2}{2} E\{V_n \mid Z_1, \cdots, Z_n\} \text{ a.s.} \tag{4.3}$$

Since $M(0) = 0$, we have, by virtue of conditions A,

$$E\{U_n \mid Z_1, \cdots, Z_n\} \leqq 0 \text{ a.s.}, \qquad E\{V_n \mid Z_1, \cdots, Z_n\} \leqq V \text{ a.s.},$$

both for all n. Hence

$$E\{Z_{n+1} - Z_n \mid Z_1, \cdots, Z_n\} \leqq \tfrac{1}{2}a_n^2 V \text{ a.s.} \tag{4.4}$$

We may assume V to be nonnegative. Using this fact together with conditions A_1 and A_2, we may apply the corollary of Section 3 to obtain

$$P\{Z_n \text{ converges}\} = 1. \tag{4.5}$$

Taking expectations on both sides of (4.3) and iterating, we have

$$E\{Z_{n+1}\} = Z_1 + \sum_{j=1}^{n} a_j E\{U_j\} + \sum_{j=1}^{n} \tfrac{1}{2}a_j^2 E\{V_j\}.$$

From what has been said above it follows that

$$E\{Z_n\} \geqq 0, \qquad E\{U_n\} \leqq 0, \qquad E\{V_n\} \leqq V, \qquad n = 1, \cdots.$$

Since V is nonnegative and the series $\sum_1^\infty a_n^2$ converges, the nonpositive term series $\sum_1^\infty a_n E\{U_n\}$ also converges. By virtue of the fact that $\sum_1^\infty a_n = \infty$ we have

$$\limsup_{n\to\infty} E\{U_n\} = 0, \qquad \liminf_{n\to\infty} E\{| U_n |\} = 0.$$

Let $\{n_k\}$ be an infinite sequence of integers such that $\lim_{k\to\infty} E\{|U_{n_k}|\} = 0$. Then U_{n_k} converges to zero in probability and there exists a further subsequence say $\{U_{m_k}\}$ such that

$$P\{\lim_{k\to\infty} U_{m_k} = 0\} = 1.$$

From condition A_3 it follows that $P\{\lim_{k\to\infty} X_{m_k} = 0\} = 1$. Since Z_n is a continuous function of X_n it follows from (4.5) that

$$P\{\lim_{n\to\infty} Z_n = Z_0\} = 1. \tag{4.6}$$

Now consider a sample sequence $\{X_n\}$ such that for the corresponding sequence $\{Z_n\}$ we have $\lim_{n\to\infty} Z_n = Z_0$. From condition A_4 it is clear that for such a sequence we must have $\lim_{n\to\infty} X_n = 0$. Hence (4.6) gives the desired result.

We may obtain the same result by assuming a slightly different set of conditions: A′, changing A_3 and A_5 to:

A_3': There exists $\epsilon > 0$ such that $\sup_{0 \leqq \|x\| < \epsilon} V_a(x) \leqq V < \infty$ for every number a;

A_5': There exists $\lambda > 0$, with $\lambda > \frac{1}{2}a_n$ for each n, such that $\sup_{\delta \leqq \|x\|} [U(x) + \lambda V_a^+(x)] < 0$ for every $\delta > 0$ and every number a.

Then we have

THEOREM 2. *If the sequence $\{a_n\}$ satisfies condition A_1 and if there exists a real-valued function $f(x)$ with continuous first and second partial derivatives satisfying A_2, A_3', A_4, and A_5, then the sequence $\{X_n\}$ defined by (4.2) converges* a.s. *to zero.*

The proof of this theorem follows very closely that of Theorem 1, and so is omitted.

5. Examples. In this section we illustrate the results of the previous section by a few simple examples. Assume that the problem is as described in (A) of Section 2. Then to each $x \varepsilon E_k$ corresponds to a random vector $Y_x \varepsilon E_k$ with coordinates $Y_x^{(i)}$ for $i = 1, \cdots, k$. Let $M(x)$ be the vector of conditional expectations, when x is given. Without loss of generality we assume that $\alpha_i = \theta_i = 0$ for $i = 1, \cdots, k$.

EXAMPLE I. Let B be a negative definite $k \times k$ matrix and assume

(i) for some $\rho > 0$, $\|x\| \leqq \rho$ implies $M(x) = Bx$;
(ii) $\|x\| > \rho$ implies $M(x) = M([\rho/\|x\|]x)$;
(iii) $\sigma_x^{2(i)} \leqq \sigma^2 < \infty$ for each $x \varepsilon E_k$, and each $i = 1, \cdots, k$, where $\sigma_x^{2(i)}$ is the variance of the ith component of Y_x.

Under these conditions it is clear that both $\|M(x)\|$ and $E\{\|Y_x\|^2\}$ are bounded uniformly in x. Now define $f(x)$ by $f(x) = \|x\|^2$. If we choose the sequence $\{a_n\}$ to satisfy condition A_1, we can easily verify that the remainder of condition A is satisfied. To do this we note that A_2 and A_4 are obviously satisfied from the choice of $f(x)$. Further we have

$$U(x) = \begin{cases} 2\langle x, Bx\rangle & \|x\| \leqq \rho; \\ 2[\rho/\|x\|]\,\langle x, Bx\rangle & \|x\| > \rho; \end{cases}$$

$$V_a(x) = 2E\{\|Y_x\|^2\} \qquad \text{for every number } a.$$

From the boundedness of $E\{\|Y_x\|^2\}$ it is clear that A_5 if also satisfied. It remains to check A_3. To do this we recall that for every negative definite matrix B there exists a positive number b such that $\langle x, Bx\rangle \leqq -b\|x\|^2$. Thus if ϵ is any positive number with $0 < \epsilon \leqq \rho$, we have

$$\langle x, Bx\rangle \leqq -b\epsilon^2 \text{ if } \epsilon \leqq \|x\| \leqq \rho, \qquad [\rho/\|x\|]\,\langle x, Bx\rangle \leqq -b\rho^2 \text{ if } \|x\| > \rho.$$

Hence A_3 is also satisfied and Theorem 1 applies.

EXAMPLE II. Consider a negative definite matrix B and assume

(i) $M(x) = Bx$;
(ii) there exist $\epsilon > 0$ and $C > 0$ such that $\|x\| \leqq \epsilon$ implies $E\{\|Y_x\|^2\} \leqq C$
(iii) there exists $\rho > 0$ such that $\|x\| > \epsilon$ implies

$$\langle x, Bx\rangle + \rho E\{\|Y_x\|^2\} \leqq 0.$$

With $f(x)$ again defined by $f(x) = \|x\|^2$, we have

$$U(x) = 2\langle x, Bx\rangle, \qquad V_a(x) = 2E\{\|Y_x\|^2\} \qquad \text{for all } a.$$

Hence it is clear that if we choose the sequence $\{a_n\}$ to satisfy condition A_1, we need only verify A_5', since the other conditions follow immediately. To do this, assume first that $\|x\| \leqq \epsilon$ as determined by assumption (ii) of this example, and let λ be any positive number. Let $b > 0$ be such that $\langle x, Bx\rangle \leqq -b\|x\|^2$.

Then we have

$$U(x) + \lambda V^+(x) = 2[\langle x, Bx\rangle + E\{\| Y_x \|^2\}]$$
$$\leqq 2[\langle x, Bx\rangle + \lambda C] \leqq 2[-b \| x \|^2 + \lambda C].$$

Hence it is clear that if $0 < \delta \leqq \| x \| \leqq \epsilon$, we can choose λ_1 such that

$$U(x) + \lambda_1 V^+(x) \leqq 2[-b\delta^2 + \lambda_1 C] < 0,$$

and if $\| x \| > \epsilon$, choose $0 < \lambda_2 < \rho$, where ρ is determined by assumption (iii) of the example. Then

$$\frac{[U(x) + \lambda_2 V^+(x)]}{2} = \left(\frac{\rho - \lambda_2}{\rho}\right)\langle x, Bx\rangle + \frac{\lambda_2}{\rho}[\langle x, Bx\rangle + \rho E\{\| Y_x\|^2\}]$$
$$\leqq \left(\frac{\rho - \lambda_2}{\rho}\right)\langle x, Bx\rangle \leqq -\left(\frac{\rho - \lambda_2}{\rho}\right) b\epsilon^2 < 0.$$

Hence by choosing $\lambda = \min(\lambda_1, \lambda_2)$ we satisfy condition A_4 and Theorem 2 applies.

6. The maximum of a regression function in several variables. In this section we turn to problem (B) of Section 2. Assume once more that x is a variable point in E_k and to each x corresponds a random variable Y_x, with corresponding regression function $M(x)$. Assume, without loss of generality, that $M(x)$ has a unique maximum at $x = 0$. The problem becomes one of constructing a sequence $\{X_n\}$ of random vectors with the property

$$P\{\lim_{n\to\infty} X_n = 0\} = 1.$$

Let $\{a_n\}$ and $\{c_n\}$ be two infinite sequences of positive numbers satisfying conditions B:

$$B_1: \lim_{n\to\infty} c_n = 0, \qquad B_2: \sum_{n=1}^{\infty} a_n = \infty, \qquad B_3: \sum_{n=1}^{\infty} a_n c_n < \infty,$$
$$B_4: \sum_{n=1}^{\infty}\left(\frac{a_n}{c_n}\right)^2 < \infty,$$

Suppose now $x \in E_k$ and let c be a positive number. Let $u_1, \cdots, u_k$ be the orthonormal set spanning E_k. We construct a random vector $Y_{x,c}$ by taking $k + 1$ independent observations on the random variables $Y_x, Y_{x+cu_1}, \cdots, Y_{x+cu_k}$ and defining

$$Y_{x,c} = [(Y_{x+cu_1} - Y_x), \cdots, (Y_{x+cu_k} - Y_x)].$$

We proceed to construct a recursive sequence of random vectors by choosing X_1 arbitrarily and defining

$$X_{n+1} = X_n + a_n Y_n/c_n, \tag{6.1}$$

where Y_n has the distribution of Y_{x,c_n} when X_n yields the observation x. The intuitive reason for (6.1) is fairly clear, since Y_n/c_n is the vector in the direction of the maximum slope of the plane determined by the $k + 1$ vectors

$$(X_n, \; Y_{X_n}), \; (X_n + c_n u_1, \; Y_{X_n + c_n u_1}), \; \cdots, \; (X_n + c_n u_k, \; Y_{X_n + c_n u_k}).$$

We denote the vector of first partial derivatives and the matrix of second partial derivatives of $M(x)$ by $D(x)$ and $A(x)$, respectively. We write D_n for $D(X_n)$ and A_n for $A(X_n)$, and denote by $\bar{A}_n$ the vector whose coordinates are the diagonal entries of A_n, by Δ_n the vector $E\{Y_n \mid X_n\}$, and by σ_x^2 the variance of Y_x. Without loss of generality we assume that $M(0) = 0$ so that $M(x) \leqq 0$ for all x. Then we have

THEOREM 3. *Suppose the sequences* $\{a_n\}$ *and* $\{c_n\}$ *satisfy conditions B and further that*

(i) $M(x)$ *is continuous with continuous first and second derivatives;*

(ii) $\sigma_x^2 \leqq \sigma^2 < \infty$;

(iii) *for every positive number* ϵ *there exists a positive number* $\rho(\epsilon)$ *such that*

$$\| x \| \geqq \epsilon \quad \textit{implies} \quad M(x) \leqq -\rho(\epsilon) \quad \textit{and} \quad \| D(x) \| \geqq \rho(\epsilon).$$

(iv) *The second partial derivatives* $\partial^2 M(x)/\partial x_i \partial x_j$ *are bounded for* $i,j = 1, \cdots, k$

Then the sequence $\{X_n\}$ *defined by* (6.1) *converges* a.s. *to zero.*

PROOF. Expanding $-M(X_{n+1})$ we obtain, with $0 \leqq \theta \leqq 1$,

$$-M(X_{n+1}) = -M(X_n) - \frac{a_n}{c_n} \langle D_n, Y_n \rangle - \frac{a_n^2}{2c_n^2} \left\langle Y_n, A\left(X_n + \theta \frac{a_n}{c_n} Y_n\right) Y_n \right\rangle.$$

Taking conditional expectation for given X_n we have

$$E\{-M(X_{n+1}) \mid X_n\} = -M(X_n) - \frac{a_n}{c_n} \langle D_n, \Delta_n \rangle - \frac{a_n^2}{2c_n^2} E\left\{ \left\langle Y_n, A\left(X_n + \theta \frac{a_n}{c_n} Y_n\right) Y_n \right\rangle \mid X_n \right\} \text{ a.s.}$$

Since $A(x)$ is a bounded matrix and σ_x^2 is bounded, we have

$$\left| E\left\{ \left\langle Y_n, A\left(X_n + \theta \frac{a_n}{c_n} Y_n\right) Y_n \right\rangle \mid X_n \right\} \right| \leqq K_1 \| \Delta_n \|^2 + K_2,$$

where K_1 and K_2 are suitably chosen positive constants. By virtue of the hypothesis we obtain

$$\Delta_n^{(i)} = c_n \langle D_n, u_i \rangle + \tfrac{1}{2} c_n^2 \langle u_i, A(X_n + \theta^{(i)} c_n u_i) u_i \rangle, \quad i = 1, \cdots, k,$$

where $\Delta_n^{(i)}$ is the ith component of Δ_n and $0 \leqq \theta^{(i)} \leqq 1$ for $i = 1, \cdots, k$. Hence

$$\langle D_n, \Delta_n \rangle = c_n \| D_n \|^2 + \tfrac{1}{2} c_n^2 \langle D_n, \bar{A}_n \rangle$$

$$\| \Delta_n \|^2 = c_n^2 \| D_n \|^2 + c_n^3 \langle D_n, \bar{A}_n \rangle + \tfrac{1}{4} c_n^4 \| \bar{A}_n \|^2.$$

Now by hypothesis, $\| \bar{A}_n \|$ is bounded, say $\| \bar{A}_n \|^2 \leqq K_3$. Then

$$\| \langle D_n, A_n \rangle |^2 \leqq K_3 \| D_n \|^2.$$

After some computation we find

$$E\{-M(X_{n+1}) \mid X_n\} \leqq -M(X_n) - a_n\{\| D_n \|^2[1 - \tfrac{1}{2}K_1a_n] - \| D_n \| K_3^{1/2}[\tfrac{1}{2}c_n - \tfrac{1}{2}K_1a_nc_n]\} + \tfrac{1}{8}K_1K_3a_n^2c_n^2 + \tfrac{1}{2}K_2a_n^2/c_n^2 \quad \text{a.s.},$$

where n is chosen so large that $[1 - \frac{1}{2}K_1a_n]$ and $[c_n - K_1a_nc_n]$ are both nonnegative.

Let λ_n be a sequence of random variables defined by

$$\lambda_n = \begin{cases} 1 & \text{if } \| D_n \| \geqq 1, \\ 0 & \text{otherwise.} \end{cases}$$

We note that for n sufficiently large we have

$$a_n\{\| D_n \|^2 [1 - \tfrac{1}{2}K_1a_n] - \lambda_n \| D_n \| K_3^{1/2}[\tfrac{1}{2}c_n - \tfrac{1}{2}K_1a_nc_n]\} \geqq 0. \tag{6.2}$$

Hence, for such n we obtain

$$E\{-M(X_{n+1}) \mid X_n\} \leqq -M(X_n) + a_nc_n(1 - \lambda_n) \| D_n \| K_3^{1/2} \mid \tfrac{1}{2} - \tfrac{1}{2}K_1a_n \mid + \tfrac{1}{8}K_1K_3a_n^2c_n^2 + \tfrac{1}{2}K_2a_n^2/c_n^2 \quad \text{a.s.}$$

This inequality clearly is still preserved if we take conditional expectations with respect to $M(X_n)$ on both sides. But now we note that

$\sum_{j=1}^n a_jc_jK_3^{1/2}[\frac{1}{2} - \frac{1}{2}K_1a_n]\, E\{(1 - \lambda_n) \| D_n \| \mid M(X_n)\}$ converges a.s.;

$\sum_1^n \frac{1}{8}K_1K_3a_j^2c_j^2$ and $\sum_1^n \frac{1}{2}K_2a_j^2/c_j^2$ both converge.

These follow from conditions B and the definitions of λ_n. Hence, we may again apply the corollary of Section 3 to obtain that $M(X_n)$ converges a.s. to a random variable. Now we note that $\sum_1^n a_j$ diverges to $+\infty$ and that $M(X_n) \leqq 0$. Hence the series

$$\sum_{j=1}^n a_jE\{\| D_j \|^2 [1 - \tfrac{1}{2}K_1a_j] - \lambda_j \| D_j \| K_3^{1/2}[\tfrac{1}{2}c_j - \tfrac{1}{2}K_1a_jc_j\}$$

converges. This, together with (6.2), insures the existence of a subsequence D_{n_k} with the property $P\{\lim_{k\to\infty} D_{n_k} = 0\} = 1$. Hence X_{n_k} converges a.s. to zero. Since $M(x)$ is continuous and $M(0) = 0$, we have $P\{\lim_{k\to\infty} M(X_n) = 0\} = 1$, which implies the desired result.

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