The Annals of Mathematical Statistics
1968, Vol. 39, No. 2, 457–465

ON THE CHOICE OF DESIGN IN STOCHASTIC APPROXIMATION METHODS

By Václav Fabian

Michigan State University, and Czechoslovak Academy of Sciences

1. Summary. In a previous paper [Fabian (1967)], we have shown that the Kiefer-Wolfowitz procedure—for functions f sufficiently smooth at θ, the point of minimum—can be modified in such a way as to be almost as speedy as the original Robbins-Monro method. The modification consists of taking more observations at every step and utilizing these (according to a design d) so as to eliminate the effect of all derivatives $\partial^j f/[\partial x^{(i)}]^j$, $j = 3, 5, \cdots, s-1$. Let δ_n be the distance of the approximating value to the approximated θ after n observations taken. Under some regularity conditions it was shown that $E\delta_n^2 = O(n^{-s/(s+1)})$. There are many designs d achieving this speed. For selection of the best one, i.e. the one which minimizes $\lim n^{s/(s+1)}E\delta_n^2$ we have to derive the dependence of this limit on the design d, which is done in Section 4. The best choice of the design $d = [u, \xi]$ is that which minimizes the right-hand side of (2.7) below; here $u = [u_1, u_2, \cdots, u_m]$, $\xi = [\xi_1, \cdots, \xi_m]$ with $0 < u_1 < u_2 < \cdots < u_m \leqq 1$, $\xi_i \geqq 0$, $\sum_{i=1}^m \xi_i = 1$; ξ_i indicates how many observations should be taken (roughly speaking) at u_i. The vector $v = [v_1, \cdots, v_m]$ is determined by $v = \frac{1}{2}U^{-1}e_1$ ($e_1 = [1, 0, \cdots, 0]$, $[\cdots]$ denotes column vectors), $U^{(ij)} = u_j^{2i-1}$, $i, j = 1, \cdots, m$.

It seems difficult to minimize (2.7) given K_0, K_1. Moreover we usually do not know these constants. So in this paper we solve the question of minimizing the first term $\sum_{i=1}^m (v_i^2/\xi_i)$ only. The result is formulated in Theorem 5.1.

2. Introduction. The result on $\lim n^{s/(s+1)} E\delta_n^2$ is very similar to the results for the original Kiefer-Wolfowitz method as given by Dupač (1957) and Sacks (1958). The proofs are similar to those used by Dupač. There are, however, some differences beside the difference between the stochastic approximation methods considered. Sacks derives moments of asymptotic distribution and not the asymptotic moments, Dupač deals only with the one-dimensional case. Both consider only such a choice of eligible constants which ensures that, with X_n the approximating value at the nth step, the mean of $X_n - \theta$ is negligible in comparison with $(E\|X_n - \theta\|^2)^{\frac{1}{2}}$ for large n. This then makes it impossible to achieve the above result $E\delta_n^2 = O(n^{-s/(s+1)})$.

We shall frequently refer to Fabian (1967) and Kiefer and Wolfowitz (1959) by using symbols I and KW in an obvious way. We keep notations introduced in Section I.2 and Theorem I.3.1. All random variables are supposed to be defined on a probability space (Ω, S, P). If h_n is a sequence of random variables (or, in particular, numbers) we use the notation $O(h_n)$ and $o(h_n)$ for denoting

Received June 19, 1967; revised October 5, 1967.

sequences of random variables such that there is a constant C and a number sequence $\delta_n \to 0$ such that $|O(h_n)| \leqq C|h_n|$ and $|o(h_n)| \leqq \delta_n|h_n|$ with probability one. Throughout the paper we confine ourselves to the situation of Theorem I.5.1 with some slight additional requirements. The following Assumptions 2.1 and 2.2 will be supposed valid throughout the paper.

ASSUMPTION 2.1. f is a real function on R^k. There is a point $\theta \varepsilon R^k$, and $\epsilon > 0$ and an even positive integer s such that D_{s+1} exists and is continuous on the closed 2ϵ-neighborhood $C(2\epsilon)$ of θ. The Hessian H of f exists and is bounded on R^k, continuous at θ and $H(\theta)$ is positive definite (with λ_0 the smallest eigenvalue), $D(\theta) = 0$. There is a positive number K_0 such that

$$K_0\|x - \theta\|^2 \leqq (x - \theta)'D(x). \tag{2.1.1}$$

ASSUMPTION 2.2. The sequence X_n of random vectors satisfies

$$X_{n+1} = X_n - a_n Y_n \tag{2.2.1}$$

with X_0 a constant, with random vectors Y_n satisfying conditions (I.3.1.2) to (I.3.1.5) with given u_i, v_i,

$$a_n = an^{-\alpha}, \qquad c_n = cn^{-\gamma}, \tag{2.2.2}$$

$$a > 0, \quad c > 0, \quad 0 < \alpha \leqq 1, \quad \beta = \alpha s/(s + 1), \quad \gamma = \tfrac{1}{2}\alpha/(s + 1), \tag{2.2.3}$$

$$2K_0 a > \beta \quad \text{if} \quad \alpha = 1. \tag{2.2.4}$$

REMARK 2.3. The special choice of γ corresponds to the optimal value of γ for a given α (see Remark I.5.2). Assumptions 2.1 and 2.2 imply all conditions of Theorem I.5.1 (see also Remark I.3.7). Hence $E\|X_n - \theta\|^2 = O(n^{-\beta})$. Note that condition $E_{\mathbf{X}_n}\|Z_n\|^p \leqq Kc_n^{-p}$, used in Lemma 3.1, means that the pth conditional moments of the original estimates $Y_{n,i}^{(j)}$ in Lemma I.3.1 are bounded. Note that $\beta = \alpha - 2\gamma = 2\gamma s$, a relation which will be used frequently.

Under a slight additional condition Corollary 4.4 gives the result

$$\lim n^{\beta}E\|X_n - \theta\|^2 = 2^{-1}a^2c^{-2} \operatorname{tr} (C^{-1}\Sigma) + c^{2s}q\|C^{-1}D_{s+1}(\theta)\|^2 \tag{2.4}$$

with C depending on $H(\theta)$, α and a (see (4.1.2)) and

$$q = ((s + 1)!)^{-1}a^2 \textstyle\prod_{i=1}^{m} u_i^4. \tag{2.5}$$

The matrix Σ is the limit of the covariance matrix $c_n^2E_{\mathbf{X}_n}Z_nZ_n'$ as $X_n \to \theta$, $n \to \infty$ (see Theorem 4.3 for a precise meaning of Σ), where $Z_n = Y_n - E_{\mathbf{X}_n}Y_n$. If $Y_n = c_n^{-1}\sum_{i=1}^{m} v_iY_{n,i}$ with conditionally $(\mathbf{X}_n)$ independent $Y_{n,i}^{(j)}$ $(i = 1, \cdots, m;\ j = 1, \cdots, k)$ then Σ is diagonal. Constructing each $Y_{n,i}^{(j)}$ from n_i elementary conditionally $(\mathbf{X}_n)$ independent estimates with conditional $(\mathbf{X}_n)$ variances $2\sigma^2$, we get that the conditional variance of $Y_{n,i}^{(j)}$ is $2\sigma^2/n_i$, and

$$\Sigma = 2\textstyle\sum_{i=1}^{m} (v_i^2/n_i)\sigma^2 I \tag{2.6}$$

with I the identity matrix. The number of observations needed to construct Y_n is then $k\sum_{i=1}^{m} n_i$.

If δ_t is the square of the distance of X_n from θ after t observations taken (i.e. if $t = kNn$ with $N = \sum_{i=1}^m n_i$) then

$$t^\beta E\delta_t \to (kN)^\beta a^2 c^{-2} \sum_{i=1}^m (v_i^2/n_i)\sigma^2 \operatorname{tr}(C^{-1}) + (kN)^\beta c^{2s} q\|C^{-1}D_{s+1}(\theta)\|^2.$$

Limiting ourselves now to the optimal value $\alpha = 1$ which implies $\beta = s/(s+1)$, writing $\xi_i = n_i/N$ and choosing c to depend on N by putting $c = c_0 N^{-1/(2s+2)}$ we obtain

$$t^\beta E\delta_t \to k^\beta[a^2 c_0^{-2}\sigma^2 \operatorname{tr}(C^{-1}) \sum_{i=1}^m (v_i^2/\xi_i) + c_0^{2s} q\|C^{-1}D_{s+1}(\theta)\|^2]$$

which does not depend on N. So

$$\lim_{t\to\infty} t^\beta E\delta_t = K_0 \sum_{i=1}^m (v_i^2/\xi_i) + K_1 \prod_{i=1}^m u_i^4 \tag{2.7}$$

with $K_0 = k^\beta a^2 c_0^{-2}\sigma^2 \operatorname{tr}(C^{-1})$, $K_1 = ((s+1)!)^{-2} k^\beta c_0^{2s} a^2 \|C^{-1}D_{s+1}(\theta)\|^2$.

It is difficult to minimize (2.7) by a choice of u, ξ; moreover K_0, K_1 involve unknown characteristics of the function f, namely C and $D_{s+1}(\theta)$. Of the two terms, the second is bounded by K_1 for any design u, ξ, but the first term may become quite large for unsuitable u. That is why it seems to be of interest to find a design minimizing just the first term in (2.7).

3. Preliminary lemmas.

LEMMA 3.1. *If, for a $p_0 > 0$, $E_{\mathbf{X}_n}\|Z_n\|^{p_0} \leqq O(n^{\gamma p_0})$, then for all $0 \leqq p \leqq p_0$*

$$E\|X_n - \theta\|^p = O(n^{-p\beta/2}). \tag{3.1.1}$$

PROOF. The proof will be similar to that used by Dupač (1957), only we do not assume all moments of $\|Z_n\|$ are finite and this makes it necessary to split the proof into two parts. Note that for every sequence of non-negative random variables ξ_n if (i) $E\xi_n^p = O(n^{-ph})$ for an $h \geqq 0$, and $p = \pi > 0$, then (i) holds for every $0 \leqq p \leqq \pi$. So we can assume $p_0 > 2$ because $E\|X_n - \theta\|^2 = O(n^{-\beta})$ by Theorem I.5.1.

Without loss of generality we may assume that $\theta = 0$. By (2.2.4) there is an $\eta > 0$ such that $a_n(2-\eta)K_0 \geqq \kappa n^{-\alpha}$ with $1 > \kappa > 0$, and with $\kappa > \beta$ if $\alpha = 1$. From Lemma I.4.1 it then follows (see (I.4.1.2) and use expressions following (I.4.1.9)) that

$$\|X_{n+1}\|^2 \leqq (1 - \kappa n^{-\alpha})\|X_n\|^2 + Q_{n,1} + Q_{n,2} \tag{3.1.2}$$

where

$$Q_{n,1} = -2a_n Z_n'(X_n - a_n M_n(X_n)), \quad Q_{n,2} = a_n^2\|Z_n\|^2 + Cn^{-\alpha-\beta} \tag{3.1.3}$$

with a positive constant C.

Note that by (I.4.1.5) $|Q_{n,1}| \leqq \|a_n Z_n\| O(\|X_n\| + n^{-\beta/2})$ and for $0 \leqq q \leqq p_0$

$$E_{\mathbf{X}_n} Q_{n,1} = 0, \quad E_{\mathbf{X}_n}|Q_{n,1}|^q \leqq O(\|X_n\|^q + n^{-\beta q/2}) n^{-q(\alpha+\beta)/2}; \tag{3.1.4}$$

for $0 \leqq q \leqq p_0/2$

$$E_{\mathbf{X}_n} Q_{n,2}^q = O(n^{-q(\alpha+\beta)}). \tag{3.1.5}$$

Now put $e_{n+1,i} = (1 - \kappa n^{-\alpha})e_{n,i} + Q_{n,i}$, $e_{1,1} = \|X_1\|^2$, $e_{1,2} = 0$ so that $\|X_n\|^2 \leqq e_{n,1} + e_{n,2}$ and it suffices to prove

$$E|e_{n,i}|^q = O(n^{-q\beta}) \tag{3.1.6}$$

for $q = p_0/2$. For $i = 2$ we have of course $e_{n,i} = |e_{n,i}|$. Note that $e_{n,i}$ are measurable with respect to the smallest σ-algebra generated by $\mathbf{X}_n$.

First consider $i = 2$ and let $1 \leqq p \leqq p_0/2$, let (3.1.6) hold for $q = p - 1$ (this is true if $p = 1$). Then using Taylor expansion for $h(u) = u^p$, and noting that $(1 - \kappa n^{-\alpha})^p = 1 - p\kappa_n n^{-\alpha}$ with $\kappa_n \to \kappa$,

$$\begin{aligned} Ee_{n+1,2}^p &\leqq (1 - p\kappa_n n^{-\alpha})Ee_{n,2}^p + EE_{\mathbf{X}_n} p|Q_{n,2}|(e_{n,2} + |Q_{n,2}|)^{p-1} \\ &\leqq (1 - p\kappa_n n^{-\alpha})Ee_{n,2}^p + EO(e_{n,2}^{p-1} n^{-\alpha-\beta} + n^{-\alpha-p\beta}) \\ &\leqq (1 - p\kappa_n n^{-\alpha})Ee_{n,2}^p + O(n^{-\alpha-p\beta}) \end{aligned}$$

and Chung's lemma (Lemma I.4.2) implies (3.1.6) for $q = p$. By induction (3.1.6) holds for $i = 2$ and every $0 \leqq p \leqq p_0/2$.

Now consider $i = 1$, write e_n for $e_{n,1}$, suppose $2 \leqq p \leqq p_0/2 + 1$ and suppose (3.1.6) holds for $i = 1$ and $q = p - 1$. Because then (3.1.6) holds for $i = 2$, $q = p - 1$ by the previous part of the proof, we have $\|X_n\|^2 \leqq f_n = \sum_{i=1}^2 |e_{n,i}|$, $Ef_n^{\,q} = O(n^{-q\beta})$ for $0 \leqq q \leqq p - 1$. From (3.1.4), which holds for $0 \leqq q \leqq p$ because $p_0/2 + 1 < p_0$, we get

$$EQ_{n,1}^2[|e_n| + |Q_{n,1}|]^{p-2} = O(n^{-\alpha-p\beta});$$

note that this relation obtains for $p = 2$ even without assuming (3.1.6) for $q = p - 1$. Then, however, using (3.1.4)

$$\begin{aligned} E|e_{n+1}|^p &\leqq (1 - p\kappa_n n^{-\alpha})E|e_n|^p + pEQ_{n,1}(1 - \kappa n^{-\alpha})^{p-1}|e_n|^{p-1} \operatorname{sign} e_n \\ &\quad + \tfrac{1}{2}p(p - 1)E|Q_{n,1}|^2[|e_n| + |Q_{n,1}|]^{p-2} \\ &= (1 - p\kappa_n n^{-\alpha})E|e_n|^p + O(n^{-\alpha-\beta p}) \end{aligned}$$

and Chung's lemma implies (3.1.6) for $q = p$ and $i = 1$. By induction, starting with $p = 2$, we obtain that (3.1.6) holds for $i = 1$ and all $0 \leqq p \leqq p_0/2 + 1$ which is more than was necessary to prove the lemma.

Lemma 3.2. *If $E_{\mathbf{X}_n}\|Z_n\|^p = O(n^{\gamma p})$ for a positive p, then for every $0 \leqq q \leqq p$ and every positive δ*

$$Ec\{\|X_n - \theta\| \geqq \delta\}\|X_n - \theta\|^q = O(n^{-\beta p/2}). \tag{3.2.1}$$

holds with c the characteristic function of the indicated set.

Proof. $c\{\|X_n - \theta\| \geqq \delta\}\|X_n - \theta\|^q \leqq \delta^{q-p}\|X_n - \theta\|^p$ and (3.2.1) follows from Lemma 3.1.

Remark 3.3. A direct formula for $v = \frac{1}{2}U^{-1}e_1$ can be obtained without difficulty since U is a Vandermonde matrix multiplied by a diagonal matrix. In particular

(3.3.1) $$\sum_{i=1}^{m} v_i u_i^{s+1} = (-1)^{m-1} 2^{-1} \prod_{i=1}^{m} u_i^2.$$

To see it we observe that $2v = U^{-1}e_1$ is the first column of the matrix U^{-1}. Therefore $2v_i|U|$ is the cofactor of the $(1, i)$th element in the matrix U (with $|U|$ denoting the determinant of U) and $2|U| \sum_{i=1}^{m} v_i u_i^{s+1}$ is the determinant of the matrix U_1 which is obtained by replacing the first row in U by $[u_1^{s+1}, u_2^{s+1}, \cdots, u_m^{s+1}]'$. But $|U_1| = (-1)^{m-1}|U_2|$ where $U_2^{(i,j)} = u_i^2 U^{(i,j)}$. Hence $|U_1| = (-1)^{m-1}|U| \prod_{i=1}^{m} u_i^2$ and this implies (3.3.1).

4. Asymptotic first two moments of X_n.

REMARK 4.1. Some additional notation will be useful. We denote $A = H(\theta)$. Because A is positive definite, there is an orthogonal matrix P and a diagonal matrix Λ with $\Lambda^{(ii)}$ positive, such that $\Lambda = P'AP$. We denote

(4.1.1) $$h = (-1)^{m-1}((s+1)!)^{-1} ac^s \prod_{i=1}^{m} u_i^2.$$

To achieve a greater simplicity we introduce also the notation

(4.1.2) $$\beta_+ = 0 \quad \text{if} \quad \alpha < 1, \qquad C = aA - (\beta_+/2)I,$$
$$= \beta \quad \text{if} \quad \alpha = 1;$$

where I is the identity matrix.

THEOREM 4.2.

(4.2.1) $$\lim_{n\to\infty} n^{\beta/2}(EX_n - \theta) = -hC^{-1}D_{s+1}(\theta).$$

PROOF. Assume again $\theta = 0$. From Assumption 2.1 we obtain that $\Lambda^{(ii)} \geqq K_0$ for every $i = 1, 2, \cdots, k$ and thus because of (2.2.4) the inverse of C exists. By Lemma 3.2 we have $Ec\{\|X_n\| \geqq \delta\}(\|X_n\| + 1) = O(n^{-\beta})$ for every $\delta > 0$ and surely we can choose a sequence $\delta_n \to 0$ such that $Ec\{\|X_n\| \geqq \delta_n\}(\|X_n\| + 1) = o(n^{-\beta/2})$ holds.

Because $D(x) = H(\xi)x$ with a $\|\xi\| < \|x\|$, we have $D(X_n) = [A + o(1)]X_n = AX_n + o(\|X_n\|)$ on $\Omega_n = \{\|X_n\| \leqq \delta_n\}$. From (I.3.1.4) together with the expression for Q_n just preceding Remark I.3.2, and from the continuity of D_{s+1} at 0, we get, noting that $\gamma s = \beta/2$,

(4.2.2) $$M_n(X_n) = AX_n + n^{-\beta/2}a^{-1}hD_{s+1}(0) + \Psi_n$$

with $\Psi_n = o(\|X_n\| + n^{-\beta/2})$ on Ω_n and $\Psi_n = O(\|X_n\| + n^{-\beta/2})$ outside of Ω_n[1] (see I.4.1.5)). Hence $E\Psi_n = o(n^{-\beta/2})$ and

$$EX_{n+1} = E(I - an^{-\alpha}A)X_n - n^{-\alpha-\beta/2}hD_{s+1}(0) + o(n^{-\alpha-\beta/2}).$$

Put $e_n = P'EX_n$ and multiply the preceding equation by P' to obtain

$$e_{n+1} = (I - an^{-\alpha}\Lambda)e_n - n^{-\alpha-\beta/2}hP'D_{s+1}(0) + o(n^{-\alpha-\beta/2}).$$

A coordinatewise application of Chung's lemma (Lemma I.4.2) gives

[1] Note, for the use in the next proof, that for fixed n, Ψ_n is a function of X_n and therefore $E\Psi_n Z_n = 0$.

$$\lim n^{\beta/2} e_n = -h(a\Lambda - (\beta_+/2)I)^{-1}P'D_{s+1}(0)$$

and this implies (4.2.1).

THEOREM 4.3. *Suppose* $E_{X_n}\|Z_n\|^{2+\eta} = O(n^{\gamma(2+\eta)})$ *for an* $\eta > 0$ *and suppose there is a matrix* Σ *such that* $\sup_{\|X_n-\theta\|<\delta_n} \|c_n^2 E_{X_n} Z_n Z_n' - \Sigma\| \to 0$ *for any sequence* $\delta_n \downarrow 0$. *Then*

$$\lim n^{\beta} E(X_n - EX_n)(X_n - EX_n)' = PMP' \tag{4.3.1}$$

with

$$M^{(ij)} = a^2c^{-2}(P'\Sigma P)^{(ij)}/[a(\Lambda^{(ii)} + \Lambda^{(jj)}) - \beta_+]. \tag{4.3.2}$$

PROOF. Assume again $\theta = 0$. Similarly as in the preceding proof we conclude there is a sequence $\delta_n \downarrow 0$ such that $Ec(\Omega - \Omega_n)(\|X_n\|^2 + \|X_n\| + 1) = o(n^{-\beta})$ with $\Omega_n = \{\|X_n\| \leqq \delta_n\}$. Using (4.2.2) and denoting $\xi_n = X_n - EX_n$ we get

$$\xi_{n+1} = \xi_n - an^{-\alpha}A\xi_n - an^{-\alpha}Z_n - an^{-\alpha}\varphi_n$$

where $\varphi_n = \Psi_n - E\Psi_n$. We have $E\|Z_n\| = O(n^{\gamma})$, $E_{X_n}Z_n = 0$ and $EZ_nZ_n' = E[c(\Omega_n)c^{-2}n^{2\gamma}(\Sigma + o(1)) + c(\Omega - \Omega_n)O(n^{2\gamma})] = c^{-2}n^{2\gamma}\Sigma + o(n^{2\gamma}) = c^{-2}n^{\alpha-\beta}\Sigma + o(n^{\alpha-\beta})$. Also $E\varphi_n^2 \leqq E\Psi_n^2 = o(n^{-\beta})$ and thus

$$E\xi_{n+1}\xi_{n+1}' = E(I - an^{-\alpha}A)\xi_n\xi_n'(I - an^{-\alpha}A)' + a^2c^{-2}n^{-\alpha-\beta}\Sigma + o(n^{-\alpha-\beta}).$$

Denoting $e_n = P'E\xi_n\xi_n'P$, we get

$$\begin{aligned} e_{n+1} &= (I - an^{-\alpha}\Lambda)e_n(I - an^{-\alpha}\Lambda)' + a^2c^{-2}n^{-\alpha-\beta}P'\Sigma P + o(n^{-\alpha-\beta}) \\ &= e_n - an^{-\alpha}(\Lambda e_n + e_n\Lambda) + a^2c^{-2}n^{-\alpha-\beta}P'\Sigma P + o(n^{-\alpha-\beta}). \end{aligned}$$

An application of Chung's lemma shows

$$\lim n^{\beta}e_n^{(ij)} = a^2c^{-2}(P'\Sigma P)^{(ij)}/[a(\Lambda^{(ii)} + \Lambda^{(jj)}) - \beta_+] = M^{(ij)}$$

and this implies (4.3.1).

COROLLARY 4.4. *Under the assumptions of Theorem* 4.3

$$\lim n^{\beta}E\|X_n - \theta\|^2 = 2^{-1}a^2c^{-2}\operatorname{tr}(C^{-1}\Sigma) + h^2\|C^{-1}D_{s+1}(\theta)\|^2. \tag{4.4.1}$$

PROOF. From Theorem 4.2 $\lim n^{\beta}\|EX_n - \theta\|^2 = h^2\|C^{-1}D_{s+1}(\theta)\|^2$. From Theorem 4.3,

$$\begin{aligned} \lim n^{\beta}E\|X_n - EX_n\|^2 &= \lim n^{\beta}\operatorname{tr} E(X_n - EX_n)(X_n - EX_n)' \\ &= \operatorname{tr} PMP' = \operatorname{tr} M = \operatorname{tr} a^2c^{-2}(2a\Lambda - \beta_+I)^{-1}P'\Sigma P \\ &= \operatorname{tr} 2^{-1}a^2c^{-2}P(a\Lambda - \tfrac{1}{2}\beta_+I)^{-1}P'PP'\Sigma PP' \\ &= 2^{-1}a^2c^{-2}\operatorname{tr} C^{-1}\Sigma \end{aligned}$$

and (4.4.1) follows from the relation $E\|X_n\|^2 = E\|X_n - EX_n\|^2 + \|EX_n\|^2$.

5. The design minimizing $\sum_{j=1}^m v_j^2/\xi_j$.

THEOREM 5.1. *The problem of minimizing* $\sum_{j=1}^m v_j^2/\xi_j$ *has the unique solution*

$$(5.1.1) \qquad u_j = \cos[(m-j)\pi/(2m-1)], \qquad j = 1, 2, \cdots, m,$$

$$(5.1.2) \qquad \xi_j = [s(m-1) + \tfrac{1}{2}]^{-1} u_j^{-2}(1 - \tfrac{1}{2}\delta_{mj}), \qquad j = 1, 2, \cdots, m,$$

with δ_{ij} *the Kronecker symbol.*

For this design

$$(5.1.3) \qquad v_j = (s-1)^{-1}(-1)^{j-1} u_j^{-2}(1 - \tfrac{1}{2}\delta_{mj}), \qquad j = 1, 2, \cdots, m,$$

and

$$(5.1.4) \qquad \textstyle\sum_{j=1}^{m} v_j^2/\xi_j = \tfrac{1}{4}(s-1)^2, \qquad \prod_{j=1}^{m} u_j^4 = 2^{-4(m-1)}.$$

PROOF. Consider the regression problem with a random vector y satisfying

$$(5.1.5) \qquad Ey = U'\alpha, \qquad (E(y-Ey)(y-Ey)')^{(ij)} = \delta_{ij}/\xi_j$$

with α unknown.

The linear unbiased estimate η of $\alpha^{(1)}$ is of form $\eta = w'y$; unbiasedness means $Ew'y = w'U'\alpha = \alpha^{(1)}$ for every α; this implies $Uw = e_1$, $w = 2v$. The variance of this estimate is $4\sum_{j=1}^{m}(v_j^2/\xi_j)$. Thus our problem is equivalent to that of minimizing the variance of η by the choice of ξ_j and u_j. This problem can be solved using results of Kiefer and Wolfowitz (1959), especially their Theorem 3, KW. In the terminology of Section 2, KW, let $\mathfrak{X}$ be the closed interval $[\epsilon, 1]$, with an $0 < \epsilon < \cos[(m-1)/(2m-1)\pi]$, $f_i(u) = u^{s+1-2i}$, $i = 1, 2, \cdots, m$. Functions $f_{m-1}, f_{m-2}, \cdots, f_1$, i.e. $u^3, u^5, \cdots, u^{s-1}$ form a Čebyšev system on $\mathfrak{X}$, because every non-trivial linear combination of these functions can be written as $u^3h(u)$ with an even polynomial h of order at most $s-4$ and has, therefore, at most $m-2$ roots in $\mathfrak{X}$.

If T is the Čebyšev polynomial of order $s-1$, $T(u) = \sum_{j=1}^{m} d_j u^{2j-1}$ acquires its maximal absolute value 2^{2-s} at the points u_i defined in (5.1.1) with alternating signs. Thus $T_1(u) = -\sum_{j=2}^{m}(d_j/d_1)u^{2j-1}$ is the best Čebyšev approximation to u on $\mathfrak{X}$ because $|T_1(u) - u|$ is maximal and equal to $2^{2-s}/|d_1|$ at the points u_i and $T_1(u) - u$ alternates sign in these points. From Theorem 3, KW it follows that our problem has a unique solution with u_i as given in (5.1.1) and with ξ_j which must satisfy the condition

$$(5.1.6) \qquad \textstyle\sum_{j=1}^{m}(-1)^j u_j^{2i-1}\xi_j = 0 \quad \text{for} \quad i = 2, 3, \cdots, m.$$

((5.1.6) is equivalent to condition (2.10, KW) and also to (2.14, KW).) It can be shown that

$$(5.1.7) \qquad \textstyle\sum_{j=0}^{2m-2}(-1)^j(\cos^i[\pi j/(2m-1)] = 0 \quad \text{for} \quad i = 1, 3, \cdots, 2m-3$$

(see (3.4, KW) with $h = 2m-1$; there is a printing error in KW which would imply that (5.1.7) holds also with $i = h$). The values $\cos[\pi j/(2m-1)]$ for $j = m, m+1, \cdots, 2m-2$, are just number $-u_1, -u_2, \cdots, -u_{m-1}$ so that for any odd integer i, the left-hand side of (5.1.7) becomes $2\sum_{j=1}^{m-1}(-1)^j u_{m-j}^i + u_m^i$ and (5.1.7) then implies that (5.1.6) is satisfied with $\xi_j = \lambda^{-1}u_j^{-2}(1 - \tfrac{1}{2}\delta_{mj})$ and with a constant λ determined by the requirement $\sum_{j=1}^{m}\xi_j = 1$.

As for the vector v, it is easy to see that $v_j = \gamma^{-1}\lambda(-1)^{j-1}\xi_j$ because we have to have $\sum_{j=1}^m u_j^{2i-1}v_j = 0$ for $j = 2, \cdots, m$; the condition $\sum_{i=1}^m v_i u_i = \frac{1}{2}$ determines then γ and, because $|v_i u_i| \geqq |v_{i+1}u_{i+1}|$, it follows that $\gamma > 0$.

These u, ξ are optimal on $[\epsilon, 1]$ for every $0 < \epsilon < \cos[(m-1)\pi/(2m-1)]$ and hence also on the original interval $(0, 1]$ open from the left and (5.1.1) to (5.1.3) are proved but for the values of λ and γ which remain to be computed.

The polynomial $T(u) = \sum_{i=1}^m d_i u^{2i-1}$ can be written as

$$T(u) = 2^{2-s}\sum_{0\leqq\alpha\leqq j\leqq m-1}(-1)^\alpha\binom{2m-1}{2j}\binom{j}{\alpha}u^{2m-2\alpha-1}$$

and so

$$(5.1.8)\quad d_1 = (-1)^{m-1}2^{2-s}(s-1), \qquad d_2 = (-\tfrac{1}{3}d_1 s(m-1), \qquad d_m = 1.$$

The polynomial T has its extremes at the points $\pm u_i$, $i = 1, 2, \cdots, m-1$, its derivative T' has zeros at these points and the polynomial P given by $P(u) = u^{m-1}T'(u^{-\frac{1}{2}})$ for $u > 0$ has $m-1$ zeros at $u_1^{-2}, u_2^{-2}, \cdots, u_{m-1}^{-2}$ and is given by

$$P(u) = \sum_{i=0}^{m-1}(2i+1)\,d_{i+1}u^{m-1-i} = d_1\prod_{j=1}^{m-1}(u - u_j^{-2}).$$

This implies $d_1(-1)^{m-1}\prod_{j=1}^{m-1}u_j^{-2} = (2m-1)\,d_m$ and $-d_1\sum_{j=1}^{m-1}u_j^{-2} = 3\,d_2$ and by (5.1.8) we obtain

$$(5.1.9)\quad \sum_{j=1}^m u_j^{-2}(1-\delta_{jm}) = s(m-1) + \tfrac{1}{2}, \quad \prod_{j=1}^m u_j^2 = 2^{2-s}.$$

Moreover $4\sum_{j=1}^m v_j^2/\xi_j$ for the optimal design is equal to the reciprocal of the maximum square deviation of T_1 from u on $(0, 1]$ which is $(s-1)^2$, this with (5.1.9) establishes (5.1.4). On the other hand, $\sum_{j=1}^m v_j^2/\xi_j = \sum_{j=1}^m \lambda^2\gamma^{-2}\xi_j = \lambda^2\gamma^{-2}$ so that $\gamma = 2\lambda/(s-1)$. By (5.1.9) $\lambda = (s(m-1) + \frac{1}{2})$ which gives $\gamma = [2m(2m-2)+1]/(2m-1) = 2m-1$. This completes the proof of (5.1.2) and (5.1.3) and of the whole theorem.

Example 5.2. With $m = 3$, the design minimizing $\sum v_j^2/\xi_j$ is given by

$$u = [\cos\tfrac{2}{5}\pi, \cos\tfrac{1}{5}\pi, \cos 0] = [0.30902, 0.80902, 1],$$

$$\xi = 12.5^{-1}[u_1^{-2}, u_2^{-2}, \tfrac{1}{2}u_3^{-2}] = [0.83777, 0.12223, 0.04],$$

$$v = 5^{-1}[u_1^{-2}, -u_2^{-2}, \tfrac{1}{2}u_3^{-2}] = [2.09439, -0.30557, 0.1],$$

$$\prod_{j=1}^3 u_j^4 = 2^{-8}, \qquad \sum_{j=1}^3 v_j^2/\xi_j = 25/4.$$

The constant 12.5 for ξ was obtained as $s(m-1) + \frac{1}{2} = 6 \times 2 + \frac{1}{2}$, the constant 5 for v as $s - 1$.

Remark 3.3. In practical situations we will be forced to use only approximations to the optimal ξ. Unhappily, unlike in case of estimating the leading coefficient of a polynomial, the optimal ξ is far from the uniform distribution. It is not clear, whether the problem of minimizing $\sum_{i=1}^m v_i^2/\xi_i$ with ξ restricted to a given class (in particular with $\xi_i = 1/m$) would admit a simple solution.

REFERENCES

DUPAČ, V. (1957). O Kiefer-Wolfowitzově aproximační metodě. *Časopis Pěst. Mat.* **82** 47–75.

FABIAN, V. (1967). Stochastic Approximation of Minima with Improved Asymptotic Speed. *Ann. Math. Statist.* **38** 191–200.

KIEFER, J. and WOLFOWITZ, J. (1959). Optimum designs in regression problems. *Ann. Math. Statist.* **30** 271–294.

SACKS, J. (1958). Asymptotic distribution of stochastic approximation procedures. *Ann. Math. Statist.* **29** 373–405.