SYMMETRIC SEQUENTIAL MINIMAX SEARCH FOR A MAXIMUM

LEATON T. OLIVER and DOUGLASS J. WILDE
University of Texas, Austin, Texas

1. INTRODUCTION

Kiefer[1] has given a sequential method for seeking the maximum of a unimodal (single-peaked) function of one variable in a finite interval. This procedure is minimax in the sense that no matter where the peak may happen to be, the final interval within which the peak will be known with certainty to lie will be as small as possible. In this technique the last experiment must be located as closely as possible to the experiment giving the greatest value among those previously run. If this distance ϵ is negligibly small, then Kiefer's procedure is indeed minimax. When on the other hand ϵ cannot be neglected, which is often the case in practical problems, then Kiefer's method can be modified to give a shorter final interval of uncertainty.

Kiefer's original technique is asymmetric in the sense that the last two experiments are not located symmetrically with respect to each other. The modified procedure is symmetric, since it permits the last experiment to be placed symmetrically with respect to the most effective previous experiment. In the extreme case when as many experiments as possible are run, the symmetric technique gives a final interval only two-thirds as long as for the asymmetric method. Formulae are given for the maximum number of experiments which can profitably be performed for a finite resolution ϵ. Analysis of them shows that the symmetric method can occasionally make use of at most one more experiment than the asymmetric procedure.

Problem: Let y be a single-valued function of x having a maximum y^* at the unknown point x^* somewhere in the interval $a \leq x \leq b$. Suppose that in this interval y is unimodal, i.e., that $a \leq x_1 < x_2 \leq x^*$ implies $y(x_1) < y(x_2)$, and $x^* \leq x_1 < x_2 \leq b$ implies $y(x_1) > y(x_2)$. If observations of y are taken at the k points $x_1 < x_2 < \cdots < x_k$, and if the greatest value of y is found at x_j, then the unimodality implies that $x_{j-1} < x^* < x_{j+1}$, with the convention

*Currently at Stanford University, Stanford, California.

that $x_o \equiv a$ and $x_{k+1} \equiv b$. Let

(1) $$x_{j+1} - x_{j-1} \equiv L_k$$

the length of the interval of uncertainty after k observations ($L_o = L_1 = b-a$). For $k > 1$, L_k will become smaller as more measurements are taken, and we wish to locate them in such a way that the length L_n of the final interval of uncertainty after n sequential observations will be as small as possible, no matter where x^* actually happens to be. If $\{x_n\}$ represents any sequence of n observations, then the minimax sequence $\{x_n^*\}$ is the one which gives this smallest interval L_n^*. Formally,

(2) $$L_n^*/L_o = \min_{(\{x_n\}} - \max_{a \leq x^* \leq b)} \{L_n/L_o\}$$

2. DISTINGUISHABILITY

Even when the function is known to be unimodal it may not be possible to detect, in a physical problem, the difference between the outcomes of two measurements that are too close together. When this happens, the experimenter is unable to reduce the interval of uncertainty, and one of the observations is useless. Thus in designing a sequential search technique one must take into account the minimum spacing ϵ for which two outcomes are distinguishable. The smallest interval of uncertainty obtainable practically is therefore 2ϵ.

(3) $$L_n = x_{j+1} - x_{j-1} = (x_{j+1} - x_j) - (x_j - x_{j-1}) = 2\epsilon.$$

Although the resolution ϵ is usually negligible compared to the original interval of uncertainty L_o, it is often a large fraction of the final interval L_n if the search is at all efficient.

3. RESULTS OBTAINED BY NEGLECTING RESOLUTION

Kiefer[1] has given a search procedure based on the Fibonacci sequence (1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, ...), where the nth Fibonacci number is given by

(4) $$F_o = F_1 = 1; \quad F_n = F_{n-1} + F_{n-2} \quad \text{for } n = 2, 3, \ldots$$

One places the first two experiments at distances L_oF_{n-1}/F_n from one end of the original interval. By equations (1) and (4) the better observation will be a distance L_oF_{n-3}/F_n from one end of the new interval of uncertainty, whose length will be $L_2 = L_oF_{n-2}/F_n$. The third observation is made symmetrically with respect to the one already in the interval, i.e., a distance L_oF_{n-3}/F_n from the other end. This procedure is continued until all but one experiment has been run and the interval of uncertainty has length $L_{n-1} = L_oF_2/F_n = 2L_o/F_n$. The best observation will be exactly in the center of this interval, because $L_oF_1/F_n = L_o/F_n = L_{n-1}/2$. Thus if the final observation were placed symmetrically it would be completely indistinguishable from the one already in the interval. It must therefore be located a distance ϵ to one side or the other of the midpoint. For this reason we shall call this asymmetric minimax method.

If the experimenter's luck is bad he will be left with an interval of uncertainty of length

(5) $$L^*_n = L_o/F_n + \epsilon$$

The asterisk has been added to L_n because Kiefer has shown that this interval is ϵ-minimax among all non-randomized procedures. If one randomizes the placement of the last experiment, the expected final interval is slightly less

(6) $$E\left\{L^*_n\right\} = L_o F_n + \epsilon/2$$

These results were obtained essentially by neglecting the resolution and minimaxing the other term. Thus as ϵ approaches zero L^*_n approaches the true minimax length.

A SHORTER INTERVAL

By taking proper account of the resolution ϵ we can obtain a shorter interval of uncertainty L^{**}_n. In establishing this result we can avoid a long proof by using an intermediate result of Johnson reported in [3]. Johnson showed, in an independent alternate proof of Kiefer's result, that the minimax procedure must be such that after k trials,

(6') $$L^{**}_k = L^{**}_{k-2} - L^{**}_{k-1}\ ; \quad k = 2, 3, \ldots, n$$

Both Kiefer and Johnson have demonstrated that the final two experiments should be a distance ϵ apart in the center of the remaining interval, whose length is L^{*}_{n-1}. Our procedure will be called <u>symmetric</u> because it preserves this symmetry. With this spacing, the final interval is

(7) $$L^{**}_{n} = L^{**}_{n-1}/2 + \epsilon/2$$

Equations (6') and (7) together give

(8) $$L^{**}_{n-2} = L^{**}_{n} + L^{**}_{n-1} = L^{**}_{n} + (2L^{**}_{n} - \epsilon) = 3L^{**}_{n} - \epsilon$$

By iterating the recursion relation (6) we obtain

(9) $$L^{**}_{k} = F_{n-k+1} L^{**}_{n} - F_{n-k-1}\epsilon$$

which can be proven readily by mathematical induction on the indices. When in particular $k = 1$, then

$$L_{1} = F_{n} L^{**}_{n} - F_{n-2}\epsilon$$

whence, since $L_{o} = L_{1}$,

(10) $$L^{**}_{n} = L_{o}/F_{n} + F_{n-2}\epsilon/F_{n}$$

This interval is shorter than that of the asymmetric technique by an amount

(11) $$L^{*}_{n} - L^{**}_{n} = (1 - F_{n-2}/F_{n})\epsilon = F_{n-1}\epsilon/F_{n}$$

As n becomes large, the ratio F_{n-1}/F_{n} approaches $(\sqrt{5}-1)/2 = 0.618033989\ldots$ [1], [2], [3], and so the resolution term in the symmetric method is only about 38% as large as for the asymmetric procedure.

4. PLACEMENT OF THE EXPERIMENTS

Although we have given the final interval obtainable by the symmetric minimax method, we have not yet described how to locate the experiments. The symmetric procedure is similar to the asymmetric one in that each new experiment is placed symmetrically with respect to the observation already in the remaining interval of uncertainty.

Hence the technique is completely defined when the location of the first two experiments is specified. This is accomplished by noting that the interval remaining after these two experiments will be L_2^{**}, which is, from equation (9),

$$L_2^{**} = F_{n-1}L_n^{**} - F_{n-3}\epsilon \tag{12}$$

Equations (10) and (12) together give this length in terms of L_o.

$$L_2^{**} = \left[F_{n-1}L_o + (F_{n-2}F_{n-1} - F_nF_{n-3})\epsilon\right]/F_n \tag{13}$$

The coefficient of ϵ can be rearranged

$$\begin{aligned} F_{n-2}F_{n-1} - F_nF_{n-3} &= (F_{n-2} + F_{n-3})F_{n-2} - (F_{n-1} + F_{n-2})F_{n-3} = \\ &F_{n-2}^2 - F_{n-1}F_{n-3} \end{aligned} \tag{14}$$

so that it can be simplified by a result of Simson[3] [4]

$$F_{n-2}^2 - F_{n-1}F_{n-3} = (-1)^n \tag{15}$$

Equations (13), (14), and (15) together give the optimal placement of the first two experiments

$$L_2^{**} = F_{n-1}L_o/F_n + (-1)^n\epsilon/F_n \tag{16}$$

Thus for an odd number of experiments the first pair is slightly closer together than for an asymmetric search. Conversely when n is even they are slightly farther apart.

5. MAXIMUM NUMBER OF EXPERIMENTS

The need for distinguishability puts an upper bound on the number of experiments that can be performed profitably. Let m be this maximum number for a symmetric search. Equations (3) and (10) together give

$$L_m^{**} = L_o/F_m + F_{m-2}\ /F_m \geq 2\epsilon,$$

from which one can show that

$$F_{m+1} \leq L_o/\epsilon < F_{m+2} \tag{17}$$

Thus if ϵ is only one percent of L_o, there is no advantage in performing more than nine experiments because $89 = F_{10} < 100 < F_{11} = 144$. When n is large, Lucas' relation [3] [5] gives approximately

$$F_{m+1} \approx (1.618)^{m+2}/\sqrt{5},$$

which can be used to obtain, from equation (17),

$$m \le 4.785 \log (L_o/\epsilon) - 0.328 \tag{18}$$

For an asymmetric search the final observation, which is a distance ϵ from the center, can be no closer than ϵ to the end of the interval. Hence the final asymmetric interval L_n^* can be no shorter than 3ϵ

$$L_n^* \ge 3\epsilon , \tag{19}$$

which is 50% longer than the limit on L_n^{**} for symmetric search. Equations (5) and (19) together give a limit on the number m' of asymmetric experiments that can be performed.

$$F_{m'} \le L_o/2\epsilon < F_{m'+1} \tag{20}$$

When $L_o = 100\epsilon$, $m' = 8$, one less experiment than for symmetric search.

It is not always possible for the symmetric search to employ more experiments than the asymmetric scheme (when $L_o = 12\epsilon$, $m = m' = 4$). Moreover, the difference will never be more than one experiment, as can be seen by combining the equalities (17) and (20) with the definition (4) of the Fibonacci sequence.

$$2F_{m-1} < F_m + F_{m-1} = F_{m+1} \le \frac{L_o}{\epsilon} < 2F_{m'+1} ,$$

whence

$$F_{m-1} < F_{m'+1} ,$$

or

$$F_{m-1} \le F_{m'} .$$

It follows that

$$m - m' \leq 1 \quad . \tag{21}$$

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