OPTIMAL DESIGNS FOR MULTIVARIATE POLYNOMIAL EXTRAPOLATION¹

By W. J. STUDDEN

Purdue University

1. Introduction. Let $f = (f_1, f_2, \dots, f_k)$ be a vector of linearly independent continuous functions on a compact set X in Euclidean m-space. For each "level" x in X an experiment can be performed whose outcome is a random variable Y(x) with mean value $\sum_{i=1}^k \theta_i f_i(x)$ and variance σ^2 , independent of x. The functions f_1, f_2, \dots, f_k are called the regression functions and assumed known to the experimenter, while the vector of parameters $\theta = (\theta_1, \theta_2, \dots, \theta_k)$ and σ^2 are unknown. We will be concerned here with the problem of estimating the regression function $\sum_{i=1}^k \theta_i f_i(\bar{x})$, at a point \bar{x} outside of X, by means of a finite number of uncorrelated observations $Y(x_i)$. The design problem is one of selecting the levels x_i in X at which to experiment. The result here is approximate in that we consider a design to be an arbitrary probability measure on X. For a more complete discussion of the model see Kiefer (1959) or Karlin and Studden (1966).

For the case X = [-1, 1] and $\sum_{i=1}^k \theta_i f_i(x) = \sum_{i=1}^k \theta_i x^{i-1}$, Hoel and Levine (1964) showed that the optimum design for estimating $\sum_{i=1}^k \theta_i \bar{x}^{i-1}$ (for any $\bar{x} \notin [-1, 1]$) was supported on the points $x_v = -\cos v\pi/(k-1)$, $v = 0, 1, \dots, k-1$. Kiefer and Wolfowitz (1965), Studden (1968) and Studden and Karlin (1966) give further results for the case where the system $\{f_i(x)\}_1^k$ is a Tchebycheff system. Hoel (1965) gives a discussion of the extrapolation problem in multidimensions when the regression function is essentially of a product type.

In the present paper we consider the case where the regression function is a polynomial in m dimensions of degree less than or equal to n. The domain X will be a compact convex subset of the Euclidean m-space. Thus we take our f_i to be the functions $x_1^{\alpha_1} \cdots x_m^{\alpha_m}$ where the α_j are nonnegative integers and $\sum_{j=1}^m \alpha_j \leq n$. The number of such functions is $k = \binom{n+m}{m}$ and we assume that they are arranged in some fixed order.

2. Optimal design. The optimal extrapolating design is described as follows. Consider a line through \bar{x} which intersects the convex set X at two points, say a and b, such that the tangent hyperplanes at a and b are parallel. (The line in question exists but is not necessarily unique). The optimal design for extrapolating to \bar{x} is now obtained by using the one-dimensional result for polynomials of degree n on the line through a and b. Thus we consider the transformation $x(\alpha) = [(1-\alpha)a+(1+\alpha)b]/2$, such that x(-1)=a and x(+1)=b. The optimal design concentrates on the points $x_v=x(\alpha_v)$ where $\alpha_v=-\cos v\pi/n$, $v=0,1,\cdots,n$. The optimal weights p_v , $v=0,1,\cdots,n$ can be found as in the one-dimensional case

Received February 11, 1970.

¹ This research was supported by the National Science Foundation Contract GP-8986.