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GEOMETRIC AND GAME-THEORETIC APPROACHES TO OPTIMUM ALLOCATION

By

G. ELFVING

TECHNICAL REPORT NO. 68

February 17, 1961

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CONTRACT Nonr-225(52) (NR-342-022)
WITH THE OFFICE OF NAVAL RESEARCH

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This work was sponsored by the Army, Navy and Air Force
through the Joint Services Advisory Group for Research
Groups in Applied Mathematics and Statistics by Contract
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1. Introduction

The purpose of this paper is to draw attention to certain relatively recent developments in the theory of experimental design. The emphasis will be on ideas and connections rather than on actual techniques.

We shall throughout be concerned with linear experiments, i.e., experiments composed of independent observations of form

$$y_\nu = a'_\nu \alpha + \eta_\nu \qquad \nu = 1, \dots , n , \tag{1.1}$$

where $\alpha = (\alpha_1, \dots , \alpha_k)'$ is an unknown parameter vector, the $a_\nu = (a_{\nu 1}, \dots , a_{\nu k})'$ known coefficient vectors, and the independent error terms η_ν have mean 0 and a common variance which we may, for convenience, take to be 1. In matrix notation, the equation (1.1) may be written $y = A\alpha + \eta$. Provided that A is of full rank k, it is well-known that the least-squares estimator vector $\hat{\alpha}$ is given by

$$\hat{\alpha} = (A'A)^{-1} A'y = \alpha + (A'A)^{-1} A'\eta \tag{1.2}$$

and has covariance matrix $\text{cov}\ \hat{\alpha} = (A'A)^{-1}$. The matrix

$$M = A'A = \sum_{\nu=1}^{n} a_\nu\ a'_\nu \tag{1.3}$$

is termed the <u>information matrix</u> of the experiment, and essentially determines its estimatory properties.

So far we have been concerned with a <u>given</u> experiment. On the design level, of course, the experiment has to be composed of observations from out of a set of potentially available ones. Since an observation, in our set-up, is described by the corresponding coefficient vector a_ν , we shall assume that there is given a bounded and closed set $\mathcal{A}$ in k-space from out of which the observations a_ν have to be selected, each one being independently repeatable any number of times. It is no restriction to assume $\mathcal{A}$ to be symmetric about the origin, since the observation $-y$ is automatically available along with y . The set $\mathcal{A}$ may be finite (as is mostly the case in analysis of variance, the coefficients being 0 or 1), or it may be described, e.g., by means of a continuous parameter x (as in polynomial or trigonometric regression models).

An actual experiment, then, is described by its <u>spectrum</u> $a = (a_1, \ldots, a_r)$, $a_j \in$, indicating the different observations selected, and its <u>allocation</u> $(n_1, \ldots, n_r)$ indicating the number of times that each selected observation is to be repeated. The number r is, of course, part of the design. Denoting by $n = \sum n_j$ the total of actual observations, and writing $p_j = n_j/n$, we may essentially describe the experiment by the pair $e = (a,p)$ where $p = (p_1, \ldots, p_r)$ $p_j > 0$, $\sum p_j = 1$. The p_j are the relative allocations, to be chosen by the experimental designer, whereas n usually is fixed by cost considerations. In practice, the p_j run over multiples of $1/n$; in a large sample theory we may, however, consider them as continuous.

The information matrix of an experiment $e = (a,p)$ of size n is, by (1.3),

$$M = M(e) = \sum_{a} n_j a_j a_j' = n \sum_{a} p_j a_j a_j' . \tag{1.4}$$

$M(e)$ determines the value of any particular goodness criterion, such as the variance of the least-squares estimator of a particular parameter, the sum of all such variances, the largest variance, or the like. The solution of the design problem depends, of course, on what criterion we have in mind.

2. Estimating a single parametric form

Consider a particular linear form $\theta = c'\alpha$ in the parameters. The variance of its least-squares estimator $\hat{\theta} = c'\hat{\alpha}$ is

$$\operatorname{var} \hat{\theta} = c' M^{-1} c , \tag{2.1}$$

and depends through M on the design e. The straight forward minimization of (2.1) with respect to the design is difficult due to the complex character of $e = (a,p)$. Two indirect methods have been devised and will be briefly presented below, their interrelation being at the same time pointed out. Both are essentially based on interchanging extremizations.

Geometric method. This approach, suggested by Elfving [1], works primarily in the case of two or at most three parameters.

The information matrix $M = n \sum p_j a_j a_j'$ is that of r independent observations $\bar{y}_j$ with means $a_j'\alpha$ and error variances $(np_j)^{-1/2} (j=1,\ldots,r)$.

The least-squares estimator $\hat{\theta}$ is a linear combination $\theta = \sum_a q_j \bar{y}_j$ fulfilling the unbiasedness condition (note: a vector equation)

$$(2.2) \qquad Q_c: \quad \sum_{a_j \in a} q_j a_j = c$$

and the minimum variance condition

$$(2.3) \qquad \text{var} \left(\sum q_j y_j \right) = \sum_a \frac{q_j^2}{np_j} = \min_{q \in Q_c} .$$

Hence we are, in our design problem, faced with the double minimization

$$(2.4) \qquad \min_{(a,p)} \quad \min_{q \in Q_c} \quad \sum_a \frac{q_j^2}{p_j}$$

the minimizing $e = (a,p)$ being the desired optimal experiment.

Now we interchange the order of minimization: To an arbitrary spectrum a, and an arbitrary corresponding set of non-vanishing coefficients q_j, we find the minimizing $p = p(a,q)$ and the least variance; this will, in turn, be minimized by a certain choice a^*, q^*, from which finally $p^* = p(a^*,q^*)$ is obtained.

Minimizing the sum in (2.4) with respect to p, under the conditions $p_j > 0$, $\sum p_j = 1$, gives elementarily

$$(2.5) \qquad p_j = \frac{|q_j|}{\sum_a |q_h|} , \qquad \min_p \sum_a \frac{q_j^2}{p_j} = \left(\sum_a |q_j| \right)^2 .$$

In order to minimize the latter expression with respect to a, q under condition (2.2), we shall write this condition in the form

$$\text{(2.6)} \qquad \sum_h |q_h| \cdot \sum_j \frac{|q_j|}{\sum |q_h|} \cdot \operatorname{sgn} q_j \cdot a_j = c \quad ,$$

where all sums are over the spectrum a . Call the point represented by the latter sum c_q . For any a and any q , this is a point inside, or on the boundary of, the convex polyhedron spanned by the vectors $\pm a_j \in a$, and hence, within the convex hull $\mathcal{A}^*$ of the set $\mathcal{A}$ of available observations. Conversely, choosing the spectrum and the relative size of the $|q_j|$ appropriately, we may make c_q equal any vector in $\mathcal{A}^*$. The condition (2.6) requires that c_q be proportional to c ; this condition being fulfilled, we have $\sum |q_h| = \|c\|/\|c_q\|$. In order to make the minimum in (2.5) as small as possible, we obviously have to choose for c_q the intersection point c^* between the vector c and the boundary of the convex hull $\mathcal{A}^*$. The vector c^* may be expressed as a convex combination of r points $a_j \in \mathcal{A}$, $r \leq k$. The points form the spectrum a of the desired experiment, the allocations $p_j = |q_j|/\sum |q_h|$ being the barycentric coordinates of c^* with respect to $a_1, \ldots , a_r$.

The situation is illustrated in Fig. 1, where $k = 2$, $c = (0,1)$; consists of 6 (pairwise opposite) points, and $\mathcal{A}^*$ is a hexagon. The desired spectrum is $a = (a_1, a_2)$, and the allocation $p_1{:}p_2$ is given by the ratio of the segments $c^* a_2$, $c^* a_1$.

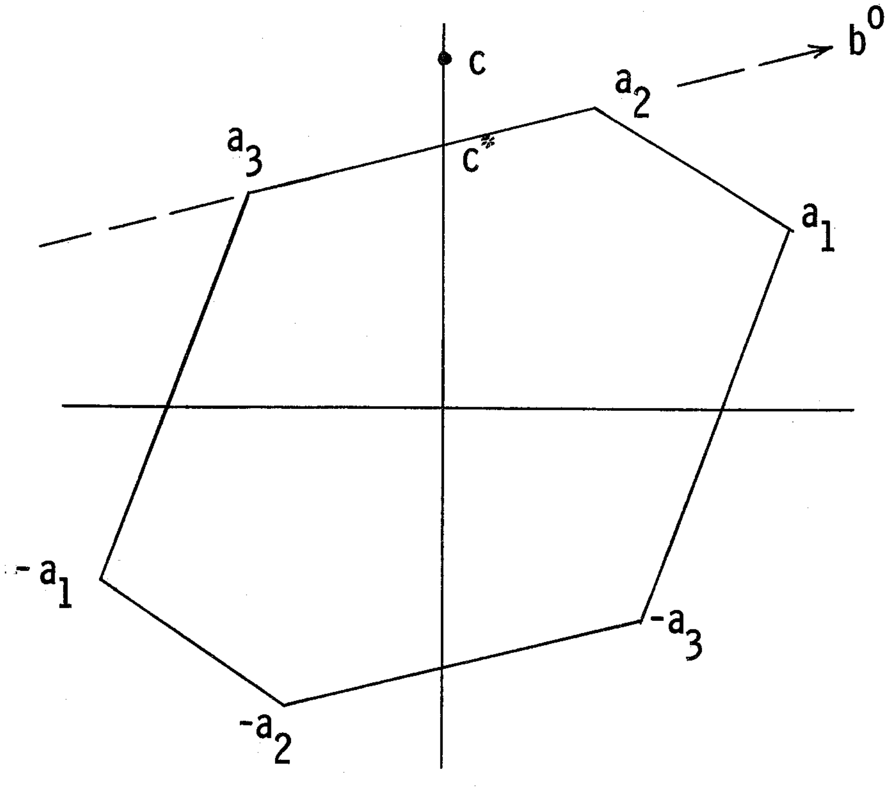

Figure 1

Game-theoretic method. In 1959, Kiefer and Wolfowitz [3] suggested a game-theoretic approach to the allocation problem. Following these authors, we shall show how to find the optimal design for estimating, say, the parameter α_k .

Using a convenient transformation of the parameters $\alpha_1, \dots, \alpha_{k-1}$, it can easily be shown that for any design $e = (a,p)$

$$\frac{1}{n \operatorname{var} \hat{\alpha}_k} = \min_b K(e,b) \tag{2.7}$$

where

$$K(e,b) = \sum_a p_j \, [a_{jk} - b_1 a_{j,} - \cdots - b_{k-1} \, a_{j,k-1}]^2 \ ,$$

$b = (b_1, \dots, b_{k-1})$ denoting a vector in $(k-1)$ - space. Since we wish $\operatorname{var} \hat{\alpha}_k$ to be as small as possible, the design problem consists in maximizing the right-hand side of (2.7).

This formulation suggests the use of game theory. Consider the game with pay-off function $K(e,b)$. This function is convex in b . If by the convex combination (q_1,q_2) of two designs e^1, e^2 we understand the design with spectrum $a = a^1 \cup a^2$ and allocation $p = \{p_j\}$, $p_j = q_1 p_j^{(1)} + q_2 p_j^{(2)}$, it is obvious that $K(e,b)$ is linear in e . As a consequence, the game is completely determined, and we may interchange the extremizations. More precisely, we may adopt the following procedure:

1° For arbitrary b, find $e = e(b)$ so as to maximize $K(e,b)$; let the maximum be $m^2(b) = K(e(b),b)$. The response $e(b)$ will in certain cases (and notably, in the relevant ones) not be uniquely determined.

2° Find b° such as to minimize $m^2(b)$.

3° Find $e^\circ = e(b^\circ)$ and (in case of non-uniqueness) such that conversely $b^\circ = b(e^\circ)$, i.e., b° is a response to e° in the sense $K(e^\circ, b) = \min$ for $b = b^\circ$.

Then, e°, b° constitute a pair of equilibrium strategies, and e° is minimax, as desired.

Let us see how this program works out in our particular situation.

The function (2.8) is maximized with respect to e if we include in the spectrum any finite number of observations a_j for which

$$(2.9) \qquad |a_{jk} - b_1 a_{j1} - \cdots - b_{k-1}\, a_{j,k-1}| = \max_{a_j} = m(b^\circ)$$

and provide them with weights p_j adding up to 1. For b's , the response spectrum will contain just one observation. In the case $k = 2$, the geometric interpretation of this operation is the following (Fig. 1): Let a straight line of slope b_1 move parallel to itself, and consider the outermost positions in which it has points in common with the symmetric set $\mathcal{a}$. Let $B(b_1)$ be the set of these points. For most b_1, $B(b_1)$ contains only two (opposite) elements; when b_1 is the slope of a side in the convex hull $\mathcal{a}^*$ of $\mathcal{a}$, there will be four or more.

Next, the maximum in (2.9) has to be minimized by a proper choice of b. It is clear geometrically that this occurs when the hyperplane determined by b is a supporting plane to $\mathcal{a}^*$ in the point c^* where $\mathcal{a}^*$ is cut by the a_k - axis. When $\mathcal{a}$ is finite, $B(b^\circ)$ will normally contain k points on each side of the origin.

In the case where $B(b^o)$ contains more than one element (as it usually does), it remains to determine $e^o = (a^o, p^o)$ such that $b^o = b(e^o)$. For this to hold, we must have

$$(2.10) \qquad -\frac{1}{2}\frac{\partial K}{\partial b_i} = \sum_a p_j a_{ji} [a_{jk} - b_1 a_{ji} - \cdots - b_{k-1} a_{j,k-1}] = 0 \qquad i = 1, \ldots , k-1 .$$

The expressions in brackets have the same absolute value $m(b^o)$ for all $a_j \in B(b^o)$; it is no restriction to assume this value to be positive, since otherwise we just have to replace a_j by $-a_j$. The conditions (2.10) then boil down to

$$(2.11) \qquad \sum_a p_j a_{ji} = 0 \qquad i = 1, \ldots , k-1 .$$

That is, the spectrum a, and the allocation p, have to be chosen in such a way that the compound vector $\sum p_j a_j$ coincides with the a_k-axis, i.e., with the direction of the coefficient vector $c = (0, \ldots , 0, 1)$ of the parametric form $\theta = \alpha_k$. We see, thus, that the game-theoretic approach leads to the same procedure as the geometric one, whenever this is practicable.

It should be noted, however, that Kiefer and Wolfowitz primarily aimed at the situation where $\mathcal{a}$ is described by means of a continuous parameter x , say $a = a(x)$, $x \in \mathcal{X}$. The second step of the procedure then consists in minimizing

$$\max_x \left| a_k(x) - \sum_{i=1}^{k-1} b_i a_i(x) \right| .$$

Hence, the b_i have to be the Chebyshev coefficients of the function $a_k(x)$ with respect to the basis $a_1(x), \dots, a_{k-1}(x)$; for their determination, ready-made results may often be available.

3. Minimax estimation

For another example of the kind of methods we have in mind, assume that we do not know what parameter, or what linear combination of parameters, is eventually going to be relevant. In such a situation, a reasonable approach seems to be to minimize, with respect to the design e, the largest estimator variance of any standardized linear form in the parameters, i.e., the quantity

$$(3.1) \qquad \max_{\|c\|=1} \operatorname{var} c'\hat{\alpha} = \max_{\|c\|=1} c'M^{-1}c ,$$

$\|c\|$ denoting the length of the vector c. The quantity (3.1) obviously depends on e through M according to (1.4). In order for this approach to make any sense, one must, of course, have the parameters measured on such scales as to make the desired accuracy the same for all of them.

Consider the game - between the Statistician and Nature - with pay-off

$$(3.2) \qquad K(e,c) = c'M^{-1}c = c'\left(\sum_{a} p_j a_j a_j' \right)^{-1} c .$$

The Statistician's set of strategies is obviously that of all $e = (a,p)$, $a \in \mathcal{A}$. The function (3.2) is convex in e, i.e.,

$$K(q_1 e^1 + q_2 e^2, c) \leqq q_1 K(e^1,c) + q_2 K(e^2,c)$$

where the weighted average of two e's is interpreted as in the previous section. Hence no extension of the e-set is necessary. Nature's set of strategies is the unit sphere in the k-dimensional c-space. On this set, there can be no question of forming linear combinations, so we have to extend it by introducing mixed strategies. A general mixed strategy, say γ^*, would be a probability distribution on the unit sphere S, and the corresponding pay-off would be

$$(3.3) \qquad K^*(e,\gamma^*) = \int_S c'M^{-1}\, d\gamma^* .$$

However, γ^* may always be replaced by a discrete distribution assigning positive probability only to the end-points of k orthogonal diameters in the sphere. As a matter of fact, if we factorize M^{-1} into a sum $\sum m_\mu m'_\mu$ of rank one matrices, we have

$$(3.4) \qquad K^*(e,\gamma^*) = \sum_\mu \int_S c'm_\mu m'_\mu c d\gamma^* = \sum_\mu \left(\int_S cc'd\gamma^* \right) m_\mu .$$

The integral is the expected value of a non-negative definite matrix with trace 1, hence is itself a matrix of the same kind, and can be written $\sum_\nu \gamma_\nu c_\nu c'_\nu$ where the c_ν $(\nu = 1, \ldots , k)$ are the column vectors of an orthogonal matrix, and where $\gamma_\nu \geqq 0$, $\sum \gamma_\nu = 1$. Inserting this result in (3.4), and inverting the order of summation, we find

$$(3.5) \qquad K^*(e,\gamma^*) = \sum_\mu m'_\mu \left(\sum_\nu \gamma_\nu c_\nu c'_\nu \right) m_\mu = \sum_\nu \gamma_\nu \sum_\mu c'_\nu m_\mu m'_\mu c_\nu$$

$$= \sum_\nu \gamma_\nu c'_\nu M^{-1} c_\nu = K^*(e,\gamma) \qquad \text{(say)}$$

which shows that we may restrict ourselves to the particular set of "orthogonal mixed strategies" γ. Statistically, the extension of Nature's strategies means that we use for loss function not only the squared error in the estimate of a single parameter, but rather a standardized quadratic form in the estimation errors, this form being described by a non-negative definite matrix with trace one.

After this extension, the fundamental theorem in game theory is applicable. Interchanging the extremizations, we are then faced with the following program:

1^o For an arbitrary γ, find the response $e = e(\gamma)$ maximizing $K(e,\gamma)$. The response may be non-unique.

2^o Find γ^o such as to minimize $K(e(\gamma),\gamma)$.

3^o Find $e^o = e(\gamma^o)$ and (in case of non-uniqueness) such that conversely $\gamma^o = \gamma(e^o)$.

The carrying out of this program may be no less complex than the original problem. Already the first step involves solving the allocation problem for an arbitrary quadratic loss function. It can be shown (see [2]) that no more than $\frac{1}{2}k(k+1)$ different observations will ever have to be included in the optimal design for any estimation problem within the framework of least squares. Generally, then, one will have to try out all "promising" spectra with $\frac{1}{2}k(k+1)$ or less observations, to solve equally many equations for the optimal p, to pick the best spectrum, and finally to find the minimizing γ. We have no simple technique to offer in the general case. There are, however, situations in which shortcuts are possible.

First assume that we are able to find an admissible design e^o such that $M(e^o) = \lambda I$ (e^o being admissible means that there is no e making the difference $M(e) - M(e^o)$ non-negative definite). In practice, this can often be achieved by making the design sufficiently symmetric. It can be shown that any admissible design is optimal for some quadratic loss problem, i.e., is a response to some γ^o. On the other hand, since $M = \lambda I$, we have $c'M^{-1}c = c'c/\lambda = \text{const.}$ on the unit sphere, and hence any γ, and in particular γ^o, is a response to e^o. This implies that e^o is minimax.

Another simple situation is the following, representing in a way the opposite of the former one. Assume that there is no e such that the smallest eigenvalue κ_{min} of $M(e)$ be multiple. Since

$$\max_{\|c\| = 1} c'M^{-1}c = \left[\min_{\|c\| = 1} c'Mc\right]^{-1} = \left[\kappa_{min}(M)\right]^{-1}$$

it is seen that the maximum on the left-hand side is always attained in a single pair of points $\pm c$ on the unit sphere. In this case, thus, we do not have to worry about mixed strategies, but may apply the one-parameter technique of Sec. 2 to find $e(c)$. The corresponding pay-off $K(e(c)\ c)$ is the inverted and squared distance from the origin to the boundary of $\mathcal{A}^*$, in the direction c. The least favorable direction c^o is that in which the boundary of $\mathcal{A}^*$ is closest to the origin. The minimax allocation, finally, is obtained as the response to c^o using the methods of Sec. 2 – it is, however, not trivial to decide whether the minimum eigenvalue will always be simple. For the case $k = 2$, a simple geometric criterion is indicated in [2], Theorem 3.3.

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