

OPTIMUM ALLOCATION IN LINEAR REGRESSION THEORY

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Summary. If for the estimation of β_1, β_2 different observations ("sources") of form (1.1) are potentially available, each of them being repeatable as many times as we please, the question arises which of them the experimenter should utilize, and in what proportions. With appropriate optimality conventions the answer is the following. For the estimation of a single quantity of form $\theta = a_1\beta_1 + a_2\beta_2$ the optimum allocation comprises two sources only; for the estimation of both parameters, the corresponding number is two or three; the best proportions are indicated in Sections 2 and 4 below. Generalizations to more than two parameters and to observations at different costs are briefly discussed.

The problem is related to Hotelling's weighing problem [2] and to the topics treated by David and Neyman in [1].

1. Introduction. Consider an experimenter who wants to determine two unknown quantities β_1, β_2 . We assume that for this purpose a certain number r of different *potential* observations are at his disposal, the outcomes of which are of form

$$(1.1) \quad y_i = x_{i1}\beta_1 + x_{i2}\beta_2 + \eta_i \quad (i = 1, \dots, r);$$

here x_{i1}, x_{i2} denote known coefficients and η_i a random variable (the error term) with mean zero and standard deviation σ . (If the standard deviations of the different observations are proportional to known numbers k_1, \dots, k_r , we have only to divide the equations (1.1) by these numbers in order to restore the situation of the text.) We assume, furthermore, that the experimenter may perform each of the observations as many times as he pleases, or not at all, all actual observations being uncorrelated. If he has decided upon a certain total n of actual observations, he is faced with the problem which of the potential ones should be performed, and in what number. As an application, the reader may think of a surveyor who wants to find the coordinates of a point by observing the direction to it from given surrounding points of known position; in this case the regression is, of course, only differentially linear.

In order to distinguish between the potential and the actual observations, we will in the following refer to the former as *sources* (of information), to the latter as *observations*. Since a source is essentially described by the coefficient vector $\mathbf{x}_i = (x_{i1}, x_{i2})$, we will also briefly speak of the source \mathbf{x}_i or simply the source i . In the solution of any particular optimum allocation problem, those sources which are actually utilized will be called *relevant*, the others *irrelevant*.

The following normalization and idealization of our problem is mathematically convenient. Let the required number of observations on the i th source be

$n_i = np_i$; the p_i 's are obviously multiples of $1/n$ fulfilling the conditions

$$(1.2) \quad p_i \geq 0, \quad \sum p_i = 1.$$

The mean of the observations on the i th source then has a regression equation which may be written

$$(1.3) \quad \bar{y}_i = x_{i1} \beta_1 + x_{i2} \beta_2 + \frac{\eta_i}{\sqrt{p_i}} \quad (i = 1, \dots, r),$$

where η_i has variance σ^2/n . If a certain p_i is zero, the corresponding equation has to be left out of the system. For large n , the p_i 's may be varied practically continuously over the range (1.2). Idealizing this feature we get a large-sample problem, which is essentially independent of σ and n . For simplicity we may finally assume $\sigma^2/n = 1$; in order to restore full generality we have only to reintroduce this factor in all variance and covariance formulas below. We are then faced with the following question:

Consider a planned set of observations of form (1.3) with $E(\eta_i) = 0$, $D^2(\eta_i) = 1$, and with the weights p_i at our disposal, subject only to the conditions (1.2). What are the optimal p_i 's?

The solution of this problem obviously presupposes a specification of the word "optimal," that is, a specification of the estimation problem at hand.

When applying the solution to practical problems, one has to remember that our large-sample p_i 's must be approximated by multiples of $1/n$; here, a fine-structure study might be necessary.

2. Estimation of a single quantity. In this section we shall deal with the case where the interest of the experimenter is centered upon a particular linear combination of the parameters, say

$$(2.1) \quad \theta = a_1 \beta_1 + a_2 \beta_2.$$

Particularly we may have $\theta = \beta_1$ or $\theta = \beta_2$.

Consider all linear forms $t = \sum c_i \bar{y}_i$ yielding unbiased estimates of the quantity (2.1). For this purpose the c_i 's have to make the equality

$$E(t) = \sum c_i (x_{i1} \beta_1 + x_{i2} \beta_2) = a_1 \beta_1 + a_2 \beta_2$$

identical in β_1, β_2 , that is, they must satisfy the vector equation

$$(2.2) \quad \sum c_i \mathbf{x}_i = \mathbf{a}.$$

For $r > 2$ there are infinitely many sets $\{c_i\}$ fulfilling this condition. Among the corresponding estimates t there is, for every fixed set of p_i 's, one with least variance; this statistic is, according to a theorem by Gauss, obtained by substituting in (2.1) the least-squares estimates $\hat{\beta}_1, \hat{\beta}_2$ of the parameters, that is, the values β_1, β_2 that minimize the weighted square sum

$$(2.3) \quad \sum p_i (\bar{y}_i - x_{i1} \beta_1 - x_{i2} \beta_2)^2.$$

The variance of this t is, of course, a function of p_1, \dots, p_r . We want to find those weights p_i which yield the smallest minimum variance.

The solution of this problem can be found by a simple geometric argument. For this purpose we first notice that the smallest minimum variance, by definition, equals $\min_p \min_c D^2 \{ \sum c_i \bar{y}_i \}$, the c_i 's and p_i 's being subject to the conditions (2.2) and (1.2). Inverting the order of minimization and calculating, to begin with, the minimum with respect to the p_i 's for fixed c_i 's, we easily find

$$(2.4) \quad \min_p D^2 \{ \sum c_i \bar{y}_i \} = \min_p \sum \frac{c_i^2}{p_i} = k_c^2,$$

where $k_c = \sum |c_j|$. The minimizing p_i values are $p_{ci} = |c_i|/k_c$.

It remains to minimize (2.4) with respect to the c_i 's, remembering the condition (2.2) which we rewrite in the form

$$(2.5) \quad \mathbf{a} = k_c \sum p_{ci} \cdot \text{sgn } c_i \cdot \mathbf{x}_i = k_c \mathbf{a}_c \text{ (say).}$$

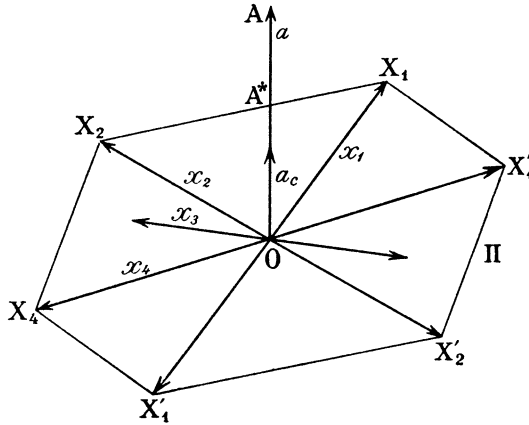


FIG. 1

The factor k_c being a positive scalar, the sum on the right-hand side represents a vector \mathbf{a}_c with the same direction as \mathbf{a} . The weights p_{ci} being nonnegative with sum one, it is clear that the endpoint of this vector lies on or within the convex polygon Π spanned by the vectors $\pm \mathbf{x}_1, \dots, \pm \mathbf{x}_r$ (Fig. 1). Since by (2.5), k_c is the length ratio of the vectors \mathbf{a} and \mathbf{a}_c , it is obvious that (2.4) reaches its minimum when the endpoint of \mathbf{a}_c coincides with the intersection A^* of the vector \mathbf{a} (or its extension) with the polygon Π . If this point lies, for example, between the corners X_1 and X_2 of Π (see Fig. 1), it is seen that the coefficients p_{ci} in (2.5)—and hence the optimum weights—must be in the ratio $A^*X_2 : A^*X_1$ for $i = 1, 2$, and zero for $i = 3, \dots, r$. The smallest minimum variance is given by $(OA/OA^*)^2$. In terms of our original problem we may state this result as follows:

For the estimation of a single quantity (2.1), two and only two of the sources (1.1) are relevant; they have to be used in the proportion shown by the geometric argument above. (There are obvious modifications of this statement in the cases where \mathbf{a} passes through a corner of Π , or where three or more of the \mathbf{x}_i 's have their endpoints on the same line.)

If the vector of a certain source falls entirely inside the polygon spanned by the remaining vectors, this source is of no use for the estimation of any single quantity (2.1).

The fact that, with optimum allocation, only two of the potential observations are actually performed, has a somewhat surprising consequence. The square sum (2.3) reducing to two terms only, its absolute minimum, zero, is reached when β_1 and β_2 are chosen so as to make both terms vanish. The estimates $\hat{\beta}_1$, $\hat{\beta}_2$ are thus obtained simply by dropping the error terms in (1.3) and solving for the parameters.

Example. Consider the case where the potential observations are of form

$$y_i = \alpha + X_i\beta + \eta_i, \quad X_1 < X_2 < \cdots < X_r,$$

that is, the case of linear regression in the elementary sense. Here the polygon Π is a parallelogram spanned by the vectors $(1, X_1)$, $(1, X_r)$, and their opposite vectors. If the interest of the experimenter is centered upon β alone, it is seen that he has to use only the extreme sources 1 and r ; the observations on them have to be equal in number. If α alone is to be estimated and if all X_i 's have the same sign, the extreme ones should again be used, this time in proportion $X_r : X_1$. If the X_i 's include both positive and negative numbers, then the values of the p_i 's are arbitrary with the sole condition that the weighted average $\sum p_i X_i = 0$. Since in practice the p_i 's have to be multiples of $1/n$, n being the number of observations, it is usually impossible to arrange the p_i 's so that the condition mentioned is exactly fulfilled. In such circumstances, one can still make a useful choice between different approximations¹.

Generalization. The generalization to three parameters is obvious. The polygon Π is replaced by a convex polyhedron with triangular side-planes. In any estimation problem concerned with a single linear combination of the parameters there will in general be three relevant sources. For more than three parameters, the geometric rule must be replaced by an algebraic procedure.

3. Estimation of both parameters. For a set of actual observations, that is, for fixed p_1, \dots, p_r , the least-squares technique yields minimum variance estimates of both parameters as well as of all linear combinations of them; nothing is gained in the accuracy of one estimate by giving up accuracy in another. In the present setup where the weights p_i are variable, some information is needed concerning the desired relative accuracy of different estimates. A reasonable approach seems to be to choose an appropriate positive definite quadratic form in the estimation errors $\hat{\beta}_1 - \beta_1$, $\hat{\beta}_2 - \beta_2$ and minimize its expectation by proper choice of the weights. By a linear transformation of the parameters (and a corresponding transformation of the coefficient vectors) the problem can always be reduced to the minimization of the particular form

$$(3.1) \quad q = E\{(\hat{\beta}_1 - \beta_1)^2 + (\hat{\beta}_2 - \beta_2)^2\} = D^2(\hat{\beta}_1) + D^2(\beta_2)$$

with respect to p_1, \dots, p_r .

¹ Cf. [1], p. 116. I am indebted to the referee for this and several other valuable remarks.

It is well known that the covariance matrix Λ of $\hat{\beta}_1, \hat{\beta}_2$ is the inverse of the information matrix

$$(3.2) \quad \mathbf{M} = \begin{bmatrix} \sum p_i x_{i1}^2 & \sum p_i x_{i1} x_{i2} \\ \sum p_i x_{i1} x_{i2} & \sum p_i x_{i2}^2 \end{bmatrix} = \sum p_i \mathbf{x}'_i \mathbf{x}_i.$$

Our object is to minimize the trace

$$q = \lambda_{11} + \lambda_{22} = \mu^{11} + \mu^{22}$$

of this inverse with respect to the p_i 's. A peculiar feature of this problem is that the minimum point usually will lie on the boundary of the region (1.2), some of the p_i 's being actually equal to zero.

Consider a point $P = (p_1, \dots, p_r)$ in (1.2) in which q reaches its minimum. If i and j are two relevant sources, that is, if $p_i > 0, p_j > 0$, any differential variation

$$dp_i = -\delta, \quad dp_j = \delta, \quad dp_h = 0 \quad (h \neq i, j)$$

of the coordinates leads to another point in (1.2). Accordingly, in order for P to be a minimum point, we must have $(\partial q/\partial p_j - \partial q/\partial p_i) \delta \geq 0$ for all δ , that is, we must have $\partial q/\partial p_i = \partial q/\partial p_j$ for any two relevant sources i, j . If, on the other hand, i is a relevant and j an irrelevant source (i.e., $p_i > 0, p_j = 0$), then p_j can be varied only in the positive direction, and we must, by the same argument as above, have $(\partial q/\partial p_j - \partial q/\partial p_i) \delta \geq 0$ for any positive δ ; hence $\partial q/\partial p_j \geq \partial q/\partial p_i$. In conclusion: to any solution of our minimization problem there exists a constant $-\kappa^2$ such that $\partial q/\partial p_i = -\kappa^2$ for all relevant sources, whereas $\partial q/\partial p_i \geq -\kappa^2$ for irrelevant sources.

As far as the relevant sources are concerned, κ^2 is the ordinary Lagrange multiplier. Since q is a homogeneous function of order -1 of p_1, \dots, p_r , and since, by the above result,

$$\sum_1^r p_i \frac{\partial q}{\partial p_i} = -\kappa^2 \sum_1^r p_i = -\kappa^2,$$

we conclude from Euler's identity that κ^2 equals the minimum value of q . This also establishes the sign of κ^2 as positive, as already anticipated in the notation.

We shall now compute the derivatives $\partial q/\partial p_i$. This is easily done by differentiating the matrix identity $\mathbf{M}\Lambda \equiv \mathbf{I}$ with respect to $p_i (i = 1, \dots, r)$. Since by (3.2), $\partial \mathbf{M}/\partial p_i = \mathbf{x}'_i \mathbf{x}_i$, a short calculation gives

$$\frac{\partial \Lambda}{\partial p_i} = -\Lambda \mathbf{x}'_i \mathbf{x}_i \Lambda = -(\Lambda \mathbf{x}'_i)(\Lambda \mathbf{x}'_i)'$$

Hence

$$(3.3) \quad \frac{\partial q}{\partial p_i} = \frac{\partial \text{sp } \Lambda}{\partial p_i} = -\text{sp } \{(\Lambda \mathbf{x}'_i)(\Lambda \mathbf{x}'_i)'\} = -\|\Lambda \mathbf{x}'_i\|^2,$$

where $\|\Lambda \mathbf{x}'_i\|$ denotes the length of the vector $\Lambda \mathbf{x}'_i$. We note that $\|\Lambda \mathbf{x}'_i\|^2$ is a

positive definite quadratic form in the components of \mathbf{x} ; hence, the equation $\|\mathbf{A}\mathbf{x}'\|^2 = \text{Const.}$ represents an ellipse centered at the origin.

Combining the results of the three preceding paragraphs we have the following theorem.

THEOREM. *To any set $\{p_i\}$ that minimizes the function (3.1) there corresponds an ellipse E , centered at the origin, such that all points \mathbf{x}_i representing relevant sources lie on E and none of the points representing irrelevant sources lie outside of E .*

Since three points determine a conic centered at the origin, we conclude that, in general, *there are at most three relevant sources.* Even in the case where four or more source-points happen to lie on the same ellipse, and the rest inside it, it may be shown by a continuity argument that three relevant sources are enough for the minimization of q .

Generalization. The preceding arguments apply to an arbitrary number s of parameters, the ellipse being replaced by an $(s - 1)$ -dimensional ellipsoid or hyperellipsoid in R_s . Hence, there will be at most $\frac{1}{2}s(s + 1)$ relevant sources. However, already for $s = 3$ the computation of the optimum allocation becomes rather complicated.

4. Finding the weights. Simple examples show that the cases with two and with three relevant sources both actually occur. Assuming for the time being that we know how to pick these sources, we now want to find the weight distribution between them as well as the minimum value of q .

If there are two relevant sources corresponding, say, to $i = 1, 2$, we find the estimates $\hat{\beta}_1, \hat{\beta}_2$ simply by solving the equations $\bar{y}_i = x_{i1}\beta_1 + x_{i2}\beta_2$, $i = 1, 2$. Performing the solution, taking the variances, and introducing polar coordinates r, θ for the vectors $\mathbf{x}_1, \mathbf{x}_2$, we find

$$(4.1) \quad q = D^2(\hat{\beta}_1) + D^2(\hat{\beta}_2) = \frac{r_2^2 p_1^{-1} + r_1^2 p_2^{-1}}{r_1^2 r_2^2 \sin^2(\theta_2 - \theta_1)}.$$

The minimum of this expression is attained for

$$(4.2) \quad p_1 = r_2/(r_1 + r_2), \quad p_2 = r_1/(r_1 + r_2),$$

and the minimum value itself is

$$(4.3) \quad q_{\min} = \left\{ \frac{r_1^{-1} + r_2^{-1}}{\sin(\theta_2 - \theta_1)} \right\}^2.$$

The case with three relevant sources $i = 1, 2, 3$ is somewhat more complicated. The derivatives (3.3) being less convenient for actual computation of the minimizing p_i values, we replace q by the homogeneous rational function L/M , where M is the determinant of the matrix (3.2) and L is the trace of M multiplied by $p_1 + p_2 + p_3$. On the set $p_1 + p_2 + p_3 = 1$ we obviously have $q = L/M$. Instead of minimizing L/M on the set mentioned, we may find the required ratio $p_1:p_2:p_3$ by minimizing L under the restriction $M = \text{Const.}$ Introducing a Lagrange multiplier λ and differentiating $L - \lambda M$ we find the equations

$$(4.4) \quad \sum_{j=1}^3 (l_{ij} - \lambda m_{ij})p_j = 0 \quad (i = 1, 2, 3),$$

where

$$(4.5) \quad l_{ij} = r_i^2 + r_j^2, \quad m_{ij} = r_i^2 r_j^2 \sin^2 (\theta_j - \theta_i).$$

If λ is any eigenvalue of the system (4.4) and P a corresponding eigenvector, a well known argument shows that λ is the value of L/M in P . Hence, *the minimum value of q on (1.2) is equal to the smallest eigenvalue of (4.4) for which all components of the eigenvector have same sign. The required optimum allocation is given by these components normalized to sum one.*

5. Selection of sources. There remains the question how to pick the relevant sources from a given set of potential observations.

From the theorem in Section 3 it is immediately seen that a source is certainly irrelevant if it is represented by a point inside the convex polygon spanned by all \mathbf{x} 's. A source i is, furthermore, irrelevant if for any two subscripts j, k ($\neq i$), the ellipse passing through $\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k$ and centered at the origin leaves some fourth \mathbf{x}_h outside it. After discarding all such sources there might still be more than three left. It is in principle always possible to examine these "eligible sources" three by three, determine the corresponding minimum values of q according to Section 4, and pick the triplet with the smallest value. Most of the triplets will actually reduce to pairs, one of the three sources being irrelevant in combination with the others. The occurrence of this case is most easily detected by means of the following criterion, which we mention without proof:

A source \mathbf{x}_3 is irrelevant in combination with \mathbf{x}_1 and \mathbf{x}_2 if and only if \mathbf{x}_3 lies inside or on a certain ellipse, centered at the origin and passing through \mathbf{x}_1 and \mathbf{x}_2 , with parametric equation

$$(5.1) \quad \mathbf{x} = \frac{\mathbf{x}_1 \sin (t - \theta_1) + \mathbf{x}_2 \sin (t - \theta_2)}{\sin (\theta_2 - \theta_1)} \quad (0 \leq t \leq 2\pi).$$

In most practical situations, two sources picked by inspection will probably do without much loss of accuracy.

Example. Take three sources with polar coordinates $(r, \theta), (r, -\theta),$ and (ρ, ϕ) respectively. We consider the two first as fixed, the third as variable. The equation of the ellipse (5.1) becomes in rectangular coordinates $\xi^2 \tan^2 \theta + \eta^2 \cot^2 \theta = r^2$. When \mathbf{x}_3 is inside this ellipse, the source 3 is irrelevant in combination with 1 and 2. There are, on the other hand, regions in which \mathbf{x}_3 "knocks out" one of the other sources. Writing (5.1) explicitly and interchanging the subscripts 1 (2) and 3 one finds, after some calculations, that source 1 (2) becomes irrelevant when \mathbf{x}_3 moves outside the curve $\rho |\sin 2\phi| = r |\sin 2\theta|$ in the first or third (second or fourth) quadrant. As a result we have a cross-shaped figure: in the center only sources 1, 2 are relevant, in the angle-fields only 2, 3 or 1, 3; along the axes all three sources are relevant.

6. Observations at different costs. The preceding theory can easily be adapted to the case where the potential observations are at different costs, say $\$v_1, \dots, v_r$ per unit. Let n_1, \dots, n_r be the number of times that the different

observations are repeated. If the total costs have to equal a prescribed amount C , we have the restriction $\sum n_i v_i = C$ instead of $\sum n_i = n$. Dividing the regression equations for the averaged observations \bar{y}_i by $\sqrt{v_i}$ ($i = 1, \dots, r$) we get a new set of regression equations

$$(6.1) \quad \bar{y}_i^* = x_{i1}^* \beta_1 + x_{i2}^* \beta_2 + \frac{\eta_i^*}{\sqrt{p_i^*}} \quad (i = 1, \dots, r),$$

where

$$(6.2) \quad y_i^* = \bar{y}_i / \sqrt{v_i}, \quad x_{ij}^* = x_{ij} / \sqrt{v_i}, \quad p_i^* = v_i n_i / C,$$

where η_i^* is a random variable with mean zero and standard deviation σ / \sqrt{C} , and where the weights p_i^* are subject to the restrictions (1. 2). This is precisely the previous situation. One has only to enter the procedure with the modified sources x_i^* and to remember that the outcoming p_i^* 's give the optimum allocation of the costs, not of the observations themselves.

REFERENCES

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- [2] H. HOTELLING, "Some improvements in weighing and other experimental techniques," *Annals of Math. Stat.* Vol. 15 (1944), pp. 297-306.