EXPERIMENTAL DETERMINATION OF THE MAXIMUM OF A FUNCTION[1]

By Harold Hotelling

Columbia University, New York City

1. The necessary background for efficient experimental determinations. We shall deal with the problem of arranging an experiment for determining the value of x for which an unknown function $f(x)$ is a maximum or minimum. This problem is to be distinguished from those of estimating the maximum or minimum itself, and of studying the distributions of such estimates, problems to which Bernstein [1] and Rice [2] have contributed.

The range of applications in which determinations of maximizing and minimizing values are important is extremely wide. Among these are the determination of the time of year at which the number of algae or bacilli in a lake is a maximum, and the amount of fertilizers and of irrigation water making the yield of a crop a maximum. The magnetic permeabilities of permalloys, perminvars and permendurs as functions of the induction, and the hardness of a copper-iron alloy as a function of the time of aging at 500°C., possess smooth maxima having interest in telephony, [3], [4]. The effective range of a gun is a function of the speed of burning of the powder, a variable which can be controlled. Almost every entrepreneur has a fervent desire to know the selling prices that will yield a maximum profit, and a few have undertaken controlled experiments with a view to finding out. There are also numerous practical problems of minimizing costs; for example, the cost of operating a ship as a function of its speed possesses a minimum. We shall confine our attention chiefly to the experimental determination of maxima, since such problems seem to occur naturally with greater frequency in applications; there is no loss of generality in this, since $f(x)$ has a maximum where $-f(x)$ has a minimum.

We shall assume that, for each value of x in the set we shall select, one or more observations will be made on $y = f(x)$, and that these observations are afflicted with errors which are independently distributed about zero with a common variance σ^2. From this it follows that if $f(x)$ is a linear function of known functions of x, with unknown coefficients β_0, β_1, $\cdots$, β_p (for example a polynomial in x), the most efficient method of fitting is the method of least squares, which yields unbiased estimates $b_0, \cdots, b_p$ of $\beta_0, \cdots, \beta_p$ having the least possible variances; this is true whether or not the errors are normally distributed. If the fourth moment of the errors is finite, and if the number N

[1] Presented at the joint meeting of the Institute of Mathematical Statistics and the American Mathematical Society at Hanover, September 10, 1940.

of observations is large, the estimated coefficients will be distributed in an approximately normal manner; and so also will any function of them that is regular in a fixed neighborhood of its "population value." By the "population value" of a function $\phi(b_0, \cdots, b_p)$ we mean $\phi(\beta_0, \cdots, \beta_p)$. In particular, if

$$f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 \cdots \beta_p x^p$$

has a maximum for $x = \xi$ of the simplest type, such that $f'(\xi) = 0$ and $f''(\xi) < 0$, so that ξ is a simple root of the equation

$$f'(\xi) = \beta_1 + 2\beta_2\xi + \cdots + p\beta_p\xi^{p-1} = 0,$$

and if x_0 is an estimate of ξ found from the polynomial fitted by the method of least squares, so that

$$b_1 + 2b_2x_0 + \cdots + pb_px_0^{p-1} = 0,$$

this last equation defines x_0 as a function of $b_1, \cdots, b_p$. The function is, to be sure, multiple-valued when $p > 2$; but for sufficiently large values of N the probability will become arbitrarily great that the roots obtained from a random experiment will each differ by an arbitrarily small quantity from one of the roots of $f'(x) = 0$. Then *provided we have a sufficient preliminary approximate knowledge of* ξ, we may choose the root nearest ξ; and the probability distribution of this root, which in nearly all experiments will be a single-valued function

$$\phi(b_1, \cdots, b_p),$$

will approach normality of form, with standard error of order $N^{-1/2}$, about a mean differing from

$$\xi = \phi(\beta_1, \cdots, \beta_p)$$

at most by terms of order N^{-1}, which are thus negligible in comparison with the standard error. The situation will be effectively the same if, without knowing ξ in advance even approximately, we choose the root x_0 giving the greatest value $f(x_0)$, provided $f(\xi)$ is greater than any other value of $f(x)$.

From these considerations it appears advisable, whenever the unknown function is capable of being represented adequately by a polynomial of degree p considerably less than the number N of observations, to fit a polynomial of degree p by least squares, and from it to determine the maximizing value by differentiation. In practice, however, there are obstacles to carrying out such a procedure with confidence. The form of the function is usually not known; it is far from clear what value should be given p even if the function is to be regarded as a polynomial; the use of a polynomial which does not give a sufficiently good fit, with observations taken at a considerable distance from the maximizing value, perhaps separated from it by other maxima and minima, appears to be a highly dubious proceeding; and if p is taken large, the labor of calculation becomes excessive. For all these reasons it is desirable to assign the values of x which are to be the basis of the experimental work close enough to the maximizing value ξ so that a polynomial of very low degree will fit adequately in the neighborhood.

We shall restrict ourselves to functions having continuous derivatives of all relevant orders[2] in a neighborhood of ξ. Such a function can in a sufficiently small neighborhood be approximated by a polynomial of the second degree. The necessity of using a polynomial of higher degree can therefore be avoided, *when a fairly good knowledge of the function is already in hand*, and when the number N of observations that can be made is large enough, by choosing all the values of x in a sufficiently small neighborhood of ξ. We shall suppose that this is done; that is, a regression equation

$$Y = b_0 + b_1x + b_2x^2$$

is fitted by least squares to a large number of observations after choosing the values of x quite close to the true maximizing value ξ; and the estimate x_0 of ξ is a solution of $dY/dx = b_1 + 2b_2x = 0$, so that

$$x_0 = -\frac{b_1}{2b_2}.$$

We shall examine the errors in x_0 arising both from the inadequacy that may exist in the quadratic approximation and from the random errors of observation, and shall consider what distribution of x may most appropriately be chosen to reduce the errors of both kinds, and to place them in a suitable balance with each other.

It will be observed that a fairly definite preliminary knowledge of the function under investigation is required for such a program. Any criterion for the selection of values of x for experimentation must involve not only the value of ξ but also the values of the first few derivatives in a neighborhood of ξ, or some similar information. The requirement of preliminary information is essential for the efficient design of experiments in general. For instance the efficiency of an agricultural field experiment depends on the correctness of the appraisal, before the experiment is laid down, of the general nature of the fertility gradients likely to exist in the field and of the variances due to error and main effects which will be revealed more accurately by the experiment itself. If the pre-

[2] Other cases may well arise in practice and deserve separate consideration in connection with the particular investigations in which they arise. For example various physical properties of alloys, regarded as functions of the proportion of a particular constituent, have maxima, but may have discontinuous derivatives because of the phenomena of crystallization and solution of one metal in another. The assumptions appropriate to an investigation, parallel to that of the present paper, of the proper organization of experiments for finding such metallurgical maxima must be drawn from metallurgy. The case of continuous derivatives is however of widespread importance. If *no* regularity assumption is made about the function, one set of N values of x is as good as another, and no set is likely to tell us very much about the function if it is one of the violently irregular ones utilized in the theory of functions to emphasize the necessity of studying that subject.

liminary information is incorrect, a properly arranged self-contained experiment will nevertheless give results which are *valid*, in the sense that the significance probabilities calculated from them by accurate methods are correct, but will be *inefficient*, in the sense that another experiment of the same cost, based on better preliminary information, would be more likely to detect real effects through the smallness of such a calculated probability. The efficient conduct of experimentation thus proceeds in stages of ascending magnitude. A large-scale investigation should be preceded by a smaller one designed primarily to obtain information for use in designing the large one. The small preliminary investigation may well in turn be preceded by a still smaller pre-preliminary investigation, and so on,[3] like an army marching after an advance guard, which follows a more advanced smaller detachment, which follows a still smaller and still more advanced unit, which follows a "point." At the very beginning of the process of chain experimentation will stand work based on little or no clear information of the kind required for efficient design. This first phase will be speculative and exploratory in character. Neither its cost nor its accuracy can well be estimated in advance. It is a favorite, but not exclusive, preoccupation of men of genius. Many of its results turn out to be worthless. But it is an essential preliminary to well-organized research directed to definite aims defined qualitatively in advance.

After the first speculative and unsystematic phase in the knowledge of a subject is past, but before the careful, economical organization of an accurate investigation, an intermediate type of exploration is needed to supply estimates of the parameters required for the design of the full-scale investigation. In the present case such a systematic though small-scale experiment might perhaps consist in dividing a range within which the desired maximizing value ξ is known to lie into equal parts, making at least two observations at each of the ends of these intervals, and fitting a polynomial of at least the fifth degree by least squares. This will make possible estimates of the parameters $\sigma, \beta_1, \beta_2, \cdots, \beta_5$ (and hence of ξ) required for using the efficient designs which we shall obtain. At least six different values of x are required for fitting the polynomial of the fifth degree. The fitting process is facilitated by taking them in arithmetic progression and using orthogonal polynomials.

---

[3] A remarkable example of such a series of investigations is the chain of sample censuses of area of jute in Bengal carried out for the Indian Central Jute Committee under the direction of Prof. P. C. Mahalanobis annually beginning in 1937. Each year's work is designed primarily to obtain information for planning the next year's, and a sequence of four or five such investigations, each considerably larger than the preceding, is planned to lead up to an eventual annual sampling of the whole immense jute area in the province. A partial account of this is given in [5], a fuller one in confidential but printed reports of the Indian Central Jute Committee, Calcutta.

Certain multiple-sample schemes in manufacturing inspection also provide good examples of chain experiments, [6].

2. Sampling errors and bias in the quadratic approximation. Let us measure all values of x from the value ξ under investigation which makes $f(x)$ a maximum. Then $\xi = 0$, and in the expansion

$$f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \cdots \tag{1}$$

we shall have $\beta_1 = 0$ and $\beta_2 \leq 0$; we shall assume that $\beta_2 < 0$. An observation y_α corresponding to a chosen value x_α will have, by assumption, an error Δ_α of zero expectation and variance σ^2, such that

$$y_\alpha = f(x_\alpha) + \Delta_\alpha . \tag{2}$$

A quadratic estimate

$$Y = b_0 + b_1 x + b_2 x^2 \tag{3}$$

of $f(x)$ is obtained by means of normal equations which may be written

$$\begin{aligned} a_0 b_0 + a_1 b_1 + a_2 b_2 &= Sy \\ a_1 b_0 + a_2 b_1 + a_3 b_2 &= Sxy \\ a_2 b_0 + a_3 b_1 + a_4 b_2 &= Sx^2 y, \end{aligned} \tag{4}$$

where S stands for summation over all the observations, so that, for example, $Sy = \Sigma y_\alpha = y_1 + y_2 + \cdots + y_N$, and where

$$a_k = Sx^k. \tag{5}$$

In particular, $a_0 = N$. A determinate solution is possible only if there are at least three distinct values of x; we shall always suppose therefore that this is the case. This is equivalent to assuming that the determinant a of the coefficients in (4) is not zero. A greater number of observations y is necessary to obtain an estimate of the variance σ^2, and furthermore we shall suppose this number large in our approximations, but since repeated observations may be made for each value of x, it is not essential that there be more than three values of x in the distribution to be selected.

If we put

$$\delta b_k = b_k - \beta_k , \qquad \gamma_k = Sx^k \Delta, \tag{6}$$

for $k = 0, 1, 2$, substitute (1) in (2) and the result in (4), and utilize (5) and (6), we obtain

$$\begin{aligned} a_0 \delta b_0 + a_1 \delta b_1 + a_2 \delta b_2 &= \gamma_0 + a_3 \beta_3 + a_4 \beta_4 + \cdots \\ a_1 \delta b_0 + a_2 \delta b_1 + a_3 \delta b_2 &= \gamma_1 + a_4 \beta_3 + a_5 \beta_4 + \cdots \\ a_2 \delta b_0 + a_3 \delta b_1 + a_4 \delta b_2 &= \gamma_2 + a_5 \beta_3 + a_6 \beta_4 + \cdots \end{aligned} \tag{7}$$

From these equations it follows that the errors δb_k are homogeneous linear functions of the right-hand members and will therefore be small if the quantities on the right are small. Of these quantities, the γ_k's will be stochastically of the order $N^{1/2}$ for large samples with any fixed set of values of x. When the equations are solved, their coefficients will be of the order of N^{-1}, so that the product is of order $N^{-1/2}$, and becomes negligible if N is large enough. The coefficients a_k of $\beta_3, \beta_4, \cdots$ can be kept small if the values of x are chosen to lie within a sufficiently restricted range. Of course the coefficients a_k in the *left* members of (7) will also be small in this case, but not small enough to offset fully the smallness of those on the right. To see this, we observe that if all the values of x be multiplied by any quantity g, a_k is multiplied by g^k, while

$$(8) \qquad a = \begin{vmatrix} a_0 & a_1 & a_2 \\ a_1 & a_2 & a_3 \\ a_2 & a_3 & a_4 \end{vmatrix}$$

is multiplied by g^6. The cofactors of the last column are proportional respectively to g^4, g^3 and g^2. Hence, in the expression for δb_2, the coefficient of β_3 is of order g, that of β_4 is of order g^2, and so on, the coefficients of the β's of higher orders vanishing more and more rapidly with g as we go on in the sequence. The like is true of δb_1 and δb_0, which vanish even more rapidly with g. Thus we may, by restricting sufficiently the range of x on the basis of the assumed preliminary knowledge of the function, and taking a sufficiently large sample of observations, bring it about that the probability will be arbitrarily close to unity that the δb_k's are less than any assigned limits.

Let us, in particular, restrict the range sufficiently and take a large enough sample to make it reasonable to regard δb_2 as negligible in comparison with β_2 The error in the estimate

$$(9) \qquad x_0 = -\frac{b_1}{2b_2}$$

of the maximizing value ξ will, since we are taking $\xi = 0$, be x_0 itself, and may be written

$$\delta x_0 = -\frac{\delta b_1}{2(\beta_2 + \delta b_2)} = -\frac{1}{2}\frac{\delta b_1}{\beta_2}\left(1 - \frac{\delta b_2}{\beta_2} + \cdots\right),$$

where the terms other than 1 in the last parentheses are negligible. The problem of minimizing the error δx_0 is then virtually equivalent to minimizing the error δb_1. In section 5 it will be shown that it is not until we reach terms of the order of g^5 that the errors δb_2 need be taken into account. We shall first discuss the errors in x_0 of lower orders in g, and thus confine the discussion to δb_1. For the present we shall take as the quantity to be made as small as possible the expectation of the square of this last error, $E(\delta b_1)^2$. This is not the same as the variance of b_1, since $E\delta b_1$ is not in general zero. We have, in fact, by transposing a familiar formula for the variance,

$$(10) \qquad E(\delta b_1)^2 = (E\delta b_1)^2 + \sigma_{b_1}^2,$$

thus dividing our minimand into two parts, due respectively to the bias arising from the neglect of terms of third and higher orders, and to the usual sampling errors.

By the usual least-square theory, the sampling variance of b_1 is

$$\sigma_{b_1}^2 = \mu\sigma^2, \tag{11}$$

where μ is the cofactor of the central element in a, divided by a, that is,

$$\mu = (a_0 a_4 - a_2^2)/a. \tag{12}$$

Since μ is of the order of g^{-2}, we may reduce the sampling variance as much as we please by taking the values of x sufficiently far removed from ξ. If $f(x)$ is definitely known to be only of the second degree, a wide dispersion of the desirable values of x is thus indicated, since in this case $E\delta b_1 = 0$, as appears by taking the expectation of each term in (7). But if, as will usually be the case, $f(x)$ has terms of higher orders than the second, an excessively wide dispersion may increase the bias $E\delta b_1$ to such an extent as to render the quadratic approximation inapplicable.

In taking the expectation of each term of (7) and then solving for $E\delta b_1$ we obtain, since $E\gamma_k = 0$ according to the definition of γ_k, and because $E\Delta = 0$, a result of the form

$$E\delta b_1 = B_3\beta_3 + B_4\beta_4 + B_5\beta_5 + \cdots. \tag{13}$$

We shall call B_3, B_4, and B_5 respectively the cubic, quartic and quintic components of the bias, or simply biases. If we denote by λ, μ, ν, the ratios to a of the cofactors of the second column of a, so that

$$\lambda a_1 + \mu a_2 + \nu a_3 = 1, \tag{14}$$

we shall have for the components of bias,

$$\begin{aligned} B_3 &= \lambda a_3 + \mu a_4 + \nu a_5 \\ B_4 &= \lambda a_4 + \mu a_5 + \nu a_6 \\ B_5 &= \lambda a_5 + \mu a_6 + \nu a_7, \end{aligned} \tag{15}$$

and so forth. Since λ, μ, and ν are of respective orders -1, -2 and -3 in a multiplier g of all the values of x, B_3 is of order 2, B_4 is of order 3, and the higher biases are of higher orders. Thus if we begin with any particular distribution of x and apply a sufficiently small multiplier g, we can make the quartic bias negligible in comparison with the cubic, the quintic in comparison with the quartic, and so forth, provided none of these biases is zero. But in reducing g we increase the sampling variance, which is of the order of g^{-2}.

Under these conditions it is reasonable to consider what types of distribution having a fixed value of the sampling variance make the cubic bias a minimum in absolute value; then if there is more than one distribution of this kind, to seek among them a class minimizing the absolute value of the total of cubic and quartic biases; and among these a class minimizing the absolute value of the total of cubic, quartic and quintic biases, with the modified meaning of the quintic bias taking account of δb_2.

3. The cubic and quartic biases. We find, somewhat unexpectedly, that there exists a class of distributions of x for which the cubic bias is actually zero. To exemplify this we need give the variable no more than three different values, which we may call x, y and z, and we may assign to them the arbitrary frequencies k, m, n of experiments ($k + m + n = N$). If we put

$$P = \begin{vmatrix} 1 & 1 & 1 \\ x & y & z \\ x^2 & y^2 & z^2 \end{vmatrix} = (x - y)(y - z)(z - x), \tag{16}$$

and consider a matrix of three rows and N columns, of which k columns are identical with the first column of P, m with the second, and n with the third, it is evident that the sum of the squares of the three-rowed determinants in this matrix is $kmnP^2$. But this sum of squares is also equal to the determinant formed from the sums of products of the three rows, and this is a (formula (8)). Thus $a = kmnP^2 \neq 0$, since x, y, z are all different. Together with the foregoing $3 \times N$ matrix consider another,

$$\begin{Vmatrix} 1 \cdots & 1 \cdots\cdots & 1 \cdots \\ x^2 \cdots & y^2 \cdots\cdots & z^2 \cdots \\ x^3 \cdots & y^3 \cdots\cdots & z^3 \cdots \end{Vmatrix}, \tag{17}$$

having k columns identical with that first written, m identical with the second written, and n identical with the third. The only non-vanishing three-rowed determinants in this matrix are formed of these three different columns, and equal $(xy + yz + zx)P$; there are kmn of them. The sum of products of corresponding three-rowed determinants in the two matrices is therefore $kmnP^2(xy + yz + zx)$. But this sum is also equal to the determinant, formed from the sums of products of corresponding rows,

$$\begin{vmatrix} a_0 & a_2 & a_3 \\ a_1 & a_3 & a_4 \\ a_2 & a_4 & a_5 \end{vmatrix},$$

which, by (15), equals $-aB_3$. It follows that

$$-B_3 = xy + yz + zx. \tag{18}$$

There are many real solutions of the equation

$$xy + yz + zx = 0, \tag{19}$$

with the three values all different, for example $-2, 3, 6$. If we assign such values to our variable, and an arbitrary number of experimental determinations to each of these values, the cubic bias B_3 will be zero.

It will be noticed that such a solution cannot have zero for one of the values. If, for example, $z = 0$ in (19), then x or y must also vanish, in violation of the condition that there must be at least three distinct values. Moreover a solution cannot be symmetrical about zero; if $x + y = 0$ it follows from (19) that $x = y = 0$. A solution may or may not be symmetrical about a value other than zero. The values $3 - 2\sqrt{3}$, $(3 - \sqrt{3})/2$, $\sqrt{3}$ satisfy the equation and are in arithmetic progression, while the solution $-2, 3, 6$ is asymmetrical.

If we modify (17) by replacing the cubes of the variables by their fourth powers, and apply the same procedure to the modified matrix, we find that

$$B_4 = -(x + y)(y + z)(z + x). \tag{20}$$

Thus there exist sets of three distinct real values making the quartic bias vanish, for example any set for which $x + y = 0$; but no such set can at the same time nullify the cubic bias (18). Since it is ordinarily more important for the cubic than for the quartic bias to vanish, distributions nullifying (20) are not in general to be recommended. But in exceptional cases it may be known that β_3 is zero, or very small in comparison with β_4, and then the vanishing of B_4 is a more valuable property than that of B_3. It will be shown that no distribution of three or more values exists such that both the cubic and quartic components of bias are zero.

Let us denote by D_p the p-rowed determinant having a_{i+j-2} as the element in its ith row and jth column. Thus D_3 is the same determinant which we have in (8) called a, and

$$D_4 = \begin{vmatrix} a_0 & a_1 & a_2 & a_3 \\ a_1 & a_2 & a_3 & a_4 \\ a_2 & a_3 & a_4 & a_5 \\ a_3 & a_4 & a_5 & a_6 \end{vmatrix}. \tag{21}$$

For every distribution, every $D_p \geq 0$; and a necessary and sufficient condition that a distribution have p or more distinct values is that D_p be *greater* than zero. [7, p. 362]. If D_p is positive, so is each of its principal minors. In particular, since we are requiring at least three values in a distribution, $D_3 = a > 0$, and therefore

$$a_2a_4 - a_3^2 > 0, \tag{22}$$

and

$$a_0a_4 - a_2^2 > 0. \tag{23}$$

We shall now consider distributions for which the cubic bias B_3 is zero, and consequently, by (15),

$$\lambda a_3 + \mu a_4 + \nu a_5 = 0, \tag{24}$$

and expand D_4. From the definition of λ, μ, ν, we have

$$\lambda a_2 + \mu a_3 + \nu a_4 = 0. \tag{25}$$

Multiply the last row of the determinant (21) by ν, and add to it λ times the second row and μ times the third. The last row is thus, by (14), (25), (24) and (15) transformed into

$$1 \quad 0 \quad 0 \quad B_4,$$

while the determinant has been multiplied by ν. Let this new determinant be expanded with respect to its last row. The cofactor of the first element 1 is

$$G = -\begin{vmatrix} a_1 & a_2 & a_3 \\ a_2 & a_3 & a_4 \\ a_3 & a_4 & a_5 \end{vmatrix}.$$

Let the last row of this determinant be multiplied by ν, an operation having the effect of multiplying the whole determinant by ν; and let λ times the first row and μ times the second row then be added to the last. The last row is thus, by (14), (25) and (24) reduced to

$$1 \quad 0 \quad 0.$$

Hence

$$\nu G = -(a_2 a_4 - a_3^2),$$

and consequently

$$\begin{aligned} \nu^2 D_4 &= \nu(aB_4 + G) \\ &= \nu a B_4 - (a_2 a_4 - a_3^2). \end{aligned} \tag{26}$$

Since the first member of this equation is positive or zero, (22) shows that it is impossible that B_4 should equal zero when $B_3 = 0$ as we have assumed. That is,

Either the cubic or the quartic bias of every distribution having three or more distinct values must be different from zero.

If ν were zero, (26) would contradict (22). Hence $\nu \neq 0$. With every distribution of x there is associated another obtained from it by changing the sign of each value of x. Such a pair of distributions we shall call *opposite.* When we pass from a distribution to its opposite, the power-sums a_k remain unchanged when k is even and change only in sign when k is odd. Since a is always positive, and since

$$\nu = (a_1 a_2 - a_0 a_3)/a, \tag{27}$$

ν has opposite signs and the same absolute value for opposite distributions. The conclusions to be reached shortly will be equally valid for a distribution and its opposite, and in reaching them we may assume $\nu > 0$. It will then follow from (22) and (26) that $B_4 > 0$.

4. Distributions nullifying cubic bias with minimum quartic bias. We can now prove the following theorem:

Among distributions for which the cubic bias vanishes and the standard error of b_1 has a fixed value, those for which the quartic bias is a minimum have exactly three distinct values of the variable. These values satisfy the equation

$$xy + yz + zx = 0. \tag{28}$$

Since the standard error σ of a single observation is not affected by the distribution chosen for x, fixation of the standard error of b_1 is equivalent by (11) to fixation of the value of the expression μ given by (12). We suppose therefore that μ has some fixed positive value and that $B_3 = 0$. Since μ, B_3 and B_4 do not involve the distribution of x excepting through the power-sums $a_0, a_1, \cdots, a_6$, we may treat these power-sums as the independent variables in trying to make B_4 a minimum. Their region of variation is limited by the inequalities referred to in the preceding section,

$$D_1 = a_0 > 0, \qquad D_2 > 0, \qquad D_3 = a > 0, \qquad D_4 \geq 0.$$

The inequalities $D_p \geq 0$ for $p > 4$ involve power-sums of orders higher than the sixth and are irrelevant to our purpose.

The definition (8) of a shows that it is independent of a_5 and a_6; consequently λ, μ, and ν are also. According to (15), B_3 involves a_5 but not a_6; while of all the expressions we have considered, only B_4 and D_4 are functions of a_6. Therefore when $a_0, a_1, \cdots, a_5$ are given any definite values, a_6 may be chosen to make B_4 a minimum without any regard to the fixed values of μ and B_3. Now (15) shows that B_4 is a linear function of a_6 with a coefficient which, at the end of the last section, we have proved not to be zero and assumed positive. Thus B_4, which is also positive, is an increasing function of a_6. Its minimum will correspond to the least value of a_6 consistent with the condition $D_4 \geq 0$. But (21) shows that D_4 is also a positive linear function of a_6 with a positive coefficient, a. The minimum of a_6, and therefore that of B_4, require therefore that $D_4 = 0$. But $D_4 = 0$ is exactly the condition that there should be no more than three distinct values in the distribution. Since there must be at least three distinct values, and since if there are only three they must satisfy (19), the theorem is proved.

The minimum value of B_4 with respect to variations of a_6 when $B_3 = 0$ may be found by putting $D_4 = 0$ in (26). Designating this minimum by b and using (27) we have

$$b = \frac{a_2 a_4 - a_3^2}{a_1 a_2 - a_0 a_3}, \tag{29}$$

where the numerator is intrinsically positive, and the denominator is positive for the class of distributions we are now considering, though we might equally well consider the opposite distributions, for which it is negative. We have also from (20),

$$(x + y)(y + z)(z + x) = -b. \tag{30}$$

Substituting for each of these binomials its value as given by (28), we may write this in the simpler form

$$xyz = b > 0. \tag{31}$$

It was shown at the beginning of section 3 that when there are only three values in the distribution, with frequencies k for x, m for y, and n for z,

$$a = kmnP^2 = kmn(x - y)^2(y - z)^2(z - x)^2. \tag{32}$$

The first two rows of (17) form a matrix such that the sum of the squares of its two-rowed determinants is

$$mn(y^2 - z^2)^2 + nk(z^2 - x^2)^2 + km(x^2 - y^2)^2. \tag{33}$$

Since this is equal to the determinant of the sums of products of the rows, namely

$$\begin{vmatrix} a_0 & a_2 \\ a_2 & a_4 \end{vmatrix},$$

it follows from (12), (32) and (33) that

$$\mu = \frac{(y + z)^2}{k(x - y)^2(x - z)^2} + \frac{(x + z)^2}{m(x - y)^2(y - z)^2} + \frac{(x + y)^2}{n(x - z)^2(y - z)^2}. \tag{34}$$

It is desired to minimize this expression, which is the factor of the variance that is independent of the accuracy of the individual observations, while holding $b = xyz$ fixed; or to minimize b while holding μ fixed. In either case the values of x, y and z are to be chosen to satisfy (28). The relations established by the solution of either of these virtually equivalent problems will fix x, y, and z except for a factor of proportionality, which must then be adjusted to provide a balance as satisfactory as possible between random errors and bias.

5. The quintic bias. Effect of δb_2. With any distribution determined in this way will be associated its opposite distribution, which will have the same minimizing properties so far as the variance and the cubic and quartic components of bias are concerned. The appropriate choice between these two opposite distributions will in general involve the quintic component of the bias. At this point we must, for the first time, take account of the errors in the denominator b_2 of x_0.

Since b_1 converges stochastically to Eb_1, and b_2 to Eb_2, the error $x_0 = -\frac{1}{2}b_1/b_2$ converges stochastically (for large samples) to $-\frac{1}{2}Eb_1/Eb_2$. By keeping our values of x close enough to ξ we may insure that Eb_2 differs as little as we please from β_2, and hence that the series

$$\frac{Eb_1}{Eb_2} = \frac{Eb_1}{\beta_2 + E\delta b_2} = \frac{Eb_1}{\beta_2}\left\{1 - \frac{E\delta b_2}{\beta_2} + \frac{(E\delta b_2)^2}{\beta_2^2} - \cdots\right\}$$

converges rapidly. Let us rearrange this series after inserting for Eb_1 and $E\delta b_2$ their values, so as to obtain a series in ascending powers of a common multiplier g which may be applied to the values of x. We recall that in the expression (13) for Eb_1, B_3 is of the second order in g, B_4 is of the third order, B_5 is of the fourth order, and so forth. In the same way, we find that

$$E\delta b_2 = C_3\beta_3 + C_4\beta_4 + \cdots,$$

where

$$C_3 = \frac{1}{a}\begin{vmatrix} a_0 & a_1 & a_3 \\ a_1 & a_2 & a_4 \\ a_2 & a_3 & a_5 \end{vmatrix}$$

is of the first order, C_4 is of the second order, and so forth. Thus in

$$\beta_2\frac{Eb_1}{Eb_2} = B_3\beta_3 + (B_4\beta_4 - B_3C_3\beta_3^2/\beta_2)$$
$$+ (B_5\beta_5 - B_4C_3\beta_3\beta_4/\beta_2 - B_3C_4\beta_3\beta_4/\beta_2 + B_3C_3^2\beta_3^3/\beta_2^2) + \cdots,$$

the first term is of the second order, those in the first parentheses are of the third order, those in the second parentheses are of fourth order, and the remaining terms are of higher orders.

We have seen that we can choose distributions for which $B_3 = 0$. In this way we get rid of the second-order term and reduce the third-order terms to $B_4\beta_4$. We shall in the next two sections show how, under various conditions, to select from among the distributions for which $B_3 = 0$ an opposite pair for each of which $|B_4|$ is a minimum. In choosing between these two opposite distributions, the criterion we shall adopt is that the terms of third order and those of fourth order shall have opposite signs; for while the fourth-order terms may be made much smaller than those of third order in absolute value, still it is desirable that they should offset them, in order to reduce the error. The terms of third and of fourth orders reduce respectively for $B_3 = 0$ to $B_4\beta_4$ and to $B_5\beta_5 - B_4C_3\beta_3\beta_4/\beta_2$. Our criterion is that these are to have opposite signs, and consequently that

$$B_4\beta_2\beta_4(B_5\beta_2\beta_5 - B_4C_3\beta_3\beta_4) < 0.$$

We shall however modify this criterion whenever σ is not negligibly small. A more precise criterion will be obtained by expanding x_0^2 in a series of powers of δb_2, taking the expectation term by term, and reducing the moments thus obtained of orders higher than the second to those of first and second orders by means of the theory of the bivariate normal distribution of b_1 and b_2. It is then necessary to make some assumption regarding the order of magnitude of x, y and z relatively to N in order to assemble terms of like magnitude in a criterion resembling that above but involving σ. The appropriate balance indicated by the results of the next two sections calls for x, y and z to be of the order of $N^{-1/8}$. This leads to the following criterion:

$$\beta_2(B_4B_5\beta_2\beta_4\beta_5 - B_4^2C_3\beta_3\beta_4^2 - C_3\beta_3\mu\sigma^2) < 0.$$

We have seen that $B_4 = b = xyz$. To evaluate C_3 and B_5, which latter may in accordance with (15) be written

$$B_5 = -\frac{1}{a}\begin{vmatrix} a_0 & a_2 & a_5 \\ a_1 & a_3 & a_6 \\ a_2 & a_4 & a_7 \end{vmatrix},$$

we proceed as in section 3, replacing the second row of (17) by the first powers to obtain C_3, and replacing the third row of (17) by the fifth powers of x, y and z to obtain B_5. In this way we find

$$C_3 = \frac{1}{P}\begin{vmatrix} 1 & 1 & 1 \\ x & y & z \\ x^3 & y^3 & z^3 \end{vmatrix}, \qquad B_5 = -\frac{1}{P}\begin{vmatrix} 1 & 1 & 1 \\ x^2 & y^2 & z^2 \\ x^5 & y^5 & z^5 \end{vmatrix}.$$

Letting Σx, Σx^2yz, etc. stand for the symmetric functions of x, y and z of which one term is written in each case after Σ, we may reduce these expressions to

$$C_3 = \Sigma x,$$

$$B_5 = -\Sigma x^3y - \Sigma x^2y^2 - 2\Sigma x^2yz.$$

With the help of (28) and (31) we find

$$\Sigma x^2yz = xyz\Sigma x = b\Sigma x,$$

$$\Sigma x^2y^2 = (\Sigma xy)^2 - 2\Sigma x^2yz = -2b\Sigma x,$$

$$\Sigma x^3y = \Sigma xy\Sigma x^2 - \Sigma x^2yz = -b\Sigma x.$$

Therefore $B_5 = b\Sigma x$. Substituting these values for B_4, C_3 and B_5 in the last inequality gives the rule:

Choose that one of a pair of opposite distributions for which

$$(x + y + z)\beta_2\{b^2\beta_4(\beta_2\beta_5 - \beta_3\beta_4) - \beta_3\,\mu\sigma^2\} < 0. \tag{35}$$

It will be remembered that β_2 is negative for a maximum of $f(x)$, positive for a minimum. The other β's can only be estimated from preliminary experimentation, or possibly in particular cases from general knowledge or theory.

Quite different algebraic methods are appropriate to minimizing μ with a fixed

b according to the limitations to be placed on the frequencies k, m, n; the methods leading very simply to a solution in one case involve troublesome complications in another. We shall deal with two of the leading cases.

6. The case of equal frequencies. Some experimental situations call for equal frequencies for all values of the variable. If $k = m = n$, then $a_0 = N = 3n$. Let $a_j' = a_j/n$. Then $a_0' = 3$ and $a_1' = \Sigma x$. Inasmuch as

$$\Sigma xy = 0 \qquad \text{and} \qquad xyz = b, \tag{36}$$

we may express a_2', a_3' and a_4' as functions of a_1' and b as follows:

$$a_2' = \Sigma x^2 = (\Sigma x)^2 - 2\Sigma xy = a_1'^2.$$

$$a_3' = \Sigma x^3 = (\Sigma x)^3 - 3\Sigma x^2 y - 6xyz;$$

and since $\Sigma x^2 y = \Sigma x \Sigma xy - 3xyz$ we have from (36),

$$a_3' = a_1'^3 + 3b.$$

We have also

$$a_4' = \Sigma x^4 = (\Sigma x)^4 - 4\Sigma x^3 y - 6\Sigma x^2 y^2 - 12\Sigma x^2 yz,$$

and since

$$\Sigma x^3 y = \Sigma xy \Sigma x^2 - \Sigma x^2 yz, \qquad \Sigma x^2 yz = xyz\Sigma x = a_1' b,$$

$$\Sigma x^2 y^2 = (\Sigma xy)^2 - 2\Sigma x^2 yz = -2a_1' b,$$

it follows that

$$a_4' = a_1'^4 + 4a_1' b.$$

Therefore

$$a = n^3 \begin{vmatrix} 3 & a_1' & a_1'^2 \\ a_1' & a_1'^2 & a_1'^3 + 3b \\ a_1'^2 & a_1'^3 + 3b & a_1'^4 + 4a_1' b \end{vmatrix}$$

Upon subtracting a_1' times the second column from the third, and a_1' times the first from the second, this becomes

$$a = n^3 b \begin{vmatrix} 3 & -2a_1' & 0 \\ a_1' & 0 & 3 \\ a_1'^2 & 3b & a_1' \end{vmatrix} = -n^3 b(4a_1'^3 + 27b).$$

Also,

$$a_0 a_4 - a_2^2 = n^2\{3(a_1'^4 + 4a_1' b) - (a_1'^2)^2\} = 2n^2(a_1'^4 + 6a_1' b).$$

Hence, by (12),

$$\mu = \frac{a_0 a_4 - a_2^2}{a} = -\frac{2}{nb}\frac{a_1'^4 + 6a_1' b}{4a_1'^3 + 27b}. \tag{37}$$

Differentiating with respect to a_1' to find a minimum, we obtain

$$0 = (4a_1'^3 + 27b)(4a_1'^3 + 6b) - 12a_1'^2(a_1'^4 + 6a_1'b) = 4a_1'^6 + 60a_1'^3 + 162b^2.$$

The minimum of μ, for b fixed, and satisfying the condition $4a_1'^3 + 27b < 0$, which is equivalent to $a > 0$ since we assume $b > 0$, is attained when $a_1'^3 = bq$ where q is the numerically greater root of the equation $4q^2 + 60q + 162 = 0$; that is,

$$q = -(15 + \sqrt{63}/2) = -11.468\ 626\ 97.$$

The elementary symmetric functions of the values x, y, z composing the distribution are

$$\Sigma x = a_1' = (bq)^{1/3}, \qquad \Sigma xy = 0, \qquad xyz = b.$$

Hence x, y and z must be the roots of the equation in u,

(38) $$u^3 - (bq)^{1/3}u^2 - b = 0.$$

If we put $u = (bq)^{1/3}v$,

$$v^3 - v^2 + q^{-1} = 0.$$

Calculation gives approximately

(39) $q^{-1} = -.087\ 194\ 396$, and for the roots of the equation in v,

.2628, $\quad -.3729$, $\quad -.8899$,

numbers which are therefore proportional to the values of the variable that should be chosen when the frequencies must be equal. If any values x, y, z proportional to these are used, the value (37) of μ is

(40) $$\mu' = -\frac{6}{N}\frac{q+6}{4q+27}q^{1/3}b^{-2/3}$$

and is the minimum consistent with any fixed value b of xyz.

Choice of the factor of proportionality will involve a compromise between the criteria of minimum sampling variance and minimum bias. If we ignore components of bias of orders higher than the fourth and recall (10) and (11) it will appear that the appropriate combined criterion is that

(41) $$b^2\beta_4^2 + \mu\sigma^2$$

shall be a minimum. Putting for μ its value μ' from (40) and differentiating with respect to b gives

$$2\beta_4^2 b + \frac{4\sigma^2 q^{1/3}}{N}\frac{q+6}{4q+27}b^{-5/3} = 0,$$

or

$$b = b' = \left(-\frac{2\sigma^2}{N\beta_4^2}\frac{q+6}{4q+27}q^{1/3}\right)^{3/8}.$$

The product of the three roots (39) is $-q^{-1}$. Numbers proportional to them and having the product b' will be obtained by multiplying them by $-(b'q)^{1/3}$, that is, by

$$\left(\frac{\sigma^2}{N\beta_4^2}\right)^{1/8}\left(2\,\frac{q+6}{4q+27}\right)^{1/8}(-q)^{3/8} = 2.3318\left(\frac{\sigma^2}{N\beta_4^2}\right)^{1/8}.$$

Multiplying (39) by 2.3318 gives numbers

$$.6128, \qquad -.8695, \qquad -2.0751, \tag{42}$$

which must still be multiplied by $\pm\ [\sigma^2/(N\beta)_4^2]^{1/8}$ to give the set minimizing $E\delta b_1^2$. The ambiguous sign is to be fixed according to the rule at the end of the last section. Thus we arrive finally at the conclusion:

If the numbers of observations are required to be the same for all the values of the variable used, these values should for greatest efficiency deviate from the estimated maximizing value by the products of the three numbers (42) *by*

$$\pm\left(\frac{\sigma^2}{N\beta_4^2}\right)^{1/8}, \tag{43}$$

choosing the ambiguous sign so as to satisfy (35).

The product b' of the three values is to be substituted for b in (40) and (35), and the value of μ thus obtained from (40) is also to be substituted in (35). These substitutions yield

$$(x + y + z)\beta_2\beta_4(\beta_2\beta_5 - 4\beta_3\beta_4) < 0$$

as the criterion for choosing the sign in (43).

The expectation of the square of the error in the estimate of the value x_0 of ξ is, according to (9) and (10), given approximately by the ratio of (41) to $4\beta_2^2$, and it is this that will be a minimum when the foregoing rule is followed. The minimum of (41) is obtained by replacing b by b' in (40) and (41), and substituting (40) for μ in (41). This gives

$$E(\delta b_1)^2 = 4\left(\frac{2}{N}\,\frac{q+6}{4q+27}\right)^{3/4}(-q)^{1/4}\beta_4^{1/2}\sigma^{3/2};$$

that is,

$$E(\delta b_1)^2 = 4.889\ N^{-3/4}\beta_4^{1/2}\sigma^{3/2}. \tag{44}$$

7. Adjustable frequencies. If the total number N of observations to be made can be distributed freely among the values of the variable, the efficiency of the experiment can be increased by a proper selection of the individual frequencies

k, m, n along with the corresponding values x, y, z. We shall choose these six unknowns, subject to the three conditions[4]

$$k + m + n = N, \tag{45}$$

$$xy + xz + yz = 0, \tag{46}$$

$$xyz = -b, \tag{47}$$

to minimize μ. The last condition fixes the quartic bias, the preceding one expresses the vanishing of the cubic bias. It is of course understood that k, m, n are all positive, and we shall, as before, suppose initially that b is positive. No two of x, y, z can be equal, and it follows that none of them, or of the sums of two of them, can be zero while satisfying the second condition. We shall lose no generality in assuming that

$$x > y > 0 > z. \tag{48}$$

Furthermore, it is easy to see that $x + y$, $x + z$, and $y + z$ are all positive. Therefore the quantities

$$r = \frac{y + z}{(x - y)(x - z)}, \quad s = \frac{x + z}{(x - y)(y - z)}, \quad t = \frac{x + y}{(x - z)(y - z)} \tag{49}$$

are all positive. From (34) we have

$$\mu = \frac{r^2}{k} + \frac{s^2}{m} + \frac{t^2}{n}. \tag{50}$$

The values of k, m, n making this a minimum while themselves subject to the limitation that their sum is N must if they were continuous positive variables be proportional to r, s and t. Of course the frequencies are integers, but we are supposing N large, so that the values found by differentiation will be close approximations, and we shall disregard this complication. Put therefore

$$r = k\rho, \qquad s = m\rho, \qquad t = n\rho, \tag{51}$$

where ρ is a multiplier which evidently is not zero. If we use these equations to eliminate r, s, t from μ we obtain, with the help of (45), $\mu = N\rho^2$. But if we use them to eliminate k, m, n from (50) we have instead,

$$\mu = (r + s + t)\rho.$$

Now from (49),

$$r + t = s, \tag{52}$$

[4] The condition (47) is here used instead of (31), from which it differs by the introduction of the negative sign, because it simplifies the argument of this section slightly to have the quantities (49) positive. There is no essential difference, since we are seeking a pair of opposite distributions.

so that $\mu = 2s\rho$. Therefore $N\rho = 2s$, and finally $\mu = 4s^2/N$. Therefore μ is a minimum when the positive quantity s is a minimum. In the expression (49) for s we substitute from (46) and (47)

$$\begin{aligned} x + z &= -xz/y = b/y^2, \\ (x - y)(y - z) &= (x + z)y - xz - y^2 = 2b/y - y^2, \end{aligned} \tag{53}$$

so that

$$s = \frac{b}{y(2b - y^3)}. \tag{54}$$

Since y, s and b are positive, this shows that $y^3 < 2b$. The value of y on the interval from 0 to $2b$ making s a minimum is found by differentiation to be $2^{-1/3}b^{1/3}$. Substituting this in (53) and (47) gives

$$x + z = 2^{2/3}b^{1/3}, \qquad xz = -2^{1/3}b^{2/3},$$

whence

$$x = (b/2)^{1/3}(1 + \sqrt{3}), \qquad y = (b/2)^{1/3}, \qquad z = (b/2)^{1/3}(1 - \sqrt{3}). \tag{55}$$

From (45), (51) and (52) it is seen that $k + n = m = N/2$. Thus half the total observations are to be concentrated on the middle value. From (51) and (49) we have also

$$\frac{k}{n} = \frac{r}{t} = \frac{y^2 - z^2}{x^2 - y^2},$$

wherefore

$$k = \frac{N}{2}\frac{y^2 - z^2}{x^2 - z^2}, \qquad n = \frac{N}{2}\frac{x^2 - y^2}{x^2 - z^2}.$$

With (55) this shows that

$$\begin{aligned} k &= N(2 - \sqrt{3})/8 \qquad m = N/2, \qquad n = N(2 + \sqrt{3})8 \\ &= .03349\, N, \qquad\qquad\qquad\qquad\qquad\quad = .46651\, N. \end{aligned} \tag{56}$$

We have seen that $\mu = 4s^2/N$. Substituting in (54) the value found for y gives $s = 2^{4/3}b^{-1/3}/3$. Therefore the minimum of μ for a fixed value of b is

$$\mu = (16/9N)(2/b)^{2/3} \tag{57}$$

Inserting this in the expression (41) for the total expectation of the squared error and then differentiating with respect to b gives

$$b = 2^{7/4}3^{-9/8}N^{-3/8}\beta_4^{-3/4}\sigma^{3/4}. \tag{58}$$

When this value is given to b, (41) becomes

$$3.8207N^{-3/4}\beta_4^{1/2}\sigma^{3/2}. \tag{59}$$

The greater efficiency of experiments with the frequencies (56) and the correspondingly adjusted values x, y, z, in comparison with the case in which the frequencies must be equal, corresponds to the smaller coefficient in (59) than in (44). To obtain as great accuracy with equal frequencies as with adjusted ones it is necessary to have more observations, in a ratio obtained by equating (59) with (44) after inserting different symbols for N in the two cases. In this way it is found that the number of observations required with efficient distribution of the frequencies is almost exactly 72 per cent of the number required when the frequencies are equal, if the values x, y, z are in each case given their most efficient values.

Substituting (58) in (55) gives the numbers

$$2.1520, \qquad .7877, \qquad -.2110, \tag{60}$$

multiplied by (43), with a change of signs if necessary to satisfy (35), as the values x, y, z of the variable to be used. The more concentrated character of this distribution with adjustable frequencies is emphasized by the small proportion, less than $3\frac{1}{2}$ per cent, of the frequencies (56) that pertains to the value most remote from the tentative maximizing value.

When (58) is substituted in (57) and, with the result, in (35), this inequality reduces to exactly the same form as that obtained in the preceding section for fixing the sign of (43).

8. Introduction to the two-variable problem. Functions of two or more variables are of greater practical importance than functions of one variable. The recent work on factorial experiments [8] makes it clear that in the experimental determination of maxima of functions of several variables, considerable improvements are possible over the practice of trying the effect of variations in only one variable at a time while holding the others constant. It seems likely that the methods worked out in the previous sections for experimenting with one variable are capable of generalization. However certain difficulties enter which have not yet been surmounted. The object of the present section is to indicate something of the nature of the problem of extending the foregoing results to two variables, x and y.

Let us suppose that a quadratic regression equation,

$$Z = b_{00} + b_{10}x + b_{01}y + \tfrac{1}{2}(b_{20}x^2 + 2b_{11}xy + b_{02}y^2),$$

will be fitted by least squares to observations of $z = f(x, y)$ based on N combinations of x and y, each of which represents a point in a plane. Since there are six coefficients to be determined, there must be at least six distinct points

$(x_1, y_1), \cdots, (x_6, y_6)$. The coefficients in the normal equations may be written $a_{jk} = Sx^j y^k$, so that $a_{00} = N$. The determinant

$$a = \begin{vmatrix} a_{00} & a_{10} & a_{01} & a_{20} & a_{11} & a_{02} \\ a_{10} & a_{20} & a_{11} & a_{30} & a_{21} & a_{12} \\ a_{01} & a_{11} & a_{02} & a_{21} & a_{12} & a_{03} \\ a_{20} & a_{30} & a_{21} & a_{40} & a_{31} & a_{22} \\ a_{11} & a_{21} & a_{12} & a_{31} & a_{22} & a_{13} \\ a_{02} & a_{12} & a_{03} & a_{22} & a_{13} & a_{04} \end{vmatrix}$$

must not vanish. Let the function under investigation be

$$f(x, y) = \Sigma\Sigma\beta_{jk}x^j y^k/(j + k)!,$$

and suppose that $\beta_{10} = 0 = \beta_{01}$, so that the origin is the point sought at which the first derivatives vanish. We shall assume that

$$\beta = \beta_{20}\beta_{02} - \beta_{11}^2 > 0, \qquad \beta_{20} < 0,$$

implying a definite maximum. The estimates x_0, y_0 of the maximizing (or minimizing) values obtained by differentiating Z are

$$x_0 = (b_{11}b_{01} - b_{02}b_{10})/b, \qquad y_0 = (b_{11}b_{10} - b_{20}b_{01})/b,$$

where

$$b = b_{20}b_{02} - b_{11}^2 .$$

For large samples and values of x and y taken not too far from the origin, b will approximate to β, and x_0 and y_0 respectively to

$$(\beta_{11}b_{01} - \beta_{02}b_{10})/\beta, \qquad (\beta_{11}b_{10} - \beta_{20}b_{01})/\beta.$$

Some means is needed of combining into one the two desiderata of minimizing the errors x_0 and y_0. A combined measure of these deviations is

$$\beta_{20}x_0^2 + 2\beta_{11}x_0y_0 + \beta_{02}y_0^2 .$$

This expression is constant except for terms of higher order when x_0 and y_0, while remaining small, vary in such a way that $f(x, y)$ maintains a constant value. Substituting in it the approximate values of x_0 and y_0 gives β^{-1} times

$$\beta_{02}b_{10}^2 - 2\beta_{11}b_{10}b_{01} + \beta_{20}b_{01}^2 .$$

The expectation of this measure of error may be separated into two parts by means of the formulae for the variances and covariance,

$$\sigma_{b_{10}}^2 = Eb_{10}^2 - (Eb_{10})^2, \qquad \sigma_{b_{10}b_{01}} = Eb_{10}b_{01} - (Eb_{10})(Eb_{01}), \quad \text{etc.}$$

One of these parts is a generalized sampling variance,

$$\beta_{02}\sigma^2_{b_{10}} - 2\beta_{11}\sigma_{b_{10}b_{01}} + \beta_{20}\sigma^2_{b_{01}},$$

and tends to zero with order N^{-1} as N increases provided the values (x_k, y_k) are fixed. The other part,

$$\beta_{02}(Eb_{10})^2 - 2\beta_{11}(Eb_{10})(Eb_{01}) + \beta_{20}(Eb_{01})^2, \tag{61}$$

is a bias which does not tend to zero as N increases, but which may be kept arbitrarily small, at the expense of the sampling variance, by restricting the values (x_k, y_k) to be sufficiently small. This expression is a negative definite quadratic form in Eb_{10} and Eb_{01}, and therefore cannot be zero unless both these components of bias vanish separately.

We may proceed as in paragraph 2 to express Eb_{10} and Eb_{01} in terms of the coefficients of $f(x, y)$ of orders higher than the second, among which those of third order will be of leading importance. In this way it may be shown that, if we neglect terms in $f(x, y)$ of orders higher than the third, Eb_{10} and Eb_{01} are given by the ratios to a constant multiple of a of determinants obtained from a by replacing respectively the second and the third columns by the column

$$\begin{matrix} \beta_{30}a_{30} + 3\beta_{21}a_{21} + 3\beta_{12}a_{12} + \beta_{03}a_{03} \\ \beta_{30}a_{40} + 3\beta_{21}a_{31} + 3\beta_{12}a_{22} + \beta_{03}a_{13} \\ \beta_{30}a_{31} + 3\beta_{21}a_{22} + 3\beta_{12}a_{13} + \beta_{03}a_{04} \\ \beta_{30}a_{50} + 3\beta_{21}a_{41} + 3\beta_{12}a_{32} + \beta_{03}a_{23} \\ \beta_{30}a_{41} + 3\beta_{21}a_{32} + 3\beta_{12}a_{23} + \beta_{03}a_{14} \\ \beta_{30}a_{32} + 3\beta_{21}a_{23} + 3\beta_{12}a_{14} + \beta_{03}a_{05}\,. \end{matrix}$$

It is desirable to select a distribution of points (x_k, y_k) such that these components of bias will vanish, no matter what may be the values of β_{30}, β_{21}, β_{12} and β_{03}. For this it is necessary and sufficient that all the determinants vanish that are obtained from these two by replacing the column written above by the terms in it that multiply any one of the four β_{jk}'s. The single-variable analogy suggests using a distribution having the smallest possible number of points, which in this case is six. Let us now take $N = 6$. The eight determinants will all be multiples of

$$P = \begin{vmatrix} 1 & x_1 & y_1 & x_1^2 & x_1y_1 & y_1^2 \\ 1 & x_2 & y_2 & x_2^2 & x_2y_2 & y_2^2 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & x_6 & y_6 & x_6^2 & x_6y_6 & y_6^2 \end{vmatrix}.$$

To save space we shall indicate determinants of this character merely by writing a single row without subscripts, thus:

$$P = |\,1 \quad x \quad y \quad x^2 \quad xy \quad y^2\,|.$$

If we define

$$A'_{jk} = | 1 \quad x^j y^k \quad y \quad x^2 \quad xy \quad y^2 |,$$
$$A''_{jk} = | 1 \quad x \quad x^j y^k \quad x^2 \quad xy \quad y^2 |,$$

and multiply each of these determinants for which $j + k = 3$ $(j, k = 0, 1, 2, 3)$ by P, columns by columns, we shall have exactly the determinants whose vanishing is the condition for nullification of the cubic bias. If we multiply P by itself in the same way we have $P^2 = a$. Therefore $P \neq 0$. Therefore the required condition is that the distribution satisfy the eight equations

$$A'_{30} = 0, \quad A'_{21} = 0, \quad A'_{12} = 0, \quad A'_{03} = 0,$$
$$A''_{30} = 0, \quad A''_{21} = 0, \quad A''_{12} = 0, \quad A''_{03} = 0,$$

and the inequality $P \neq 0$.

In seeking distributions nullifying the cubic bias we have twelve unknowns $x_1, \cdots, x_6, y_1, \cdots, y_6$ which must satisfy these eight equations. This suggests that we give arbitrary values to four of them and then solve for the other eight by straightforward elimination. Unfortunately, since the eight equations are each of the tenth degree, reducing to the ninth degree when coordinates of two of the points are given numerical values, a straightforward elimination would seem to lead to an equation of degree $9^8 = 43{,}046{,}711$. The number of algebriac operations in performing the elimination, solving the equation for one of the unknowns, substituting back, and solving for the others, would be a large multiple of this number, and would doubtless be sufficient to occupy a large and efficient computing project for many millenniums. At the end of this period it might be found that the roots corresponding to the original arbitrary values chosen were all complex or made $P = 0$, and were therefore unusable. Thus indirect and less elementary methods are called for, and some qualitative investigations of such distributions, if they exist (which is not certain), are in order.

The set of conditions as a whole is invariant under all non-singular homogeneous linear transformations of x and y, as is easily proved by making linear combinations of the columns of each of the determinants A'_{jk}, A''_{jk} and P, and by making linear combinations of these determinants themselves. These linear transformations leave the origin invariant. They have four degrees of freedom, which is exactly the right number to take care of the excess of unknowns over equations. This points to the possible existence of a finite number of fundamental solutions, from which all solutions may be obtained by linear homogeneous transformations. Geometrical properties of the configuration will be represented by invariants under linear transformations. Thus the condition $P \neq 0$ means that the six points must not all lie on any conic section. From this it follows at once that no four of them can lie on a straight line, since this line, with the line through the other two, would constitute a degenerate conic. As a matter of fact, we can go further and prove that no three of the points may lie on a straight line. In the proof of this and other properties of the distribution it is convenient to use the arbitrariness provided by a linear transformation to pass the axes (which may be oblique) through any two of the six points, and then to adjust the scales of measurement so that the coordinates of these points become (1, 0) and (0, 1), except that one of them might conceivably be the origin. If three points are collinear, their line can be taken to be the x-axis if it passes through the origin, or the line $y = 1$ if it does not. Even with the help provided by such procedures the proofs are rather long, though straightforward. We shall content ourselves here with stating, without proof, the following properties necessary for sets of six points for which $P \neq 0$ and all components of the cubic bias vanish:

No three of the points can lie on a straight line.

No two straight lines through the origin can contain four of the points.

No four of the points can lie on the vertices of a parallelogram.

The set cannot consist of the origin and the vertices of a regular pentagon with center at the origin.

These conditions have been established by calculations of a rather straightforward and laborious sort, too long to be reproduced.

If $z_k = x_k + iy_k$ and $\bar{z}_k = x_k - iy_k$, the conditions $P \neq 0$, $A'_{jk} = 0 = A''_{jk}$, may be written

$$| 1 \; z \; \bar{z} \; z^2 \; z\bar{z} \; \bar{z}^2 | \neq 0, \qquad | 1 \; z^j\bar{z}^k \; \bar{z} \; z^2 \; z\bar{z} \; \bar{z}^2 | = 0, \qquad | 1 \; z \; z^j\bar{z}^k \; z^2 \; z\bar{z} \; \bar{z}^2 | = 0.$$

9. Some further unsolved problems. Since it is useful to demarcate the frontiers of knowledge by pointing out what lies a little outside them as well as what is within, a few of the many questions may be mentioned which this paper falls short of answering. Besides the extension to two variables mentioned in the last section, and to an arbitrary number of variables, it is desirable that the whole theory should be developed from an exact, or small-sample, point of view rather than on the basis of the large-sample approximations used here. This however appears to be an extremely large enterprise. A simpler, but still quite difficult, problem is to modify the criteria obtained in paragraphs 6 and 7 so as to fit problems of economic experimentation, such as those of determination of maximum monopoly profit or minimum cost, in which the cost of each observation consists largely of the lost profit, or excess cost over the minimum, occasioned by the deviation from the value sought. In such a case the limitation of cost replaces the limitation of the total number of observations.

Another important problem is to take account of the inaccuracy of the preliminary information on which the design of the experiment is based, and to utilize the relations thus involved to design efficient sequences of experiments.

Determination of limits of error in terms of the maxima *over an interval* of the derivatives of $f(x)$ should be a fairly straightforward problem in analysis and have practical importance. With this are associated various problems dealing with maxima of functions having discontinuities in the first or higher derivatives at or near the maximum.

An important extension would deal with the case in which the maximum is estimated from a least-squares polynomial of degree three or more. This might be a connected with the difficult wider problem of deciding on the degree of a polynomial to be fitted in a particular case.

10. Summary. In determining the value ξ of x for which $f(x)$ is a maximum or minimum, a quadratic polynomial may be fitted to observations made for chosen values of x. The errors considered are of two kinds: sampling errors resulting from the inaccuracy in each observation, which diminish as the number of observations is increased, but increase if the values of x are chosen too close to the value sought; and biased errors resulting from the fact that $f(x)$ is not truly quadratic, which do not decrease when the number of observations increases with a fixed set of values of x, but do decrease when the deviations of x from the value sought are reduced. The biased errors may be separated into components corresponding to the third, fourth and higher powers of $x - \xi$ in the expansion of $f(x)$, and these components will ordinarily be of diminishing importance as we go on in the sequence. However it is possible to choose values of x making the cubic component zero and the quartic component at the same time a minimum. Such a set consists of only three values of x. These values may be further adjusted to minimize the expectation of the square of the total error in ξ, as far at least as the term of fourth order in the bias, by a proper balance between the sampling variance and the quartic bias. The values of x satisfying these conditions, measured from the true maximizing or minimizing value ξ, are the products of $[\sigma^2/(N\beta_4^2)]^{1/8}$ by the values u in the table below. Since the root will usually be extracted by logarithms, the common logarithms of the values are given. The first set are the most efficient when the frequencies must be equal. The second set is appropriate when the frequencies are made proportional to the quantities in the last column; in this case only about 72 per cent as many observations are required for any specified accuracy as when the frequencies must be equal. The approximate expected squared errors in the estimates of ξ in the two cases are given respectively by formulae (44) and (59). All these results are approximations of the kind appropriate to large numbers of observations.

Equal frequencies		*Adjustable frequencies*		
u	$\log_{10} u$	u	$\log_{10} u$	Frequency
−.6128	−.21267	−.2110	−.67572	.46 651 N
.8695	−.06071	.7877	−.10364	.50 000 N
2.0751	.31704	2.1520	.33284	.03 349 N

The signs of u should be reversed if $\beta_2\beta_4(\beta_2\beta_5 - 4\beta_3\beta_4) > 0$. Here β_k is the coefficient of $(x - \xi)^k$ in the expansion of $f(x)$, and σ^2 is the error variance of an individual observation. For designing an efficient experiment it is necessary to have some knowledge of these quantities. It may be gained from preliminary experiments of smaller scale.

A suitable preliminary experiment, where knowledge of the function is extremely scanty, might consist of a fixed small number, greater than one, of observations on $f(x)$ corresponding to each of a set of six or more values of x in arithmetic progression covering an interval that includes the value ξ sought, and selected with a view to getting ξ in the center of it as nearly as possible. A polynomial of the fifth degree at least should be fitted by least squares, in which process all the quantities desired for the design of the later, larger experiment can be estimated, together with their accuracies. Since the values of x are taken in arithmetic progression, the fitting can be carried out with extreme ease by the method of orthogonal polynomials.

Numerous subsidiary questions promise to have both practical importance and mathematical interest.

REFERENCES

[1] FELIX BERNSTEIN, *Hartmann and Bauer Handbuch der Erblichkeitslehre*, Vol. 1, Berlin, 1928.

[2] S. O. RICE, "The distribution of the maximum of a random curve," *Am. Jour. of Math.*, Vol. 61 (1939), pp. 409–416.

[3] G. W. ELMEN, "Magnetic alloys of iron, nickel and cobalt in communication circuits," *Elec. Eng.*, Vol. 54 (1935), pp. 1292–1299.

[4] E. E. SCHUMACHER AND A. G. SOUDEN, "Some alloys of copper and iron," *Metals and Alloys*, Vol. 7 (1936), pp. 95–101.

[5] P. C. MAHALANOBIS, "A sample survey of the acreage under jute in Bengal, with discussion on planning of experiments," *Proc. 2nd Ind. Stat. Conf.*, Calcutta, Statistical Publishing Soc. (1940).

[6] H. G. ROMIG, *Allowable average in sampling inspection*, Columbia Univ. thesis, privately printed, 1939.

[7] J. V. USPENSKY, *Introduction to mathematical probability*, New York, McGraw-Hill, 1937.

[8] R. A. FISHER, *The design of experiments*, London and Edinburgh, Oliver and Boyd, 1935, Chap. 6.