OPTIMAL SPACING IN REGRESSION ANALYSIS[1]

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1. Introduction and summary. When a response (or dependent) variable y can be observed for a continuous range of values of the independent variable x, which is at the control of the experimenter, the question arises as to how a given number of observations should be spaced. It will be assumed that x is measurable without error and that y differs from the true response function $f(x)$ by a random term z with mean zero and constant variance σ^2. We suppose that the aim of the experimenter is to estimate $f(x)$, or possibly the mean response $\overline{f(x)}$, on the basis of n observations (x_i, y_i).

Various aspects of this problem of optimal spacing have been studied for the case where $f(x)$ is known apart from some parameters (see e.g. Elfving [3], Chernoff [1], de la Garza [2], and Kiefer and Wolfowitz [8]). However, the functional form of $f(x)$ is often unknown or only approximately known. In the absence of a specific model to the contrary, polynomial approximations to $f(x)$ provide a convenient approach. Section 2 deals briefly with the non-statistical case $\sigma = 0$ when the problem of choosing n abscissae in order to approximate to $f(x)$ by a polynomial of degree $n - 1$ reduces to one of optimum interpolation and that of integrating $f(x)$ reduces to Gaussian quadrature. For a fuller account of this part see Hildebrand [5] or Kopal [6].

If the response contains a random element, a polynomial of degree $n - 1$ or less may be fitted to the n observations by least squares. The error of approximation will now be due, in general, both to random error and the use of an incorrect approximating function. We confine ourselves to the case of fitting a straight line when the true response, while roughly linear, may contain a quadratic component. Two criteria are considered in arriving at the two abscissae resulting in an optimal fit. The first of these criteria ((3.2) below) has also been discussed in a recent paper by Box and Draper [7] who have extended its use to the case of several independent variables.

It is shown in Section 6 that for x-values symmetrically spaced about the centre of the region of interest nothing is gained in fitting a straight line by the use of more than two such abscissae. These optimal abscissae are determined in Sections 3 and 4.

The emphasis of the present approach is on attaining an optimal straight line fit with a small number of observations, rather than on detecting departures from linearity. For the latter purpose more than two abscissae would, of course, be needed, but the number of observations required may well be uneconomically large. In Section 7 comparisons with some other simple spacings are made.

Received August 25, 1958; revised February 18, 1959.

[1] This paper was prepared with the support of the Office of Ordnance Research, U.S. Army, under Contract DA-36-034-ORD-1527 RD.

As an illustration, consider the calibration of a large number of instruments for a range of x in which $f(x)$ is known to be approximately linear. In this case adequate accuracy may be attainable by the use of two observations only. If σ is not negligibly small several observations may be taken at each of two appropriately selected settings, especially if it is much easier to repeat measurements at a given setting than to turn to a new one (compare de la Garza [2]).

An example illustrating the methods proposed is given in Section 8.

2. Optimal spacing in the absence of random error. We suppose that the region of interest of the independent variable is finite and that it has been transformed into the closed interval $(-1, 1)$. If $g_{n-1}(x)$, a polynomial of degree $n - 1$, agrees with $f(x)$ at the n abscissae $x_1, x_2, \cdots x_n$, and if $f(x)$ has n continuous derivatives in $(-1, 1)$ the remainder $R(x) = f(x) - g_{n-1}(x)$ may be expressed as

$$R(x) = \pi(x) \frac{f^{(n)}(\xi)}{n!},$$

where $\pi(x) = (x - x_1)(x - x_2) \cdots (x - x_n)$, and $|\xi| < 1$. In order to make $g_{n-1}(x)$ a desirable approximating function it is natural to attempt to minimize $|R(x)|$ in some sense by an appropriate choice of abscissae. However, ξ depends, in general, not only on the abscissae but also on x and the nature of the function $f(x)$. It is therefore customary to content oneself with the minimization, in the sense chosen, of $|\pi(x)|$. If $f(x)$ is a polynomial of degree n, $|R(x)|$ will also be minimized, but more generally the minimization of $|R(x)|$ will be only approximate (compare [5], Section 9.6).

We consider the following two alternative requirements:

$$\int_{-1}^{1} \pi^2(x)\, dx = \min, \tag{2.1}$$

$$\max_{(-1,1)} |\pi(x)| = \min. \tag{2.2}$$

The first is a criterion of closest overall fit and gives the abscissae as the n zeros of the Legendre polynomial $P_n(x)$ of degree n; the second results in abscissae which are the zeros of the Tchebysheff polynomial $T_n(x) = \cos(n \cos^{-1} x)$. Corresponding to these two cases we shall speak of Legendre and Tchebysheff spacing. Generally, the latter would be regarded as more appropriate in the problem of calibration outlined in the introduction.

Criteria (2.1) and (2.2) may also be given a statistical interpretation. To this end we note that (2.2) can be shown (e.g. [5], Section 9.6) to be equivalent to

$$\int_{-1}^{1} \frac{\pi^2(x)}{(1 - x^2)^{\frac{1}{2}}}\, dx = \min. \tag{2.3}$$

Suppose $g_{n-1}(x)$ is required for a value of x chosen randomly in $(-1, 1)$. Then, clearly, $\mathcal{E}[\pi^2(x)]$ is minimized by (2.1) if x is uniformly distributed in $(-1, 1)$ and by (2.2) if $\cos^{-1} x$ is uniformly distributed in $(0, \pi)$.

A further advantage of the above spacings is that the integral approximation

$$\int_{-1}^{1} w(x)f(x)\,dx \doteqdot \int_{-1}^{1} w(x)g_{n-1}(x)\,dx \tag{2.4}$$

is a Gaussian quadrature formula with weight function $w(x) = 1$ for Legendre spacing and $w(x) = (1 - x^2)^{-\frac{1}{2}}$ for Tchebysheff spacing (see e.g. [6], Chapter VII). Thus if the integral of $f(x)$ over $(-1, 1)$ is required it is given by

$$\sum_{k=1}^{n} H_k f(x_k) + E_n , \tag{2.5}$$

where the H_k are tabulated weights, the x_k are the zeros of the Legendre polynomial of degree n, and the error of integration E_n is given by

$$\frac{2^{2n+1}(n!)^4}{(2n+1)[(2n)!]^3} f^{(2n)}(\eta). \tag{2.6}$$

The integration formula (2.5), although it uses only n ordinates, is therefore of degree of precision $2n - 1$, i.e., the integration is exact if $f(x)$ is a polynomial of degree $2n - 1$ or less. For a general function $f(x)$, (2.5) can be shown to be optimal in the sense that the coefficient of $f^{(2n)}(\eta)$ in (2.6) is smaller than for any other integration formula of degree of precision $2n - 1$.

3. Criteria for optimal spacing in the presence of random error in the observed response. We take the observed response to be

$$y(x) = f(x) + z$$

where $f(x)$ is the true response and z is a variate with zero mean and variance σ^2 independent of x. As stated in the introduction we shall consider specifically the case where $f(x)$ is a quadratic while the fitted curve is a straight line. We suppose that $\frac{1}{2}n$ observations are taken at each of x_1, $x_2 (x_1 < x_2)$ and that the corresponding observed mean responses are $\bar{y}_1$, $\bar{y}_2$. The use of more than two abscissae is discussed in Section 6.

The fitted straight line is then

$$Y(x) = \hat{c}_0 + \hat{c}_1(x - \bar{x}),$$

where

$$\hat{c}_0 = \bar{y}, \qquad \hat{c}_1 = (\bar{y}_2 - \bar{y}_1)/(x_2 - x_1). \tag{3.1}$$

For $\sigma = 0$ we know from Section 2 that taking x_1, x_2 as the zeros of $P_2(x) = \frac{1}{2}(3x^2 - 1)$ or of $T_2(x) = 2x^2 - 1$ will minimize respectively

$$\int_{-1}^{1} [f(x) - Y(x)]^2\,dx,$$

$$\max_{(-1,1)} |f(x) - Y(x)|.$$

Of course, in this case we would take $n = 2$.

If $\sigma \neq 0$ it is a natural extension to try to choose x_1, x_2 so as to minimize respectively the expected mean square error $\bar{E}$ given by

$$\bar{E} = \frac{1}{2} \mathcal{E} \int_{-1}^{1} [f(x) - Y(x)]^2 \, dx = \frac{1}{2} \int_{-1}^{1} \mathcal{E}[f(x) - Y(x)]^2 \, dx \tag{3.2}$$

or the *maximum expected squared error*

$$E_{\max} = \max_{(-1,1)} \mathcal{E}[f(x) - Y(x)]^2. \tag{3.3}$$

These criteria are equally applicable to the case where $f(x)$ is a polynomial of degree $p \leqq n$ while $Y(x)$ is of degree $p - 1$, there being n locations. If $f(x)$ and $Y(x)$ are of the same degree, (3.3) reduces to the minimization of the maximum variance which has been considered by de la Garza [2], Guest [4], and Kiefer and Wolfowitz [8].

4. Legendre and Tchebysheff spacing for $\sigma \neq 0$. Before obtaining the abscissae x_1, x_2 satisfying (3.2) or (3.3) we consider briefly the effects of using Legendre or Tchebysheff spacing when $\sigma \neq 0$. For the former case it is convenient to express $f(x)$ in terms of Legendre polynomials, viz.,

$$f(x) = c_0 + c_1 P_1(x) + c_2 P_2(x).$$

Then for any two symmetrical locations $(-x_1 = x_2)$ we have from (3.1)

$$\mathcal{E}(\hat{c}_0) = c_0 + c_2 P_2(x_2), \qquad \mathcal{E}(\hat{c}_1) = c_1 \tag{4.1}$$

and

$$\operatorname{var} \hat{c}_0 = \frac{\sigma^2}{n}, \qquad \operatorname{var} \hat{c}_1 = \frac{\sigma^2}{n x_2^2}, \qquad \operatorname{cov}(\hat{c}_0, \hat{c}_1) = 0. \tag{4.2}$$

Thus, if $x_2 = 1/\sqrt{3}$, $\hat{c}_0$ and $\hat{c}_1$ are unbiased estimators of c_0 and c_1. In this case

$$\mathcal{E}[f(x) - Y(x)] = c_2 P_2(x)$$

and

$$\int_{-1}^{1} \mathcal{E}[f(x) - Y(x)] \, dx = 0. \tag{4.3}$$

Thus $Y(x)$ may be said to be "unbiased on the average" as an estimator of $f(x)$. Interchanging the integration and expectation signs in (4.3) we see that the expected area under $Y(x)$ is equal to the area under $f(x)$, a result which continues to be true if $f(x)$ is a cubic, in line with the optimal integration properties of Legendre spacing. With Legendre spacing we have also

$$\begin{aligned} \mathcal{E}[f(x) - Y(x)]^2 &= \operatorname{var} \hat{c}_0 + x^2 \operatorname{var} \hat{c}_1 + c_2^2 P_2^2(x) \\ &= \tfrac{1}{2}\sigma'^2 + \tfrac{3}{2} x^2 \sigma'^2 + c_2^2 P_2^2(x), \end{aligned}$$

where $\sigma'^2 = 2\sigma^2/n$, so that the expected mean square error is

$$\bar{E}_L = \sigma'^2 + \tfrac{1}{5} c_2^2. \tag{4.4}$$

The results (4.1), (4.2) but not (4.3) hold also with obvious changes when $f(x)$ is expressed in terms of Tchebysheff polynomials, viz.,

$$f(x) = b_0 + b_1 T_1(x) + b_2 T_2(x).$$

In this case $\hat{c}_0$ and $\hat{c}_1$ are unbiased estimators of b_0 and b_1 if $x_2 = 1/\sqrt{2}$.

5. Optimal spacing with two locations. We consider first the minimization of $\bar{E}$ in (3.2) and to this end show that the search for optimal values of x_1 and x_2 may be confined to the symmetrical spacing $-x_1 = x_2$.

In place of (4.1) and (4.2) we now have

$$\mathcal{E}(\hat{c}_0) = c_0 + c_1\bar{x} + c_2\bar{P}_2(x), \qquad \mathcal{E}(\hat{c}_1) = c_1 + 3c_2\bar{x}$$

and

$$\operatorname{var} \hat{c}_0 = \tfrac{1}{2}\sigma'^2, \qquad \operatorname{var} \hat{c}_1 = \frac{2\sigma'^2}{(x_2 - x_1)^2}, \qquad \operatorname{cov}(\hat{c}_0, \hat{c}_1) = 0,$$

where $$\bar{P}_2(x) = \tfrac{1}{2}[P_2(x_1) + P_2(x_2)].$$

It follows that

$$\mathcal{E}[f(x) - Y(x)] = c_2[P_2(x) - \bar{P}_2(x) - 3\bar{x}(x - \bar{x})]$$

and

$$\mathcal{E}[f(x) - Y(x)]^2 = \tfrac{1}{2}\sigma'^2 + \frac{2\sigma'^2}{(x_2 - x_1)^2}(x - \bar{x})^2 + \{\mathcal{E}[f(x) - Y(x)]\}^2. \tag{5.1}$$

Hence

$$\bar{E} = \tfrac{1}{2}\sigma'^2 + \frac{\sigma'^2}{3(x_2 - x_1)^2}[(1 - \bar{x})^3 + (1 + \bar{x})^3] + c_2^2 X, \tag{5.2}$$

where

$$X = \{\tfrac{1}{5} + \bar{P}_2^2(x) + \tfrac{3}{2}\bar{x}^2[(1 - \bar{x})^3 + (1 + \bar{x})^3] - 6\bar{P}_2(x)\bar{x}^2\}.$$

Let $x_2 - x_1 = 2\alpha$; then $|\bar{x}| \leqq 1 - \alpha$. Writing also $\bar{x} = y$, $x_1 = y - \alpha$, $x_2 = y + \alpha$, we have

$$X = \tfrac{1}{5} + \tfrac{1}{4}(3y^2 + 3\alpha^2 - 1)^2 + 6y^2 - 9y^2\alpha^2,$$

and for any given α this may be shown to have a single minimum at $y = 0$ provided $|y| \leqq 1 - \alpha$, $|\alpha| < 1$. Corresponding to any given α, therefore, X and hence $\bar{E}$ are minimized by taking $x_1 = -\alpha$, $x_2 = \alpha$.

From (5.2) we may now write

$$\bar{E} = \tfrac{1}{2}\sigma'^2 + \frac{\sigma'^2}{6x_2^2} + c_2^2[\tfrac{1}{5} + P_2^2(x_2)]. \tag{5.2'}$$

This is to be minimized with respect to x_2. Setting $d\bar{E}/dx_2 = 0$ we find x_2 to be a root of the equation

TABLE 1

Values of $-x_1 = x_2$ *, as a function of* $b = \sigma' / |c_2|$*, giving* (i) *generalized Legendre and* (ii) *generalized Tchebysheff spacing*

b	$-x_1 = x_2$	
	(i)	(ii)
0	0.577	0.707
0.3	.599	.721
0.6	.642	.755
0.9	.685	.800
1.2	.725	.850
1.5	.762	.899
1.8	.796	.949
2.1	.827	.997
2.4	.855	1.000
2.7	.882	...
3.0	.908	...
3.3	.932	...
3.6	.955	...
3.9	.976	...
4.2	.997	...
4.5	1.000	1.000

N.B. $x_2 = 1$ for $b \geqq 4.243$ in (i) and $b \geqq 2.121$ in (ii).

$$x_2^4(3x_2^2 - 1) = a, \tag{5.3}$$

where $a = \sigma'^2/(9c_2^2)$. Thus x_2 is a function of a or equivalently, of $b = \sigma'/|c_2|$. Equation (5.3) is a cubic in x_2^2 with only one real root which corresponds to the required minimum. For $\sigma = 0$, (5.3) gives Legendre spacing. On the other hand, if $\sigma \neq 0$ but $c_2 = 0$, so that a is infinite, $\bar{E}$ will be minimized by making x_2 as large as possible, i.e., $x_2 = 1$. In fact, $x_2^2 = 1$ for $a = 2$. For $a > 2$ or $\sigma'^2 > 18c_2^2$ we still take $x_2 = 1$. The dependence of x_2 on b is shown in Table 1.

We turn now to the minimization of the maximum expected squared error of (3.3). In this case also we may take $-x_1 = x_2$. By (5.1) it is therefore required to maximize

$$X' = \frac{\sigma'^2 x^2}{2x_2^2} + \tfrac{9}{4}c_2^2(x^2 - x_2^2)^2$$

with respect to x and subsequently to minimize this maximum with respect to x_2. If we regard X' as a quadratic in x^2 for $0 \leqq x^2 \leqq 1$, it is clear that its maximum occurs at $x^2 = 0$ or 1. For $x^2 = 0$, X' increases in x_2 from 0 to $(9/4)c_2^2$ while for $x^2 = 1$, X' decreases from ∞ to $\frac{1}{2}\sigma'^2$. Thus if $\sigma'^2 \geqq (9/2)c_2^2$, then $x_2 = 1$ is the solution. Otherwise the solution is that value of x_2 between 0 and 1 which equalizes X' for $x^2 = 0$ and $x^2 = 1$. This occurs for $x_2^4 - \frac{1}{2}x_2^2 = a$, so that for optimal spacing

$$x_2 = \tfrac{1}{2}[1 + (1 + 16a)^{\frac{1}{2}}]^{\frac{1}{2}} \text{ or } 1, \tag{5.4}$$

whichever is smaller. For $\sigma = 0$, (5.4) gives Tchebysheff spacing The dependence of x_2 on b in this case is also shown in Table 1.

The two types of spacing may conveniently be referred to as generalized Legendre and generalized Tchebysheff spacing.

6. Possible use of more than two locations. Suppose that more than two locations are available to us and that we fit a least squares straight line to the n observations. If these are taken at $x_1 \leqq x_2 \leqq \cdots \leqq x_n$, it seems natural to continue to assume symmetry of spacing, i.e., $x_i = -x_{n+1-i}$ $(i = 1, 2, \cdots, n)$, so that both $\sum x_i$ and $\sum x_i^3$ vanish. Then

$$\hat{c}_0 = \bar{y}, \qquad \hat{c}_1 = \sum x_i y_i / \sum x_i^2, \tag{6.1}$$

$$\mathcal{E}(\hat{c}_0) = c_0 + \frac{c_2 \sum P_2(x_i)}{n}, \qquad \mathcal{E}(\hat{c}_1) = c_1, \tag{6.2}$$

$$\operatorname{var} \hat{c}_0 = \frac{\sigma^2}{n}, \qquad \operatorname{var} \hat{c}_1 = \frac{\sigma^2}{\sum x_i^2}, \qquad \operatorname{cov}(\hat{c}_0, \hat{c}_1) = 0. \tag{6.3}$$

Now comparison of (6.2), (6.3) with (4.1), (4.2) shows that the two sets of equations become identical if $\sum x_i^2 = nx_2^2$. In other words, corresponding to any symmetrical configuration of n locations, a value $x_2(> 0)$ can be found such that $\frac{1}{2}n$ observations at each of $\pm x_2$ give estimators $\hat{c}_0$, $\hat{c}_1$ with the same expectations, variances and covariances. It follows that the two spacings are equivalent from this point of view as well as on the basis of any criteria depending on the first two moments only, such as (3.2) and (3.3). See also Box and Draper [7], who obtain similar results on merely taking $\sum x_i = 0$.

In certain situations it is advantageous to vary the independent variable as little as necessary. Apart from its convenience the use of two locations will obviously be optimal on this score also. Of course, more than two locations are necessary to detect departures from linearity in $f(x)$ but this is not our aim here.

As before, we have taken n even which would be the usual situation. However, if n is odd, the number of locations is reducible to three, and an odd number of observations has to be taken at $x = 0$. Clearly, the narrowest spacing is given by a single observation at $x = 0$ and $\frac{1}{2}(n - 1)$ observations at each of $\pm x_2[n/(n - 1)]^{\frac{1}{2}}$.

These equivalence results may be compared with those obtained by Elfving [3] and de la Garza [2] in the case when the fitted function and the true response are polynomials of the *same* degree, so that no bias enters. For $c_2 = 0$ the present result is a special case of theirs; the equivalence continues to hold for $c_2 \neq 0$ because by (6.2), (6.3) the bias in $\hat{c}_0$ is, like the variance of $\hat{c}_1$, a function of $\sum x_i^2$.

TABLE 2

$\bar{E}$ and $E_{\max}$ as functions of $b = \sigma'$, for various spacings

$\bar{E}$

b	(i) Generalized Legendre	(ii) Legendre $(-1/\sqrt{3}, 1/\sqrt{3})$	(iii) $(-1, 1)$	(iv) $(-1, 0, 1)$	(v) $(\pm 0.2, \pm 0.6, \pm 1)$
0	0.20	0.20	1.20	0.45	0.24
0.6	0.54	0.56	1.44	0.72	0.55
1.2	1.46	1.64	2.16	1.53	1.47
1.8	2.88	3.44	3.36	2.88	3.02
2.4	4.75	5.96	5.04	4.77	5.18
3.0	7.06	9.20	7.20	7.20	7.95
3.6	9.80	13.16	9.84	10.17	11.35
4.2	12.96	17.84	12.96	13.68	15.36
4.8	16.56	23.24	16.56	17.73	19.99

$E_{\max}$

b	(i) Generalized Tchebysheff	(ii) Tchebysheff $(-1/\sqrt{2}, 1/\sqrt{2})$	(iii) $(-1, 1)$	(iv) $(-1, 0, 1)$	(v) $(\pm 0.2, \pm 0.6, \pm 1)$
0	0.56	0.56	2.25	1.00	0.64
0.6	0.91	1.10	2.43	1.18	1.21
1.2	1.89	2.72	2.97	2.05	2.90
1.8	3.44	5.42	3.87	4.30	5.73
2.4	5.76	9.20	5.76	7.45	9.69

7. Comparison of $\bar{E}$ and $E_{\max}$ for various spacings. It is of interest to compare our two optimal spacings with other simple spacings. The results of a number of such comparisons are set out in Table 2. For definiteness, and without real loss of generality, we have taken the true quadratic response as $f(x) = c_0 + c_1P_1(x) + P_2(x)$, so that $b = \sigma'$. For various values of σ' Table 2 lists $\bar{E}$ which from (5.2′) and Section 6 is given by

$$\bar{E} = \sigma'^2(0.5 + 6\gamma^{-1}) + (0.45 - 1.5\gamma + 2.25\gamma^2),$$

where $\gamma = \sum x_i^2/n$; and also $E_{\max}$ which is the larger of $0.5\sigma'^2 + 2.25\gamma^2$ and $0.5\sigma'^2(1 + \gamma^{-1}) + 2.25(1 - \gamma)^2$.

8. An example. To illustrate Legendre and generalized Legendre spacing we suppose that the true law under study is

$$h(x') = 8 - x' + \tfrac{1}{20}x'^2, \qquad 0 \leqq x' \leqq 10. \tag{8.1}$$

Put $x' = 5 + 5x$ to transform this to

$$\begin{aligned} f(x) &= \tfrac{17}{4} - \tfrac{5}{2}x + \tfrac{5}{4}x^2, \qquad -1 \leqq x \leqq 1 \\ &= \tfrac{14}{3} - \tfrac{5}{2}P_1(x) + \tfrac{5}{6}P_2(x). \end{aligned}$$

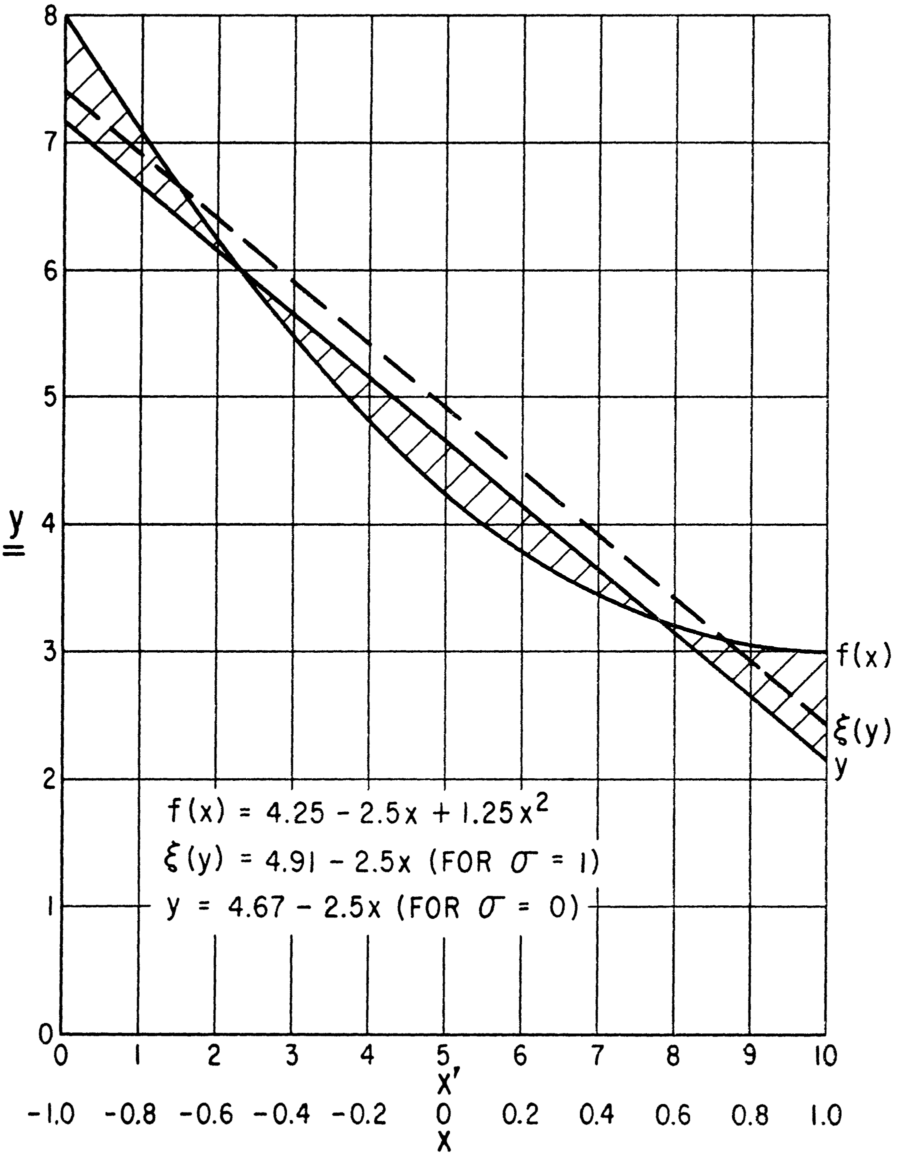

FIG. 1. Illustrating Legendre and generalized Legendre spacing

If this function may be observed for only two values of x the closest overall fit in the case of no random error ($\sigma = 0$) is obtained by taking $-x_1 = x_2 = 1/\sqrt{3}$, which results in the straight line of approximation

$$Y(x) = \tfrac{14}{3} - \tfrac{5}{2}x.$$

The average error is zero and the mean square error is by (4.4) simply $c_2^2/5 = 5/36$.

When $\sigma \neq 0$ the optimal spacing is given by Table 1 with $b = 6\sigma'/5$. Thus for $\sigma' < \frac{1}{2}$ the spacing is only slightly wider than the Legendre spacing while for $\sigma' > 3$ the observations should be taken at $x = -1, 1$. The *expected* line still has slope $c_1 = -5/2$ but is displaced upwards through a vertical distance $c_2P_2(x_2)$.

For $\sigma' = 1$ the situation is shown in Figure 1. In this case $x_2 = 0.725$ and the expected mean square error $\bar{E} = 1.014$ by (5.2′) or from Table 2 ($1.46 \times (5/6)^2$). This may be compared with $\bar{E}_L = 1.139$. For $\sigma' = 2$, we have $x_2 = 0.855$ and $\bar{E} = 3.298$, $\bar{E}_L = 4.139$.

In this example we have taken $h(x')$ as known so that the results could be presented graphically. However, it is clear that the optimal locations are determined completely by the coefficient of x'^2 in (8.1), the specified range of x' and the standard deviation σ'. Thus the same results hold approximately when all that is known is that the response function is linear in the range (0, 10) apart from a quadratic term with coefficient of the order 0.05.

9. Acknowledgments. We are grateful to James L. Dolby, who drew our attention to the kind of problem considered, to the authors of papers [7] and [8] for letting us see these in advance of publication, and to the referees for a number of very helpful suggestions.

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