Design Aspects of Scheffé's Calibration Theory Using Linear Splines

by

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1. INTRODUCTION

In this report some design aspects of the calibration problem are considered. Following Scheffé [1973] a statistical relationship is being considered between two quantities U and V where V is generally more expensive or difficult to measure than U. For a given value of v, observations on U are assumed to be random with a mean value

$$m(v) = m(v,\beta) = \sum \beta_i g_i(v) \tag{1.1}$$

and variance σ^2 independent of v. Here the regression functions g_i are known while $\beta = (\beta_0, \beta_1, \ldots, \beta_{k+1})^t$ and σ are unknown. For a given value U_0, one is interested in finding the corresponding v_0. To do this the system is "calibrated". That is, accurate values $v_1, v_2, \ldots, v_n$ are chosen for v and corresponding readings $U_1, U_2, \ldots, U_n$ are taken. The regression coefficients β are then estimated by $\hat{\beta}$ and for a given value $U_0 = u_0$ the corresponding v_0 is found by solving $u_0 = m(v_0, \hat{\beta})$.

Scheffé [1973] shows how a "calibration chart" can be constructed which results in a band around the curve $u = m(v,\hat{\beta})$. (Throughout we shall view u and v as plotted in the vertical and horizontal directions respectively.) In this way, for each measurement u, an interval estimate I(u) is constructed for the corresponding unknown value of v. The bands are constructed for a given α and δ so that "for every possible sequence of constants v_i the probability is at least $1-\delta$ that the proportion of intervals containing the corresponding v_i is in the long run at least $1-\alpha$". The reader is referred to Scheffé [1973] for further discussion of the construction and interpretation of the bands. Different aspects of the calibration problem can also be found in Lieberman, Miller and Hamilton (1967) and the National

Bureau of Standards special publication 300 on Precision Measurement and Calibration.

Scheffé's calibration charts find application in the calibration of cylindrical tanks. The problem here is to determine the volume of a certain liquid in the tank by taking pressure readings P = U at or near the bottom of the tank. The tank is closed and V is difficult or impossible to measure directly. Now if P is the pressure reading at the bottom of the tank and V is the volume of liquid in the tank then $P = Vd/\bar{A}$, where $\bar{A}$ is the average cross-sectional area of the filled portion of the tank and d is the density of the liquid in the tank. Thus the pressure-volume relationship is a straight line if the cross-sectional area $\bar{A}$ of the tank is constant. (The liquid is assumed uniform with constant density d). The tanks are generally cylindrical which would produce constant $\bar{A}$, however obstructions inside the tank prevent this from being the case. These obstructions are of the nature of cooling coils, mechanisms to agitate the liquid or supporting metal to strengthen the tank.

A simple "well defined" obstruction would abruptly change the cross-sectional area hence the slope in the volume-pressure relationship. The obstructions would in general change the area A in a more gradual manner. However the regions of change are assumed to be small, relative to the size of the tank and the accuracy of the measurements, and they are ignored.

In this case the volume-pressure relationship can be written as a linear spline

$$m(v) = a + bv + \sum_{i=1}^{k} b_i (v-\xi_i)_+ \tag{1.2}$$

where $z_+ = \max\{0,z\}$. The quantities $\xi_1 < \xi_2 < \ldots < \xi_k$ are called "knots" and these will occur whenever the cross-sectional area changes. In equation (1.2) the function is $a + bv$ for v below ξ_1. The curve is continuous and changes to slope $b + b_1$ at the point ξ_1, etc.

On occasion it will be more convenient to work with a different basis for the splines than that used in (1.2). We use ξ_0 and ξ_{k+1} for the smallest and largest volume readings respectively. Then define

$$N_0(v) = \begin{cases} \dfrac{\xi_1 - v}{\xi_1 - \xi_0} & \xi_0 < v < \xi_1 \\ 0 & \xi_1 < v \end{cases}$$

$$N_i(v) = \begin{cases} \dfrac{v - \xi_{i-1}}{\xi_i - \xi_{i-1}} & \xi_{i-1} < v < \xi_i \\ \dfrac{\xi_{i+1} - v}{\xi_{i+1} - \xi_i} & \xi_i < v < \xi_{i+1} \end{cases}$$

for $i = 1,2,\ldots,k$

$$N_{k+1}(v) = \begin{cases} \dfrac{v - \xi_k}{\xi_{k+1} - \xi_k} & \xi_k < v < \xi_{k+1} \\ 0 & v < \xi_k \end{cases}$$

These are called B-splines. They are simply triangular type functions over successive pairs of intervals. With this basis the value β_i in

$$(1.4) \qquad m(v) = \sum_{i=0}^{k+1} \beta_i N_i(v)$$

is given by the value of m(v) at ξ_i, i.e. $\beta_i = m(\xi_i)$, i = 0, 1,...,k+1. An excellent discussion of splines is given in de Boor [1978].

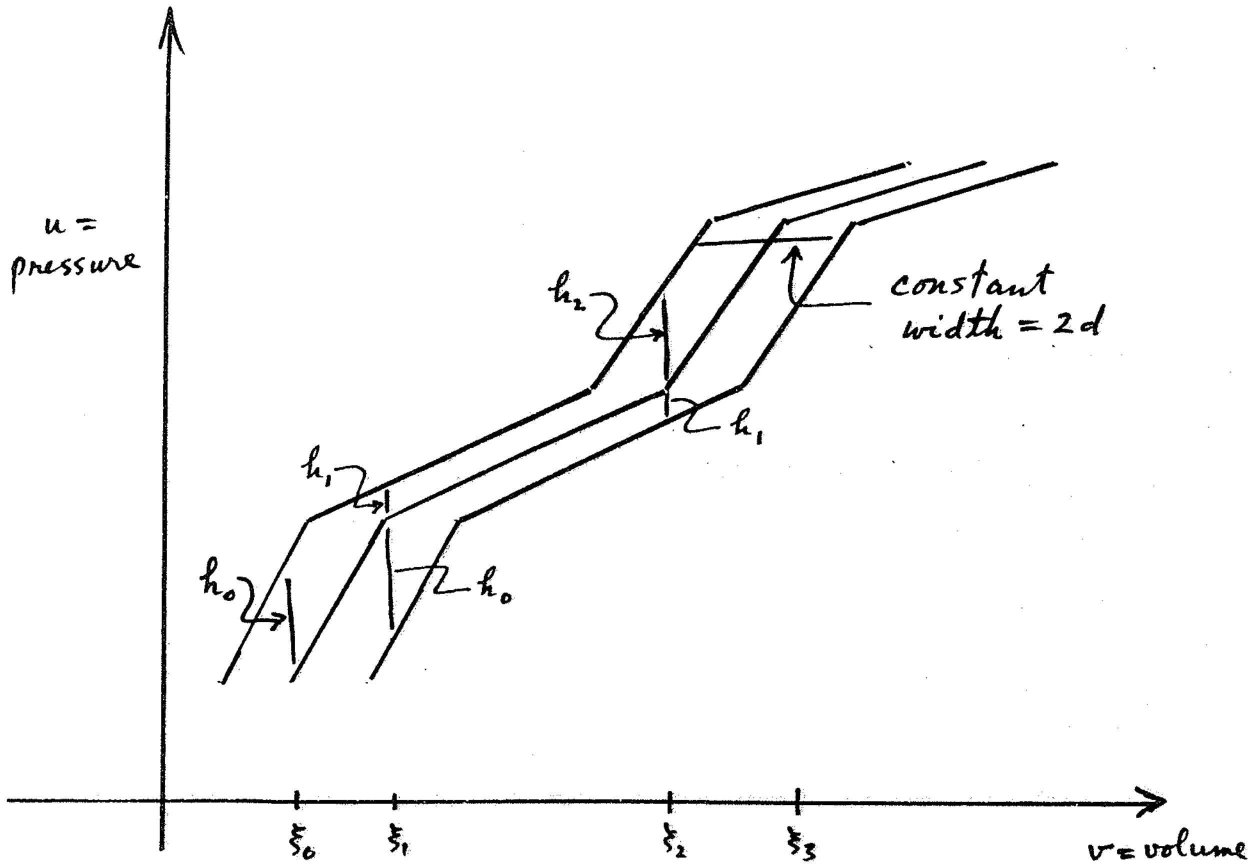
The Scheffé calibration bands around the function (1.4) produce various width inverse intervals I(u) for the corresponding unknown value v. Generally the wider the band is in the vertical u direction the wider are the horizontal intervals I(u). In addition, however, low slope values of the curve m(v) in (1.4) will produce much larger intervals I(u) than large slopes will.

For reasons which cannot be explained fully here we would like to have the maximum (over the range of u values) of the lengths of the intervals I(u) equal to a minimum. Generally one can then make a quantitive statement about the overall accuracy of the calibration. It is possible to keep the maximum of I(u) small if higher accuracy can be obtained in estimating the true curve m(v) in regions where it has lower slope. This accuracy is measured through the variance or standard deviation of our estimate of the response curve m(v). More observations are needed where the knots occur and where the slopes are low. The design problem is to see if any quantative statements can be made about where the values v_1, v_2,...,v_n should be chosen to obtain corresponding readings U_1, U_2,...,U_n in the calibration.

In Section 2 some consideration is given to the selection of v_1, v_2,...,v_n, and a procedure is proposed. An illustrative example is described in Section 3. Some discussions is given in Section 4.

2. CHOOSING THE VOLUME VALUES

As mentioned in the previous section it is desirable to keep the maximum width of the intervals I(u) at a minimum. In order to do this we consider a general curve (see Figure 1) of the form



u = pressure
h_2
constant width = 2d
h_1
h_1
h_0
h_0
ξ_0
ξ_1
ξ_2
ξ_3
v = volume

Figure 1

$$(2.1) \qquad u = m(v,\beta) = \sum_{i=0}^{k+1} \beta_i N_i(v)$$

where the β_i are all positive and increasing. (The range of v is from ξ_0 to ξ_{k+1} where generally $\xi_0 > 0$. At the bottom of the tank the volume and pressure should both be zero. However irregularities in the tank made the validity of (2.1) questionable near the bottom so we like $\xi_0 > 0$).

In order to minimize $\max_u I(u)$ we draw a band of constant horizontal width 2d about the curve. The Scheffé bands are produced by considering

$$(2.2) \qquad m(v,\hat{\beta}) \pm \hat{\sigma}[c_1 + c_2\, S(v)]$$

The notation will be explained carefully below. Our intent is to choose d so that the constant width curve contains (2.2). The value d will then be minimized by choosing the values $v_1, v_2, \ldots, v_n$, these values enter mainly through the quantity S(v).

To explain the notation, the quality $\hat{\sigma}$ is an estimate of the standard deviation σ in our pressure readings. We will assume for simplicity that σ is known and therefore take $\hat{\sigma} = \sigma$. Some discussion in Section 4 will be given to this matter. The quantities c_1 and c_2 are constants depending on the values of α and δ mentioned in the introduction. The function S(v) is, except for a factor of σ, the standard deviation of the estimate of the pressure readings for a fixed value v of the volume. If we let $N(v) = (N_0(v),\ldots,N_{k+1}(v))^t$ then

$$(2.3) \qquad S^2(v) = \frac{1}{n}\; N(v)\; M^{-1}(\mu)\; N^t(v)$$

where the matrix M(u) is given by $M(u) = \int N^t(v)\, N(v)\, d\mu(v)$. The measure μ is called the design measure and simply has mass 1/n at each observation point v_i, i = 1, 2,...,n (n = number of observations). The observations are assumed to be uncorrelated and in general some of the v_i values could be equal. In this case μ assigns mass n_i/n to distinct v_i', i = 1, 2,...,r. The elements of M = M(μ) are simply

$$m_{ab} = \frac{1}{n} \sum_i N_a(v_i)\ N_b(v_i) \tag{2.4}$$

The general problem would be to consider the maximum of the horizontal wdiths of I(u) of the Scheffé bands and minimize this maximum with respect to the values $v_1, v_2, \ldots, v_n$. This seems to be extremely difficult. We shall proceed by trying to minimize d.

To hold down the maximum width of I(u) we now require that the Scheffé bands (2.2) lie inside the bands shown in Figure 1. Since the upper and lower bands in Figure 1 are m(v+d) and m(v-d) respectively we thus require that, for all v,

$$m(v+d) - m(v) \geq \sigma[c_1 + c_2 S(v)] \tag{2.5}$$

$$m(v) - m(v-d) \geq \sigma[c_1 + c_2 S(v)] \tag{2.6}$$

It will be shown at the end of this section that $\sigma[c_1 + c_2 S(v)]$ is convex in v on each segment $[\xi_i, \xi_{i+1}]$ i = 0, 1,...,k. The right hand side of (2.5) then consists of convex segments, while the left hand side consists of linear segments. Equations (2.5) and (2.6) will then hold provided they hold at the bends of the left hand side. Thus we require (2.5) to hold for

$$\xi_i \quad i = 0, 1, \ldots, k+1 \text{ and } \xi_i - d, \ i = 1, 2, \ldots, k \tag{2.7}$$

and (2.6) should hold at the points

$$\xi_i, \quad i = 0, 1, \ldots, k+1 \text{ and } \xi_i + d, \ i = 1, 2, \ldots, k. \tag{2.8}$$

Only points in the interval (ξ_0, ξ_{k+1}) are considered. It seems clear that if

$$(2.9) \qquad \xi_{i+1} - \xi_i \geq d, \qquad i = 0, 1, \ldots, k$$

then we require that

$$\sigma[c_1 + c_2 S(\xi_0)] \leq h_0$$

$$(2.10) \qquad \sigma[c_1 + c_2 S(\xi_i)] \leq h_i \text{ and } h_{i-1} \qquad i = 1, \ldots, k$$

$$\sigma[c_1 + c_2 S(\xi_{k+1})] \leq h_{k+1}$$

where $h_i = m(\xi_i+d) - m(\xi_i) = m(\xi_{i+1}) - m(\xi_{i+1}-d)$. Let s_i denote the slope of $m(v)$ on (ξ_i, ξ_{i+1}), $i = 0, 1, \ldots, k$. Then since $h_i = ds_i$, the requirements (2.10) become

$$(2.11) \qquad \sigma[c_1 + c_2 S(\xi_i)] \leq d\ \gamma_i \qquad i = 0, 1, \ldots, k+1$$

where $\gamma_0 = s_0$, $\gamma_i = \max\{s_i, s_{i-1}\}$, $i = 1, \ldots, k$ and $\gamma_{k+1} = s_k$.

Now the design measure or the choose of $v_1, v_2, \ldots, v_n$ enters these equations in $S(v)$. The general problem is still to choose the design so that the value of d can be choosen as small as possible.

To reduce $S(v)$, observations should be choosen at the points $\xi_0, \xi_1, \ldots, \xi_{k+1}$. (Remember that the knots $\xi_1, \ldots \xi_k$ are usually unknown). If we note the dependence of $S(v)$ on μ by $S(v,\mu)$ then it is known that for a fixed set of knots and any μ_0 there is another design μ_1, concentrating on ξ_i, such that $S(v,\mu_1) \leq S(v,\mu_0)$ for all v.

Suppose, then, that we had observations only at the endpoints and knots. The matrix $M(\mu)$ in (2.3) and (2.4) can be seen to be a diagonal matrix with diagonal elements $p_0, p_1, \ldots, p_{k+1}$ where $np_i = n_i$ = the number of observations at ξ_i. The value of $S(\xi_i)$ is then

$$S(\xi_i) = \frac{1}{\sqrt{n_i}} \tag{2.12}$$

The conditions (2.11) then reduce to

$$\sigma[c_1 + \frac{c_2}{\sqrt{n_i}}] = d\gamma_i \qquad i = 0, 1, \ldots, k+1 \tag{2.13}$$

The values of n_0, $n_1, \ldots, n_{k+1}$ $(\Sigma n_i = n)$ and d which give equality in (2.13) should give a minimal value for d. Solving for n_i in (2.13) we get

$$n_i = [\frac{c_2\sigma}{d\gamma_i - \sigma c_2}]^2 \tag{2.14}$$

The general design plan would then be as follows:

(1). Take a preliminary set of m_0 observations (these may be equally spaced or wherever they appear to give a good overall robust design).

(2). With the observations from (1), estimate ξ_i, β_i, δ_i and σ, insert these in (2.14) and solve for d so that $\Sigma n_i = m_1 > m_0$.

(3). The values for n_i in (2) are roughly the number of observations that are required at ξ_i. Recall we already have m_0 observations from (1). The remaining m_1-m_0 in (2) should then be chosen to made the combined set have roughly n_i observation at ξ_i.

(4). Repeat steps (1), (2) and (3) if more stages are used to get m_2 observations etc.

(5). To help implement step (3) we may proceed as follows. For a given set of observations assign each observation to the nearest estimated ξ_i value. The new set of m_1-m_0 observations are then chosen as in (3).

The combined set m_1 are then redistributed by taking those supposedly at ξ_i to be roughly uniform from $(\xi_{i-1} + \xi_i)/2$ to $(\xi_i + \xi_{i+1})/2$.

The remainder of this section consists of a proof of the convexity of $\sigma[c_1 + c_2 S(v)]$. Consider the function $S^2(v)$ defined in (2.3) and take $v \in I_i = (\xi_i, \xi_{i+1})$ for a fixed i. The only basis functions $N_j(v)$ which are nonzero on I_i are $N_i(v)$ and $N_{i+1}(v)$. Therefore

$$nS^2(v) = a\, N_i^2(v) + 2b\, N_i(v) N_{i+1}(v) + c\, N_{i+1}^2(v) \tag{2.15}$$

where a, b and c are inverse elements in the matrix $M(\mu)$ defined in (2.4). The matrix $M(\mu)$ is tridiagonal, i.e. has nonzero elements m_{ij} only for $|i-j| \leq 1$, and has non-negative elements. The elements a and c in the inverse can be seen to be positive while b is negative. Equation (2.15) and some simple algebra then shows that (2.15) is a quadratic in v with a minimum on the interior. The convexity of $\sigma[c_1 + c_2 S(v)]$ is then equivalent to the convexity of

$$g(v) = c + d\left(1 + \left(\frac{v-\mu}{\tau}\right)^2\right)^{1/2}$$

where $c \geq 0$, $d \geq 0$, $u \in I_i$ and $\tau > 0$. However it can readily be shown that $g''(v) \geq 0$.

3. AN ILLUSTRATION

To illustrate the effect of the procedure we considered a tank which was carefully studied. The tank volume was approximately 13,500 liters. The equation of the pressure = U versus the volume = V was thought to be

$$u = -271 + 2340\ v + 11(v-1.9)_+ -27(v-4.6)_+ - 146(v-5.5)_+ -12(v-5.9)_+ - 16(v-6.5)_+ +2.2(v-7.2)_+ + 20(v-10.0)_+ -20(v-10.3)_+ + 2.5(v-12.5)_+ \tag{3.1}$$

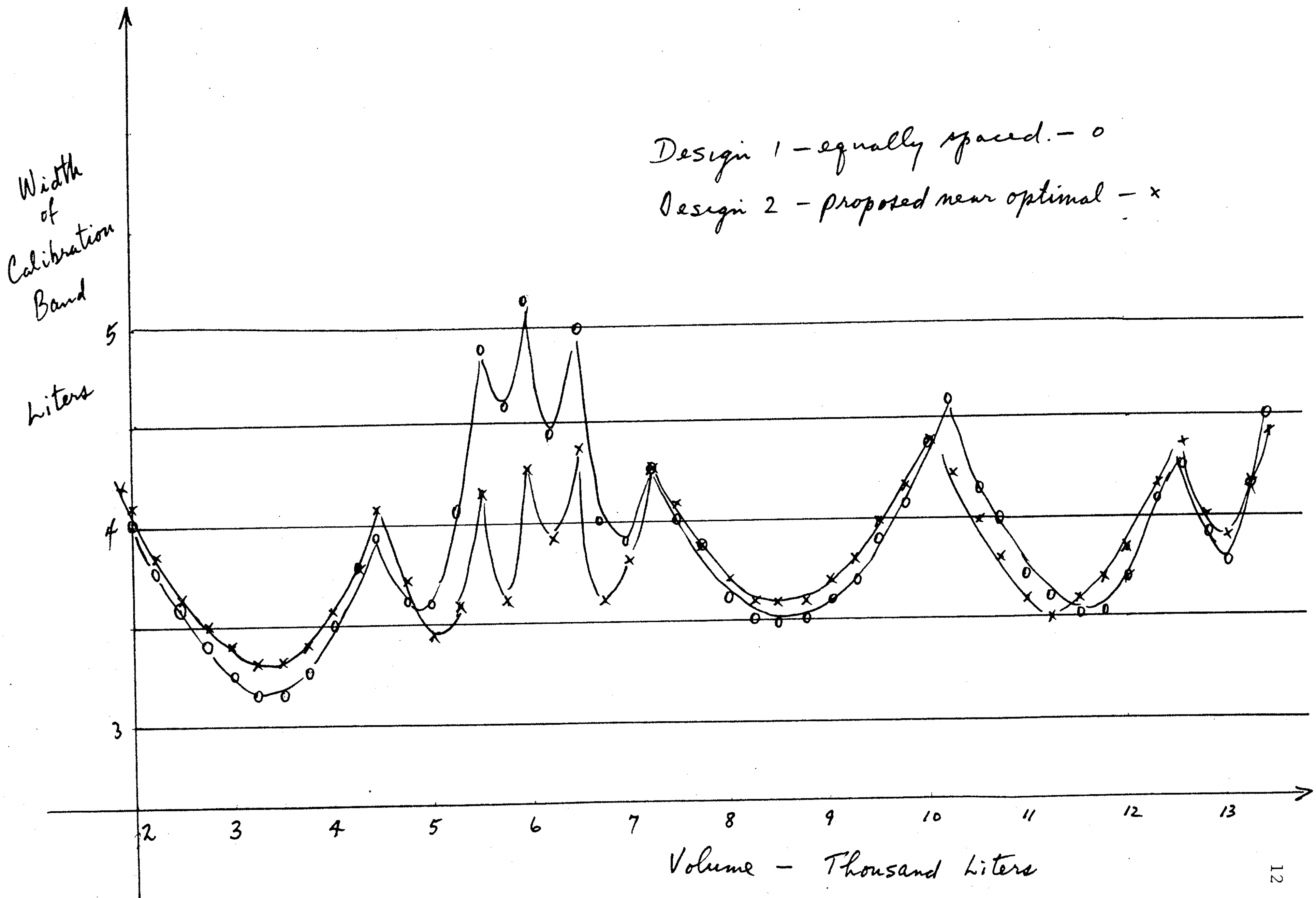
The equation was assumed to be valid over the range $\xi_0 = 1700$ litres to $\xi_{10} = 13{,}500$ litres. Throughout the example we assume that the knot position, the slopes and the standard error σ are known. In this case the effect of the design in the simplest case will be isolated. Some discussion of this will be given in the next section. The knots and slopes are then taken as in the above equation. The standard error σ was chosen as $\sigma = 0.6$. Using Scheffé, we then chose $c_1 = 2$ and $c_2 = 5$ in the equation (see (2.14))

$$n_i = \left[\frac{c_2\sigma}{d\gamma_i - \sigma c_1}\right]^2 \tag{3.2}$$

Using a trial and error method we solved (3.2) for d so that $\Sigma\, n_i = 86$. (Three runs of measurements of 30 observations each were to be taken, however 86 was more convenient than 90.) The solution for d was d = 1.03 and the corresponding n_i values were 6.2, 6.2, 6.4, 8.2, 8.6, 8.7, 8.7, 8.4, 8.7, 8.7, 8.7. Since these were roughly equal it was proposed that the number of observations around each knot should be taken equal. The following two designs were then compared.

Design 1. Take n = 86 observations equally spaced over the entire range $\xi_0 = 1700$ to $\xi_{10} = 13{,}500$

Design 2. Take n = 30 observations equally spaced over ξ_0 to ξ_{10}. The remaining are chosen to make approximately equal number around each knot. (see part (5) in the design plan in Section 2)



Design 1 - equally spaced. - o
Design 2 - proposed near optimal - x
Width of Calibration Band
Liters
5
4
3
2
3
4
5
6
7
8
9
10
11
12
13
Volume - Thousand Liters

Figure 2

Using the above two designs, we simulated observations on the pressure for the corresponding volume readings, using equation (3.1) and ran a calibration chart for each design. The graphs in Figure 2 show the width of the confidence intervals versus the volume for the two designs. It seems clear that in the area where the knots are concentrated, between 4000 and 8000 liters, the proposed design is superior to the equally spaced design.

4. DISCUSSION

The Scheffé calibration procedure involves the consideration of two bands $m(v) \pm \sigma[c_1 + c_2S(v)]$ around the curve $u = m(v)$. The bands are used in a simple inversion process, where for a given reading $U = u$ we solve $u = m(v)$ for v and find an interval $I(u)$ of possible v-values. It is required that the lengths of these intervals be short. A simple procedure is proposed whereby the two bands are bounded by "parallel" bands of uniform horizontal width and an attempt was made at minimizing the width of the outer bands. It would seem that a direct minimization of $\max_u I(u)$ would present considerable difficulty. The procedure proposed certainly needs further testing in that estimated values of ξ_i, β_i and σ should be used in step 2 of the procedure. It seems, however, that the procedure will generally give lower overall width.

The conditions in (2.9) need some attention. In our example $d = 1.03$ and the spacings $\xi_{i+1}-\xi_i$ were sometimes less than d. This, however, does not seem to crucial. In extreme situations we might revert back to (2.5)-(2.8).

The Scheffé procedure gives bands, which in our case are "square root parabolic" on segments between knots. The regression function is assumed known and probabilistic statements are made concerning statements that the true volume v, corresponding to a given reading U = u, is contained in an interval I(u). In our situation the unknown knots ξ_i prevent us from assuming that our regression functions $g_i(v)$ are known. The accuracy in any attempt at making confidence statements is then in question. Large simulation studies might remedy this.

Since blueprints of the tanks are usually available, similarities exists between tanks and other prior information is available, some sort of Bayesian analysis might be more appropriate.

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