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USE OF THE MAXIMUM LIKELIHOOD METHOD UNDER QUANTAL RESPONSES FOR ESTIMATING THE PARAMETERS OF A NORMAL DISTRIBUTION AND ITS APPLICATION TO AN ARMOR PENETRATION PROBLEM

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USE OF THE MAXIMUM LIKELIHOOD METHOD UNDER QUANTAL RESPONSES FOR ESTIMATING THE PARAMETERS OF A NORMAL DISTRIBUTION AND ITS APPLICATION TO AN ARMOR PENETRATION PROBLEM

by

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FOREWORD

The work reported in this paper was done in the Applied Mathematics section of the Science and Mathematics Research Group. The major part of the work was done under Foundational Research funds.

The problems that are resolved in this paper were first brought to the attention of the authors by Dr. Klaus Abt in connection with his work on armor penetration.

The original IBM 7030 (STRETCH) code in FORTRAN IV was developed by Mr. Travis Herring. Mr. Robert Belsky and Mr. Douglas C don produced the machine code for plotting confidence ellipses as output. Mr. Alfred Morris supplied the coefficients for two of the asymptotic expansions used in the original code. Cody's algorithm for computing the normal probability integral was analyzed and then developed as a STRAP code for STRETCH by Mr. Gordon Barker. Subsequently he incorporated this program into two versions of the main computing program. Dr. Marlin Thomas supplied one of the more interesting examples that are cited in the paper.

Released by:

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ABSTRACT

Necessary and sufficient conditions are obtained for the existence of the maximum likelihood estimates (MLE) of the parameters of a normal distribution for quantal responses. It is shown that whenever the MLE estimates exist they are unique. A modified Newton-Raphson procedure is given which will converge globally to the MLE estimates. These results are new and directly applicable to an armor plate penetration problem or any other types of experiments based on quantal responses which fall under a normal distribution.

A computer program is described which includes as output a set of plotted confidence ellipses centered about the MLE. Various examples and the corresponding computer outputs are given.

Probit analysis and confidence regions for small samples are discussed in separate appendices.

CONTENTS

I. INTRODUCTION

This report gives a mathematical analysis of maximum likelihood theory as it is used to find the "best" estimates [7, Chap. 32], $\bar{\mu}$, $\bar{\sigma}$ of the mean, μ_o, and the standard deviation, σ_o, of a normal distribution which governs the variations in measured sensitivity data. By sensitivity data, we mean a collection of measurements or determinations from experiments for which a stimulus is usually only applied once to each item, and for which the response in every case is quantal, i.e., can be described as a success or failure by some arbitrary criterion, [9], [14]. Experiments for dosage mortality studies, [13], and for armor plate evaluations are of this nature. Statisticians categorize the treatment of such problems under the general term--sensitivity analysis. The main results given in this paper are sufficiently general to include situations in which levels of stimulus cannot be precisely assigned in advance. The basic paper dealing with this particular phase was written in 1956 by Golub and Grubbs, [14].

The first objective, following [14], is to set up the sensitivity problem in mathematical terms. The theory of maximizing a likelihood function as popularized and extensively developed by Fisher, [12], plays a fundamental role. Once the problem has been defined in mathematical terms, we resolve the following mathematical questions which arise, but which have been open heretofore:

(a) Under what conditions does a maximum likelihood solution exist?

(b) When a solution exists, is it unique?

(c) Given that a solution exists, can a computational procedure be found which is guaranteed to converge globally (independent of starting values or initial estimates) to the "best" estimates, $\bar{\mu}$, $\bar{\sigma}$ of the true parameters μ_o, and σ_o?

For typographical convenience we use the notation $\bar{\mu}$, $\bar{\sigma}$ for maximum likelihood estimates instead of the more common $\hat{\mu}$, $\hat{\sigma}$.

In Section II, the hypothesis upon which maximum likelihood estimates are based is discussed. A likelihood function is derived. An armor plate penetration problem is described and is used to facilitate the derivation. In Section III questions (a), (b), (c), given above, are answered. Question (a) is answered by obtaining a set of necessary and sufficient conditions for the existence of a maximum likelihood solution. Question (b) is answered in the affirmative. Question (c) is also answered in the affirmative; a modified Newton-Raphson procedure is proved to converge globally to the maximum likelihood estimates. The main results are given by theorems 3, 4, and 5.

In Section IV, for completeness, a derivation is given of the expressions for the elements of an associated covariance matrix and of the corresponding confidence ellipses. Section V describes the

computer program as it is actually used. Several examples are given.

A discussion and a comparison of our results with those obtained from Finney's Probit Analysis, [10], are given in Appendix C. Appendix D is concerned with some remarks on small sample theory.

II. CONSTRUCTION OF THE LIKELIHOOD FUNCTION

The idea of a likelihood function is founded on the premise that if one can specify a mathematical function, $F(c_1, c_2, \ldots, c_j)$, which depends on the parameters c_k, to represent the probability of occurrence of a set of events $\{J_i\}$, then the "best" estimates, in a statistical sense, for the c_k, are those values $\bar{c}_k$ for which $F(\bar{c}_1, \bar{c}_2, \ldots, \bar{c}_j)$ is an absolute maximum. More precisely: Given the occurrence of a set of events $\{J_i\}$, the likelihood function is the mathematical function, $F(c_1, \ldots, c_j)$, which represents the probability of the occurrence of the events $\{J_i\}$ where the $c_k (k = 1,2, \ldots, j)$ are parameters whose true values are unknown. The "best" estimates in a statistical sense for the parameters are those values $\bar{c}_k$ which make F an absolute maximum. Heuristically, the reason for estimating the c_k thusly, is that since the $\{J_i\}$ have occurred, we should estimate the $\bar{c}_k$, so that the probability of their occurrence is as large as possible. This result is obtained by making F an absolute maximum. An elementary example is discussed in detail in [17; page 152].

An important problem in armor plate penetration, which gave rise to the studies reported in this paper, will be used to derive the likelihood function on which the analysis is based.

In armor plate testing, the investigator wants to know the minimum speed required by a projectile of given type to penetrate a steel plate of given size and composition. By minimum or critical penetration speed with respect to a given plate, we mean that speed below which no penetration of the plate would occur and above which penetration for that particular plate would always take place. This critical penetration speed of the projectile however will vary among a set of presumably identical plates, primarily because of random variations in steel composition, flaws, etc. from plate to plate. Hence, the experimenter settles for an average critical speed of penetration, μ_o, where the word average is used in the usual statistical sense. The real number μ_o can be estimated from a knowledge of the likelihood function which is associated with the problem.

Hence, assume there exists an infinite population of steel plates identical in form and manufactured from the same process. Each plate is characterized by its critical speed of penetration so that a mean or average critical speed, μ_o, can be associated with the population. The assumption is made that the critical speed for each plate is normally distributed about the mean μ_o with a standard deviation, σ_o. The techniques that are used to determine the validity of the normality assumption, and the transformations of variables that can often be used to approximate normality, [8], are outside the scope of the present study.

Consider the following experiment. Five plates are drawn from the infinite population, numbered one through five, and tested by firing an identical projectile once at each plate. Due to variations in gun powder, gun barrel eccentricities, etc., the desired impact speed for each projectile is generally not precisely realized, i.e., the stimuli are not completely under control, [14]. Suppose the results of the tests show that plate #1 was penetrated by the projectile traveling at a speed a_1 (from which we conclude the critical speed of plate #1 is not larger than a_1). This test is called a success. Similarly, suppose "successes" were recorded for plates #2 and #5 at projectile speeds a_2 and a_3, respectively. On the other hand, suppose "failures" were noted for plates #3 and #4 at speeds b_1 and b_2, respectively (these plates were not penetrated so that e.g., plate #3 must have a critical speed larger than b_1). Since the plates are assumed to be normally distributed with respect to their critical speeds, it is easy to express the probability, p_1, of drawing a plate with a critical speed no larger than a_1, namely

$$p_1 = p\left[(a_1 - \mu_o)/\sigma_o\right] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{(a_1 - \mu_o)/\sigma_o} \exp(-t^2/2)dt.$$

By similar reasoning, the probabilities p_2 and p_3 of drawing plates #2 and #5, respectively are

$$p_2 = p\left[(a_2 - \mu_o)/\sigma_o\right] \ , \ p_3 = p\left[(a_3 - \mu_o)/\sigma_o\right] .$$

The probability q_1 of drawing plate #3, for which a failure was recorded at a speed b_1, is given by

$$q_1 = q\left[(b_1 - \mu_o)\sigma_o\right] = \frac{1}{\sqrt{2\pi}} \int_{(b_1 - \mu_o)/\sigma_o}^{\infty} \exp(-t^2/2)dt.$$

Thus q_1 denotes the probability of drawing a plate with a critical speed no smaller than b_1. The probability of drawing plate #4 is then $q\left[(b_2 - \mu_o)/\sigma_o\right] = q_2$. Assuming all of the five cases are independent of one another, it follows directly from elementary concepts that the probability F_o of observing the events as they occurred is given by the product

$$F_o = p_1 p_2 p_3 q_1 q_2 .$$

In general, if one tests n + m plates and records n successes at penetration speeds $a_1, a_2, \ldots, a_n$, and m failures at penetration speeds $b_1, b_2, \ldots, b_m$, then the probability that this sequence of events occurs, in the order observed, is given by

$$F_o = \prod_{i=1}^{n} p_i \prod_{j=1}^{m} q_j . \qquad (1)$$

The likelihood function is simply obtained from (1) by replacing the unknown quantities μ_o and σ_o by free parameters, or variables, μ and σ, respectively. In order to keep notation to a minimum and since the expression given by (1) will not appear again, we use the same notation to express the likelihood function, F, as

$$F = \prod_{i=1}^{n} p_i \prod_{j=1}^{m} q_j, \tag{2}$$

where, hereafter,

$$p_i \equiv p[(a_i - \mu)/\sigma], \tag{3}$$

$$q_j \equiv q[(b_j - \mu)/\sigma]. \tag{4}$$

According to maximum likelihood theory, "best" estimates, $\bar{\mu}$, $\bar{\sigma}$ of the parameters μ_o and σ_o are obtained by maximizing F, in (2), as a function of the variables μ and σ. Thus, the statistical problem has been reduced to the mathematical one of maximizing a function, F, of two independent variables μ and σ, which has differentials of all orders. The mathematical problem raises the questions posed in the Introduction.

It is worth noting that the estimates $\bar{\mu}$ and $\bar{\sigma}$, obtained for μ_o and σ_o will depend on the input sequences $\{a_i\}$ and $\{b_j\}$. Hence some measure of reliability in the estimates is needed. Such measures can be obtained by considering so-called confidence regions which turn out to be ellipses in the $\mu\sigma$-plane. This phase of the study will be covered in some detail . Section IV.

III. ANALYSIS OF THE LIKELIHOOD FUNCTION

Let

$$L(\mu, \sigma) = \log_e F(\mu, \sigma) = \sum_{i=1}^{n} \log p_i + \sum_{j=1}^{m} \log q_j. \tag{5}$$

We treat L rather than F hereafter, since less notation is needed. Clearly F is a maximum at a point if and only if L is a maximum at the same point. The variables μ and σ are replaced by new variables α and β, through the 1-1 transformations:

$$\alpha = \mu/\sigma, \qquad (\mu = \alpha/\beta), \tag{6}$$

$$\beta = 1/\sigma > 0, \ (\sigma = 1/\beta). \tag{7}$$

In addition, let

$$s_i = a_i\beta - \alpha, \tag{8}$$

$$t_j = b_j\beta - \alpha, \tag{9}$$

so that in terms of the new variables, α, β, (3) and (4) become

$$p_i = p(s_i) = \int_{-\infty}^{s_i} z(t)dt, \tag{10}$$

$$q_j = q(t_j) = \int_{t_j}^{\infty} z(t)dt, \tag{11}$$

where

$$z(t) \equiv \frac{1}{\sqrt{2\pi}} \exp(-t^2/2). \tag{12}$$

We will also have need for the following partial derivatives of L:

$$L_\alpha = \frac{\partial L}{\partial \alpha} = \sum_{j=1}^{m} (y_j/q_j) - \sum_{i=1}^{n} (x_i/p_i), \tag{13}$$

$$L_{\beta} = \frac{\partial L}{\partial \beta} = \sum_{i=1}^{n} a_i (x_i/p_i) - \sum_{j=1}^{m} b_j (y_j/q_j), \tag{14}$$

$$L_{\alpha\alpha} = - \sum_{j=1}^{m} (y_j/q_j)\left[(y_j/q_j) - t_j\right] - \sum_{i=1}^{n} (x_i/p_i)\left[(x_i/p_i) + s_i\right], \tag{15}$$

$$L_{\alpha\beta} = \sum_{j=1}^{m} b_j (y_j/q_j)\left[(y_j/q_j) - t_j\right] + \sum_{i=1}^{n} a_i (x_i/p_i)\left[(x_i/p_i) + s_i\right], \tag{16}$$

$$L_{\beta\beta} = - \sum_{j=1}^{m} b_j^2 (y_j/q_j)\left[(y_j/q_j) - t_j\right] - \sum_{i=1}^{n} a_i^2 (x_i/p_i)\left[(x_i/p_i) + s_i\right], \tag{17}$$

where

$$x_i \equiv z(s_i), \tag{18}$$

$$y_j \equiv z(t_j). \tag{19}$$

The a_i and b_j are arbitrary real numbers. σ and β by their nature are positive.

The lemma which follows is stated for easy reference. The proof is not given, it follows from a well-known theorem in analysis, [2, p. 149], and elementary considerations.

LEMMA 1. Let $f(\alpha,\beta)$ have continuous second partial derivatives in an open region T of the $\alpha\beta$-plane and let there exist a point $(\bar{\alpha},\bar{\beta}) \in T$ such that at $(\bar{\alpha},\bar{\beta})$

$$f_{\alpha\alpha} < 0, \quad f_{\alpha\alpha} f_{\beta\beta} - f_{\alpha\beta}^2 > 0,$$

then $f(\alpha,\beta)$ has a maximum at $(\bar{\alpha},\bar{\beta})$ if and only if

$$f_\alpha(\bar{\alpha},\bar{\beta}) = f_\beta(\bar{\alpha},\bar{\beta}) = 0.$$

Moreover, if f has a maximum at $(\bar{\alpha},\bar{\beta})$, then the equalities must hold regardless of the above inequalities.

The possibility that all the a_i are equal (say to a), and that all the b_j are equal (say to b) is ruled out by Lemmas 2 and 3.

LEMMA 2. If L has a maximum and $a_i = a$, $b_j = b$ for each i and j, then $a = b$.

Proof: If L has a maximum at $(\bar{\alpha},\bar{\beta})$, then by Lemma 1, $L_\alpha = L_\beta = 0$ at this point. By equating the right hand sides of (13) and (14) to zero, for the arguments

$$s_i = a\bar{\beta} - \bar{\alpha}, \quad t_j = b\bar{\beta} - \bar{\alpha},$$

one obtains

$$n(x_i/p_i) = m(y_j/q_j),$$

$$na(x_i/p_i) = mb(y_j/q_j). \qquad \text{Q.E.D.}$$

LEMMA 3. If for each i and j, $a_i = b_j = c$, then L assumes its maximum at every point of the straight line

$$\alpha = c\beta - s^*, \tag{20}$$

where s^* is determined by

$$p(s^*) = n/(m+n). \tag{21}$$

Proof: Since c is a fixed constant, the function L can be considered in this case as a function of the single variable $s = c\beta - \alpha$, so that

$$L(s) = n \log p(s) + m \log q(s),$$

and

$$L'(s) = (nx/p) - (my/q) = x[(n/p) - (m/q)].$$

Since $L'' < 0$ when $L'(s) = 0$, it follows that L attains a maximum at those values of s which satisfy

$$p(s) = n/(m + n) < 1.$$

But p(s) is a positive monotone continuously increasing function of s and less than one. Therefore there exists a unique value, $s = s^*$, for which (21) holds and L takes a maximum for all (α, β) which satisfy (20).

Lemma 3 implies the obvious conclusion that best estimates cannot be determined if the stimulus is maintained at the same level for all experiments. It is also necessary that both the $\{a_i\}$ and $\{b_j\}$ sets be non-empty. If say $\{b_j\}$ were empty, then from (13), L_α would always be negative and L could not have a maximum. Hence, it is assumed hereafter that neither of the sets $\{a_i\}$, $\{b_j\}$ are empty and that at least one of the sets must contain at least two elements which differ.

The next lemma will be used to prove Theorem 1.

LEMMA 4. If $t \in (-\infty, \infty)$, then

$$[z(t)/q(t)] - t > 0, \tag{22}$$

$$[z(t)/p(t)] + t > 0. \tag{23}$$

Proof: Consider

$$f(t) = z - tq.$$

Then, since

$$z(\pm\infty) = 0,\ q(\infty) = 0,\ q(-\infty) = 1,$$

we have that

$$\lim_{t \to -\infty} f(t) = \lim_{t \to -\infty} (-t) = +\infty ,$$

$$\lim_{t\to\infty} |f(t)| = \lim_{t\to\infty} |-tq(t)| \leqslant \lim_{t\to\infty} \frac{1}{\sqrt{2\pi}} \int_t^{\infty} u\exp(-u^2/2)du$$

$$= \lim_{t\to\infty} \frac{1}{\sqrt{2\pi}} \exp(-t^2/2) = 0.$$

In addition,

$$f'(t) = -tz - q + tz = - q < 0.$$

Therefore, it follows that $f(t) > 0$, and since $q(t) > 0$

$$\frac{f(t)}{q(t)} = \frac{z(t)}{q(t)} - t > 0, \quad \forall\, t \in (-\infty,\infty).$$

The proof for (23) follows by replacing t by (-t) in (22) and using the facts that $z(t) = z(-t)$, $q(-t) = p(t)$.

THEOREM 1. If (α,β) is any point in the $\alpha\beta$-plane, then

$$L_{\alpha\alpha} < 0,\ L_{\beta\beta} < 0. \tag{24}$$

Proof: The expressions for $L_{\alpha\alpha}$ and $L_{\beta\beta}$ are given by (15) and (17). The quantities (y_j/q_j) and (x_i/p_i) are positive and from Lemma 4,

$$(y_j/q_j) - t_j > 0,$$

$$(x_i/p_i) + s_i > 0. \qquad \text{Q.E.D.}$$

Where no ambiguity will occur, it will be understood that sums over i run from one to n and sums over j run from one to m.

Another useful property of L is given by the following theorem:

THEOREM 2. The discriminant of L,

$$\Delta \equiv L_{\alpha\alpha} L_{\beta\beta} - L_{\alpha\beta}^2 , \tag{25}$$

is positive for all (α, β).

Proof: Let

$$U_i \equiv (x_i/p_i)[(x_i/p_i) + s_i] \quad (>0) \tag{26}$$

$$V_j \equiv (y_j/q_j)[(y_j/q_j) - t_j] \quad (>0). \tag{27}$$

Then Δ can be expressed in terms of the right hand sides of (15), (16), (17) accordingly:

$$\Delta = \Sigma a_i^2 U_i \Sigma U_i + \Sigma b_j^2 V_j \Sigma V_j + \Sigma a_i^2 U_i \Sigma V_j$$

$$+ \Sigma b_j^2 V_j \Sigma U_i - (\Sigma a_i U_i)^2 - (\Sigma b_j V_j)^2 - 2\Sigma a_i U_i \Sigma b_j V_j.$$

The Cauchy-Schwarz inequality requires that

$$(\Sigma a_i U_i)^2 \leqslant \Sigma a_i^2 U_i \Sigma U_i, \tag{28}$$

$$(\Sigma b_j V_j)^2 \leqslant \Sigma b_j^2 V_j \Sigma V_j. \tag{29}$$

Equality holds for (28) if and only if

$$a_i^2 \sqrt{U_i} = K \sqrt{U_i} ,$$

where K is any real positive number. Clearly, this relation implies all a_i are equal, since $U_i > 0$ by (23). Similarly, equality in (29) requires that all b_j be equal. But, by the requirement that at least two of the a_i or b_j must differ, at least one of the inequalities (28), (29) must be strict. Hence, using (28) and (29) twice,

$$\begin{aligned} \Delta &> \Sigma a_i^2 U_i \Sigma V_j + \Sigma b_j^2 V_j \Sigma U_i - 2\Sigma a_i U_i \Sigma b_j V_j \qquad (30) \\ &> (\Sigma a_i U_i)^2 (\Sigma V_j / \Sigma U_i) + (\Sigma b_j V_j)^2 (\Sigma U_i / \Sigma V_j) - 2\Sigma a_i U_i \Sigma b_j V_j \\ &= \left[(\Sigma V_j / \Sigma U_i)^{1/2} \Sigma a_i U_i - (\Sigma U_i / \Sigma V_j)^{1/2} \Sigma b_j V_j \right]^2 \geqslant 0. \end{aligned}$$

We are now able to use a well known theorem of analysis to obtain an answer to question (b) of the Introduction. The proof is given for completeness.

THEOREM 3. <u>There exists at most one point $(\bar{\alpha}, \bar{\beta})$ at which L assumes a maximum.</u>

<u>Proof:</u> Assume L has a local maximum at two different points (α_1, β_1) and (α_2, β_2). The Taylor formula for a function of two independent variables gives

$$L(\alpha_2, \beta_2) = L(\alpha_1, \beta_1) + \nabla L(\alpha_1, \beta_1) \cdot \Delta\eta + \Delta\eta^T \cdot D^2 L \cdot \Delta\eta , \tag{31}$$

where ∇L represents the gradient of L with components L_α and L_β ; D^2L is the matrix

$$D^2L \equiv \begin{pmatrix} L_{\alpha\alpha} & L_{\alpha\beta} \\ L_{\alpha\beta} & L_{\beta\beta} \end{pmatrix} , \tag{32}$$

and $\Delta\eta$ is the column vector with first and second components $\Delta\alpha = (\alpha_2 - \alpha_1)$ and $\Delta\beta = (\beta_2 - \beta_1)$, respectively. The superscript T on $\Delta\eta$ indicates the transpose. The elements of D^2L in (31) are evaluated at a point ξ, where for some $\epsilon\,(0 < \epsilon < 1)$,

$$\xi = \eta + \epsilon\Delta\eta , \qquad \eta = (\alpha_1, \beta_1).$$

By Theorems 1 and 2,

$$\begin{cases} L_{\alpha\alpha} < 0, L_{\beta\beta} < 0, \\ \Delta > 0, \end{cases} \tag{33}$$

hence D^2L is negative definite for all (α, β). But since L has a maximum at (α_1, β_1) this implies by Lemma 1 that $L_\alpha = L_\beta = 0$ at (α_1, β_1). Therefore (31) reduces to

$$L(\alpha_2, \beta_2) = L(\alpha_1, \beta_1) + (\Delta\eta)^T \cdot D^2L \cdot (\Delta\eta) < L(\alpha_1, \beta_1).$$

Interchanging the roles of (α_2, β_2) and (α_1, β_1) and applying the same arguments leads to

$$L(\alpha_1, \beta_1) < L(\alpha_2, \beta_2).$$

This inconsistency can be removed only if $\Delta\eta = 0$, which implies (α_1, β_1) and (α_2, β_2) coincide. Q.E.D.

It will be assumed hereafter that the a_i and b_j are separately ordered in increasing magnitude, i.e.,

$$\begin{aligned} a_1 &\leqslant a_2 \leqslant \cdots \leqslant a_n, \\ b_1 &\leqslant b_2 \leqslant \cdots \leqslant b_m. \end{aligned} \tag{34}$$

Question (a) as stated in the Introduction, is a natural one to raise now, i.e., under what conditions on the a_i and b_j does L have a maximum? The answer is supplied by Theorem 4. The necessity of (35) is well-known, [14], [18].

THEOREM 4. The function L has a unique maximum for $\beta > 0$ if and only if the quantities a_i and b_j satisfy the following inequalities:

$$a_1 < b_m, \tag{35}$$

$$\frac{1}{m} \Sigma b_j < \frac{1}{n} \Sigma a_i. \tag{36}$$

Proof: If L has a maximum at $(\bar{\alpha}, \bar{\beta})$, then from (13), (14), and Lemma 1, we have

$$L_\alpha(\bar{\alpha}, \bar{\beta}) = \Sigma(x_i/p_i) - \Sigma(y_j/q_j) = 0, \tag{37}$$

$$L_\beta(\bar{\alpha}, \bar{\beta}) = \Sigma a_i(x_i/p_i) - \Sigma b_j(y_j/q_j) = 0, \tag{38}$$

where all quantities are evaluated at $(\bar{\alpha}, \bar{\beta})$. From (38), and by the orderings specified in (34), it follows

$$b_1 \Sigma(y_j/q_j) < a_n \Sigma(x_i/p_i), \tag{39}$$

$$a_1 \Sigma(x_i/p_i) < b_m \Sigma(y_j/q_j). \tag{40}$$

Equality is not possible in either (39) or (40), because at least two of the a_i or two of the b_j must differ. Hence, (35) follows directly from (37), (39) and (40).

The proof for (36) is obtained by using a classical inequality which is stated in the form of a lemma.

LEMMA 5. <u>If two finite sequences of N real numbers, $\{u_k\}$ and $\{v_k\}$, are given with the properties that</u>

$$u_1 \leqslant u_2 \leqslant \cdots \leqslant u_N, \qquad v_1 \leqslant v_2 \leqslant \cdots \leqslant v_N,$$

<u>then the following inequality holds</u>

$$\sum_1^N u_k \sum_1^N v_k \leqslant N \sum_1^N u_k v_k. \tag{41}$$

<u>Moreover, if the inequalities on the elements of one of the sequences are reversed, then the inequality sign in (41) is reversed. Equality for (41) holds if and only if all the elements of at least one of the sequences are equal.</u>

<u>Proof:</u> The proof follows immediately from the identity

$$\sum_1^N u_k \sum_1^N v_k = N \sum_1^N u_k v_k + \sum_{k=1}^{N-1} \sum_{i>k}^N (u_k - u_i)(v_i - v_k). \quad \text{Q.E.D.} \tag{42}$$

In order to apply this lemma, we observe that $z(t)/q(t)$ and $z(t)/p(t)$ are monotonically increasing and decreasing functions of t, respectively. This statement is easily verified by differentiating these above quantities, using Lemma 4 and the limiting properties of the functions as $t \to \pm\infty$.

We apply Lemma 5 twice. In one case, let

$$u_j = b_j,$$

$$v_j = (y_j/q_j).$$

Then, for the point $(\bar{\alpha},\bar{\beta})$, the argument of (y_j/q_j), $t_j = b_j\bar{\beta} - \bar{\alpha}$, is an increasing function of b_j, so (y_j/q_j) is an increasing function of b_j. Hence by (34) and (41)

$$\Sigma b_j \Sigma(y_j/q_j \leqslant n\Sigma b_j(y_j/q_j). \tag{43}$$

In the other case, let

$$u_i = a_i,$$

$$v_i = x_i/p_i.$$

Then, for the fixed point $(\bar{\alpha},\bar{\beta})$, the argument of (x_i/p_i), $s_i = a_i\bar{\beta} - \bar{\alpha}$, is an increasing function of a_i, hence (x_i/p_i) is a decreasing function of a_i. Thus, by (34) and (41)

$$n\Sigma a_i(x_i/p_i) \leqslant \Sigma a_i \Sigma(x_i/p_i). \tag{44}$$

We again use the fact that either some of the a_i or some of the b_j must be different, so that by Lemma 5 either (43) or (44) must be a strict inequaiity. For definiteness, suppose (44) is strict, then from (37), (43), (38), and (44)

$$\frac{1}{n}\Sigma b_j \Sigma(x_i/p_i) = \frac{1}{n}\Sigma b_j \Sigma(y_j/q_j) \leqslant \Sigma b_j(y_j/q_j)$$

$$= \Sigma a_i(x_i/p_i) < \frac{1}{n}\Sigma a_i \Sigma(x_i/p_i). \tag{45}$$

Since $\Sigma(x_i/p_i) > 0$, the inequality (36) follows from (45).

It remains to show that (35) and (36) are sufficient to insure L has a maximum. For the proof we shall use Lemmas 6 and 7.

LEMMA 6. The function $L(\alpha, 0)$ has a unique maximum on $(-\infty,\infty)$. Moreover, this maximum occurs at $\alpha = \alpha^*$, where

$$p(-\alpha^*) = \frac{n}{m+n}, \quad q(-\alpha^*) = p(\alpha^*) = \frac{m}{m+n}. \tag{46}$$

Proof: Equation (5) is expressed in terms of α and β by using (6) and (7). Then β is set to zero to obtain the expression for $L(\alpha, 0)$,

$$L(\alpha, 0) = n \log [p(-\alpha)] + m \log[q(-\alpha)].$$

Now, differentiating $L(\alpha, 0)$,

$$\frac{dL}{d\alpha}(\alpha, 0) = -n[z(-\alpha)/p(-\alpha)] + m[z(-\alpha)/q(-\alpha)],$$

and setting the result to zero implies there exist values of α, say α^*, for which

$$[m/q(-\alpha^*)] = [n/p(-\alpha^*)].$$

However

$$q(-\alpha) = 1 - p(-\alpha),$$

so that (46) follows, and since $p(\alpha)$ is a monotonically increasing function of its argument, α^* is unique. By Theorem 1, $L_{\alpha\alpha}$ is always negative, hence $L(\alpha, 0)$ takes its maximum at $(\alpha^*, 0)$.

LEMMA 7. The quantity L_β evaluated at $(\alpha^*, 0)$ is positive, provided (36) holds, where

$$L(\alpha^*, 0) = \max L(\alpha, 0).$$

Proof. Setting $\beta = 0$ in (14) gives

$$L_\beta(\alpha, 0) = \Sigma a_i[z(-\alpha)/p(-\alpha)] - \Sigma b_j[z(-\alpha)/q(-\alpha)].$$

Evaluating this quantity at $\alpha = \alpha^*$, and using (46) and (36) gives

$$L_\beta(\alpha^*, 0) = (m+n)z(\alpha^*)\left[\frac{1}{n}\Sigma a_i - \frac{1}{m}\Sigma b_j\right] > 0. \quad \text{Q.E.D.} \quad (47)$$

The basic idea that is used to complete the sufficiency proof can be briefly described as follows: A triangular domain T (see Figure 1) is constructed in the $\alpha\beta$-plane, with the point $(\alpha^*, 0)$ in the base of the triangle but not one of its vertices, such that

$$L(\alpha, \beta) \leqslant L(\alpha^*, 0) \text{ for all } (\alpha, \beta) \in \partial T. \quad (48)$$

Then, by Lemmas 6 and 7, there exists a point (α^*, β'), an interior point of the domain T, with $\beta' > 0$, for which

$$L(\alpha^*, \beta') > L(\alpha^*, 0).$$

It will then be easy to show that the global maximum $(\bar{\alpha}, \bar{\beta})$ of the function L (not necessarily the same point as (α^*, β')) must lie in the interior of T with $\bar{\beta} > 0$ as required.

The proof of the existence of the triangular domain T follows (see Figure 1). Consider lines with equations of the form

$$a_1\beta - \alpha = -t_1, \quad t_1 > 0 \quad (49)$$

Since, by (5), $L(\alpha, \beta) = \Sigma \log p_i + \Sigma \log q_i$ and, since all these summands, logarithms of numbers on the interval (0, 1), are always negative, we have, for every point (α, β) on this line,

$$L(\alpha, \beta) < \log p_1 = \log p(a_1\beta - \alpha) = \log p(-t_1). \tag{50}$$

But, by the properties of the probability integral

$$p(x) = (1/\sqrt{2\pi}) \int_{-\infty}^{x} \exp(-t^2/2)dt, \quad p(-t_1) \to 0$$

and hence $\log p(-t_1) \to -\infty$ as $t_1 \to \infty$. Therefore we can certainly give t_1 a sufficiently large positive value so that $L(\alpha, \beta) < L(\alpha^*, 0)$ for every point of the line (49). Also, since the α-intercept of this line is $\alpha = t_1$, we can at the same time choose t_1 in such a way ($t_1 > \alpha^*$) that the α-intercept of the line lies to the right of the point $(\alpha^*, 0)$. We suppose that a fixed t_1 satisfying these conditions is chosen, and this line is designated as line ① in Figure 1.

Similarly we can show the existence of a line ②, $b_m\beta - \alpha = +t_2$

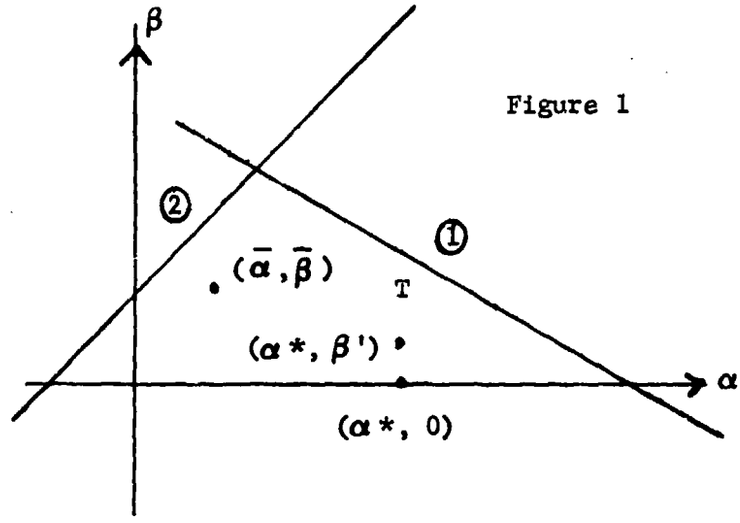

Figure 1

with $t_2 > 0$, with its α-intercept lying to the left of the point $(\alpha^*, 0)$, and such that, for all points of line ②, $L(\alpha, \beta) < L(\alpha^*, 0)$. It is easily shown by analytic geometry that these lines $a_1\beta - \alpha = -t_1$ and $b_m\beta - \alpha = +t_2$ must intersect in the upper half-plane. The solution of these equations is $\alpha = (t_1 b_m + t_2 a_1)/(b_m - a_1)$, $\beta = (t_1 + t_2/(b_m - a_1)$. Since we here have $t_1 > 0$, $t_2 > 0$, $b_m > a_1$, we must have $\beta > 0$ at the point of intersection.

Thus we have a triangle (Figure 1) formed by segments of the α-axis and lines ① and ②. This compact domain (triangle plus its interior) is denoted as T, and the interior lies in the upper half-plane, $\beta > 0$.

At all points (α, β) of the triangle itself, the boundary of T, ∂T, we have

$$L(\alpha, \beta) \leqslant L(\alpha^*, 0) \tag{51}$$

since $L(\alpha^*, 0)$ is the maximum value for the entire α-axis, and since lines ① and ② were chosen in such a way that $L(\alpha, \beta) < L(\alpha^*, 0)$ at all points of these lines.

But, by Lemmas 6 and 7, there must exist a point (α^*, β'), an interior point of the domain T with $\beta' > 0$, such that

$$L(\alpha^*, \beta') > L(\alpha^*, 0). \tag{52}$$

Combining this with (51), it is seen that $L(\alpha^*, \beta')$ is greater than $L(\alpha, \beta)$ for all points (α, β) of the boundary of T.

However, the function L must assume a maximum for the compact set T at some point of T, by elementary real analysis. This maximum cannot be assumed on the boundary of T, by what has been shown. Hence it must be assumed at some interior point, $(\bar{\alpha}, \bar{\beta})$, with $\bar{\beta} > 0$, not necessarily the same point as (α^*, β').

But, by Theorem 3, there can exist at most one maximum point for L, including local maxima, in the entire plane. Hence this maximum point, $(\bar{\alpha}, \bar{\beta})$, for the compact domain T, with $\bar{\beta} > 0$, must be the unique global maximum. This completes the proof of Theorem 4.

Our objective now is to describe a practical computational procedure by which $(\bar{\alpha}, \bar{\beta})$ can be determined to any specified accuracy. Reference will be made to the well-known Newton-Raphson procedure (abbreviated N-R) for two independent variables, [15, p. 451]. It will be shown that a modified form of the N-R algorithm will always converge globally to $(\bar{\alpha}, \bar{\beta})$, i.e., regardless of what starting point, (α^*, β^*), is chosen. We remark that α^* here is a convenient notation and has no relation to the same symbol in (47).

A point (α^*, β^*) is chosen initially (assume it is not $(\bar{\alpha}, \bar{\beta})$). The N-R algorithm is applied, with the objective of reducing L_α and L_β to zero simultaneously, to yield increments $\Delta\alpha$ and $\Delta\beta$ and a new point (α_2, β_2). We call $\Delta\alpha$ and $\Delta\beta$, N-R increments. They make up the first and second components, respectively, of the column vector $\Delta\eta$ and are found by solving the linear system

$$\Delta\alpha L_{\alpha\alpha} + \Delta\beta L_{\alpha\beta} = - L_{\alpha}, \tag{53}$$

$$\Delta\alpha L_{\alpha\beta} + \Delta\beta L_{\beta\beta} = - L_{\beta}, \tag{54}$$

where all partial derivatives are evaluated at (α^*, β^*). Hence

$$\begin{aligned} \Delta\alpha &= (L_{\beta} L_{\alpha\beta} - L_{\alpha} L_{\beta\beta})/\Delta, \\ \Delta\beta &= (L_{\alpha} L_{\alpha\beta} - L_{\beta} L_{\alpha\alpha})/\Delta, \end{aligned} \tag{55}$$

where $\Delta > 0$ as was shown in Theorem 2. In vector notation (See (31))

$$\zeta(u) = \eta + u\Delta\eta, \quad 0 < u < 1, \tag{56}$$

where $\zeta(0) = \eta = (\alpha^*, \beta^*)$, $\zeta(1) = (\alpha_2, \beta_2)$. We say the N-R algorithm is "modified" if the continuous variable u is given any value on (0, 1).

It will be shown there always exists a value of u, say u_o, such that for all $\zeta(u)$ for which $0 < u \leqslant u_o \leqslant 1$,

$$L[\zeta(u)] \equiv L(\alpha, \beta) > L(\alpha^*, \beta^*) = L(\eta) = L[\zeta(0)]. \tag{57}$$

The quantities $\Delta\alpha$ and $\Delta\beta$ that appear below are assumed to be N-R increments and are to remain fixed throughout the argument. Then, using the notation of (31) and evaluating derivatives at (α^*, β^*),

$$\nabla L \cdot \Delta\eta = \Delta\alpha L_{\alpha} + \Delta\beta L_{\beta} > 0. \tag{58}$$

The inequality follows from (55) by substituting on the right for $\Delta\alpha$ and $\Delta\beta$ so that

$$\nabla L \cdot \Delta\eta = - \frac{1}{\Delta} \left[L_{\beta}^2 L_{\alpha\alpha} - 2L_{\alpha} L_{\beta} L_{\alpha\beta} + L_{\alpha}^2 L_{\beta\beta} \right] \tag{59}$$

$$= - \frac{1}{\Delta} (g^T \cdot D^2 L \cdot g) > 0,$$

where $g \equiv (L_{\beta}, -L_{\alpha})$.

The last inequality clearly holds, because, by Theorems 1 and 2, the matrix D^2L is negative definite and Δ is always positive. Therefore, using the mean value theorem and continuity arguments, there exists a real number $u_o \in (0,1]$ such that (57) holds. By iterating this procedure, and choosing u appropriately at each step, the L values will certainly converge to some value not exceeding $L(\bar{\alpha},\bar{\beta})$ since L is increased at each step.

One difficulty in actually carrying out this procedure is that no definite rule has been given for choosing u at each step. A second, and much more serious, difficulty is the possibility that the iterates could spiral while the corresponding values of L converged to a real number bounded by $L(\bar{\alpha},\bar{\beta})$. It will be proved however that if u is properly chosen as indicated below that convergence will always be to $(\bar{\alpha},\bar{\beta})$.

A well-defined procedure is now given for choosing u. For any given step take $u = 2^{-r}$ where $r = k$ or $k + 1$ $(k = 0, 1, 2, \ldots)$ as determined by

$$r = \begin{cases} k & \text{if } L\left[\zeta(2^{-k})\right] \geqslant L\left[\zeta(2^{-k-1})\right] \\ k+1 & \text{if } L\left[\zeta(2^{-k-1})\right] > L\left[\zeta(2^{-k})\right], \end{cases} \tag{60}$$

where k is the smallest nonnegative integer for which

$$L\left[\zeta(2^{-k})\right] \geqslant L\left[\zeta(0)\right]. \tag{61}$$

In other words, the full N-R step (u = 1) is repeatedly halved until (61) is satisfied; by (58) there always exists such a k and it may be zero. Then one more halving takes place so that r, and thus u, is found

from (60). This procedure can obviously be carried out on a computer simply and efficiently. The next theorem summarizes these remarks.

THEOREM 5. <u>If $L(\bar{\alpha}, \bar{\beta})$ is a maximum and (35) and (36) are satisfied then the modified N-R algorithm as described in the preceding paragraph will always converge globally to $(\bar{\alpha}, \bar{\beta})$.</u>

The part of the theorem which remains to be proved is somewhat lengthy and is given in Appendix A.

Actually in practice, as we describe in Section V, the regular N-R algorithm (u = 1) has been used with complete success in spite of inferences to the contrary in the literature [14], [21]. Many cases of all types were tried and convergence always occurred independent of the starting values of α and β. A case was given in [21] in which divergence was reported; our program converged. (We have included this case as one of our examples (No. 2A) in Section V). We are thus led to the conjecture that the N-R algorithm always converges globally, provided sufficient accuracy is retained in all computations, but a proof has not been found.

We remark in closing this section that an implicit assumption has been carried throughout. Namely, if L has a maximum at $(\bar{\alpha}, \bar{\beta})$, then it has a maximum for the variables $(\bar{\mu}, \bar{\sigma})$, where

$$\bar{\mu} = \bar{\alpha}/\bar{\beta}, \quad \bar{\sigma} = 1/\bar{\beta}. \tag{62}$$

This assumption is clearly valid, because the variables are related by 1-1 transformations (5), (6). A detailed proof has been carried out but is not included in this report.

IV. CONSTRUCTION OF THE COVARIANCE MATRIX AND CONFIDENCE ELLIPSE

We continue to use the notation: μ_o, σ_o for the true parameters, and $\bar{\mu}$, $\bar{\sigma}$ for the estimates of the true parameters as determined from maximum likelihood theory. The notation used below follows closely that of Golub and Grubbs, [14] the analysis follows that given by Mood [17, p. 212].

The estimates $(\bar{\mu}, \bar{\sigma})$ carry no significance without some measure of the possible deviation from (μ_o, σ_o), the true parameters of the distribution. A classical procedure for obtaining an estimate of the error for large sample sizes is to determine a confidence ellipse (similar to a confidence interval for one variable). It will have meaning in the following sense: For a specified level of confidence, say 95%, an ellipse is determined in the $\mu\sigma$-plane with its center at $(\bar{\mu}, \bar{\sigma})$ such that with probability .95, the true parameter point (μ_o, σ_o) is contained in the interior of the ellipse.

We first construct a so-called covariance matrix and then show how the confidence ellipse is obtained from the elements of the inverse of this matrix. We will resort again to the armor plate penetration problem as an aid in elucidating the main ideas of this section.

Consider random variables δ_k $(k = 1, 2, \ldots, N)$ where $N = n + m$ is the number of shells fired (or experiments conducted). Each δ_k has only two possible values

$$\delta_k = \begin{cases} 1 \text{ if } k^{th} \text{ shot was a success (produced penetration)} \\ 0 \text{ if } k^{th} \text{ shot was a failure (no penetration).} \end{cases} \tag{63}$$

The probability density function for the random variable δ_k is

$$f_k = f(\delta_k; \mu, \sigma) = \left[p\left(\frac{c_k - \mu}{\sigma}\right)\right]^{\delta_k}\left[1 - p\left(\frac{c_k - \mu}{\sigma}\right)\right]^{1-\delta_k} \quad (64)$$

$$= \left[p\left(\frac{c_k - \mu}{\sigma}\right)\right]^{\delta_k} \quad \left[q\left(\frac{c_k - \mu}{\sigma}\right)\right]^{1-\delta_k}, \quad (65)$$

where p is the normal probability integral, (see (3), (4)). The quantity c_k is the stimulus (velocity of the projectile in our example) regardless of whether the k^{th} shot is a success or failure. The quantities μ (mean critical speed), σ (standard deviation) are parameters. The probability $f_k(1; \mu, \sigma)$ that the k^{th} shot was a success is determined by putting $\delta_k = 1$ in (64) and (65) to obtain $p[(c_k - \mu)/\sigma]$; similarly for a failure δ_k is set to zero in (66) to obtain $f_k(0; \mu, \sigma) = q[(c_k - \mu)/\sigma]$.

Two new quantities are introduced

$$G(\delta_k; \mu, \sigma) = G_k \equiv \frac{\partial}{\partial \mu} \log f(\delta_k; \mu, \sigma) , \quad (66)$$

$$H(\delta_k; \mu, \sigma) = H_k \equiv \frac{\partial}{\partial \sigma} \log f(\delta_k; \mu, \sigma) . \quad (67)$$

Although δ_k is a discrete variable with only two possible values, each f_k is a differentiable function of the parameters μ and σ, so these definitions are meaningful.

For the sake of a simpler notation, we drop the subscript k but it should be understood, unless otherwise noted, that all relations

that follow deal only with the k^{th} experiment, so that a fixed k subscript should be understood whenever necessary.

The expected value of G is given by

$$E(G) = \sum_{r=o}^{1} G(\delta^r; \mu, \sigma) f(\delta^r; \mu, \sigma) , \tag{68}$$

where δ^r are the values which δ (note subscript k has been dropped on δ) can take, i.e., $\delta^o = 0$, $\delta^1 = 1$. Equation (68) is the discrete analog of the expression which would be used if we had a continuous variable ϕ instead of δ, namely

$$E(G(\phi; \mu, \sigma)) \int_{-\infty}^{\infty} G(\phi; \mu, \sigma) f(\phi; \mu, \sigma) d\phi . \tag{69}$$

From (68) there follows:

$$E(G) = \sum_{r=o}^{1} \frac{\partial}{\partial \mu} f(\delta^r; \mu, \sigma) = \frac{\partial}{\partial \mu} \sum_{r=o}^{1} f(\delta^r; \mu, \sigma)$$

$$= \frac{\partial}{\partial \mu} \left[p\left(\frac{c - \mu}{\sigma}\right) + q\left(\frac{c - \mu}{\sigma}\right) \right] = \frac{\partial}{\partial \mu} (1) = 0. \tag{70}$$

Starting with the analog of (68) for H and $\partial/\partial\sigma$, instead of G and $\partial/\partial\mu$, it is shown in the same way that

$$E(H) = 0 . \tag{71}$$

The fact that every G and H (i.e., for each k = 1, 2, ..., N) has a mean or expected value of zero simplifies the calculation of the

standard deviations or variances of these functions. Let the variance of G, for any given k, be denoted by σ_G^2. Similarly σ_H^2 will denote the variance of H, and σ_{GH} the covariance of G and H. (We will have no need for the covariance of G and H for two different values of k).

The variance σ_G^2 of G is, by definition, given as

$$\sigma_G^2 \equiv \sum_{r=o}^{1} [G(\delta^r; \mu, \sigma)]^2 f(\delta^r; \mu, \sigma)$$

$$= \sum_{r=o}^{1} \frac{1}{f(\delta^r; \mu, \sigma)} \left[\frac{\partial}{\partial \mu} f(\delta^r; \mu, \sigma) \right]^2 . \qquad (72)$$

Now differentiate both sides of (68) with respect to μ to obtain

$$0 = \sum_{r=o}^{1} \frac{\partial}{\partial \mu} [G(\delta^r; \mu, \sigma)] f(\delta^r; \mu, \sigma)$$

$$+ \sum_{r=o}^{1} G(\delta^r; \mu, \sigma) \frac{\partial}{\partial \mu} [f(\delta^r; \mu, \sigma)]$$

$$= \sum_{r=o}^{1} f(\delta^r; \mu, \sigma) \frac{\partial^2}{\partial \mu^2} [\log f(\delta^r; \mu, \sigma)]$$

$$+ \sum_{r=o}^{1} \frac{1}{f(\delta^r, \mu, \sigma)} \left[\frac{\partial f(\delta^r; \mu, \sigma)}{\partial \mu} \right]^2 . \qquad (73)$$

From (72), using (73), we have

$$\sigma_G^2 = - E\left[\frac{\partial^2}{\partial \mu^2} \log f(\delta^r; \mu, \sigma)\right]. \tag{74}$$

Similarly

$$\sigma_H^2 = - E\left[\frac{\partial^2}{\partial \sigma^2} \log f(\delta^r; \mu, \sigma)\right]. \tag{75}$$

Next, we wish to obtain a useful expression for the covariance of G and H. By definition

$$\sigma_{GH} \equiv \sum_{r=0}^{1} G(\delta^r; \mu, \sigma) H(\delta^r; \mu, \sigma) f(\delta^r; \mu, \sigma)$$

$$= \sum_{r=0}^{1} \frac{1}{f(\delta^r; \mu, \sigma)} \cdot \frac{\partial f(\delta^r; \mu, \sigma)}{\partial \mu} \cdot \frac{\partial f(\delta^r; \mu, \sigma)}{\partial \sigma}. \tag{76}$$

If (68) is differentiated with respect to σ, then

$$0 = \frac{\partial}{\partial \sigma}\left[\sum_{r=0}^{1} G(\delta^r; \mu, \sigma) f(\delta^r; \mu, \sigma)\right]$$

$$0 = \sum_{r=0}^{1} \frac{\partial}{\partial \sigma}\left[G(\delta^r; \mu, \sigma)\right] f(\delta^r; \mu, \sigma) + \sum_{r=0}^{1} G(\delta^r; \mu, \sigma) \frac{\partial f(\delta^r; \mu, \sigma)}{\partial \sigma}$$

$$0 = \sum_{r=0}^{1} \frac{\partial G(\delta^r; \mu, \sigma)}{\partial \sigma} f(\delta^r; \mu, \sigma)$$

$$+ \sum_{r=0}^{1} \frac{1}{f(\delta^r; \mu, \sigma)} \frac{\partial f(\delta^r; \mu, \sigma)}{\partial \mu} \frac{\partial f(\delta^r; \mu, \sigma)}{\partial \sigma}. \tag{77}$$

From (76), using (66) and (77),

$$\sigma_{GH} = - E\left[\frac{\partial^2 \log f(\delta^r; \mu, \sigma)}{\partial \mu \partial \sigma}\right]. \tag{78}$$

It is also obvious from the definition given in (76) that

$$\sigma_{GH} = \sigma_{HG}. \tag{79}$$

We introduce the vector random variable (G,H) for a given k, k = 1, 2, ..., N. By (70) and (71) this variable has mean (0,0). We denote its covariance matrix by M, which is defined by

$$M \equiv \begin{pmatrix} \sigma_G^2 & \sigma_{GH} \\ \sigma_{GH} & \sigma_H^2 \end{pmatrix}. \tag{80}$$

Equations (74), (75), (78) give expressions for its elements which will be used later. By the multivariate central limit theorem, [7, p. 316]

$$\sum_{k=1}^{N} (G_k, H_k)$$

is, for large N, approximately multinormally distributed with mean (0, ..., 0) and covariance matrix, A^{-1},

$$A^{-1} = \sum_{k=1}^{N} M_k.$$

We denote this matrix specifically as an inverse, because this matrix, as it will be shown later, is the inverse of the covariance matrix

for the distribution of the maximum likelihood estimators $\bar{\mu}$, $\bar{\sigma}$.

Thus,

$$A^{-1} = \begin{pmatrix} \sum_{k=1}^{N} \sigma_{G_k}^2 & \sum_{k=1}^{N} \sigma_{G_k H_k} \\ \sum_{k=1}^{N} \sigma_{G_k H_k} & \sum_{k=1}^{N} \sigma_{H_k}^2 \end{pmatrix} . \tag{81}$$

In the usual terminology of statistical texts, [1, p. 19] we say

$$\left(\sum_{k=1}^{N} G_k, \sum_{k=1}^{N} H_k \right)$$

is approximately distributed according to $N(0, A^{-1})$, for large N, where 0 is the zero vector.

Recalling the likelihood function F for a given set of a_i (successes), b_j (failures) as given by (1), we can also now write F (as given in Golub and Grubbs' paper, [14]) as

$$F = \prod_{k=1}^{N} p^{\delta_k} q^{1-\delta_k} = \prod_{k=1}^{N} f\left(\delta_k^{(r)}; \mu, \sigma\right) , \tag{82}$$

where f_k is defined in (64), (65). Thus the logarithm of F, which has been previously denoted by L, is

$$L = \sum_{k=1}^{N} \log f\left(\delta_k^{r}; \mu, \sigma\right), \tag{83}$$

and by (66), (67)

$$\frac{\partial L}{\partial \mu} = L_\mu = \sum_{k=1}^{N} G_k , \tag{84}$$

$$\frac{\partial L}{\partial \sigma} = L_\sigma = \sum_{k=1}^{N} H_k \ . \tag{85}$$

We conclude that the random variable

$$\left(\sum_{k=1}^{N} G_k, \sum_{k=1}^{N} H_k \right) = (L_\mu, L_\sigma) \ , \tag{86}$$

where (L_μ , L_σ) is approximately $N(0, A^{-1})$ for large N. Moreover, by (74), (75), (78), the matrix A^{-1} can be written in the form

$$A^{-1} = \begin{pmatrix} E(-L_{\mu\mu}) & E(-L_{\mu\sigma}) \\ E(-L_{\mu\sigma}) & E(-L_{\sigma\sigma}) \end{pmatrix} \ , \tag{87}$$

and for efficiency in notation we introduce that of Golub and Grubbs by writing

$$A^{-1} = \begin{pmatrix} A_{\mu\mu} & A_{\mu\sigma} \\ A_{\mu\sigma} & A_{\sigma\sigma} \end{pmatrix} \ . \tag{88}$$

We proceed by expanding L_μ and L_σ in Taylor series about the true values μ_o and σ_o and evaluate the series at $\bar{\mu}$, $\bar{\sigma}$, the maximum likelihood estimates. Thus,

$$L_\mu(\bar{\mu}, \bar{\sigma}) = L_\mu(\mu_o, \sigma_o) + L_{\mu\mu}(\mu_1, \sigma_1)(\bar{\mu} - \mu_o)$$

$$+ L_{\mu\sigma}(\mu_1, \sigma_1)(\bar{\sigma} - \sigma_o) \ ,$$

$$L_\sigma(\bar{\mu}, \bar{\sigma}) = L_\sigma(\mu_o, \sigma_o) + L_{\mu\sigma}(\mu_2, \sigma_2)(\bar{\mu} - \mu_o)$$

$$+ L_{\sigma\sigma}(\mu_2, \sigma_2)(\bar{\sigma} - \sigma_o) \ ,$$

where (μ_1, σ_1), (μ_2, σ_2) are on the open line segment of the straight line connecting $(\bar{\mu}, \bar{\sigma})$ and (μ_o, σ_o) in the $\mu\sigma$-plane.

Since $(\bar{\mu}, \bar{\sigma})$ is the point for which L is a maximum

$$L_\mu(\bar{\mu}, \bar{\sigma}) = L_\sigma(\bar{\mu}, \bar{\sigma}) = 0,$$

so that

$$L_\mu(\mu_o, \sigma_o) = (\bar{\mu} - \mu_o)[-L_{\mu\mu}(\mu_1, \sigma_1)] + (\bar{\sigma} - \sigma_o)[-L_{\mu\sigma}(\mu_1, \sigma_1)]$$

$$L_\sigma(\mu_o, \sigma_o) = (\bar{\mu} - \mu_o)[-L_{\mu\sigma}(\mu_2, \sigma_2)] + (\bar{\sigma} - \sigma_o)[-L_{\sigma\sigma}(\mu_2, \sigma_2)] . \tag{89}$$

Now (μ_1, σ_1) and (μ_2, σ_2) converge with probability one to (μ_o, σ_o) and the second derivatives on the right hand sides of (89) converge with probability one to their expected values, [16](vol. 2, 2nd Edition, page 55). Hence (89) may be regarded as a set of linear equations in the quantities $(\bar{\mu} - \mu_o)$ and $(\bar{\sigma} - \sigma_o)$. Using vector notation, and superscript T for transpose (89) becomes

$$A^{-1}.(\bar{\mu} - \mu_o, \bar{\sigma} - \sigma_o)^T = A^{-1}\theta = \lambda = (L_\mu, L_\sigma)^T, \tag{90}$$

where $$\theta = (\bar{\mu} - \mu_o, \bar{\sigma} - \sigma_o)^T,$$

and L_μ and L_σ on the right-hand side are evaluated at (μ_o, σ_o). The matrix A^{-1} always has an inverse provided $(\bar{\mu}, \bar{\sigma})$ and (μ_o, σ_o) are not the same. This follows by Theorem 2, since

$$\text{Determinant } (A^{-1}) = \Delta > 0. \tag{91}$$

Hence

$$A \cdot \lambda = \theta . \tag{92}$$

where λ is approximately distributed as $N(0,A^{-1})$, (see page 34). We also have by another theorem from multivariate analyses, [22; p.8]:

> If X, a row vector, is distributed according to $N(v,V)$, where v is a vector and V, as usual, is a covariance matrix, then the vector Y, given by
>
> $$Y = CX^T \text{ (for any nonsingular square matrix C)} \tag{93}$$
>
> is distributed according to $N(Cv^T, CVC^T)$.

Now for $X^T = \lambda$, we have that $v = 0$, $V = A^{-1}$, and for $Y = \theta$, $C = A$. So, we conclude from the above theorem (although details are omitted) that θ is approximately distributed

$$N(0,\ AA^{-1}A^T) = N(0,A^T) = N(0,A), \tag{94}$$

where we note that $A = A^T$ since $A^{-1} = (A^{-1})^T$. Thus, for

$$\theta = (\bar{\mu} - \mu_o, \bar{\sigma} - \sigma_o)^T, \tag{95}$$

the maximum likelihood estimators for large N are approximately bivariately normally distributed about the true parameter point (μ_o, σ_o) in the $\mu\sigma$-plane with covariance matrix A, the inverse of A^{-1} of (87) or (88). We identify the elements of A with superscripts

$$A = \begin{pmatrix} A^{\mu\mu} & A^{\mu\sigma} \\ A^{\mu\sigma} & A^{\sigma\sigma} \end{pmatrix} . \tag{96}$$

The elements $A^{\mu\mu}$ and $A^{\sigma\sigma}$ are called the asymptotic variances of μ and σ respectively and $A^{\mu\sigma}$ the asymptotic covariance of μ and σ.

To determine the confidence ellipse for a given confidence level γ, we consider the quadratic form occurring in the exponent of the joint normal density function. If an M-dimensional vector variable X is distributed according to N(v,V), the joint density function f(X) is

$$f(\bar{X}) = \frac{1}{(2\pi)^{M/2}|V|^{1/2}} \exp\left[-\frac{1}{2}(X - v)\cdot V^{-1}\cdot(X - v)^T\right]. \tag{97}$$

The quadratic form

$$(X - v)\cdot V^{-1}\cdot(X - v)^T \tag{98}$$

has a chi-square distribution with M degrees of freedom since X is N(v, V), [22; p. 417]. In our case, the relevant quadratic form is

$$\theta^T\cdot A^{-1}\cdot\theta\ . \tag{99}$$

From (88) and (95)

$$\theta^T\cdot A^{-1}\cdot\theta = \left[A_{\mu\mu}(\bar{\mu} - \mu_o)^2 + 2A_{\mu\sigma}(\bar{\mu} - \mu_o)(\bar{\sigma} - \sigma_o) + A_{\sigma\sigma}(\bar{\sigma} - \sigma_o)^2\right]\ . \tag{100}$$

The confidence ellipse at the confidence level γ, say $\gamma = 0.95$, is obtained by equating the expression in brackets in (100) to $\chi^2_{1-\gamma}$ where $\chi^2_{1-\gamma}$ is obtained from a χ^2 table, [19], [20], with two degrees of freedom [22; p. 417]. In practice, the maximum likelihood

estimates $\bar{\mu}$, $\bar{\sigma}$ are available, the true parameters are unknown. So the confidence ellipse

$$A_{\mu\mu}(\bar{\mu}-\mu)^2 + 2A_{\mu\sigma}(\bar{\mu}-\mu)(\bar{\sigma}-\sigma) + A_{\sigma\sigma}(\bar{\sigma}-\sigma)^2 = \chi^2_{1-\gamma} \quad (101)$$

is plotted where μ and σ are running coordinates on the ellipse with center at $(\bar{\mu}, \bar{\sigma})$. The positive real number γ denotes the probability that the true parameter point (μ_0, σ_0) lies in the interior of the ellipse in the μ-σ plane.

The coefficients $A_{\mu\mu}$, $A_{\mu\sigma}$, and $A_{\sigma\sigma}$ are easily computed if x_i/p_i and y_j/q_j (the notation of Section II) are available, say from a computing procedure for the determination of $(\bar{\mu}, \bar{\sigma})$ in which such quantities as L_α, L_β, are needed. One computes, in addition, the quantities (x_i/q_i) and (y_j/p_j) for each i and j. Then in the notation of earlier sections we have for computation of the coefficients of $\bar{\sigma}^2 A$:

$$\bar{\sigma}^2 A_{\mu\mu} = \sum_{i=1}^{n} \frac{x_i^2}{p_i q_i} + \sum_{j=1}^{m} \frac{y_j^2}{p_j q_j}, \quad (102)$$

$$\bar{\sigma}^2 A_{\mu\sigma} = \sum_{i=1}^{n} \frac{s_i x_i^2}{p_i q_i} + \sum_{j=1}^{m} \frac{t_j y_j^2}{p_j q_j}, \quad (103)$$

$$\bar{\sigma}^2 A_{\sigma\sigma} = \sum_{i=1}^{n} \frac{s_i^2 x_i^2}{p_i q_i} + \sum_{j=1}^{m} \frac{t_j^2 y_j^2}{p_j q_j}, \quad (104)$$

where all quantities are evaluated at $(\bar{\alpha}, \bar{\beta})$ or equivalently $(\bar{\mu}, \bar{\sigma})$.

Our computer program for the determination of $(\bar{\mu}, \bar{\sigma})$ includes the calculation for confidence ellipses at $\gamma = 0.50$ and $\gamma = 0.95$ with the computer output including the ellipses in plotted form. This computer program is described in the next section.

V. COMPUTER PROGRAM

In this section we describe the actual computer program that is used to obtain $\bar{\mu}, \bar{\sigma}$ and the associated confidence ellipses as discussed in the previous section. In addition, those computations where a loss of significant digits may occur are noted and their special treatment is discussed.

Two programs exist for use on the IBM 7030 (STRETCH) computer. One is written completely in FORTRAN IV and the other only partially with the remainder in STRAP, the STRETCH machine language. The programs are designed, as mentioned previously, only for the ordinary Newton-Raphson (N-R) procedure, although it would be easy to change the programs to accommodate the modified N-R algorithm as described in Section III. The programs as they are now set up with the ordinary N-R procedure have always converged globally.

We proceed with some details of the programs, (Reference is made to only one program hereafter since the programs mentioned above differ only in programming language.). It is assumed that the input is specified as two sets of real numbers $\{a_i\}, \{b_j\}$, where $i = 1, \ldots, n$, $j = 1, \ldots, m$. At the outset the program is called upon to insure that the necessary

and sufficient conditions for the existence of a unique point at which L attains a maximum are satisfied, i.e.,

$$a_{min} < b_{max} , \tag{105}$$

$$\frac{1}{m} \sum_{j=1}^{m} b_j < \frac{1}{n} \sum_{i=1}^{n} a_i , \tag{106}$$

where $a_{min} = \min(a_i)$ and $b_{max} = \max(b_j)$. By Theorem (4) of Section III if either (105) or (106) is not satisfied there do not exist maximum likelihood estimates $\bar{\mu}$, $\bar{\sigma}$. If this is the case, an exit is made in the program.

If (105) and (106) are both satisfied by the input, the program proceeds to obtain initial approximations α^*, β^* to $\bar{\alpha}$, $\bar{\beta}$. We use the following relations, although as mentioned above α^* and β^* can actually be chosen arbitrarily,

$$\alpha^* = \mu^*/\sigma^* = \frac{1}{2}\left(\frac{1}{n}\Sigma a_i + \frac{1}{m}\Sigma b_j\right) \Big/ \left[\frac{1}{n+m}\left(\Sigma a_i^2 + \Sigma b_j^2\right) - v^2\right]^{1/2}, \tag{107}$$

$$\beta^* = 1/\sigma^* = \left[\frac{1}{n+m}\left(\Sigma a_i^2 + \Sigma b_j^2\right) - v^2\right]^{-1/2}, \tag{108}$$

where

$$v = \frac{1}{n+m}\left(\Sigma a_i + \Sigma b_j\right) . \tag{109}$$

It is understood, as before, that the sums on i run from 1 to n and those on j from 1 to m. Certainly better initial approximations could

have been obtained with more extensive analysis, however, since the N-R algorithm is a second order procedure which has always converged globally for us, little need was felt for such refinements.

If α_k and β_k denote the k^{th} approximations to $\bar{\alpha}$ and $\bar{\beta}$, respectively, then the $(k+1)^{st}$ approximations by N-R are specified by

$$\alpha_{k+1} = \alpha_k + \Delta\alpha_k \tag{110}$$

$$\beta_{k+1} = \beta_k + \Delta\beta_k, \quad k = 0, 1, \ldots, \tag{111}$$

where $\Delta\alpha_k$ and $\Delta\beta_k$ are given by (55) with all partial derivatives evaluated at (α_k, β_k). The final form for the computation of the quantities that appear in (55) are given by (115) - (119). The iterations are terminated when

$$\left|\Delta\alpha_k\right| < \epsilon_1\alpha_k, \quad \left|\Delta\beta_k\right| < \epsilon_2\beta_k \tag{112}$$

are both satisfied for some $k \geqslant 1$. The parameters ϵ_1, ϵ_2 are prescribed as part of the input. They are presently set in the program at

$$\epsilon_1 = 2.5 \times 10^{-4} = \frac{1}{2}\ \epsilon_2 \ . \tag{113}$$

Upon convergence, the program is set to proceed with the calculation of the matrix elements of A which are needed for the confidence ellipses. The equation for a confidence ellipse is given by (101). The function $X^2_{1-\gamma}$ is known as the chi-squared distribution function with two degrees of freedom; it is tabulated for various

values of γ, [17, p. 424], [19]. Values outside these tables can be determined from the incomplete gamma function, e.g.[20]. A few commonly used values of $\chi^2_{1-\gamma}$, for two degrees of freedom, are listed:

γ	$1-\gamma$	$\chi^2_{1-\gamma}$
0.50	0.50	1.39
0.90	0.10	4.61
0.95	0.05	5.99
0.99	0.01	9.21

It was shown in the previous section that for sufficiently large samples one can assert, with preassigned confidence γ, that the true parameter point (μ_o, σ_o) lies somewhere in the interior of the ellipse given by (101), with $\chi^2_{1-\gamma}$ chosen appropriately, whose center is at $(\bar{\mu}, \bar{\sigma})$. The program at present is set to compute two ellipses, one for $\gamma = 0.50$ and another for $\gamma = 0.95$. They appear in graphical form as part of the output (Examples are given at the end of this section). We remark that in order to display these ellipses to advantage somewhat more than an elementary plotting code was required. For completeness, the details of the plotting code are given in Appendix B.

The quantities $A_{\mu\mu}$, $A_{\mu\sigma}$, $A_{\sigma\sigma}$ that are needed for the ellipses in (101) can be determined from (103) - (105). However, for efficiency of calculation, as described in the next paragraph, the actual equations used in place of (103) - (105) are (120) - (122).

For efficiency, the program is designed to take advantage of the situation when some of the a_i are repeated, and likewise for the b_j. The a_i (and also b_j) are sifted so that only those a_i which are different are listed and with each such a_i an integer n(i) is also listed which denotes the number of times a_i appears as an input. For b_j the corresponding integer is denoted by m(j). One can then take advantage of the fact that the expressions for L_α, L_β, $L_{\alpha\alpha}$, $L_{\alpha\beta}$, $L_{\beta\beta}$ are linear sums in quantities such as (x_i/p_i) and (y_j/q_j) so that these quantities need only be computed for the different a_i or b_j and multiplied by n(i) or m(j), respectively. With this point of view, we introduce some additional notation and re-write all the pertinent equations as actually used in the program.

Let the k^{th} different a_i be denoted by a(k) and the r^{th} different b_j by b(r). Let K and R denote the total number of different a_i and b_j, respectively, so that

$$n = \sum_{k=1}^{K} n(k), \qquad m = \sum_{r=1}^{R} m(r), \tag{114}$$

where n, m have their usual meaning. The basic equations for the program then can be written as follows:

$$L_\alpha = \sum_{r=1}^{R} m(r)(y_r/q_r) - \sum_{k=1}^{K} n(k)(x_k/p_k) \tag{115}$$

$$L_\beta = \sum_{k=1}^{K} n(k)a(k)(x_k/p_k) - \sum_{r=1}^{R} m(r)b(r)(y_r/q_r) \tag{116}$$

$$L_{\alpha\alpha} = -\sum_{r=1}^{R} m(r)\,(y_r/q_r)\,(y_r/q_r - t_r) - \sum_{k=1}^{K} n(k)\,(x_k/p_k)\,(s_k + x_k/p_k) \qquad (117)$$

$$L_{\alpha\beta} = \sum_{k=1}^{K} n(k)\,a(k)\,(x_k/p_k)\,(s_k + x_k/p_k) + \sum_{r=1}^{R} m(r)\,b(r)\,(y_r/q_r)\,(y_r/q_r - t_r) \qquad (118)$$

$$L_{\beta\beta} = -\sum_{r=1}^{R} m(r)\,b^2(r)\,(y_r/q_r)\,(y_r/q_r - t_r) - \sum_{k=1}^{K} n(k)\,a^2(k)\,(x_k/p_k)\,(s_k + x_k/p_k) \qquad (119)$$

$$\sigma^2 A_{\mu\mu} = \sum_{k=1}^{K} n(k)\,(x_k/p_k)\,(x_k/q_k) + \sum_{r=1}^{R} m(r)\,(y_r/p_r)\,(y_r/q_r) \qquad (120)$$

$$\sigma^2 A_{\mu\sigma} = \sum_{k=1}^{K} n(k)\,s_k\,(x_k/p_k)\,(x_k/q_k) + \sum_{r=1}^{R} m(r)\,t_r\,(y_r/p_r)\,(y_r/q_r) \qquad (121)$$

$$\sigma^2 A_{\sigma\sigma} = \sum_{k=1}^{K} n(k)\,s_k^2\,(x_k/p_k)\,(x_k/q_k) + \sum_{r=1}^{R} m(r)\,t_r^2\,(y_r/p_r)\,(y_r/q_r)\,, \qquad (122)$$

where

$$s_k = a(k)\beta - \alpha$$

$$t_r = b(r)\beta - \alpha\,.$$

The total number of different a_i and b_j, K+R, is limited by the storage capacity of STRETCH to

$$K+R \leqslant 10{,}000.$$

Care must be exercised in maintaining accuracy throughout the calculations. For example, a straight-forward computation of the quantity $(x/p)[s + x/p]$, for a given a_i, will not yield an accurate result for large negative values of s. The difficulty arises because (x/p) approaches (-s) so that the quantity in square brackets is subject to a loss of its leading digits. The result may be subsequently multiplied by a large quantity x/p (or $a_i(x/p)$, $a_i^2(x/p)$) thus leading to a large error. This difficulty is easy to remedy by simply replacing (x/p) by an asymptotic expansion whose leading term is (-s) and replacing the quantity in square brackets by this asymptotic expansion with the first term (-s) removed. Similar care must be taken with the quantity $(y/q)(y/q-t)$. Losses in accuracy of this nature are one possible cause for the reported divergence of the N-R algorithm. Another may be that most subroutines for computing probability integrals retain very little accuracy over some parts of the domain $(-\infty,\infty)$. For our program, extensive efforts were made to compute probability integrals to high accuracy over the entire domain. Originally, a table of probability integrals was stored at equal increments in the argument of .0025 for the interval [-8,8], and two asymptotic series in inverse powers of the argument, each containing 27 terms, were used to evaluate (x/p) and (s+x/p) for arguments larger in absolute value than 8. In this way, all individual terms were computed to an accuracy of nearly 13 significant digits on STRETCH which uses 14 digits. Recently, however,

a method for computing p(s) (and q(s)) was published by Cody, [5] which gives, on STRETCH, at least twelve significant digits for all $s \in (-\infty, \infty)$. Cody's method was used as a basis for subroutines, after suitable modifications for the computation of $s + x/p$ for large values of s, which supplanted the table and two asymptotic series mentioned above. This resulted in a large reduction in storage requirements with no significant loss in accuracy or computing speed.

The running time for the STRETCH Fortran IV program with the tolerances chosen as in (113) averages about .007 seconds per every different item of input, i.e., a(k) or b(r). Thus the average computing time per case is about .007(K+R). The average computing time for the other program which uses some STRAP language is about .0055(K+R). These rough estimates do not include the time for plotting the confidence ellipses which are done off-line.

The output as generated off-line from a STRETCH tape is shown for 14 cases at the end of this section. Each output sheet lists, starting in the upper left-hand corner, an identification number, e.g. No. 111B, followed down the page by a listing of the different a_i and b_j and the number of times each occurs, e.g., in Case I-3-17-70, (p.61), $a_1 = -4$ occurs 6 times as input and b(3) = -5.5 occurs 4 times. Toward the top center the maximum likelihood estimates $\bar{\mu}$, $\bar{\sigma}$ are identified as mu and sigma, respectively. Below these quantities, the elements of the covariance matrix are recorded followed by the starting values α^*, β^* and μ^*, σ^* which are identified by alpha*, beta*, mu*, sigma*, respectively. Then,

a listing of the Newton-Raphson increments, for each successive iteration, $\Delta\alpha$, $\Delta\beta$, written as delta alpha, delta beta, are given as well as the associated value of F (The column is indicated incorrectly with L instead of F where F is given by (2)). Finally the two confidence ellipses are shown, at the 95% and 50% confidence levels, in the $\mu\sigma$-plane. These ellipses are constrained to a circumscribed square. The plotting was carried out so that the two axes of the ellipses lie on the diagonals of the square. The details of this graphical construction are given in Appendix B.

The various cases which are used as examples are drawn from shell penetration tests or biological experiments. In a number of the cases, the confidence ellipses include regions where σ is negative. This can probably be interpreted to mean that the sample size is too small for approximating a "large" sample. It is recalled from the previous section that the analysis for confidence ellipses was based on the hypothesis that N, the sample size, approached infinity.

Some cases are duplicated to give emphasis to the fact that N-R appears to converge globally. In particular, case No. 2A was reported in [21] to diverge. The results of case 2A are shown for four different sets of starting values. These results clearly show convergence.

Case No. 3 was taken from [14]. No. 111 and 117 are taken from NWL shell penetration tests. No. 1 is taken from [18]. Our results agree very closely with theirs. Case Jan. 19, 1970, obtained from [4],

was used to compare our results with those obtained from Finney's probit analysis. (Appendix C is devoted to a discussion of probit analysis as an alternative method for obtaining estimates of μ_o and σ_o.) Case No. 386 was supplied by Dr. Marlin Thomas. The confidence ellipses for this case also suggest that there is insufficient data for the asymptotic analysis of the previous section to apply. The remaining cases are included to give further indications of the global convergence properties of the N-R algorithm.

NO 2 A

NO.	A	NO.	B
1	.18500E+02	1	.37300E+01
1	.90500E+01	1	.37200E+01
1	.86000E+01		
1	.63000E+01		
1	.65000E+01		
1	.37200E+01		

MU= .393798E+01 SIGMA= .501148E+00

COVARIANCE MATRIX .454600E-00 .772683E+00

.772683E+00 .189650E+01

ALPHA*=.132742E+01 BETA*=.215200E-00 MU*=.616833E+01 SIGMA*=.464685E+01

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1	.651737E-01	.130657E-00	.169614E-01
2	.107884E+01	.248035E-00	.661476E-01
3	.129947E+01	.318814E-00	.101234E-00
4	.123131E+01	.317062E-00	.128409E-00
5	.970948E+00	.258911E-00	.141037E-00
6	.808594E+00	.216758E-00	.144954E-00
7	.688459E+00	.183388E-00	.146085E-00
8	.352247E-00	.946073E-01	.146366E-00
9	.107026E-00	.287469E-01	.146397E-00
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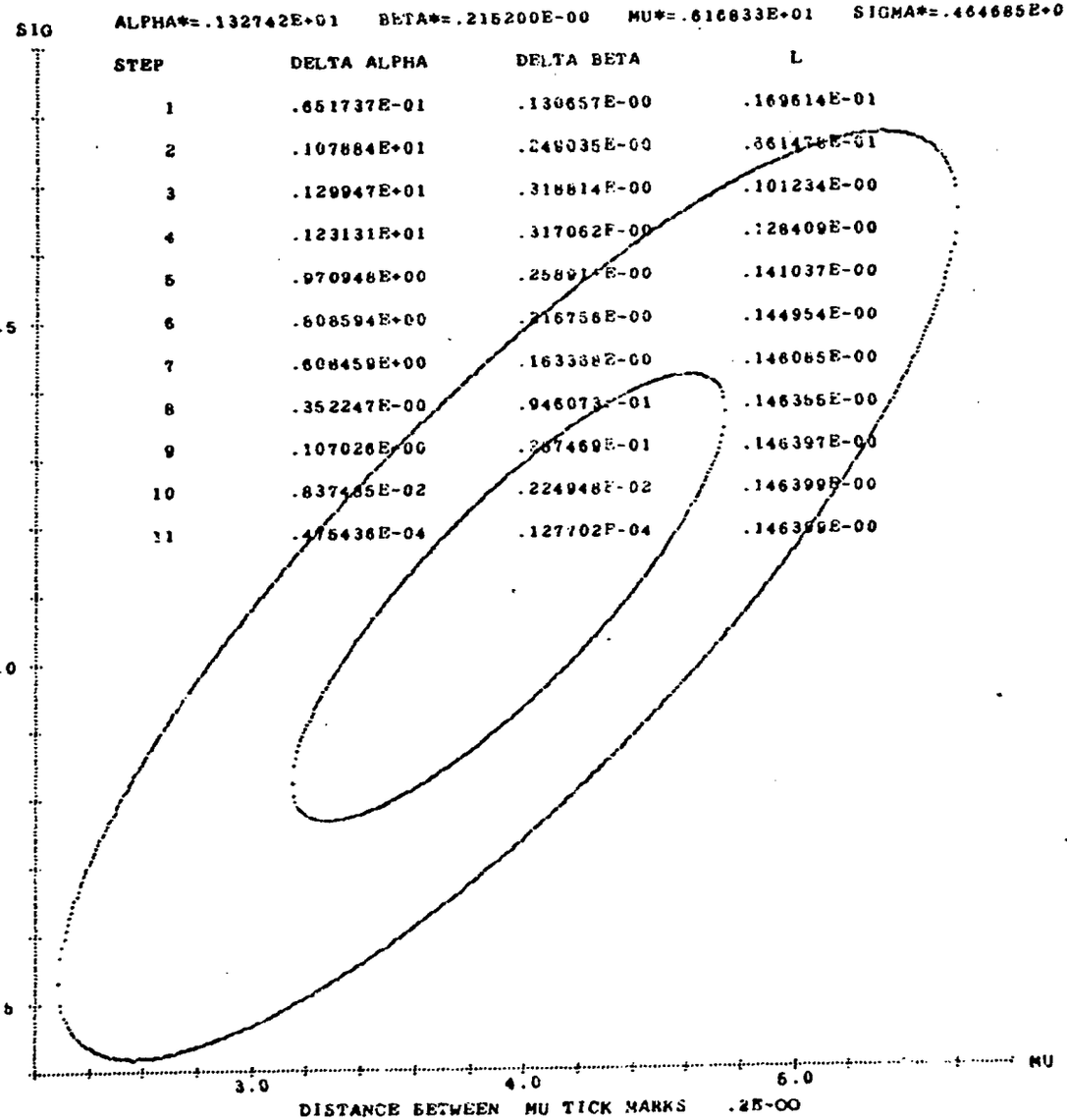
11	.476436E-04	.127702E-04	.146399E-00



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SIG= -.300000E+01

NO 2 A

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1	.90500E+01	1	.37200E+01
1	.86000E+01		
1	.63000E+01		
1	.55000E+01		
1	.37200E+01		

MU= .393798E+01 SIGMA= .501148E+00

COVARIANCE MATRIX .464460E-00 .772356E+00

.772356E+00 .189573E+01

ALPHA*=.100000E+06 BETA*=.100000E+03 MU*= 100000E+04 SIGMA*=.100000E-01

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2	.605884E+01	381244E-00	.14016[illegible]-09
3	.487519E-00	.178342E-00	.478841E-01
4	.115535E+01	.2[illegible]3419E-00	.916984E-01
5	.133879E+01	.5[illegible]8703E-00	.120973E-00
6	.102493E+01	.[illegible]72086E-00	.138590E-00
7	.860762E+00	.230506E-00	.144203E-00
8	.675430E+00	.181290E-00	.145882E-00
9	.435652E-00	.117003E-00	.146313E-00
10	.171[illegible]06E-00	.459314E-01	.146393E-00
11	.224080E-01	.[illegible]01876E-02	.146[illegible]9E-00
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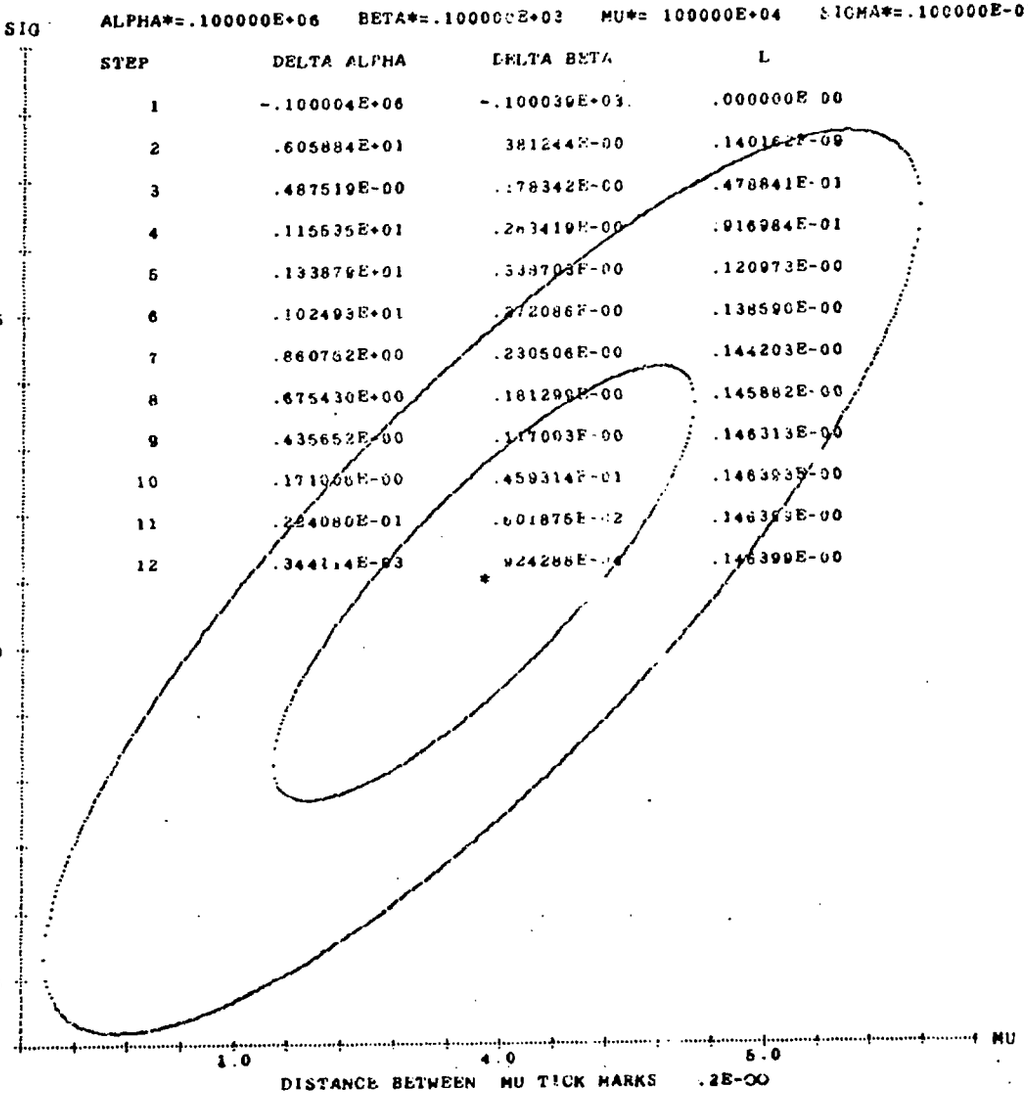

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DISTANCE BETWEEN SIG TICK MARKS .5E-00

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SIG= -.300000E+01

NO 2 A

NO.	A	NO.	B
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1	.90500E+01	1	.37200E+01
1	.86000E+01		
1	.63000E+01		
1	.55000E+01		
1	.37200E+01		

MU= .393798E+01 SIGMA= .601148E+00

COVARIANCE MATRIX .454694E-00 .772667E+00

.772667E+00 .189546E+01

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1	.199832E+04	-.100462E+03	.000000E 00
2	.167209E+01	.679076E-00	.419140E-17
3	.408566E-00	.110303E-00	.109798E-01
4	.896046E+00	.180674E-00	.323106E-01
5	.122962E+01	.266240E-00	.632492E-01
6	.129382E+01	.316115E-00	.100096E-00
7	.124616E+01	.320112E-00	.127605E-00
8	.976976E+00	.260419E-00	.140785E-00
9	.815092E+00	.218474E-00	.144878E-00
10	.616861E+00	.165619E-00	.146065E-00
11	.362427E-00	.973411E-01	.146351E-00
12	.113958E-00	.306088E-01	.146397E-00
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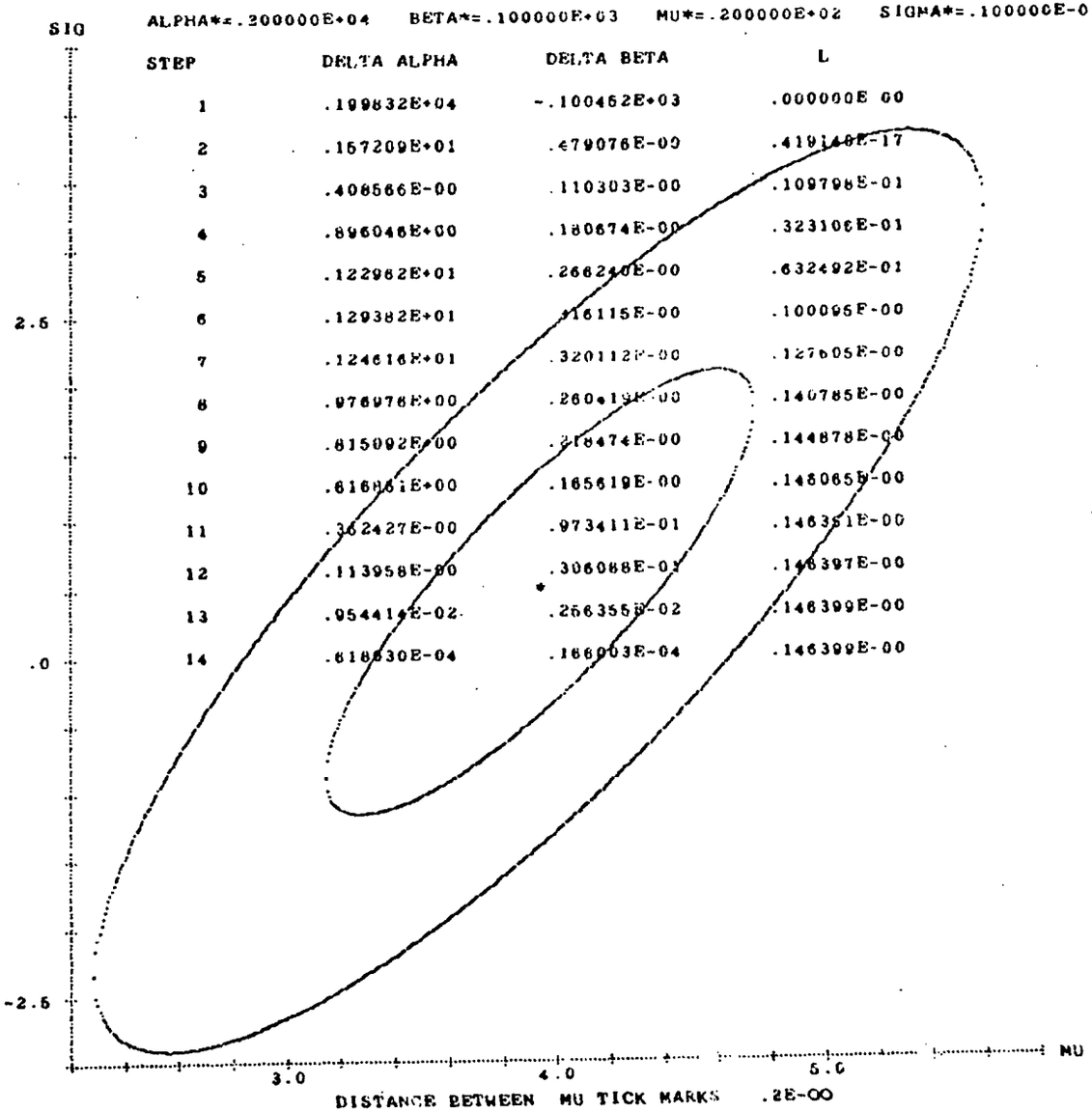

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.5E-00

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SIG= -.300000E+01

DISTANCE BETWEEN MU TICK MARKS .2E-00

NO 2 A

NO.	A	NO.	B
1	.18500E+02	1	.37300E+01
1	.90500E+01	1	.37200E+01
1	.86000E+01		
1	.63000E+01		
1	.55000E+01		
1	.37200E+01		

MU= .393798E+01 SIGMA= .501148E+00

COVARIANCE MATRIX .454498E-00 .772439E+00

.772439E+00 .189593E+01

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STEP	DELTA ALPHA	DELTA BETA	L
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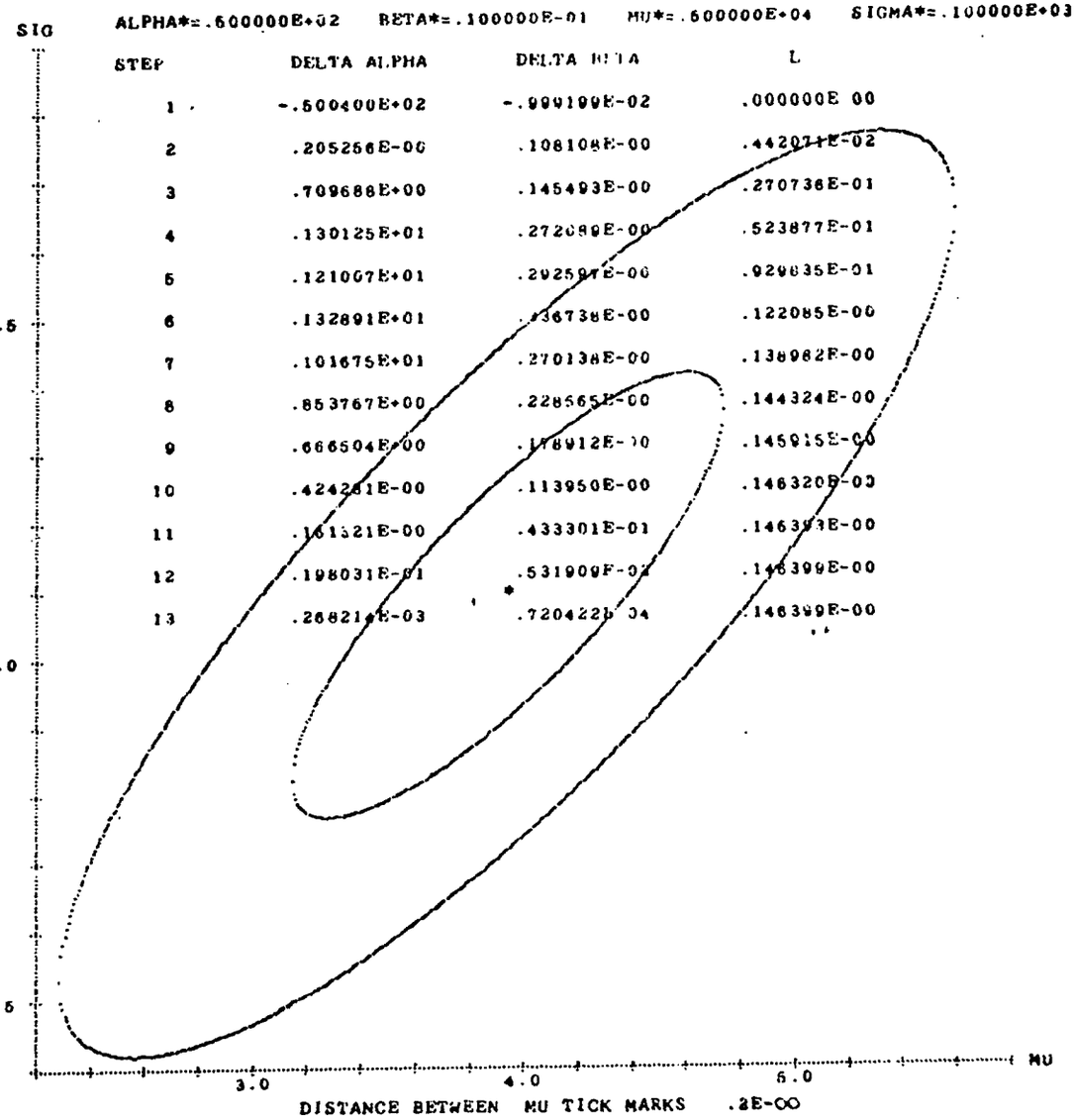
2	.205256E-00	.108108E-00	.442071E-02
3	.709688E+00	.145493E-00	.270736E-01
4	.130125E+01	.272089E-00	.523877E-01
5	.121007E+01	.292597E-00	.929835E-01
6	.132891E+01	.336738E-00	.122085E-00
7	.101675E+01	.270138E-00	.138982E-00
8	.853767E+00	.228565E-00	.144324E-00
9	.666504E+00	.178912E-00	.145915E-00
10	.424281E-00	.113950E-00	.146320E-00
11	.161521E-00	.433301E-01	.146393E-00
12	.198031E-01	.531909E-02	.146399E-00
13	.268214E-03	.720422E-04	.146399E-00



DISTANCE BETWEEN SIG TICK MARKS
.5E-00

ORIGIN MU= .220000E+01
SIG= -.300000E+01

DISTANCE BETWEEN MU TICK MARKS .2E-00

NO 3

NO.	A	NO.	B
1	.24530E+04	1	.24330E+04
1	.24230E+04	1	.24150E+04
		1	.24160E+04

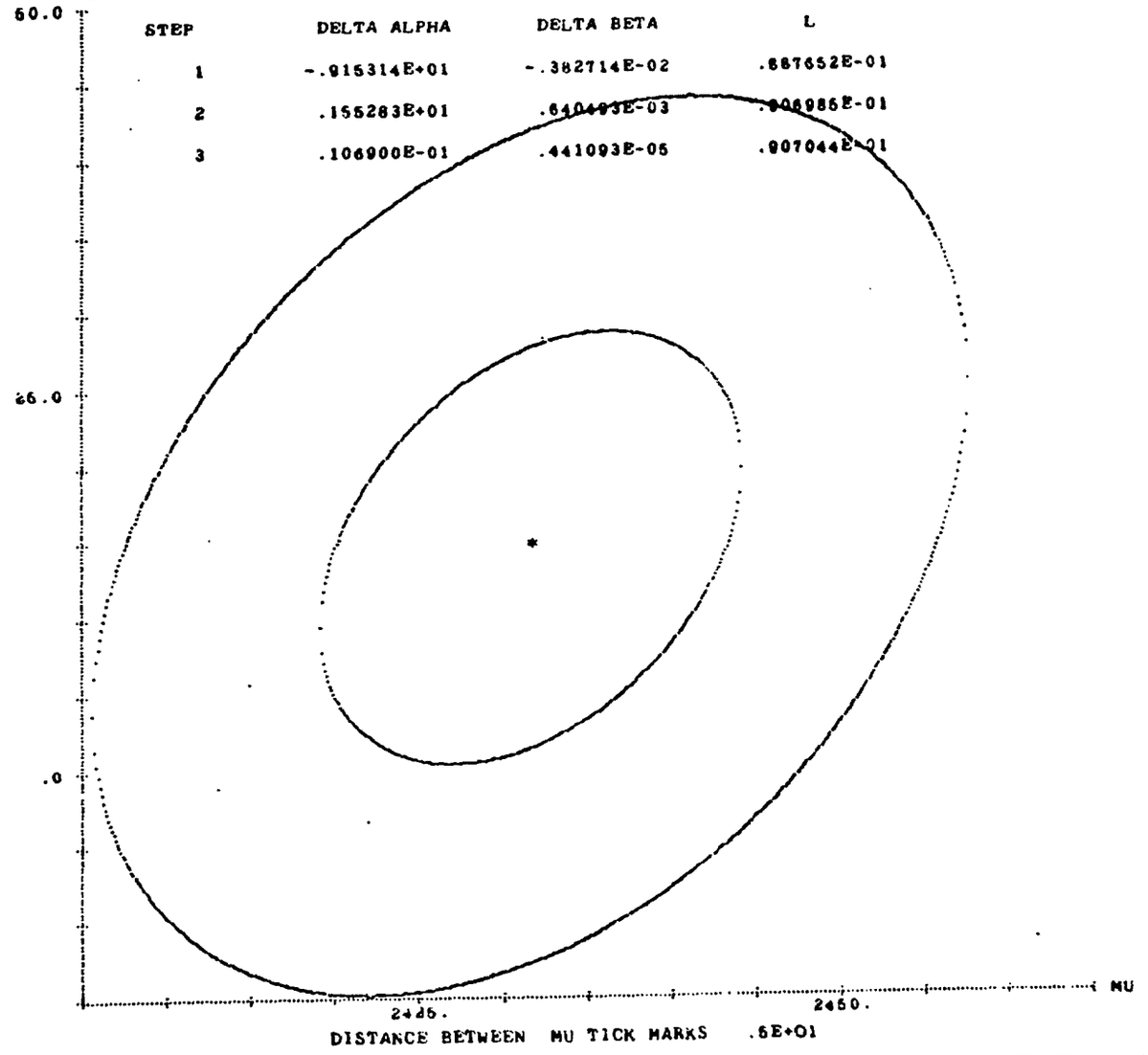
MU= .243161E+04 SIGMA= .148075E+02

COVARIANCE MATRIX .112601E+03 .465725E+02

.465725E+02 .143880E+03

ALPHA*=.170703E+03 BETA*=.702824E-01 MU*=.242950E+04 SIGMA*=.142324E+02

STEP	DELTA ALPHA	DELTA BETA	L
1	-.915314E+01	-.382714E-02	.887652E-01
2	.155283E+01	.640403E-03	.886986E-01
3	.106900E-01	.441093E-05	.887044E-01



DISTANCE BETWEEN MU TICK MARKS .5E+01

DISTANCE BETWEEN SIG TICK MARKS .5E+01

ORIGIN MU= .240500E+04
SIG= -.150000E+02

NO 111

NO.	A	NO.	B
1	.28540E+04	1	.26520E+04
1	.28360E+04	1	.27410E+04
1	.27670E+04	1	.28460E+04
1	.28140E+04	1	.27130E+04
1	.28010E+04	1	.28060E+04
1	.27920E+04	1	.27700E+04
1	.28200E+04	1	.27760E+04
1	.27410E+04	1	.27630E+04
1	.27670E+04	1	.27060E+04
1	.27610E+04	1	.27350E+04
1	.27320E+04	1	.25200E+04
1	.27730E+04	1	.26370E+04
1	.29110E+04	1	.26810E+04
1	.28240E+04	1	.26620E+04
1	.28590E+04	1	.27610E+04
1	.27460E+04	1	.28540E+04
1	.27580E+04	1	.28560E+04
1	.28480E+04		
1	.28860E+04		
1	.28920E+04		
1	.28770E+04		
1	.28560E+04		
1	.28240E+04		

DISTANCE BETWEEN SIG TICK MARKS
1.0E+01

ORIGIN MU= .271000E+04
SIG= .100000E+02

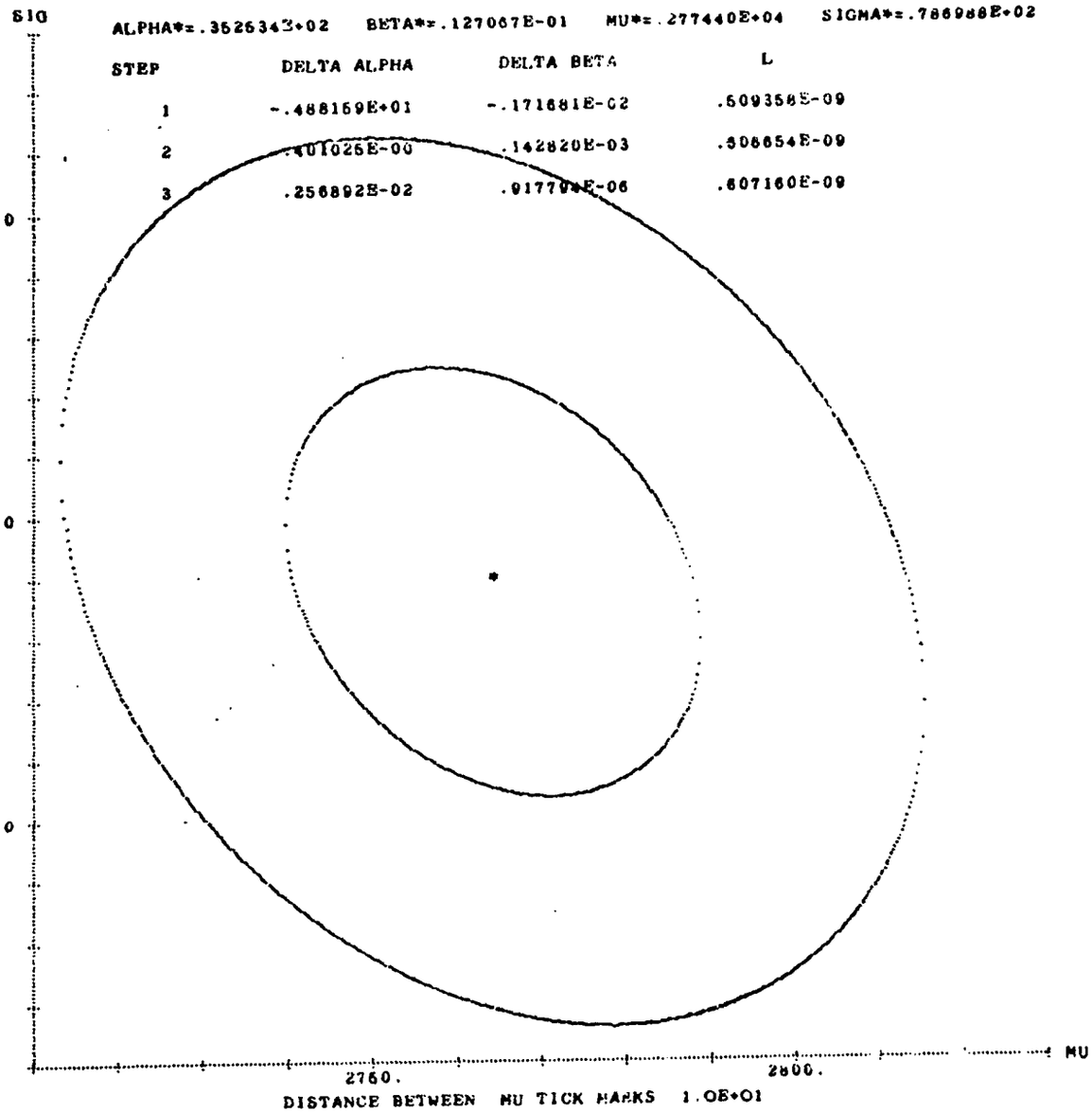
MU= .276419E+04 SIGMA= .898181E+02

COVARIANCE MATRIX .433097E+03 -.176654E+03

-.176654E+03 .893308E+03

ALPHA*=.3526343+02 BETA*=.127067E-01 MU*=.277440E+04 SIGMA*=.786988E+02

STEP	DELTA ALPHA	DELTA BETA	L
1	-.488159E+01	-.171681E-02	.509356E-09
2	-.401026E-00	.142820E-03	.508654E-09
3	.256892E-02	.91770*E-06	.507160E-09



DISTANCE BETWEEN MU TICK MARKS 1.0E+01

NO 117

NO.	A	NO.	B
1	.24810E+04	1	.24430E+04
1	.25050E+04	1	.24860E+04
1	.25330E+04	1	.24630E+04
		1	.24800E+04
		1	.25050E+04
		1	.26000E+04
		1	.26000E+04

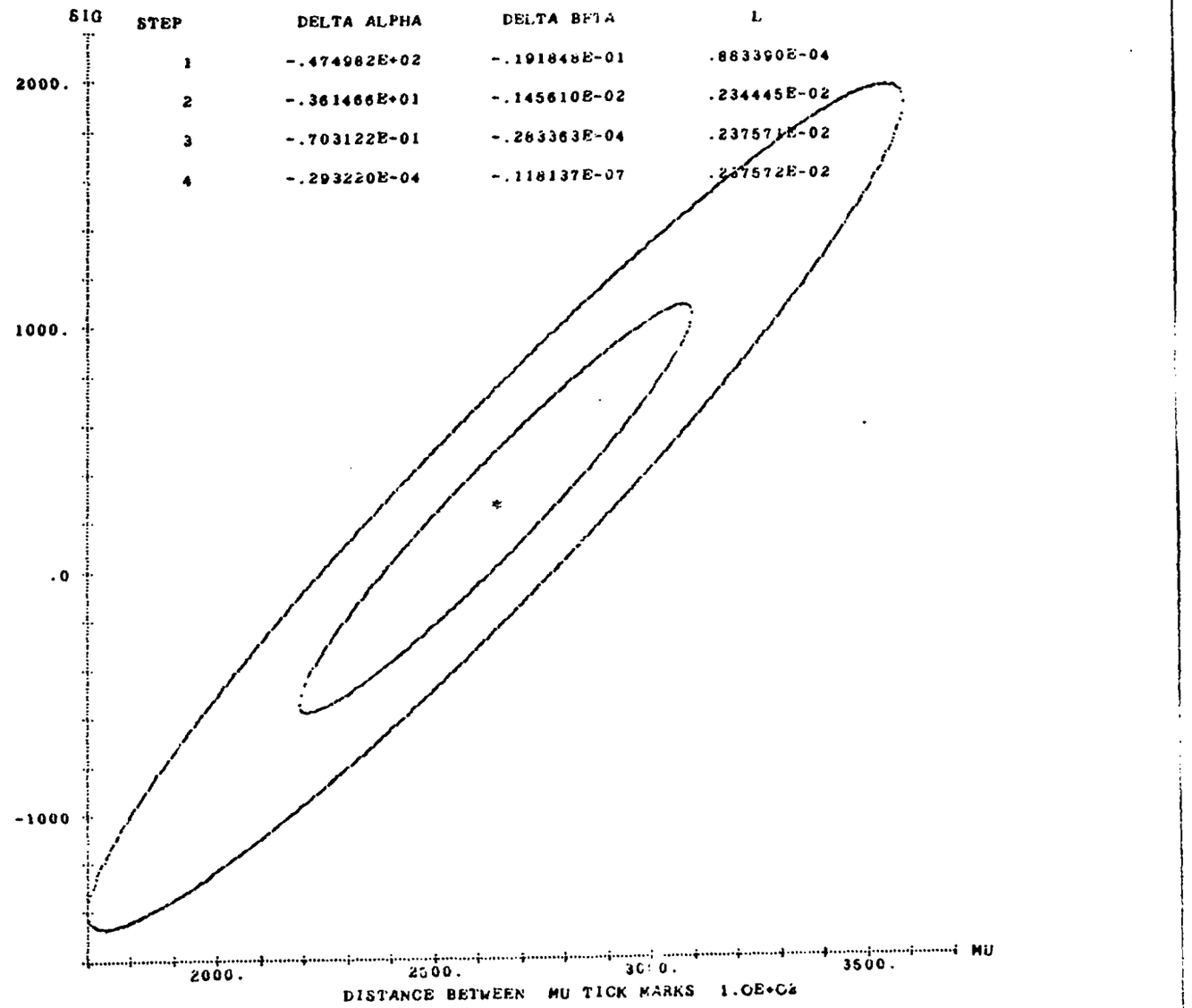
MU= .264040E+04 SIGMA= .264301E+03

COVARIANCE MATRIX .147312E+06 .257502E+06

.257502E+06 .490998E+06

ALPHA*=.611733E+02 BETA*=.244628E-01 MU*=.250169E+04 SIGMA*=.4[illegible]951E+02

STEP	DELTA ALPHA	DELTA BETA	L
1	-.474982E+02	-.191848E-01	.883390E-04
2	-.361466E+01	-.145610E-02	.234445E-02
3	-.703122E-01	-.283363E-04	.23757[illegible]E-02
4	-.293220E-04	-.118137E-07	.2[illegible]7572E-02



DISTANCE BETWEEN SIG TICK MARKS
.2E+03

ORIGIN MU= .170000E+04
SIG= -.160000E+04

NO 1

NO.	A	NO.	B
1	-.00000E 00	1	-.00000E 00
1	-.10000E+01	6	-.10000E+01
		11	-.20000E+01

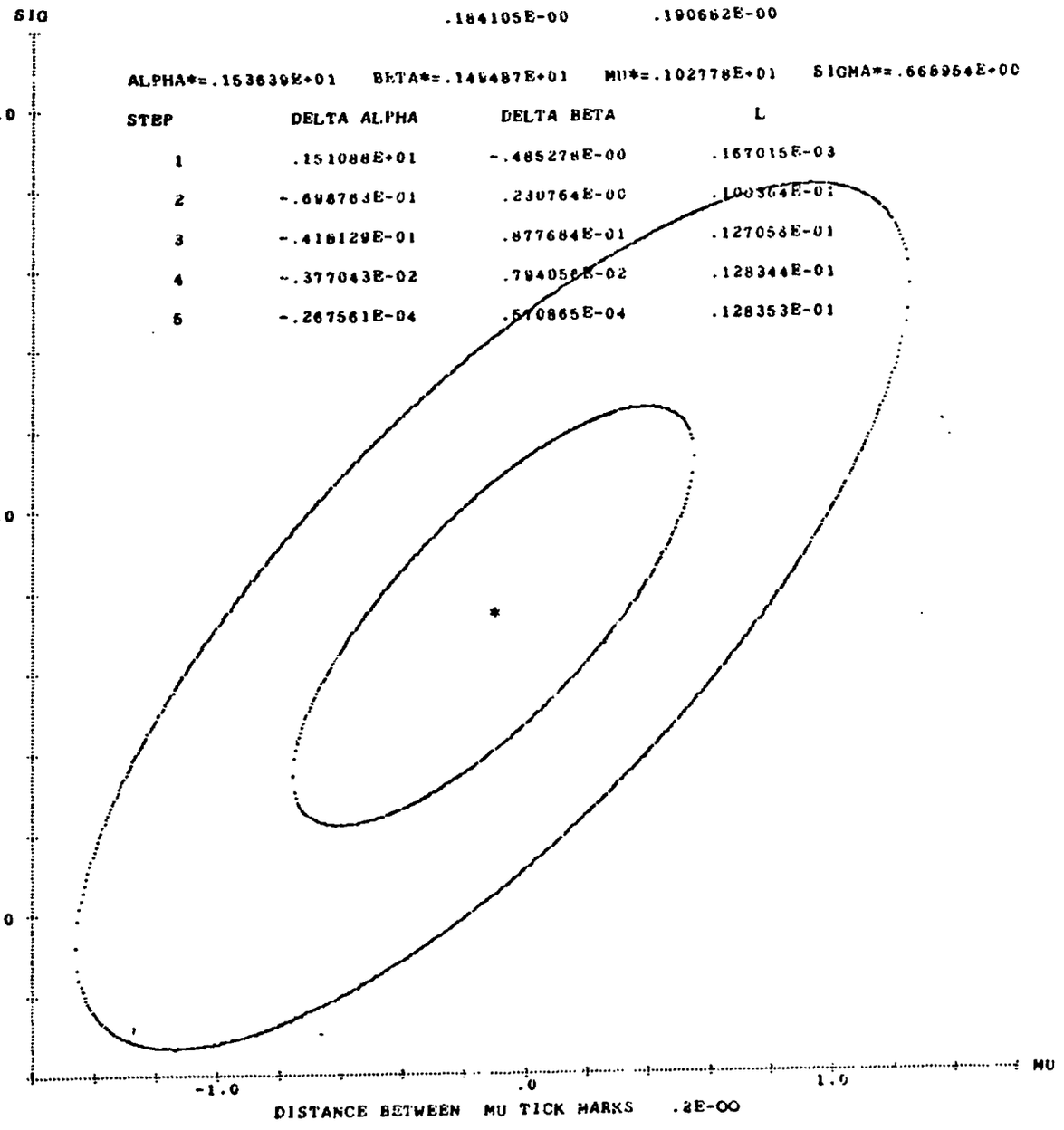
MU=-.105379E-00 SIGMA= .748435E+00

COVARIANCE MATRIX .305685E-00 .184105E-00

.184105E-00 .190662E-00

ALPHA*=.153639E+01 BETA*=.149487E+01 MU*=.102778E+01 SIGMA*=.666954E+00

STEP	DELTA ALPHA	DELTA BETA	L
1	.151088E+01	-.485278E-00	.167015E-03
2	-.698763E-01	.230764E-00	.100304E-01
3	-.416129E-01	.877684E-01	.127058E-01
4	-.377043E-02	.794056E-02	.128344E-01
5	-.267561E-04	.570865E-04	.128353E-01



DISTANCE BETWEEN SIG TICK MARKS
.2E-00

ORIGIN MU= -.160000E+01
SIG= -.400000E-00

DISTANCE BETWEEN MU TICK MARKS .2E-00

JAN. 19, 1970

NO.	A	NO.	B
1	.95424E+00	4	.77814E+00
3	.10000E+01	4	.95424E+00
3	.10432E+01	6	.10000E+01
7	.10792E+01	3	.10432E+01
6	.13979E+01	1	.10792E+01
6	.16990E+01		

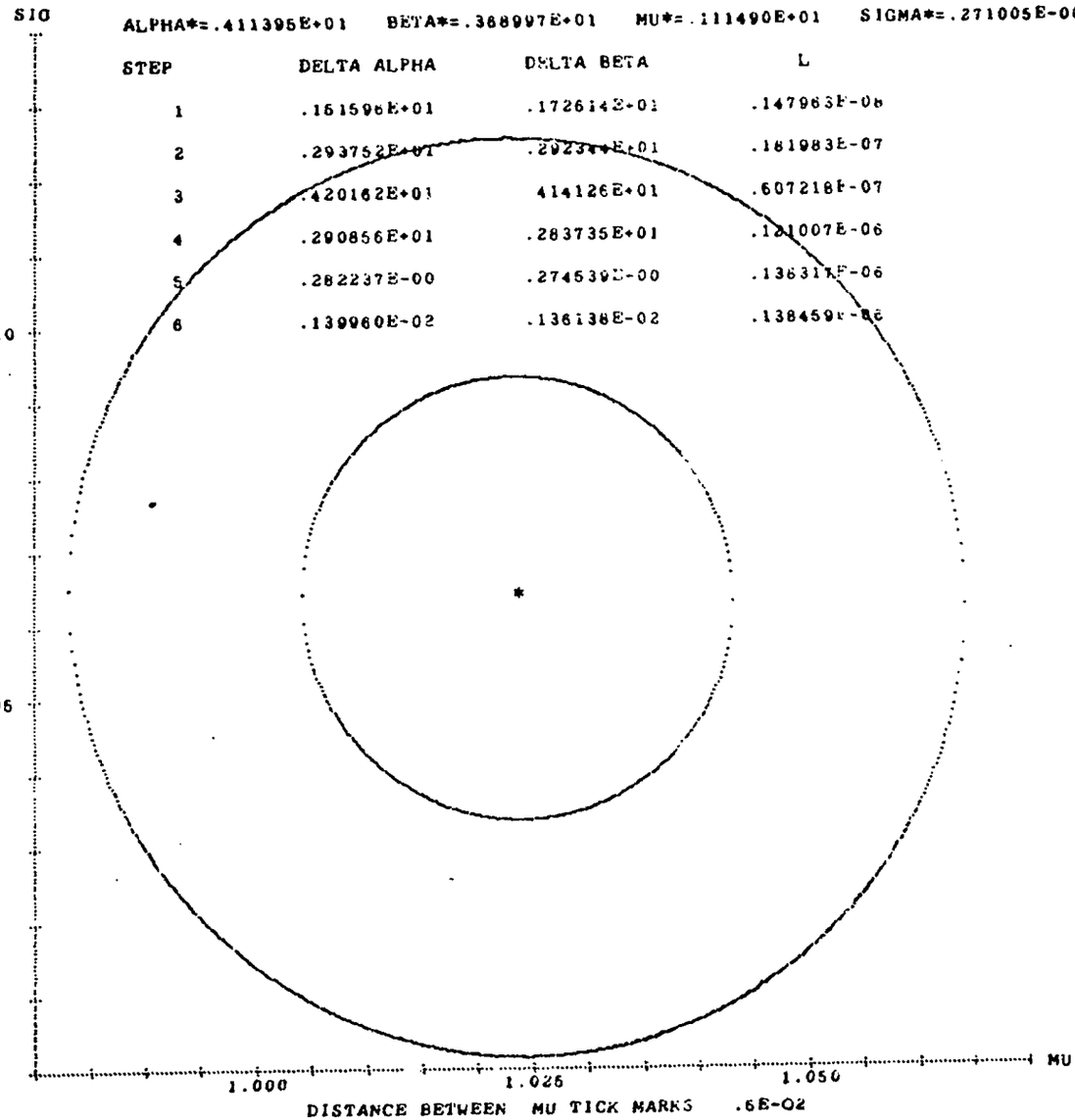
MU= .102355E+01 SIGMA= .641270E-01

COVARIANCE MATRIX .273186E-03 -.984218E-05

-.984218E-05 .638129E-03

ALPHA*=.411395E+01 BETA*=.388997E+01 MU*=.111490E+01 SIGMA*=.271005E-00

STEP	DELTA ALPHA	DELTA BETA	L
1	.161596E+01	.172614E+01	.147963E-06
2	.293752E+01	.292344E+01	.181983E-07
3	.420162E+01	.414126E+01	.607218E-07
4	.290856E+01	.283735E+01	.121007E-06
5	.282237E-00	.274639E-00	.136317E-06
6	.139960E-02	.136138E-02	.138459E-06



DISTANCE BETWEEN SIG TICK MARKS
.1E-01

ORIGIN MU= .980000E+00
SIG= .000000E 00

DISTANCE BETWEEN MU TICK MARKS .5E-02

CASE 386

NO.	A	NO.	B
1	.35500E+01	1	.24600E+01
1	.39100E+01	1	.28400E+01
1	.43300E+01	1	.40000E+01
1	.53900E+01	1	.40000E+01
		1	.56700E+01
		1	.67400E+01

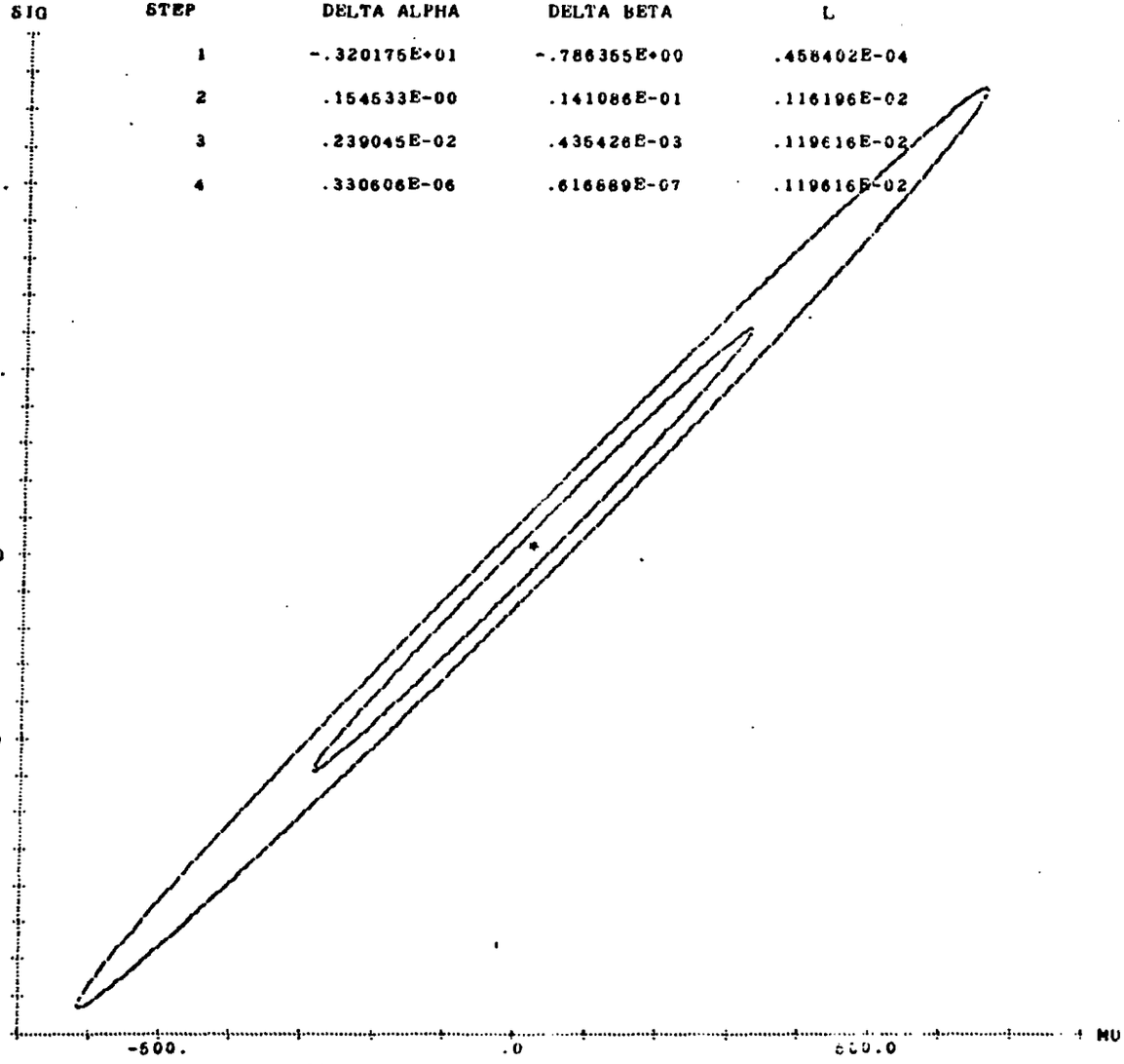
MU= .186437E+02 SIGMA= .667143E+02

COVARIANCE MATRIX .669864E+05 .262343E+06

.262343E+06 .103643E+07

ALPHA*=.337355E+01 BETA*=.789443E+00 MU*=.427333E+01 SIGMA*=.126672E+01

STEP	DELTA ALPHA	DELTA BETA	L
1	-.320175E+01	-.786365E+00	.458402E-04
2	.154533E-00	.141086E-01	.116196E-02
3	.239045E-02	.435428E-03	.119616E-02
4	.330606E-06	.616689E-07	.119616E-02



DISTANCE BETWEEN SIG TICK MARKS .2E+03

ORIGIN MU= -.700000E+03
SIG= -.260000E+04

DISTANCE BETWEEN MU TICK MARKS 1.0E+02

CASE 1

NO.	A	NO.	B
2	.41670E+02	6	.27100E+02
11	.58330E+02	9	.41670E+02
9	.81670E+02	10	.58330E+02
6	.11433E+03	1	.81670E+02

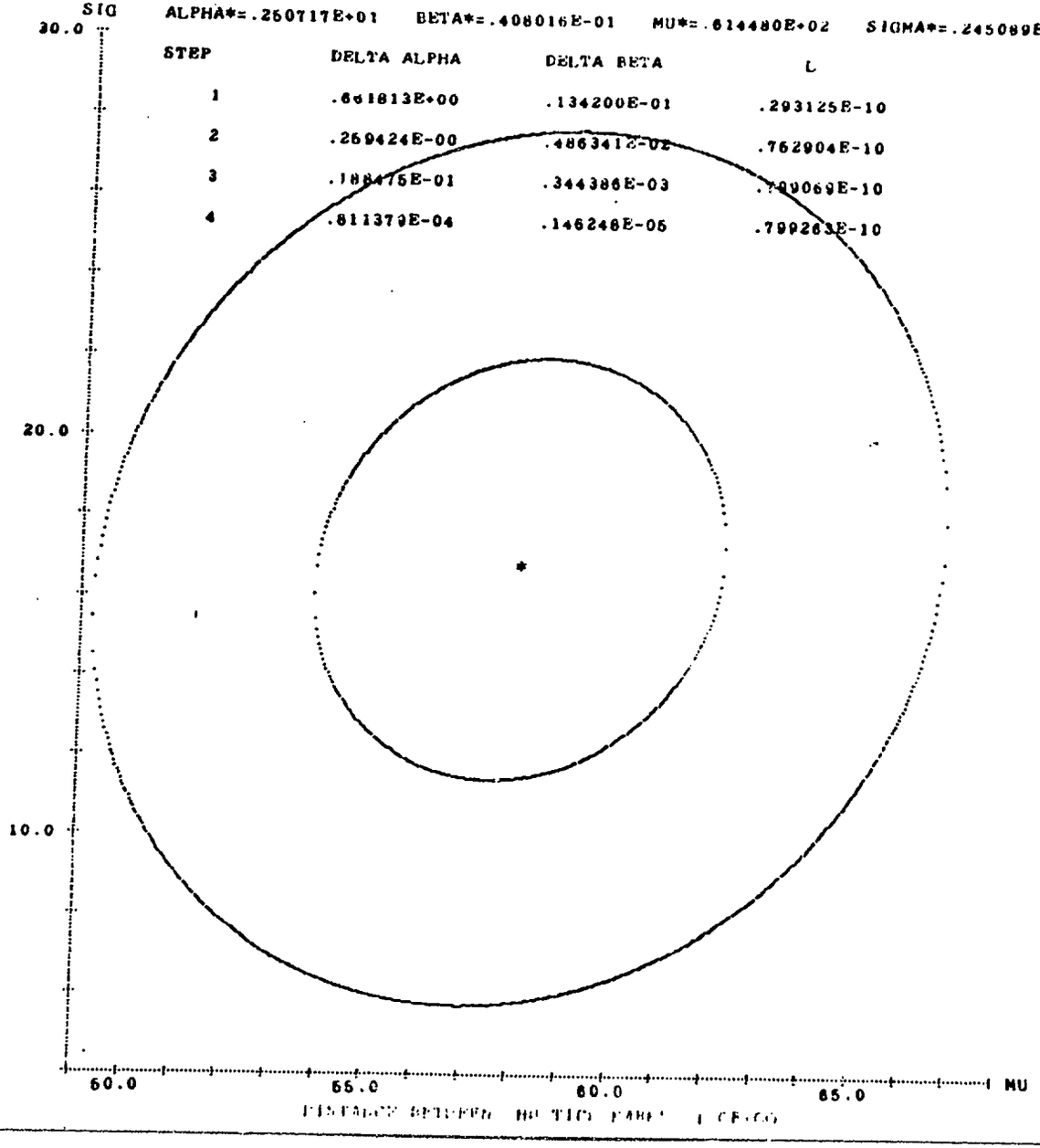
MU= .580059E+02 SIGMA= .168263E+02

COVARIANCE MATRIX .128403E+02 .185896E+01

.185896E+01 .199461E+02

ALPHA*=.250717E+01 BETA*=.408016E-01 MU*=.614480E+02 SIGMA*=.245089E+02

STEP	DELTA ALPHA	DELTA BETA	L
1	.661813E+00	.134200E-01	.293125E-10
2	.259424E-00	.4863412-02	.762904E-10
3	.1884?5E-01	.344386E-03	.789069E-10
4	.811379E-04	.146248E-05	.799263E-10



DISTANCE BETWEEN SIG TICK MARKS
.2E+01

ORIGIN MU= .490000E+02
SIG= .400000E+01

CASE 1

NO.	A	NO.	B
2	.41670E+02	6	.27100E+02
11	.58330E+02	9	.41670E+02
9	.81670E+02	10	.58330E+02
6	.11433E+03	1	.81670E+02

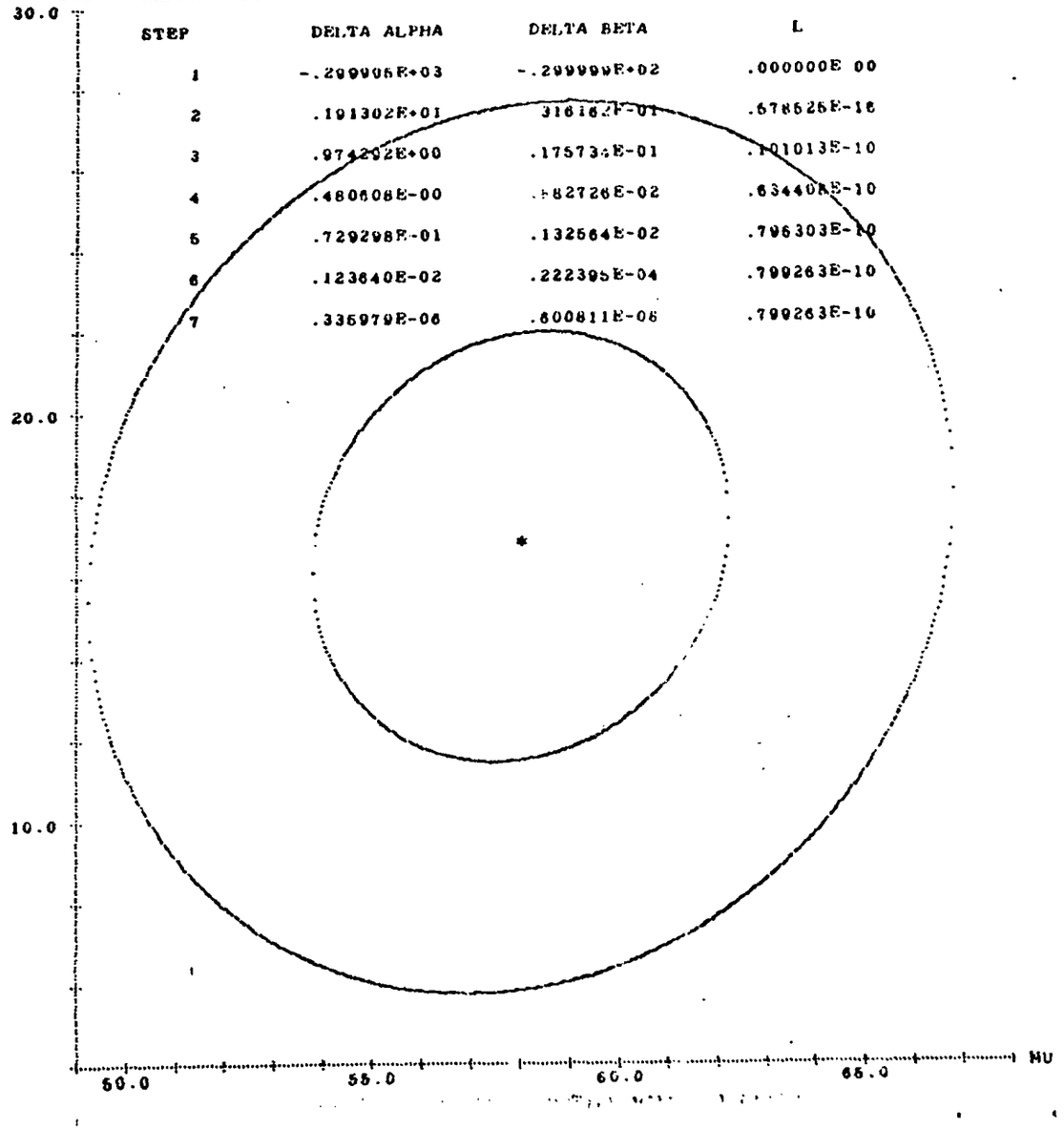
MU= .580059E+02 SIGMA=. .168263E+02

COVARIANCE MATRIX .128405E+02 .185908E+01

.185908E+01 .199470E+02

ALPHA*=.300000E+03 BETA*=.300000E+02 MU*=.100000E+02 SIGMA*=.333333E-01

STEP	DELTA ALPHA	DELTA BETA	L
1	-.299906E+03	-.299999E+02	.000000E 00
2	.191302E+01	.316162E-01	.678526E-16
3	.974292E+00	.175734E-01	.101013E-10
4	.480608E-00	.882726E-02	.634408E-10
5	.729298E-01	.132564E-02	.796303E-10
6	.123640E-02	.222395E-04	.799263E-10
7	.336979E-06	.600811E-06	.799263E-10



DISTANCE BETWEEN SIG TICK MARKS
.2E+01

ORIGIN MU= .490000E+02
SIG= .400000E+01

I. 3-17-7C

NO.	A	NO.	B
6	-.40000E+01	1	-.45000E+01
5	-.45000E+01	3	-.50000E+01
3	-.50000E+01	4	-.55000E+01
2	-.55000E+01	6	-.60000E+01

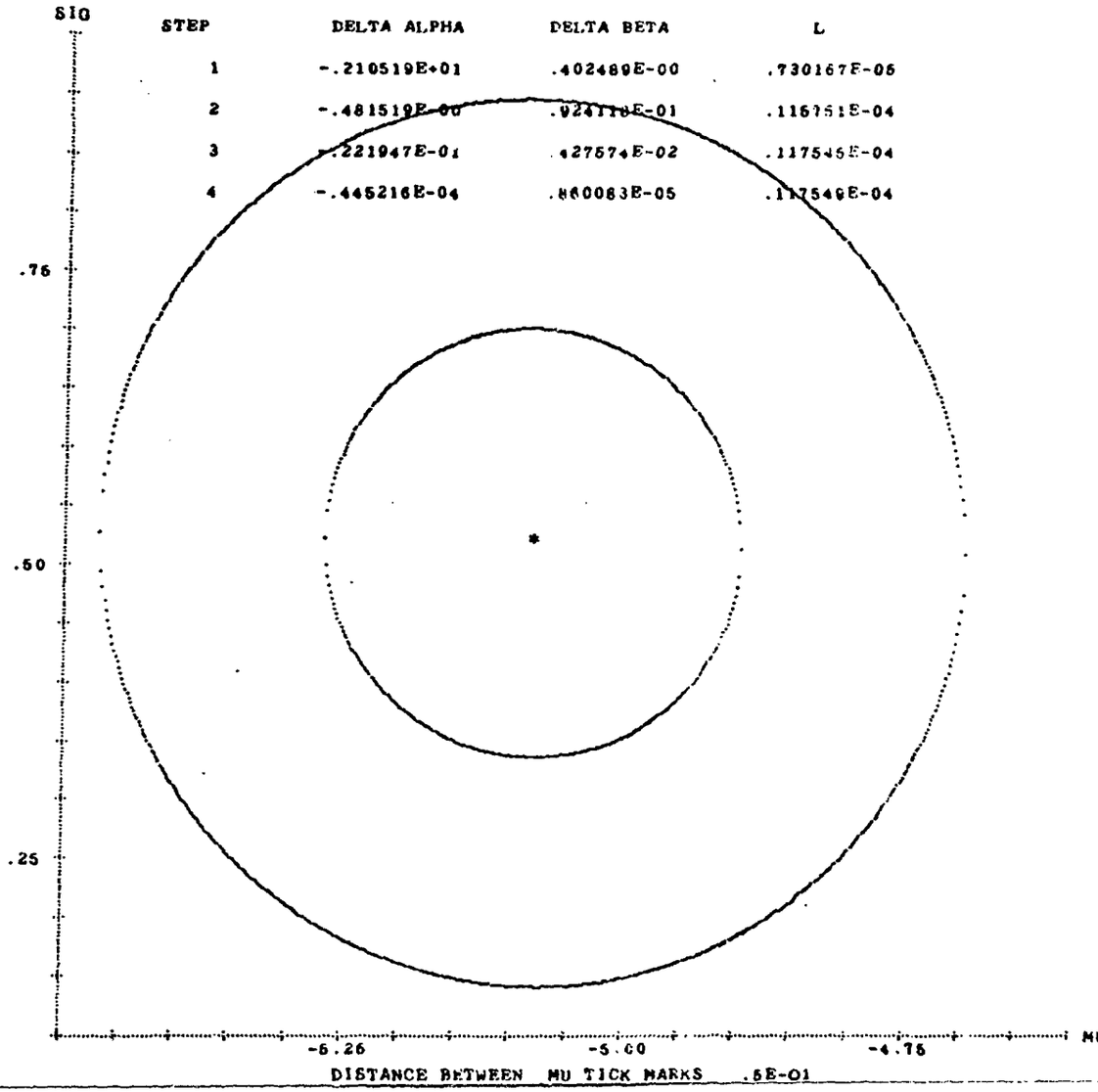
MU=-.608382E+01 SIGMA= .622630E+00

COVARIANCE MATRIX .247383E-01 -.608104E-03

-.608104E-03 .236956E-01

ALPHA*=.711842E+01 BETA*=.141421E+01 MU*=.603348E+01 SIGMA*=.707107E+00

STEP	DELTA ALPHA	DELTA BETA	L
1	-.210519E+01	.402489E-00	.730167E-05
2	-.481519E-00	.924118E-01	.116751E-04
3	-.221947E-01	.427574E-02	.117545E-04
4	-.445216E-04	.860083E-05	.117549E-04



DISTANCE BETWEEN SIG TICK MARKS
.5E-01

ORIGIN MU= -.550000E+01
SIG= .100000E-00

DISTANCE BETWEEN MU TICK MARKS .5E-01

II. 3-17-70

NO.	A	NO.	B
6	.10000E-03	1	.31250E-04
5	.31250E-04	3	.10000E-04
3	.10000E-04	4	.31250E-05
2	.31250E-05	6	.10000E-05

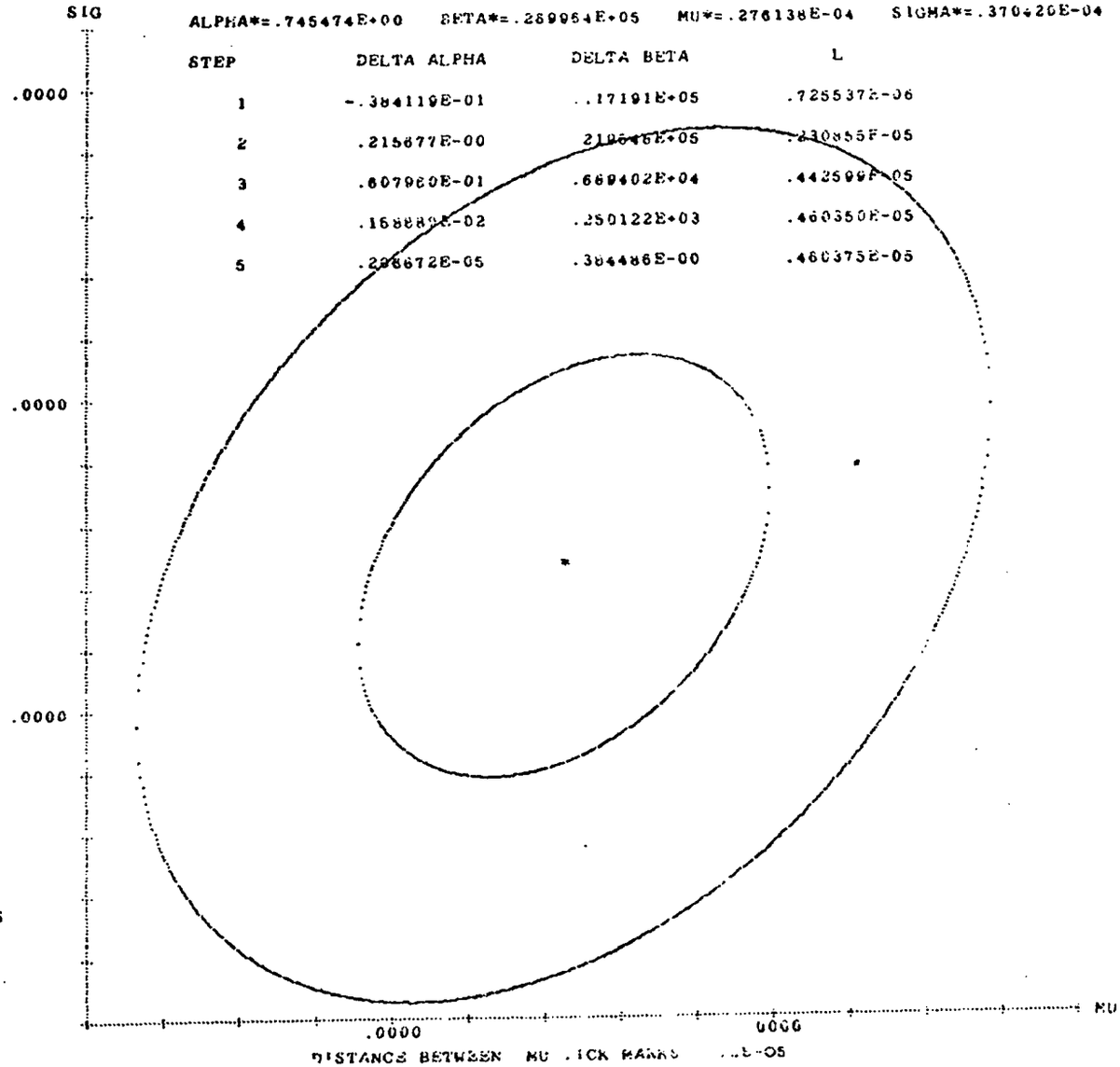
MU= .145267E-04 SIGMA= .147460E-04

COVARIANCE MATRIX .209337E-10 .938535E-11

.938535E-11 .329535E-10

ALPHA*=.745474E+00 BETA*=.289964E+05 MU*=.276138E-04 SIGMA*=.370420E-04

STEP	DELTA ALPHA	DELTA BETA	L
1	-.384119E-01	.17191E+05	.725537E-06
2	.215677E-00	2196[illegible]E+05	.430855E-05
3	.607960E-01	.669402E+04	.442599E-05
4	.168888E-02	.250122E+03	.460350E-05
5	.298672E-05	.384486E-00	.460375E-05



DISTANCE BETWEEN SIG TICK MARKS
.2E-05

ORIGIN MU= .200000E-05
SIG= .000000E 00

DISTANCE BETWEEN MU TICK MARKS [illegible]E-05

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APPENDIX A

COMPLETION OF PROOF FOR THEOREM 5.

It remains to prove that the sequence of points in E_2, $Q_i \equiv \{(\alpha_i, \beta_i)\}$, which is generated by the modified N-R procedure (See pages 23-26) actually converges to $\bar{Q} = (\bar{\alpha}, \bar{\beta})$, the point for which $L(Q) = L(\alpha, \beta)$ takes its maximum value, $\bar{L}$. It will be helpful in the analysis below to think of a point $Q \in E_2$ as a vector in E_2 which has the component form (α, β).

In the discussion of Theorem 5, in the main text of this report, a parameter u_i was associated with each modified N-R iterate, Q_i. The parameters u_i are positive real numbers defined by (60) and (61) such that for any $Q_i \neq \bar{Q}$

$$0 < u_{i+1} \leqslant 1, \tag{123}$$

$$L(Q_{i+1}) > L(Q_i), \text{ for } i = 1, 2, \ldots, \tag{124}$$

where Q_{i+1} is generated by the vector relation

$$Q_{i+1} = Q_i + u_{i+1} [\Delta Q_i], \tag{125}$$

with

$$[\Delta Q_i] \equiv (\Delta \alpha_i, \Delta \beta_i). \tag{126}$$

The quantities $\Delta \alpha_i$ and $\Delta \beta_i$ are the ordinary N-R increments which are obtained from (55) with all the derivatives which appear on the right hand side of (55) evaluated at $Q_i = (\alpha_i, \beta_i)$. A positive parameter, h_j, is associated with each consecutive pair of elements, $\{Q_j, Q_{j+1}\}$ of the sequence $\{Q_i\}$ which is defined by the relation

$$h_j \equiv L(Q_{j+1}) - L(Q_j) > 0, \quad j = 1, 2, \ldots . \qquad (127)$$

The h_j are positive for every j. This is assured by (59) which implies there always exists a u_j, as determined by (60) and (61), so that (123) and (124) hold for every j.

Clearly the procedure described can be applied to any point $P \in E_2$ (except $(\bar{\alpha}, \bar{\beta})$) with a new point generated by (125) and (126) with an associated positive increase in L indicated by h as defined by (127).

For easy reference, a result which we need is stated in the form of a lemma.

LEMMA (A-1) - The sequence $\{h_i\}$ generated by the modified N-R procedure converges to zero, i.e.

$$\lim_{i \to \infty} h_i = 0. \qquad (128)$$

Proof: We use the simpler notation L_i for $L(Q_i) = L(\alpha_i, \beta_i)$.

Then, for $k \geq 1$,

$$L_{k+1} = L_k + h_k = L_1 + h_1 + h_2 + \ldots + h_k < \bar{L}.$$

Hence, the infinite series $\sum_{i=1}^{\infty} h_i$ of positive terms is convergent,

which implies (128). Q.E.D.

LEMMA (A-2). Given an arbitrary positive real number K, there exists a quadrilateral in the $\alpha\beta$-plane, with the origin in its interior, such that $L(\alpha, \beta) < -K$ for every point (α, β) which is exterior to the quadrilateral.

Proof: The construction used here will be similar to that used following Lemma 7 (See page 20). Indeed, we can always construct a triangle here with the desired properties if it is possible to find three subscripts r, s, t such that $a_r < b_s < a_t$, or such that $b_r < a_s < b_t$. But this cannot always be done, for instance if we have $a_1 = b_1 = b_2 < a_2 = b_3$, and if we have only these five stimuli. But, in cases of interest, we always have $a_1 < b_m$ and $b_1 < a_n$, by (35), and the four stimuli appearing in these inequalities form the basis of the quadrilateral construction.

Let the positive constant K of the lemma be assigned. We determine a positive number s such that $p(-s) = \exp(-K-1)$. Such a number s exists because of the monotonic increase of p(t) from 0 to 1 on the interval $(-\infty,\infty)$. Now consider the line $a_1\beta - \alpha = -s$ in the $\alpha\beta$-plane. This is denoted as line ① in Figure 2. At every point of line ① we have $p(a_1\beta - \alpha) = p(-s) = \exp(-K-1)$, or $\log p(a_1\beta - \alpha) = -K-1 < -K$. But since, by (5), L can be expressed as a sum of negative terms, we have, for every (α, β) on line ①, $L(\alpha, \beta) < \log p_1 = \log(a_1\beta - \alpha) = \log p(-s) = -K-1 < -K$. This is similar to the corresponding analysis on pages 20-22. The α-intercept of line ①, $a_1\beta - \alpha = -s$, is $\alpha = +s$.

Now suppose (α, β) is a point to the right of line ①. By this we mean that, if (α_o, β) is the point of line ① with the same ordinate β, then $\alpha > \alpha_o$. The phrase "to the left of" will have

an analogous meaning. A line of the form $a_i\beta - \alpha = c$ or $b_j\beta - \alpha = c$ cannot be horizontal, since every a_i or b_j is finite. The point (α, β) to the right of line ① will lie on a line of the form $a_1\beta - \alpha = -s-e$ with α-intercept $\alpha = s+e$, where $e > 0$, and for this point the log p_1 term will be log p (-s-e) < log p (-s) = -K-1 < -K, and so, for this point, we have, as above, $L(\alpha, \beta) < -K$.

Thus, for every point in the $\alpha\beta$-plane which is on or to the right of line ① , we have $L(\alpha, \beta) < -K$.

Similarly, designating the line $b_m\beta - \alpha = +s$ with α-intercept -s, as line ② (see Fig. 2), we find that, for every point on line ② , $q_m = q(b_m\beta - \alpha) = q(+s) = p(-s) = \exp(-K-1)$, since the identity $q(t) = p(-t)$ holds for all real t. Hence we have, as above, $L(\alpha, \beta) < \log q_m = -K-1 < -K$. Also, any point (α, β) which is to the left of line ② is on some line $b_m\beta - \alpha = +s+e$ with α-intercept -s-e where $e > 0$, and for such a point the log q_m term will be log q (s+e) < log q (+s) = -K-1 < -K, since the function q(t), or 1-p(t), decreases as t increases. Therefore, for such a point (α, β), to the left of line ② , we have as above, $L(\alpha, \beta) < -K$. Thus, for every point in the $\alpha\beta$-plane which is on or to the left of line ② , we have $L(\alpha, \beta) < -K$.

These lines ① and ② , with equations $a_1\beta - \alpha = -s$ and $b_m\beta - \alpha = +s$ respectively, intersect, by analytic geometry, at the point $\alpha = (b_m + a_1)\, s/(b_m - a_1)$, $\beta = 2s/(b_m - a_1)$. Since $s > 0$, and $b_m - a_1 > 0$ (since $a_1 < b_m$), this point, designated as C in Figure 2, is in the upper half-plane, with $\beta > 0$.

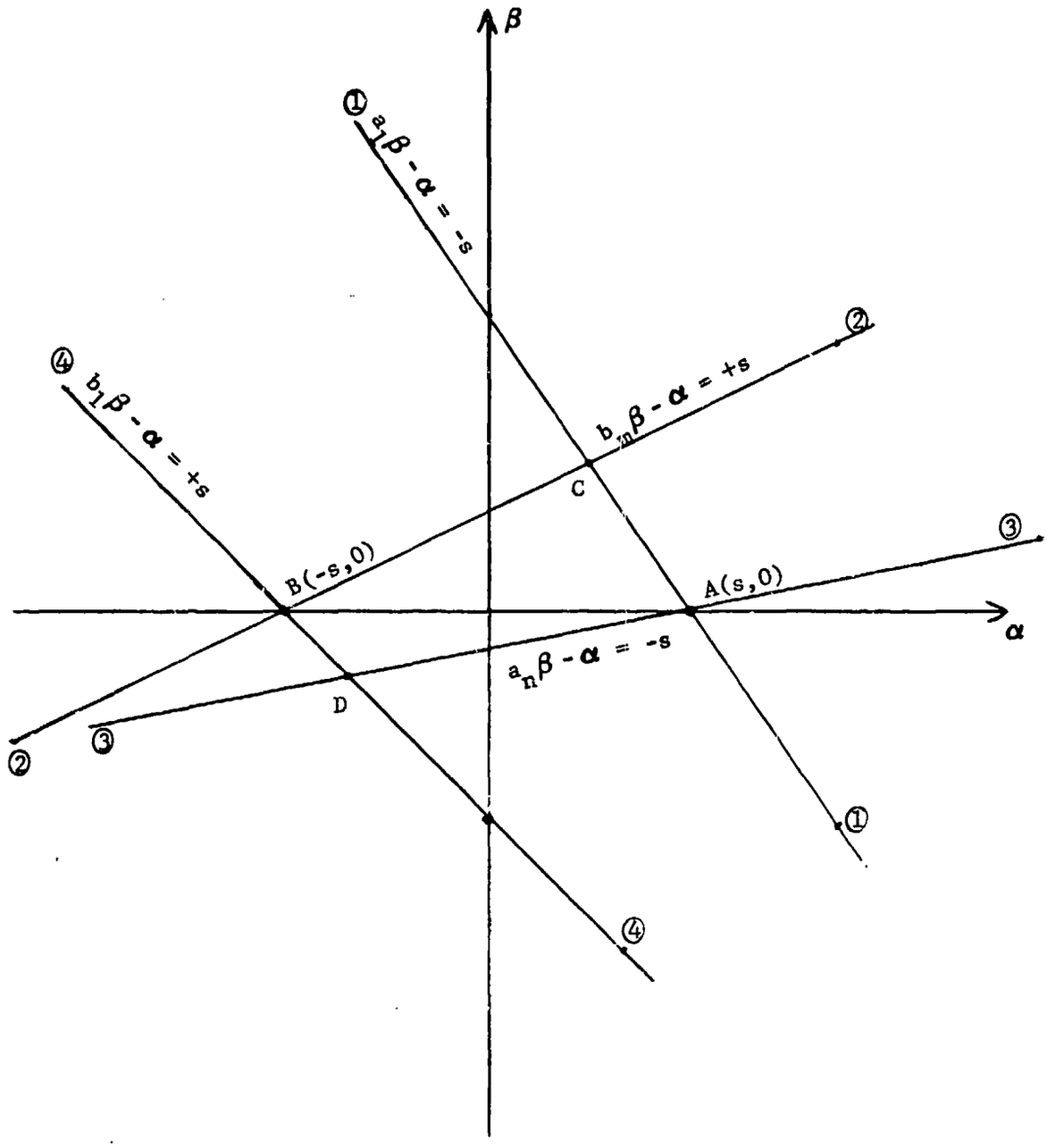
β
α
① $a_1\beta - \alpha = -s$
② $b_n\beta - \alpha = +s$
③ $a_n\beta - \alpha = -s$
④ $b_1\beta - \alpha = +s$
A(s,0)
B(-s,0)
C
D

Figure 2

We next make a very similar analysis using lines ② and ④ , Fig. 2, where line ③ by definition is the line $a_n\beta - \alpha = -s$ and line ④ is $b_1\beta - \alpha = +s$. These lines intersect at the point marked D in Fig. 2, with coordinates $\alpha = -(a_n + b_1)s/(a_n - b_1)$, $\beta = -2s/(a_n - b_1)$. Since $s > 0$ and $a_n - b_1 > 0$ (since $b_1 < a_n$ by (35)), $\beta < 0$, or the point D is in the lower half-plane. It is true, as in the foregoing analysis, that, for every point (α, β) on or to the right of line ③ , we have $L(\alpha, \beta) < -K$; and that, for every point (α, β) on or to the left of line ④ , we also have $L(\alpha, \beta) < -K$. We omit the details here as the proofs exactly parallel those for lines ① and ② .

Thus we obtain the quadrilateral ACBD of Fig. 2, where A and B as shown in the figure are the points (s,0) and (-s,0), and C and D, in the upper and lower half-planes respectively, are the points whose coordinates have been given. This quadrilateral reduces to a triangle in some cases, for instance when $b_1 < a_1 < b_2$ with $a_1 > (b_1 + b_2)/2$ and there are no other stimuli, so that $a_1 = a_n$ and lines ① and ③ coincide. But, even in such cases, A(s,0) and B(-s,0) are as shown in Fig. 2, and C and D are in the upper and lower half-planes respectively. We can in every case refer to the quadrilateral ACBD with the understanding that, in some cases, A (or B) may be collinear with C and D.

It is now not difficult to see, on the basis of the foregoing analysis, that, for every point (α, β) in the plane which is exterior to this quadrilateral, we have $L(\alpha, \beta) < -K$, as stated in Lemma (A-2).

The reader can easily convince himself, by making a copy of Fig. 2 and shading those parts of the plane where the relation $L(\alpha, \beta) < -K$ holds, that every such exterior point (α, β) satisfies <u>at least one</u> of the following conditions: it lies (1) to the right of line ①, or (2) to the left of line ②, or (3) to the right of line ③, or (4) to the left of line ④. Any one of these geometrical conditions is sufficient to ensure that the relation $L(\alpha, \beta) < -K$ holds. This completes the proof of Lemma (A-2).

Now we define a point set M in the $\alpha\beta$-plane by

$$M = \{Q \mid L(Q) \geqslant L_1\},$$

where L_1 is determined by choosing a starting point $(\alpha_1, \beta_1) = Q_1$ for the modified N-R procedure. The symbol Q here, however, refers to any point in the plane satisfying the inequality $L(Q) \geqslant L_1$, whether a member of any particular sequence of N-R iterates or not.

LEMMA (A-3). <u>The point set M is closed and bounded in E_2</u>.

Proof: M is bounded by Lemma (A-2), since one can take L_1 as the negative number -K of the lemma, and construct a quadrilateral such that $L(\alpha, \beta) < L_1$ for every point which is exterior to the quadrilateral. Hence the set M is contained in the quadrilateral plus its interior, i.e. in a bounded subset of the plane.

The set M is closed, because if a sequence of points in M converges to a point Q', we must have $L(Q') \geqslant L_1$, since L is a continuous function of its arguments α and β. Hence $Q' \in M$ by the definition of M and it has been shown that M is closed. Q.E.D.

Now consider an infinite sequence $\{Q_j\}$ of distinct modified N-R iterates with a starting point Q_1. The fact that all of the Q_j are distinct follows from the fact that L is increased at every step. For all j, $Q_j \in M$. Hence by the Bolzano-Weierstrass theorem, $\{Q_j\}$ has at least one accumulation point, say Q. Since M is closed, $Q \in M$. But Q need not be a member of the sequence $\{Q_j\}$. However, the modified N-R procedure can be applied at Q (or any other point), from which an associated h would be obtained. The quantity $h > 0$ unless $Q = \bar{Q}$, in which case $h = \bar{h} = 0$. This is easy to see because if $Q = \bar{Q}$, then from (55), since $L_{\alpha}(\bar{Q}) = L_{\beta}(\bar{Q}) = 0$, $\Delta\alpha = \Delta\beta = 0$, so that $\Delta Q = 0$ in (125) and Q is not changed by the procedure. Hence $n = 0$.

So we assume $Q \neq \bar{Q}$, consequently $h > 0$. It is always possible to choose a subsequence $\{Q_{j_w}\}$ of $\{Q_j\}$ such that $Q_{j_w} \to Q$. Hereafter, for typographical convenience, we note the elements of the subsequence by Q_w where it is understood w takes the integer values j_w. We will show the assumption $h > 0$ leads to a contradiction of Lemma (A-1). The conclusion will follow that $Q = \bar{Q}$, and that the entire original sequence $\{Q_j\}$ converges to $\bar{Q}$.

A visual aid which we call an overlaid diagram will be used to elucidate the remainder of the proof; it is briefly defined and illustrated. Pass a vertical plane V through Q and the point $Q + u\Delta Q = (\alpha + u\Delta\alpha, \beta + u\Delta\beta)$ into which Q is transformed by the modified N-R process. The intersection of V and the $L(\alpha, \beta)$ surface is a concave downward curve since the surface itself is concave downward

everywhere. This curve is indicated as the solid curve in Figure 3

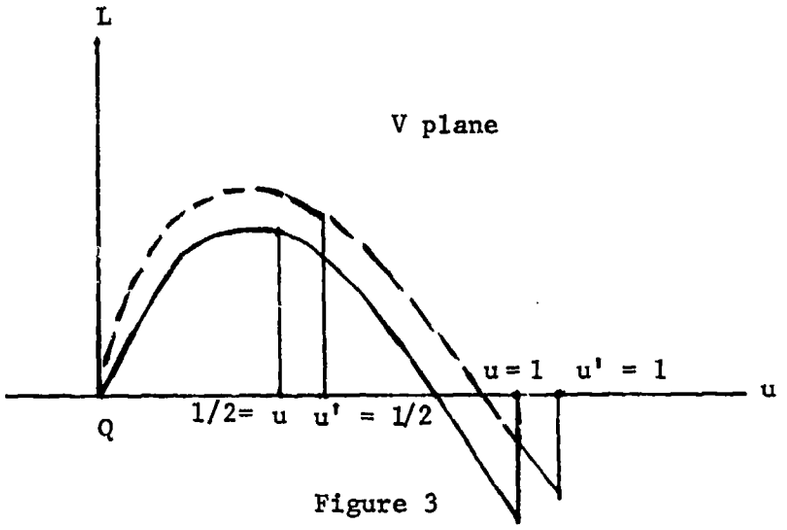

Figure 3

with Q at the origin. Points on the horizontal axis are at a height $|L(Q)|$ below (because $L < 0$) the $\alpha\beta$-plane. Points on the solid curve can be specified by appropriate values of the parameter u. Now consider a point of the subsequence, Q_w, which for large w is very near Q. Since L and all of its derivatives are continuous, the corresponding curve determined by Q_w and appropriate values of u' (we use u' here instead of u to denote a distinction from the parameter u associated with Q), in general, lies in a slightly different vertical plane from V, but will nevertheless be very near the Q curve by continuity. Now we think of the Q_w curve as translated in its plane until the projection of the point Q_w on the V plane falls exactly on the point Q. The translated Q_w curve is then projected on to the V plane and is

shown as the dashed line in the figure. The distances in the $\alpha\beta$-plane corresponding to u = 1 and u' = 1 are not exactly equal in general, but are nearly equal for large w by continuity. Figure 3 will be referred to as the overlaid diagram. The remaining arguments will assume the Q_w curves are in the V plane since the actual Q_w curves and their translated projections on the V plane can be made to differ by as little as we desire by choosing w sufficiently large.

There are two situations to consider which are distinguished by whether or not there exists a non-negative integer k for which the quantity

$$K \equiv L(Q + u\Delta Q) - L(Q)$$

is zero, where $u = 2^{-k}$, and as usual $\Delta Q \equiv (\Delta\alpha, \Delta\beta)$ with $\Delta\alpha, \Delta\beta$ the ordinary N-R increments at Q as obtained from (55).

If $K \neq 0$ for any $k \geqslant 0$, then no difficulty arises because it is easy to argue from continuity that the subsequence $\{h_w\}$ converges to h. However by Lemma (A-1), h = 0, which obviously implies $Q = \bar{Q}$ by the arguments above.

If K = 0 for some k, say for definiteness $k = 1 (u = \frac{1}{2})$ a more subtle argument is required to show h = 0. There are two possibilities to consider for the subsequence of iterates $\{Q_w\}$

(a) All but a finite number of the Q_w have the property that

$$L(Q_w + \frac{1}{2}\Delta Q_w) - L(Q_w) \geqslant 0 . \qquad (129)$$

(b) An infinite number of the Q_w have the property that

$$L(Q_w + \tfrac{1}{2}\,\Delta Q_w) - L(Q_w) < 0\ , \tag{130}$$

(This does not exclude the possibility that an infinite number of the Q_w may also satisfy (129)).

The overlaid diagram is useful here to visualize these situations keeping in mind that, for sufficiently large w, the points $Q_w + \frac{1}{2}\,\Delta Q_w$ are arbitrarily near $Q + \frac{1}{2}\,\Delta Q$.

For case (a), the arguments are essentially the same as those used above for $K \neq 0$. Briefly, since (129) holds for all w, when w is sufficiently large,

$$0 < h = \lim_{w\to\infty} \left[L(Q_w + \tfrac{1}{4}\,\Delta Q_w) - L(Q_w)\right] = \lim_{w\to\infty} (h_w), \tag{131}$$

where the factor ($\frac{1}{4}$) occurs because $K = 0$ for $k = 1$ so that by (60) and (61) we require $r = k + 1$ where $u = 2^{-r} = \frac{1}{4}$. Again we arrive at a contradiction by employing Lemma (A-1), since it requires $\lim_{w\to\infty} h_w = 0$. We note the first equality in (131) must hold because $\{Q_w\}$ converges to Q, L is continuous in Q and

$$h = \left[L(Q + \tfrac{1}{4}\,\Delta Q) - L(Q)\right]. \tag{132}$$

The second equality must hold for (131), because, for sufficiently large w, the quantity

$$L(Q_w + \tfrac{1}{2}\,\Delta Q_w) - L(Q_w)$$

approaches zero (since $K = 0$), so that the factor $\frac{1}{2}$ must eventually be changed to $\frac{1}{4}$ as w increases.

For case (b), we assume that (130) holds for an infinite number of elements Q_{w_z} of $\{Q_w\}$. We identify this subsequence by $\{Q_z\}$ where z takes the integer values w_z. By the modified N-R procedure, the h_z for each element in $\{Q_z\}$ will be the larger of $L(Q_z + \frac{1}{4} \Delta Q_z) - L(Q_z)$ and $L(Q_z + \frac{1}{8} \Delta Q_z) - L(Q_z)$. If the latter is the larger of the two, then $\{h_z\}$ will converge to $L(Q + \frac{1}{8} \Delta Q) - L(Q)$. So that by (132) and Lemma (A-1),

$$0 < h < \lim_{z \to \infty} h_z = 0 ,$$

which again leads to the desired contradiction. Certainly if

$$L(Q + \tfrac{1}{8} \Delta Q) - L(Q) > L(Q + \tfrac{1}{4} \Delta Q) - L(Q), \qquad (133)$$

then for sufficiently large w the above situation will hold. On the other hand, if this inequality is reversed or equality would hold, then $\{h_z\}$ would converge to h for which a contradiction will again follow.

The situations described by cases (a) and (b) exhaust the possibilities of what may occur for the subsequence $\{Q_w\}$. In every case we have shown h = 0, which implies $Q = \bar{Q}$. By elementary analysis it will now follow that the entire original sequence $\{Q_j\}$ must converge to the unique solution point, $\bar{Q}$. Indeed, suppose this is not the case. Then there exists an open circular region R, with center at $\bar{Q}$, such that an infinite number of Q_j lie outside R and hence in the closed

set $M_1 = M \cap (E_2 - R)$. The set M_1 is not only closed but it is also bounded because $M_1 \subseteq M$. Applying the Bolzano-Weierstrass theorem again, the set of $Q_j \in M_1$ must have an accumulation point $\bar{Q}_1$. But it has just been shown above that any convergent subsequence of $\{Q_j\}$ must converge to $\bar{Q} \notin M_1$. This is a contradiction. We conclude $\{Q_j\}$ converges to $\bar{Q}$.

APPENDIX B

ANALYSIS FOR GRAPHS OF CONFIDENCE ELLIPSES

The equation of the confidence ellipse for a given confidence level $1 - \gamma$ (for example, $\gamma = .05$ for 95% confidence) is

$$A_{\mu\mu}(\mu - \bar{\mu})^2 + 2A_{\mu\sigma}(\mu - \bar{\mu})(\sigma - \bar{\sigma}) + A_{\sigma\sigma}(\sigma - \bar{\sigma})^2 = D \equiv \chi^2_{1-\gamma}, \quad (134)$$

where $(\bar{\mu}, \bar{\sigma})$ is the computed maximum likelihood estimate for the position of the true parameter point, (μ_o, σ_o) in the $\mu\sigma$-plane. The quantity D(or $\chi^2_{1-\gamma}$) is the value obtained from a chi-square table at the γ level, for two degrees of freedom and $A_{\mu\mu}$, $A_{\mu\sigma}$, $A_{\sigma\sigma}$ are the elements of the inverse of the covariance matrix which is determined by the main program. The equations for $A_{\mu\mu}$, $A_{\mu\sigma}$, $A_{\sigma\sigma}$ are given as equations (102), (103), (104), or as actually used in the computer program, they are given by (120), (121), (122). The values of D for 95% and 50% confidence, the values at which the NWL program is presently set, are 5.99 and 1.39, respectively, (See p. 42).

We emphasize here the necessity of distinguishing between the coefficients $A_{\mu\mu}$, $A_{\mu\sigma}$, $A_{\sigma\sigma}$ of (134) and the elements $A^{\mu\mu}$, $A^{\mu\sigma}$, $A^{\sigma\sigma}$ of the covariance matrix A. Let E denote the matrix associated with the ellipse, so that

$$E = A^{-1} = \begin{pmatrix} A_{\mu\mu} & A_{\mu\sigma} \\ A_{\mu\sigma} & A_{\sigma\sigma} \end{pmatrix}, \quad (135)$$

where

$$A = \begin{pmatrix} A^{\mu\mu} & A^{\mu\sigma} \\ A^{\mu\sigma} & A^{\sigma\sigma} \end{pmatrix} \text{(Covariance matrix).} \qquad (136)$$

The elements of E are computed in the main program and those of A by numerical inversion of E. Hence, it is not necessary to reinvert A (the elements of which are printed out by the program) in order to compute E.

We simplify the notation by writing (134) in the form

$$ax^2 + 2bxy + cy^2 = D\ , \qquad (137)$$

where

$$a = A_{\mu\mu}\ ,\ b = A_{\mu\sigma}\ ,\ c = A_{\sigma\sigma}\ ,\ x = (\mu - \bar{\mu}),\ y = (\sigma - \bar{\sigma}). \qquad (138)$$

From (102) and (104), clearly a and c are positive, and it can be shown by the methods used in Theorem 2 that

$$\Lambda \equiv ac - b^2 > 0. \qquad (139)$$

Thus, (134) represents an ellipse for any positive value of D.

Our first objective is to establish the points of maximum and minimum ordinates and maximum and minimum abscissas on the ellipse. This is easily accomplished by equating successively to zero (dy/dx) and (dx/dy) as determined from (137). Substituting the linear relation

$$y = -ax/b, \qquad (140)$$

which remains into (137), one obtains

$$x^2 = \frac{b^2 D}{a\Lambda}\ , \qquad (141)$$

and from (140)

$$y^2 = \frac{aD}{\Lambda} \quad . \tag{142}$$

In this way, two points are determined (not four) from (140), (141), (142) with the possibility b may be of either sign. If b = 0, (137) represents an ellipse with vertical and horizontal axes and the points of maximum and minimum ordinates are $(0, \pm \sqrt{D/c})$.

From (142) we see that

$$S(y) \equiv \text{Span in ordinates} = 2\sqrt{\frac{aD}{\Lambda}} \quad , \tag{143}$$

where S(y) denotes difference between the extreme ordinates. By setting b = 0 in (143), we see that (143) reduces to $2\sqrt{D/c}$. Thus (143) gives the correct result for all b.

The span in abscissas, S(x), is determined by differentiating (137) with respect to y and setting $x'(= dx/dy) = 0$. It will follow, similar to the case of S(y), that

$$S(x) = 2\sqrt{\frac{cD}{\Lambda}} \quad . \tag{144}$$

The ellipse represented by (137) for a given D may be very slender and elongated as well as being too large or too small for convenient plotting, if no coordinate scaling is done. Hence, it is desirable to scale the coordinates in such a way as to avoid these undesirable characteristics as much as possible in the machine plotting.

Our next objective is to derive transformations which take the ellipse of (137) into an ellipse inscribed in a square of fixed size. The resulting ellipse may still be elongated, with eccentricity near unity, but nothing is done about this. No rotation of axes is carried out at any time.

We assume the square will have sides of M units (inches, centimeters or some other convenient unit). Thus we will require in new coordinates X and Y

$$S(X) = S \quad M. \tag{145}$$

Since it is the D_{95}(=5.99) ellip... whose size we wish to control, we hereafter let $D = D_{95}$. The scaling transformations, from μ, σ to X, Y are

$$\mu = \frac{2}{M}\sqrt{\frac{cD}{\Lambda}}\ X = \frac{S(x)}{M}\ X, \tag{146}$$

$$\sigma = \frac{2}{M}\sqrt{\frac{aD}{\Lambda}}\ Y = \frac{S(y)}{M}\ Y. \tag{147}$$

If these formulas are substituted into (137), the result is

$$(X - \bar{X})^2 + \frac{2b}{\sqrt{ac}}\ (X - \bar{X})(Y - \bar{Y}) + (Y - \bar{Y})^2 = \frac{M^2\Lambda}{4ac}\ , \tag{148}$$

where $\bar{X}$ and $\bar{Y}$ correspond to $\bar{\mu}, \bar{\sigma}$ as given by (146) and (147). If the spans S(X) and S(Y) for this transformed ellipse are computed as was done for (137), it is found that (145) holds.

Some plotters, such as those used at NWL, have a basic unit for the horizontal axis which is not equal to the basic unit for the vertical

axis. Thus, we now consider transformations to actual plotter coordinates (ξ, η) such that (145) is maintained. Let c_1 denote the number of plotter units per inch on the horizontal scale and c_2 the corresponding number on the vertical scale. On the NWL plotter, for example, there are 1024 units in about 11 inches horizontally and 1024 units in about 9 inches vertically, so that, in this case, $c_1 = 93.1$, $c_2 = 113.8$.

The scaling transformations from X, Y (in inches) to ξ, η (in plotter units) are then

$$\xi - \bar{\xi} = c_1(X - \bar{X}) \tag{149}$$

$$\eta - \bar{\eta} = c_2(Y - \bar{Y}) \, . \tag{150}$$

Here we denote by $\bar{\xi}, \bar{\eta}$ the coordinates on the arbitrary plotter scales, of the point which is selected to be the center of the confidence ellipse. In other words, $\bar{\xi}, \bar{\eta}$ are not computed from $\bar{X}$, $\bar{Y}$, but rather they are conveniently chosen to locate the ellipse as desired. Hence, although c_1 and c_2 are scale factors as indicated by (149) and (150) it would not be correct, in general, to write

$$\xi = c_1 X \text{ and } \eta = c_2 Y \, , \tag{151}$$

since $\bar{X}$ and $\bar{Y}$ are fixed while $\bar{\xi}$ and $\bar{\eta}$ are arbitrarily chosen.

Substituting from (149) and (150) into (148) gives

$$\frac{1}{c_1^2}(\xi - \bar{\xi})^2 + \frac{2}{c_1 c_2}\frac{b}{\sqrt{ac}}(\xi - \bar{\xi})(\eta - \bar{\eta}) + \frac{1}{c_2^2}(\eta - \bar{\eta}) = \frac{M^2 \Lambda}{4ac}. \tag{152}$$

Letting $\xi - \bar{\xi} = \xi'$, $\eta - \bar{\eta} = \eta'$, we have

$$(\xi'/c_1)^2 + \frac{2b}{\sqrt{ac}}(\xi'/c_1)(\eta'/c_2) + (\eta'/c_2)^2 = \frac{M^2\Lambda}{4\,ac}\,. \qquad (153)$$

Eq. (153) holds for any positive D although we have been assuming here $D = D_{95} = 5.99$. If we require the 50% level ellipse so that $D = D_{50} = 1.39$, then the right hand side of (153) is simply replaced by

$$\frac{M^2\Lambda}{4\,ac}\,\frac{D_{50}}{D_{95}}\,. \qquad (154)$$

This follows easily by simply recasting the preceding analysis in terms of D_{50} rather than D_{95}.

Solving (153) for η'/c_2, the result is

$$\eta'/c_2 = -\frac{b}{\sqrt{ac}}\,(\xi'/c_1) \pm \sqrt{\frac{M^2\Lambda}{4\,ac} - \frac{\Lambda}{ac}(\xi'/c_1)^2}\,, \qquad (155)$$

or

$$\eta = \eta' - \frac{b}{\sqrt{ac}}\left(\frac{c_2}{c_1}\right)(\xi - \xi') \pm c_2\sqrt{\frac{M^2\Lambda}{4\,ac} - \frac{\Lambda}{ac}\frac{1}{c_1^2}(\xi - \xi')^2}\,. \qquad (156)$$

The 95% ellipse can be plotted from (156) in plotter coordinates ξ, η and the 50% ellipse by the modification indicated in (154).

It remains to discuss the problem of markings on the axes in the plotted figure for the reader's convenience in interpreting the graph. These markings must indicate measurements in the original coordinates, μ, σ.

The span in abscissas and ordinates in terms of μ and σ are given by (144) and (143), respectively. Hence, the minimum (subscript 1)

and maximum (subscript 2) abscissas and ordinates are given by

$$\mu_1 = \bar{\mu} - \sqrt{\frac{cD}{\Lambda}}, \qquad \mu_2 = \bar{\mu} + \sqrt{\frac{cD}{\Lambda}},$$

$$\sigma_1 = \bar{\sigma} - \sqrt{\frac{aD}{\Lambda}}, \qquad \sigma_2 = \bar{\sigma} + \sqrt{\frac{aD}{\Lambda}}, \tag{157}$$

where we continue to assume $D = D_{95}$. These four numbers determine the boundary lines of the square in which the 95% ellipse is inscribed. In our figures the square is not explicitly indicated, but the four numbers are used to determine the scale markings in the figure.

Numbers d_1, k_1, d_2, k_2 are determined such that

$$2\sqrt{\frac{cD}{\Lambda}} = d_1 \times 10^{k_1} \tag{158}$$

$$2\sqrt{\frac{aD}{\Lambda}} = d_2 \times 10^{k_2}, \tag{159}$$

where k_1, k_2 are integers and d_1, d_2 are numbers such that

$$0.1 \leqslant d_1 < 1, \qquad 0.1 \leqslant d_2 < 1.$$

The right hand side of (158), (159) are simply representation of numbers in "normal form" for FORTRAN numbers. Thus

$$1226.4 = 0.12264 \times 10^4 \text{ with } d_1 = .12264,\ k_1 = 4.$$

Next, we determine units z_1 (horizontal) and z_2 (vertical) for marking the axes in the plotted figure. The following rule is used:

$$\begin{aligned} z_i &= .01 \times 10^{k_i} && \text{if } 0.1 \leqslant d_i < 0.2, \\ z_i &= .02 \times 10^{k_i} && \text{if } 0.2 \leqslant d_i < 0.5, \quad (i = 1, 2) \\ z_i &= .05 \times 10^{k_i} && \text{if } 0.5 \leqslant d_i < 1. \end{aligned} \tag{160}$$

To illustrate, suppose $2\sqrt{\frac{cD}{\Lambda}} = 642 = .642 \times 10^3$. Then $d_1 = .642$, $k_1 = 3$, therefore $z_1 = .05 \times 10^3 = 50$. Hence, the horizontal scale will be marked every 50 units (in μ coordinates), or since the span is 642, there will be about 13 divisions or perhaps 14 or 15 including the relatively small extensions of the axes beyond the ellipse as discussed below.

We next consider appropriate values to assign μ and σ on the axes at the left and right and lower and upper limits of the figure itself. We wish these values to be integral multiples of z_1 (horizontal) and z_2 (vertical). The following rule is used in which [x] indicates the algebraically greatest integer not exceeding x:

$$\left.\begin{aligned}
\mu_L &\equiv \left[\frac{\mu_1}{z_1}\right] z_1 \ , \\
\mu_R &= \begin{cases} \mu_2 \text{ if } \mu_2/z_1 \text{ is an integer} \\ \left(\left[\frac{\mu_2}{z_1}\right] + 1\right) z_1 \text{ otherwise} \ , \end{cases} \\
\sigma_L &= \left[\frac{\sigma_1}{z_2}\right] z_2 \ , \\
\sigma_R &= \begin{cases} \sigma_2 \text{ if } \sigma_2/z_2 \text{ is an integer} \\ \left(\left[\frac{\sigma_2}{z_2}\right] + 1\right) z_2 \text{ otherwise} \ . \end{cases}
\end{aligned}\right\} \qquad (161)$$

The subscript L refers to the left and lower boundaries of the figure and the subscript R to the right and upper boundaries. The quantities μ_1, μ_2, σ_1, σ_2, z_1, z_2 are defined in (157) and (160).

After μ_1, μ_2, μ_L, μ_R, σ_1, σ_2, σ_L, σ_R are determined, we next compute the corresponding plotter coordinates ξ_i, η_i. From (146), (147), (149), (150) we have

$$\mu - \bar{\mu} = r_1(\xi - \xi'), \qquad \sigma - \bar{\sigma} = r_2(\eta - \eta') , \quad (162)$$

where

$$r_1 = \frac{2}{Mc_1}\sqrt{\frac{cD}{\Lambda}} , \qquad r_2 = \frac{2}{Mc_2}\sqrt{\frac{aD}{\Lambda}} . \quad (163)$$

Finally, from (162)

$$\xi = (\xi' - \frac{\bar{\mu}}{r_1}) + (\mu/r_1)$$
$$\eta = (\eta' - \frac{\bar{\sigma}}{r_2}) + (\sigma/r_2) . \quad (164)$$

From these equations we compute ξ_i, η_i (i = 0, 1, 2, 3) giving the left and right and upper and lower boundaries of the 95% ellipse and of the entire plotted figure in plotter coordinates.

Markings on the horizontal axis, "tick marks", are to be inserted for the following values of μ: μ_L, $\mu_L + z_1$, $\mu_o + 2z_1$, ..., μ_R. The ξ coordinates of these points are given by the first of (164). Similarly, we use the second equation of (164) to compute the η coordinates for the "tick marks" on the vertical axis corresponding to σ_L, $\sigma_L + z_2$, $\sigma_L + 2z_2$, ..., σ_R.

Every fifth "tick mark" on both axes is identified with numerals, i.e., numerals are printed at multiples of $5z_1$ (horizontal) and $5z_2$ (vertical). For example if $z_1 = 50$, $\mu_o = 1250$, $\mu_3 = 2000$, then

numerals are printed at marks indicating 1250, 1500, 1750, 2000 and "tick marks" are printed at 1250, 1300, 1350, ..., 2000.

In general, we wish the numerals to be well chosen for easiest interpretation of the figure. In order to insure this, we determine numbers μ_4 and σ_4, where μ_4 is the μ coordinate of the first "tick mark" where a numeral is to be placed, by the rule given below, and similarly σ_4 is the σ-coordinate of the lowest "tick mark" on the σ-axis where a numeral is to be placed. This rule is:

$$\mu_4 = \begin{cases} \mu_o & \text{if } (\mu_o/5z_1) \text{ is an integer} \\ \left(\left[\frac{\mu_o}{5z_1}\right] + 1\right)(5z_1) & \text{otherwise,} \end{cases}$$

$$\sigma_4 = \begin{cases} \sigma_o & \text{if } (\sigma_o/5z_2) \text{ is an integer} \\ \left(\left[\frac{\sigma_o}{5z_2}\right] + 1\right)(5z_2) & \text{otherwise.} \end{cases}$$

The notation [x] again denotes the greatest integer function.

Hence, numerals are placed at

$$\mu_4,\ \mu_4 + 5z_1,\ \ldots,\ (\mu_4 + n_1 5z_1),\ \mu_4 + (n_1+1)5z_1 > \mu_3$$

$$\sigma_4,\ \sigma_4 + 5z_2,\ \ldots,\ (\sigma_4 + n_2 5z_2),\ \sigma_4 + (n_2+1)5z_2 > \sigma_3,$$

where n_1 and n_2 are integers.

APPENDIX C

PROBIT METHOD

The probit method is used in the statistical analysis of tests of the effectiveness of insecticides and other poisons, and in other problems of biological assay. Like the NWL statistical sensitivity program, it is used in tests where responses to stimuli are quantal, that is, every response to a stimulus can be characterized as a success or a failure according to some arbitrary criterion. Like the NWL program, it determines the maximum likelihood estimates of the mean and standard deviation of a statistical distribution which is assumed to be normal. The probit method is well adapted to, and was designed for, hand calculations, the first edition of [10], Finney's book on the method, having been published in 1947, before electronic computers were in general use. It involves fitting a sequence of increasingly accurate straight lines to the empirical data, the calculations being relatively simple, but the speed of convergence being heavily dependent on the skillful choice of a line representing a first approximation. Finney in [10] recommends that this be done by eye, and states that a statistician experienced in the method will ordinarily get results of sufficient accuracy for practical purposes in two further iterations. See further discussion below, page 104. If great accuracy is desired, the NWL statistical sensitivity program, with the quadratic convergence of the Newton-Raphson method, would be

superior. But the numerical work in the NWL program, with exact calculation of all second derivatives (as compared with approximations in the probit method) would be very laborious by hand. We mention that a useful table for carrying out a probit analysis by hand is given in [11].

In a typical insecticide test of the type discussed by Finney in [10], 50 insects might be given a dose of the poison of which the concentration is 10.2 milligrams per liter, 40 insects a dose of 7.7 mg./l., etc., and the number of insects killed for each dose or concentration is recorded. Finney actually works with the logarithm to base 10 of the concentration (or of 100 times the concentration if necessary in order to make all logarithms positive), which he calls the dosage, rather than with the concentration itself, which he calls the dose. He assumes that the critical dosages (rather than doses) of the individual insects, as commented on in more detail below, are normally distributed about a mean μ with standard deviation, σ . This appears to be purely an assumption. Extensive experience with tests of this type indicates that the critical dosages are in fact approximately normally distributed.

Suppose that a given dosage, say x_1, following Finney's notation of x for dosage, kills 40 per cent of the insects subjected to it, and another dosage, x_2, kills 70 per cent. To give intuitive content to these results, we hypothesize the existence of a random variable

called the critical dosage of an individual insect, defined as the dosage just sufficient to kill him. If the critical dosage for a particular insect is 1.2, he will be killed by a dosage of 1.2 or 1.5, but not by a dosage of 1.1. We assume that those individual critical dosages are normally distributed about a mean critical dosage, μ, with standard deviation σ. The results cited above for dosages x_1 and x_2 are interpreted as meaning that, for a randomly selected individual insect, the probability that his critical dosage is less than x_1, or less than x_2, is 0.4 or 0.7 respectively. Hence for a large random sample, about 40 per cent will be killed by a dosage x_1, and 70 per cent by a dosage x_2. In the language of normal probability integrals, we can write

$$\frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{x_1} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right] dx$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\frac{x_1-\mu}{\sigma}} \exp\left[-\frac{1}{2}u^2\right] du = 0.4 \ , \qquad (165)$$

$$\frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{x_2} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right] dx$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\frac{x_2-\mu}{\sigma}} \exp\left[-\frac{1}{2}u^2\right] du = 0.7 \ . \qquad (166)$$

If the normal deviates of the form $(x-\mu)/\sigma$ are replaced by Y-5, the quantity Y is called the probit. Thus, in these two cases we would have

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{Y_1-5} \exp\left[-\frac{1}{2}u^2\right] du = 0.4 \ , \tag{167}$$

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{Y_2-5} \exp\left[-\frac{1}{2}u^2\right] du = 0.7, \tag{168}$$

and from a probability integral table we easily determine the approximate values

$$Y_1 = 4.74665, \qquad Y_2 = 5.52440. \tag{169}$$

The term -5 has no theoretical significance, but has the effect of making the probit Y always positive in practical cases, since virtually all of a normal distribution is within $\pm 5\sigma$ of the mean. Thus the probit Y is related to the dosage x by the relation

$$Y - 5 = \frac{x-\mu}{\sigma} \ . \tag{170}$$

The probit Y of Eqs. (167) and (168), where the probability, 0.4 or 0.7 or some other value, is deduced from experimental data (for example, the killing of 40% of the insects who receive a given

dosage of poison), is called the empirical probit, to distinguish it from the expected probit, also denoted by the letter Y, which is introduced later. There exists still another probit, the working probit Eq. (204), denoted by the symbol y. The empirical probit can have the value $\pm\infty$. Suppose that 25 insects receive a certain dosage and all are killed. Then the equation corresponding to (167) is

$$(1/\sqrt{2\pi}\,)\int_{-\infty}^{Y-5} \exp(-u^2/2)du = 1 \ ,$$

of which the solution is $Y = \infty$. Similarly, if no insects are killed at a given dosage, the empirical probit is $Y = -\infty$.

Later Finney introduces new parameters α and β to express the relationship between the probit Y and the dosage or stimulus x by the formula

$$Y = \alpha + \beta x \ . \qquad (171)$$

The variable Y here is called the expected probit and the expression $\alpha + \beta x$ is similar to the expressions $\beta a_i - \alpha$ and $\beta b_j - \alpha$ in the NWL analysis (see Eqs. (5) through (8)), or $\beta c_k - \alpha$ for any stimulus c_k whether a success or a failure. To clarify this similarity, we point out that the symbols β play exactly analogous roles in the two systems of notation, but Finney's α, which we temporarily denote as α_F, differs from the NWL α, α_N, by an algebraic sign and the additive term -5. For, equating the stimuli x and c, we have

$$Y-5 = \alpha_F + \beta x - 5 = \frac{x-\mu}{\sigma} = \frac{c-\mu}{\sigma} = \beta c - \alpha_N ,$$

from which it follows that

$$\alpha_F - 5 = -\alpha_N . \tag{172}$$

Considering now Finney's notation only, from (170) and (171) we deduce

$$\left.\begin{aligned} \alpha &= 5 - \frac{\mu}{\sigma} \\ \beta &= \frac{1}{\sigma} , \end{aligned}\right\} \tag{173}$$

and

$$\left.\begin{aligned} \mu &= (5 - \alpha)/\beta \\ \sigma &= 1/\beta . \end{aligned}\right\} \tag{174}$$

The <u>expected</u> probit Y as in Eq. (171) is always finite for a finite dosage x, since this equation merely expresses a linear relationship between Y and x which is a line of best fit in some sense when the optimum values of the parameters α and β have been determined. This is in contrast to the <u>empirical</u> probit, which can have a value of $\pm\infty$ as pointed out above.

Now for the next few steps, following Finney's analysis on pages 246-248 of [10], we suppose that we have a general probability distribution, not necessarily normal, of critical dosages. We will suppose that L, the logarithm of the likelihood function, is a function of two parameters θ and ϕ, and make certain comments on maximizing L, and derive Finney's method for approximating the second derivatives of L with respect to the parameters θ and ϕ. Later we specialize to the normal distribution and identify θ and ϕ with α and β as discussed above (see Eqs. (171), (173), (174)).

Suppose that a dosage λ_o has a probability P of killing a randomly selected insect and let Q = 1 - P = probability of failure, and suppose that it is observed in a test that r out of n insects receiving the dosage λ_o are killed. Thus r/n is what can be called the <u>empirical probability</u> p of success, while P is a function of the parameters θ and ϕ as well as the dosage x and depends on the assumed probability distribution (not necessarily normal). The object is to determine the values of θ and ϕ which maximize the probability of obtaining the observed or empirical probabilities, r/n at dosage λ_o and other empirical probabilities at other dosages in the experiment. In short, we wish to determine the maximum likelihood estimates, $\bar{\theta}$ and $\bar{\phi}$, for the parameters θ and ϕ.

The probability that r out of n insects will be killed by dosage λ_o is

$$P(r) = \binom{n}{r} P^r Q^{n-r} , \tag{175}$$

$\binom{n}{r}$ being a binomial coefficient with value n!/[r!(n-r)!]. Suppose that a series of K dosages is tested in an experiment with empirical probabilities of the form r/n for each dosage. Then the logarithm, L, of the probability of obtaining all of the observed results, dropping from L constant terms (not depending on θ and ϕ) of the form $\log \binom{n}{r}$, is

$$L = \Sigma r \log P + \Sigma (n-r) \log Q , \tag{176}$$

Σ denoting summation over all dosages (Finney uses the notation S for Σ).

We remark here that n in this equation is only the number of insects subjected to one given dosage. If the values for the K different dosages are denoted by $n_1, n_2, \ldots, n_K$, the grand total N is $N = n_1 + n_2 + \ldots + n_K$. Similarly we would have $r_1, r_2, \ldots, r_K$; $P_1, P_2, \ldots, P_K$; and $Q_1, Q_2, \ldots, Q_K$. But in Eq. (176) we follow Finney's analysis (with Σ substituted for his S).

For the values of θ and ϕ which maximize L we will have

$$\frac{\partial L}{\partial \theta} = \frac{\partial L}{\partial \phi} = 0. \tag{177}$$

Now, from Eq. (176),

$$\frac{\partial L}{\partial \theta} = \Sigma \frac{r}{P} \frac{\partial P}{\partial \theta} + \Sigma \frac{n-r}{Q} \frac{\partial Q}{\partial \theta} . \tag{178}$$

Putting $\frac{\partial Q}{\partial \theta} = - \frac{\partial P}{\partial \theta}$ (since Q = 1-P), r = pn, and performing some simple algebraic steps, we easily show that

$$\frac{\partial L}{\partial \theta} = \Sigma \left[\frac{n(p-P)}{PQ} \frac{\partial P}{\partial \theta} \right], \tag{179}$$

and similarly

$$\frac{\partial L}{\partial \phi} = \Sigma \left[\frac{n(p-P)}{PQ} \frac{\partial P}{\partial \phi} \right] . \tag{180}$$

Suppose that, at an intermediate stage in the calculation, θ and ϕ have values θ_1, ϕ_1 which make the derivatives $\partial L/\partial \theta$ and $\partial L/\partial \phi$ numerically small but not exactly zero. The corrections $\delta\theta$, $\delta\phi$

are given approximately, by Taylor's theorem, by

$$\frac{\partial L}{\partial \theta_1} + \delta\theta \frac{\partial^2 L}{\partial \theta_1^2} + \delta\phi \frac{\partial^2 L}{\partial \theta_1 \partial \phi_1} = 0 \qquad (181)$$

$$\frac{\partial L}{\partial \phi_1} + \delta\theta \frac{\partial^2 L}{\partial \theta_1 \partial \phi_1} + \delta\phi \frac{\partial^2 L}{\partial \phi_1^2} = 0, \qquad (182)$$

where the subscript 1 indicates that the derivatives are to be evaluated at $\theta = \theta_1$, $\phi = \phi_1$.

Finney now states ([10], page 248) that the second derivatives "may be simplified by putting p = P after differentiation, in order to give expected instead of empirical values", and derives approximations for the second derivatives in terms of the first derivatives. These appear to depend for their validity on the assumption that the particular value P_1 is near the empirical probability p (=r/n), whereas, in fact, p may be a value which is not approximated closely when the final maximum likelihood estimates $\bar{\theta}$, $\bar{\phi}$ are obtained. Yet the method evidently has worked well in practice. Indeed, it is proved later in this appendix, pages 108-112 , that, if Finney's method converges at all, it must converge to the true maximum likelihood estimates $\bar{\theta}$, $\bar{\phi}$, as determined by the NWL program, in spite of the inexactness of the approximations which Finney makes at intermediate stages. A convergence proof has not been worked out, nor does Finney give such a proof in [10]. But a little computational experience with the method soon convinces one that the method does converge, at any rate for sufficiently good initial approximations.

The following is an attempt to obtain the expressions at which Finney arrives for the second derivatives. We suppose, following Finney's notation, that (θ_1, ϕ_1) is a point in the $\theta\phi$-plane, at which we wish to approximate the second derivatives, which will be denoted by $(\partial^2 L/\partial\theta^2)_1$, $(\partial^2 L/\partial\theta\partial\phi)_1$, $(\partial^2 L/\partial\phi^2)_1$. We will illustrate with $(\partial^2 L/\partial\theta^2)_1$, but similar considerations will apply in the cases of the other second derivatives.

We shall simply differentiate, with respect to θ, the first derivative as given by Eq. (179), and for convenience, in the next few steps, we drop the subscript 1, since this differentiation will apply to any point (θ, ϕ) including (θ_1, ϕ_1). Primes will denote partial derivatives with respect to θ; thus P'' represents $\partial^2 P/\partial\theta^2$.

Eq. (179) states

$$\frac{\partial L}{\partial \theta} = \Sigma \frac{n(p-P)}{PQ} P' , \tag{183}$$

or

$$\frac{\partial L}{\partial \theta} = \Sigma \frac{(np-nP)P'}{P - P^2} , \tag{184}$$

since $Q = 1 - P$.

Derivative of numerator of (184) $= -n(P')^2 + (np-nP)P''$. (185)

Derivative of denominator of (184) $= P' - 2PP' = P'(1-2P)$. (186)

Hence,

$$\frac{\partial^2 L}{\partial\theta^2} = \Sigma \frac{PQ[-n(P')^2 + (np-nP)P''] - (np-nP)P'P'(1-2P)}{P^2Q^2}$$

$$\frac{\partial^2 L}{\partial\theta^2} = \Sigma \frac{n}{PQ} \left\{ -(P')^2 + (p-P)\left[P'' - \frac{(P')^2(1-2P)}{PQ} \right] \right\} . \tag{187}$$

From this it is seen that we get a simplified expression for $\partial^2 L/\partial\theta^2$, although not necessarily an extremely close approximation, by assuming that p = P for every dosage x. Probably, in the majority of practical cases, the positive errors in the summation approximately balance the negative errors. Further comments on this are given below. Making this assumption that p = P in all cases, we have

$$\frac{\partial^2 L}{\partial\theta^2} \cong \Sigma \frac{n}{PQ} [- (P')^2] \tag{188}$$

or, putting in the subscript 1, since, following Finney, we wish this to apply at a point designated as (θ_1, ϕ_1),

$$\left(\frac{\partial^2 L}{\partial\theta^2}\right)_1 \cong \Sigma \left[- \frac{n}{P_1 Q_1} \left(\frac{\partial P}{\partial\theta}\right)_1^2 \right] . \tag{189}$$

Similarly we have the approximations

$$\left(\frac{\partial^2 L}{\partial\phi^2}\right)_1 \cong \Sigma \left[- \frac{n}{P_1 Q_1} \left(\frac{\partial P}{\partial\phi}\right)_1^2 \right] , \tag{190}$$

$$\left(\frac{\partial^2 L}{\partial\theta\partial\phi}\right)_1 \cong \Sigma \left[- \frac{n}{P_1 Q_1} \left(\frac{\partial P}{\partial\theta}\right)_1 \left(\frac{\partial P}{\partial\phi}\right)_1 \right] . \tag{191}$$

From this development it appears that Finney simply accepts the errors which undoubtedly occur in using (189) - (191), trusting that in the long run the positive errors will approximately balance

the negative errors. Experience indicates that the method does converge satisfactorily in practice in realistic cases, especially in the hands of an investigator who is experienced in the method and who makes a skilled first approximation. If it converges at all, it must converge to the true maximum likelihood estimates $\bar{\theta}$, $\bar{\phi}$, as shown in Theorem C-1 in this appendix. However, it is possible that artificial or unrealistic cases exist in which the probit method fails to converge, since no general convergence proof has been given so far as the present authors are aware.

Using the approximations represented by (189) - (191), and for convenience dropping the "$\cong$" signs although they are understood here, Eqs. (181) and (182) for $\delta\theta$ and $\delta\phi$ take the form

$$\delta\theta \Sigma \frac{n}{P_1Q_1}\left(\frac{\partial P}{\partial \theta}\right)_1^2 + \delta\phi \Sigma \frac{n}{P_1Q_1}\left(\frac{\partial P}{\partial \theta}\right)_1\left(\frac{\partial P}{\partial \phi}\right)_1$$

$$= \Sigma \frac{n(p-P_1)}{P_1Q_1}\left(\frac{\partial P}{\partial \theta}\right)_1 , \qquad (192)$$

$$\delta\theta \Sigma \frac{n}{P_1Q_1}\left(\frac{\partial P}{\partial \theta}\right)_1\left(\frac{\partial P}{\partial \phi}\right)_1 + \delta\phi \Sigma \frac{n}{P_1Q_1}\left(\frac{\partial P}{\partial \phi}\right)_1^2$$

$$= \Sigma \frac{n(p-P_1)}{P_1Q_1}\left(\frac{\partial P}{\partial \phi}\right)_1 . \qquad (193)$$

For given values, θ_1, ϕ_1 of the parameters (assuming they are near the maximum likelihood estimates $\bar{\theta}, \bar{\phi}$), resulting in values P_1, Q_1, and the first derivatives $(\partial P/\partial\theta)_1$, $(\partial P/\partial\phi)_1$, at the various stimulus levels, we solve Eqs. (192), (193) for corrections $\delta\theta, \delta\phi$ to give improved values $\theta_1 + \delta\theta$, $\phi_1 + \delta\phi$.

So far this is very general, as remarked after Eq. (174), and the probability distribution is arbitrary and not necessarily normal. But now suppose we have a normal distribution, with

$$P = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{Y-5} \exp(-u^2/2)du \ , \tag{194}$$

$$Y = \alpha + \beta x \ , \tag{195}$$

(195) being the same as (171). Then

$$\frac{\partial P}{\partial Y} = \frac{1}{\sqrt{2\pi}} \exp\left[-(Y-5)^2/2\right] \equiv Z \ , \tag{196}$$

$$\frac{\partial P}{\partial \alpha} = Z \ , \tag{197}$$

$$\frac{\partial P}{\partial \beta} = xZ \ . \tag{198}$$

Hence, if c_1 and d_1 of

$$Y = c_1 + d_1 x \tag{199}$$

are first approximations to the maximum likelihood estimates of (195), corrections δc, δd, to c_1, d_1 are given by (192), (193) as

specialized to the present normal case. Using the first derivatives as given by (197), (198), the equations become

$$\delta c \, \Sigma \frac{nZ^2}{PQ} + \delta d \, \Sigma \frac{nZ^2}{PQ} x = \Sigma \frac{nZ^2}{PQ} \left(\frac{p-P}{Z} \right) \tag{200}$$

$$\delta c \, \Sigma \frac{nZ^2}{PQ} x + \delta d \, \Sigma \frac{nZ^2}{PQ} x^2 = \Sigma \frac{nZ^2}{PQ} x \left(\frac{p-P}{Z} \right) , \tag{201}$$

Z, P and Q being determined from (194) and (196) by the value of Y from (199), i.e. with $\alpha = c_1$, $\beta = d_1$.

Defining the weighting coefficient, w, by

$$w = \frac{Z^2}{PQ} , \tag{202}$$

Eqs. (200) and (201) are the equations for the estimation of the weighted linear regression of the variable (p-P)/Z on x, the weight nw being assigned to each value of (p-P)/Z.

This is briefly shown as follows. Suppose we have a set of K points $\{(x_i, y_i)\}$ and a set of corresponding weights $\{v_i\}$ (y_i will be identified with (p-P)/Z for the various stimuli in the present situation, and v_i with the corresponding weight nw). It is desired to find the line $y = c + dx$ such that the weighted sum $S = \Sigma v_i (c + dx_i - y_i)^2$ is minimized. We put

$$\left\{ \begin{array}{l} \frac{1}{2} \frac{\partial S}{\partial c} = \Sigma v_i (c + dx_i - y_i) = 0 \\ \\ \frac{1}{2} \frac{\partial S}{\partial d} = \Sigma v_i (c + dx_i - y_i) x_i = 0, \end{array} \right\}$$

from which follow the normal equations,

$$\left\{ \begin{array}{l} c\Sigma v_i + d\Sigma v_i x_i = \Sigma v_i y_i \\ c\Sigma v_i x_i + d\Sigma v_i x_i^2 = \Sigma v_i x_i y_i . \end{array} \right\} \tag{203}$$

Letting c, d, y_i, v_i here correspond to δc, δd, $(p-P)/Z$, $nw = \frac{nZ^2}{PQ}$, respectively, the similarity of (203) to (200) and (201) is clear.

We now introduce the working probit, y, [10, p. 250], defined by

$$y = Y + \frac{p - P}{Z} . \tag{204}$$

The working probit y depends on both the expected probit Y (which determines P and Z) and the per cent kill p. Convenient tables for determining y as a function of these arguments are given in [10].

Replacing $(p - P)/Z$ in Eqs. (200) and (201) by $y - Y$, by (204), transposing the terms containing Y to the left, and replacing $Z^2/(PQ)$ by w, by (202), Eqs. (200) and (201) give

$$\delta c\Sigma nw + \delta d\Sigma nwx + \Sigma nwY = \Sigma nwy \tag{205}$$

$$\delta c\Sigma nwx + \delta d\Sigma nwx^2 + \Sigma nwxY = \Sigma nwxy . \tag{206}$$

But the expected probits, Y, are determined in each cycle of the calculation from the equation of the line determined in the previous cycle, $Y = c_1 + d_1 x$, Eq. (199), in the present situation. In the first cycle of calculations, c_1 and d_1 would depend on the line fitted by eye (see further comments on this following Eq. (210)) to the

experimental data, and the improved values resulting from the cycle would be $c_2 (= c_1 + \delta c)$ and $d_2 (= d_1 + \delta d)$. Logically, we should have c_n and d_n at the start of our cycle, and improved values c_{n+1} and d_{n+1}, but we will stick with our notation c_1, d_1 for the initial values as in (199). Thus each expected probit Y is determined from the corresponding stimulus x by Eq. (199), and so we have

$$\Sigma nwY = c_1 \Sigma nw + d_1 \Sigma nwx \tag{207}$$

$$\Sigma nwxY = c_1 \Sigma nwx + d_1 \Sigma nwx^2 \ . \tag{208}$$

Putting these results in (205) and (206), and recalling that $c_2 = c_1 + \delta c$, $d_2 = d_1 + \delta d$, we have

$$c_2 \Sigma nw + d_2 \Sigma nwx = \Sigma nwy \tag{209}$$

$$c_2 \Sigma nwx + d_2 \Sigma nwx^2 = \Sigma nwxy \tag{210}$$

for the direct determination of the improved values c_2 and d_2.

The skillful determination of a first approximation $Y \equiv c_1 + d_1 x$ by fitting a line "by eye" to the empirical data is a matter of experience and defies exact analysis. Finney states, [10, page 248], "care and experience in the choice of first approximations will usually ensure that two cycles give a numerical accuracy sufficient for practical purposes." The dosages x are known and the empirical probits, Y, which are determined from the empirical probabilities p(= r/n), putting p in place of P in Eq. (194), are plotted against x. The subsequent fitting of a line to these plotted points is similar to

"least squares by eye", which is well known in obtaining "quick and dirty" solutions to practical problems. But the difficulties are compounded here by the fact that some of the empirical probits may be $\pm\infty$. If, for a certain dosage x, all of the subjects are killed, or r = n, then the empirical probability p is 100% or 1.0, and consequently, by (194), the empirical probit Y is ∞. Similarly if, for a given x, p is 0 (i.e. none of the subjects is killed), then the empirical probit Y is $-\infty$. Presumably, users of the method learn through experience how much to raise or lower the line $Y = c_1 + d_1 x$, corresponding to empirical probits of ∞ and $-\infty$, respectively, so as to get a reasonably good first approximation and thus justify the quoted statement from [10] that two subsequent cycles of calculation will usually give a numerical accuracy sufficient for practical purposes.

In solving this linear system (209) and (210), for c_2 and d_2, we introduce, with Finney, [10, pp. 55 and 250], symbols $\bar{x}$, $\bar{y}$, S_{xx}, S_{xy}, defined as follows:

$$\bar{x} = \frac{\Sigma nwx}{\Sigma nw} , \tag{211}$$

$$\bar{y} = \frac{\Sigma nwy}{\Sigma nw} , \tag{212}$$

$$S_{xx} = \Sigma nw(x - \bar{x})^2 , \tag{213}$$

$$S_{xy} = \Sigma nw(x - \bar{x})(y - \bar{y}) . \tag{214}$$

We can then show by algebraic manipulations, of which we omit the details, that

$$S_{xx} = \Sigma nwx^2 - \frac{(\Sigma nwx)^2}{\Sigma nw} \tag{215}$$

$$S_{xy} = \Sigma nwxy - \frac{(\Sigma nwx)(\Sigma nwy)}{\Sigma nw} . \tag{216}$$

The determinant, Δ, of the linear system (209), (210), is

$$\Delta = \Sigma nw \Sigma nwx^2 - (\Sigma nwx)^2 = S_{xx} \Sigma nw, \tag{217}$$

the last expression following by (215). Clearly, $\Delta > 0$, by (213) and the fact that the weights nw are positive. The solution of the system (209), (210), for c_2 and d_2 by Cramer's rule from linear algebra is then given by

$$\Delta \cdot c_2 = \Sigma nwy \cdot \Sigma nwx^2 - \Sigma nwx \cdot \Sigma nwxy \tag{218}$$

$$\Delta \cdot d_2 = \Sigma nw \cdot \Sigma nwxy - \Sigma nwx \cdot \Sigma nwy , \tag{219}$$

and from (216), (217) and (219) we obtain

$$\Delta \cdot d_2 = S_{xy} \Sigma nw ,$$

or

$$d_2 = \frac{S_{xy} \Sigma nw}{S_{xx} \Sigma nw} = \frac{S_{xy}}{S_{xx}} . \tag{220}$$

We can then show that

$$c_2 = \bar{y} - d_2 \bar{x} \tag{221}$$

by evaluating $\Delta \cdot (\bar{y} - d_2\bar{x})$ by means of several of the equations starting with (211), carrying out the necessary algebra, of which again we omit the details, and showing that the resulting expression is equivalent to $\Delta \cdot c_2$ as given by (218).

The improved values c_2 and d_2 are thus given by Eqs. (220), (221), and the resulting equation at the end of the computing cycle is

$$Y = c_2 + d_2 x, \tag{222}$$

as an improvement on Eq. (199); that is, (222) in general leads to a larger value of the likelihood function than (199).

This analysis leads to an efficient algorithm for use with a desk calculator, and such calculations have been carried out by one of the present authors. The experimentally determined values of the logarithms of the stimuli, x, are entered, and the corresponding values of n, r and p(= r/n). The values of Y are then calculated by Eq. (199), $Y = c_1 + d_1 x$, from the previous cycle or from the line fitted by eye. The values of w and nw can then be computed from Eq. (202), from the values of P, Q and Z, all of which depend on Y, but [10] gives tables for w which are accurate and extensive enough for most practical work. The working probits, y (see Eq. (204)), are then found from tables in [10]. We next compute Σnwx, Σnwy, Σnwx^2, and $\Sigma nwxy$, all of which are efficiently computed on a desk calculator. The values of $\bar{x}$, $\bar{y}$, S_{xx} and S_{xy} are then found by Eqs. (211), (212), (215) and (216), d_2 by (220) and c_2 by (221), and we then have the improved equation, (222).

After several such computing cycles, usually not more than four or five cycles unless the $\{c_i\}$ and $\{d_i\}$ are computed to high precision, say to more than five significant digits, the values start repeating themselves, with (for some n) $c_n = c_{n+1} = c_{n+2} = \ldots$ to the number of digits carried, and similarly for the $\{d_i\}$, indicating that convergence has occurred. We show in the following theorem that in such a case, denoting the final regression equation so obtained as $Y = \alpha + \beta x$ (see Eq. (171)), then the corresponding values of μ and σ, computed by Eqs. (174), must be identical with the maximum likelihood values $\bar{\mu}$, $\bar{\sigma}$ computed by the NWL program.

THEOREM C-1

Assume that the parameters c_n, d_n in the Finney method converge to values, α, β, with (1) $c_n \to \alpha$, $d_n \to \beta$ as $n \to \infty$, (2) if $c_1 = \alpha$ and $d_1 = \beta$ in the cd-plane, the increments δc, δd as given by Eqs. (200) and (201) both vanish, and (3) by continuity, δc and δd are arbitrarily close to zero if (c_1, d_1) is arbitrarily close to (α, β) in the cd-plane. Assume further that the experiment is such that (35), (36) in the NWL theory are satisfied, guaranteeing the existence of a unique pair $\bar{\mu}$, $\bar{\sigma}$ of maximum likelihood estimates.

Then if μ, σ are computed from this pair α, β by Eqs.(174), these values μ, σ are identical with the values $\bar{\mu}, \bar{\sigma}$ as computed by the NWL method.

Proof. The proof consists simply of showing that, if we have values α, β such as are described in the hypothesis, then for the

corresponding values in the NWL theory (corresponding to the same values of μ and σ, but with α_N in general different numerically from α_F, as indicated by Eq. (172)) we will have $L_\alpha = L_\beta = 0$, which can be true only for the unique maximum point $(\bar{\alpha}, \bar{\beta})$ or $(\bar{\mu}, \bar{\sigma})$ in cases where the conditions (35), (36) are satisfied. Hence the point (α_F, β) of the hypothesis must correspond to the point $(\bar{\alpha}_N, \bar{\beta})$ or $(\bar{\mu}, \bar{\sigma})$ of the NWL theory. Naturally there are many details, which we proceed to give.

From Eqs. (200) - (201), the corrections δc and δd both vanish, indicating that convergence has occurred in the probit method, if and only if the right-hand sides of these equations vanish. This linear system has a nonsingular matrix, since it has been shown following Eq. (217) that $\Delta > 0$. These right-hand sides are equivalent to $\partial L/\partial\alpha$ and $\partial L/\partial\beta$ in the probit system, as is easily shown. Hence convergence occurs, and $\delta c = \delta d = 0$, if and only if a point is reached at which $\partial L/\partial\alpha = \partial L/\partial\beta = 0$, and this result is to be expected on general principles as well as on the specific analysis given here. Hence our object is to show that, if a point is reached where $\partial L/\partial\alpha = \partial L/\partial\beta = 0$ in the probit system, then we also have $\partial L/\partial\alpha = \partial L/\partial\beta = 0$ in the NWL system, so that we are at the maximum likelihood parameter point $(\bar{\alpha}, \bar{\beta})$ or $(\bar{\mu}, \bar{\sigma})$.

In comparing the probit and NWL systems, we have to deal with the univariate probability integral $p(x)$, $q(x) = 1 - p(x)$ and $z(x)$, with Finney's P, Q, Z and P_k, Q_k, Z_k corresponding to a specific dosage x_k,

with his $p = r/n$ = empirical probability for a given dosage, and with the expressions p_i and q_j in the NWL system. Hence we comment here on these various notations.

The probability integrals $p(x)$, and $q(x)$ and $z(x)$, are given by Eqs. (10) - (12) with slightly different notation from that which is used here, and also the functions $P(x)$ and $Q(x)$ are defined earlier, page 95 . The NWL expressions p_i and q_j are defined in Eqs. (3), (4) in terms of these p and q functions of certain arguments.

We now suppose that, in a sequence of iterations of the probit method, a situation has been reached in which $\partial L/\partial\theta = \partial L/\partial\phi = 0$, or, Eqs. (179) - (180) are satisfied, implying that a maximum of Finney's likelihood function L has been reached. Supposing further that the underlying distribution is normal, we use Eqs. (197) - (198) and obtain

$$\frac{\partial L}{\partial \alpha} = \Sigma \frac{n(p - P)}{PQ} Z = 0 \qquad (223)$$

$$\frac{\partial L}{\partial \beta} = \Sigma \frac{n(p - P)}{PQ} xZ = 0 \ . \qquad (224)$$

These obviously imply that the right-hand sides vanish in Eqs. (200) - (201), the equations which are actually used in the iterations, so that further iterations would merely repeat the values already obtained.

Our object is to show that, in this situation, we must also have $\partial L/\partial\alpha = \partial L/\partial\beta = 0$ in the NWL method, so that we must have arrived at the unique maximum likelihood point $(\bar{\alpha}, \bar{\beta})$ or $(\bar{\mu}, \bar{\sigma})$ in the NWL system, using the (μ, σ) system as a common coordinate system for purposes of comparison.

By Eqs. (194) and (196),

$$P_k = p\left(\frac{x_k - \mu}{\sigma}\right), \quad Z_k = z\left(\frac{x_k - \mu}{\sigma}\right), \tag{225}$$

since Y-5 is equivalent to $(x_k - \mu)/\sigma$, and similarly

$$Q_k = 1 - P_k = q\left(\frac{x_k - \mu}{\sigma}\right) . \tag{226}$$

Now the derivative L_α in the NWL system is, by Eqs. (10), (11), (13), (18) and (19), given by

$$L_\alpha = \sum_{j=1}^{m} \frac{z\left(\frac{b_j - \mu}{\sigma}\right)}{q\left(\frac{b_j - \mu}{\sigma}\right)} - \sum_{i=1}^{n} \frac{z\left(\frac{a_i - \mu}{\sigma}\right)}{p\left(\frac{a_i - \mu}{\sigma}\right)} , \tag{227}$$

and by Eqs. (225), (226), this is equivalent to

$$L_\alpha = m\frac{Z_k}{Q_k} - n\frac{Z_k}{P_k} , \tag{228}$$

(referring only to subjects receiving the stimulus x_k).

Here we have the NWL derivative L_α and the i and j summations as in Eq. (5), but Finney's P_k, Q_k and Z_k corresponding to the dosage x_k. At a given x_k, n_k insects receive the stimulus and r_k of them are killed. Hence the contribution to the NWL L_α from these n_k insects is

$$\frac{(n_k - r_k)Z_k}{Q_k} - \frac{r_k Z_k}{P_k} , \tag{229}$$

and taking all of the K stimuli into account, the NWL L_α is

$$L_\alpha = \sum_{k=1}^{K} \left[\frac{(n_k - r_k)Z_k}{Q_k} - \frac{r_k Z_k}{P_k} \right] , \qquad (230)$$

which simplifies to

$$\Sigma \left[\frac{n_k P_k Z_k - r_k Z_k}{P_k Q_k} \right] . \qquad (231)$$

Putting $r_k = p_k n_k$ and simplifying further,

$$L_\alpha = \sum_{k=1}^{K} \frac{n_k Z_k}{P_k Q_k} (P_k - p_k) , \qquad (232)$$

and this by Eq. (223) is $-L_\alpha$ in the probit system.

Hence L_α(NWL) = 0 if and only if L_α(probit method) = 0, and a similar analysis shows that the L_β derivatives vanish together. Hence Finney's maximum likelihood point (μ, σ) must be identical with the NWL maximum likelihood point $(\bar{\mu}, \bar{\sigma})$, and this completes the proof of Theorem C-1.

In [4], [10] and other books and papers dealing with experiments in which the probit method is used, we often find expressions such as LD50, LD99, etc., signifying the lethal dose (or dosage) for 50% of the subjects, for 99%, etc. Finney in [10] also uses expressions such as ED50, the letters meaning "effective dose", in cases where effects other than the deaths of the subjects are considered successes. Once the maximum likelihood values $\bar{\mu}, \bar{\sigma}$ have been determined, values such as LD50 and LD99 are very simply determined from a table of

probability integrals. Since

$$p(0) = 0.50, \quad p(2.3263) = 0.99, \tag{233}$$

where p(x) is the probability integral,

$$p(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} \exp(-u^2/2)du, \tag{234}$$

then, if x_{50} and x_{99} represent LD50 and LD99 respectively, we have

$$\frac{x_{50} - \bar{\mu}}{\bar{\sigma}} = 0, \quad \frac{x_{99} - \bar{\mu}}{\bar{\sigma}} = 2.3263 \ , \tag{235}$$

(compare with Eqs. (165), (166)), from which we find

$$x_{50} = \bar{\mu} \ , \quad x_{99} = \bar{\mu} + 2.3263 \, \bar{\sigma} \ , \tag{236}$$

and similarly for other expressions such as LD25, LD90, or LD95.

Reference [4] deals with an experiment in which poison (cobra venom) was administered to dogs. The input values including calculated values of x or log (100 · dose), are as follows:

Dose mg/kg	x = log(100 dose)	n	r
0.06	0.77815	4	0
0.09	0.95424	5	1
0.10	1.00000	9	3
0.11	1.04319	6	3
0.12	1.07918	8	7
0.25	1.39794	6	6
0.50	1.69897	6	6

The dose is in milligrams of poison per kilogram of the dog's weight.

The maximum likelihood values $\bar{\mu}$, $\bar{\sigma}$, using the dosages, x, were calculated at NWL by two distinct methods, (1) by desk calculator, using the probit method as discussed in this appendix, and (2) on an IBM 7030 (STRETCH) computer, using the NWL method as described in the main body of this report. The results of the STRETCH calculation are shown on page 115 of this report on which it will be observed that values of the dosage x to 5 decimal digits were used (with one trivial discrepancy in the smallest value of x, in that published tables of logarithms give 0.77815 as the value of log 6, whereas the value printed by the computer was 0.77814). In the NWL hand calculations, rounded values of the x's were used, 0.78, 0.95, etc. The LD99 values were also computed by Eqs. (236) above. Then the results were expressed in terms of the doses (in mg./kg. as discussed above), by taking antilogarithms. The values of $\bar{\sigma}$ so obtained are of doubtful significance, since the doses are not normally distributed if the dosages are so distributed. But the results were expressed in terms of the doses for purposes of comparison with the results in [4].

It is not known to the present authors how the authors of [4] performed their calculations. But it is assumed that they used the probit method, since they used such terminology as LD50 and LD99, and gave a figure showing the line $Y = \alpha + \beta x$ and curves determining 95% confidence limits, which are similar to the corresponding curves

in [10]. It is stated in [4] that the LD50 and LD99 doses are 0.105 and 0.148 mg./kg. respectively. The remaining results on the line "Edgewood, ref. [4]" in the table below were deduced by the present authors by means of Eqs. (236) and by taking logarithms to express results in terms of dosages. In view of the uncertainty as to the methods used in [4], close agreement between the Edgewood and NWL results was not necessarily to be expected.

However, a comparison between the two lines of NWL results, for dosages rather than doses, is meaningful. The input values of x were slightly different, as has been explained. Additional slight differences may be attributable to roundoff error and similar causes at intermediate stages, the NWL and probit methods being quite different. But theoretically the final results should be identical (for identical input), by Theorem C-1 of this appendix.

The results of these calculations were as shown in the following table.

	$\bar{\mu}$ = LD50 x	$\bar{\sigma}$ x	LD99 x	$\bar{\mu}$ = LD50 mg/kg	$\bar{\sigma}$ mg/kg	LD99 mg/kg
Edgewood, ref.[4]	1.02119	.064051	1.17026	.105	.11589	.148
NWL Hand Calc.	1.02309	.064432	1.17214	.10525	.11599	.14864
NWL STRETCH Calc.	1.02355	.064127	1.17273	.10557	.11591	.14884

In this table, the first three columns refer to the output in dosages, and the last three to the output in doses, milligrams of poison per kilogram of the dog's weight.

Also, 90% confidence limits for the NWL hand calculations were computed by Eq. (4.6), page 63 in [10], which is repeated here as (237). For a given Y, for which the corresponding x is computed from the equation $Y = \alpha + \beta x$, the limits are

$$x + \frac{g}{1-g}(x-\bar{x}) \pm \frac{t}{\beta(1-g)} \sqrt{\frac{1-g}{\sum nw} + \frac{(x-\bar{x})^2}{S_{xx}}}\ , \qquad (237)$$

where

$$g = t^2/(\beta^2 S_{xx})\ , \qquad (238)$$

and t is the value such that the standard t-variate in the Student t distribution, with K-2 degrees of freedom, with probability 0.90 (in the case of 90% limits) lies in the interval (-t, t). In the present case, in which K = 7 and hence there are 5 degrees of freedom, the value of t is 2.02. The positive and negative signs, in the double sign in (237), give the upper and lower confidence limits respectively.

These curves and the line $Y = \alpha + \beta x$, are shown in Figure 4.

If $g > 1$, expression (237) will clearly have a negative radicand when $x = \bar{x}$, and for this reason 95% confidence limits cannot be computed for this example by this method. For probability 0.95, the value of t as discussed above is 2.57, and for this example we have $\beta = 15.52013$, $S_{xx} = .02732$, and hence $g = 1.004 > 1$. It is not known to the present authors how the 95% confidence limits of [4] were computed.

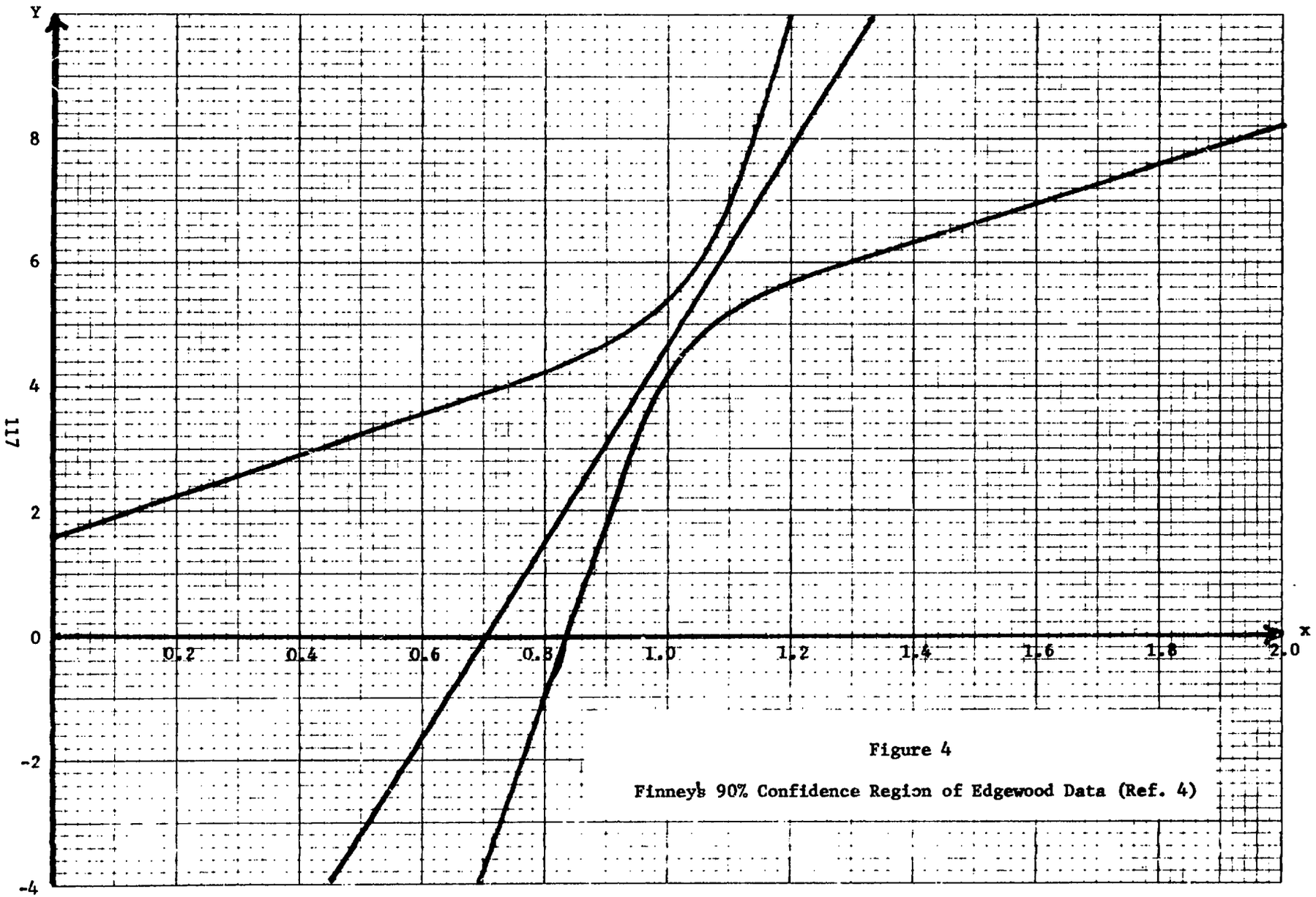

Figure 4

Finney's 90% Confidence Region of Edgewood Data (Ref. 4)

APPENDIX D

SMALL SAMPLE THEORY

For determining confidence regions, the method recommended by Golub and Grubbs in [14] (see Section IV of the present report) and used in the existing NWL program, is that based on the asymptotic normality of the distribution of the maximum likelihood estimates $\bar{\mu}$ and $\bar{\sigma}$ for large samples. Since the experimental cases received at NWL usually contain 30 results or more (firings at armor plate), this asymptotic or large sample method is reliable.

Also, this asymptotic method is relatively simple and straightforward to program for a computer. It is not exact, however, except in the limit as the sample size becomes infinite.

In this appendix, a method is outlined by which confidence regions could be set up, which would be exact for finite samples of any size. Unfortunately, it appears that it would take a great deal of computer time. But we feel that it is worth giving this method for completeness. If computationally feasible, it would be of greatest interest and usefulness for small samples of say 4 or 5 results, for which the asymptotic large sample method would give results substantially in error. For this reason, such a method or theory is often referred to as a small sample theory. It could equally well be called an exact theory, giving exact results for samples of any size, which the asymptotic theory fails to do.

The confidence regions generated by the exact method discussed here would be connected sets in the plane, but not ellipses in general. These point sets, each containing infinitely many points, could be approximated by working with finite grids of small mesh size.

We begin with some definitions and generalities about confidence regions for experiments of the type here considered, and many of these remarks apply to the asymptotic large sample theory, or to any method of setting up confidence regions for these experiments, as well as to the exact theory to be presented in detail in this appendix.

We are given a set of stimulus levels (projectile speeds in the case of the armor plate experiment), $c_1, c_2, \ldots, c_N$ in the notation of this report, Section IV, where $N = n + m$. We could have, for instance, $c_1 = 1153$ ft./sec., $c_2 = 1161$, etc. These c_i are constants which serve to define the experiment. They are not random variables. In setting up confidence regions we conceive of a large number of replications of the experiment, with exactly the same set of $\{c_i\}$ each time, but with different outcomes, and analyze the distribution of these outcomes by probabilistic methods. The fact that in many experimental situations it is not possible to control the stimuli exactly, in particular in the case of projectile speeds, is immaterial from the theoretical point of view. Once we are given the constants of the experiment, the set of $\{c_i\}$, we can compute the functions $f(\delta_k; \mu, \sigma)$ of Eq. (65), each f_k depending on the constant c_k, the

random variable δ_k, and the variables μ and σ. If we changed any of the $\{c_i\}$, we would have a different experiment, with a different set of confidence regions corresponding to the various possible outcomes.

The random variables are the $\{\delta_k\}$ of Section IV, δ_k being given the value 1 if the k-th shot, of speed c_k, produced penetration, and a value of 0 if there was no penetration. Since there are N of these random variables, each having two possible values, there are 2^N possible outcomes of the experiment, or 2^N values in the joint distribution of the random variables. When we conduct an actual firing experiment, determining whether or not penetration occurs at 1153 ft./sec., at 1161 ft./sec., etc., in the armor plate experiment, we are taking a sample from the joint distribution of the set $\{\delta_k\}$. In practice we could not without many trials repeat the experiment even once, because of the impossibility of precisely controlling the stimuli, but we can conceive of a large number of replications, always with the same constants $\{c_i\}$.

Those members of the set $\{c_i\}$ for which penetration occurs form the set $\{a_i\}$ in the notation of this report, and the "failures" form the set $\{b_j\}$. In some of the 2^N possible outcomes, for a given set of constants $\{c_i\}$, Eqs. (35) and (36), the necessary and sufficient conditions for the existence of a unique maximum of the likelihood function, with $\sigma = 1/\beta > 0$, will be satisfied. These will be called <u>valid outcomes</u>. The remaining outcomes, in which Eqs. (35) - (36) are not satisfied, will be called <u>degenerate outcomes</u>. Thus the number of valid outcomes, plus the number of degenerate outcomes, is 2^N.

It is a trivial matter to construct examples of both types of outcome say for N = 3, the minimum value of N for a possible valid outcome.

In any experiment, where the set $\{c_i\}$ is specified, with $N \geqslant 3$, degenerate outcomes will necessarily exist, for instance by taking every "success", a_i, greater than every b_j, so that (35) is not satisfied. Also, valid outcomes must exist, in every experiment of interest at any rate. Hence if we denote the numbers of valid outcomes and degenerate outcomes by N_v and N_d respectively, we have

$$\left.\begin{aligned} N_v + N_d &= 2^N \\ 0 < N_v &< 2^N, \end{aligned}\right\} \tag{239}$$

where $N(= n + m)$, as before, is the number of members of the set $\{c_i\}$, or, in the armor plate experiment, the number of projectiles fired.

For any one of the N_v valid outcomes of the experiment, say the t-th one, there exists by Theorem 4 a unique point $\bar{A}_t(\bar{\mu}_t, \bar{\sigma}_t)$ in the $\mu\sigma$-plane, representing the maximum likelihood estimates of the parameters μ and σ determined by the t-th outcome. The calculation of these values $\bar{\mu}_t$ and $\bar{\sigma}_t$ to a preassigned accuracy is of course the principal object of the program described in this report. The $\mu\sigma$-plane and three of these points are shown in Figure 5. In actual experiments N_v may be very large, but is always less than 2^N and therefore finite. If N = 30, a realistic value in armor plate firings, $2^N > 10^9$.

For any method which may be used for determining confidence regions, there is associated with each point $\bar{A}_t(\bar{\mu}_t, \bar{\sigma}_t)$ a corresponding

confidence region R_t. For the asymptotic large sample method which is used in the program (Section IV), each of these regions is an ellipse with $\bar{A}_t$ at its center, and for convenience the confidence regions are shown as ellipses in Figure 5. But for the exact or small sample method to be described in this appendix, the regions are in general not ellipses. However, with each point $\bar{A}_t(\bar{\mu}_t, \bar{\sigma}_t)$ there is associated a corresponding confidence region R_t.

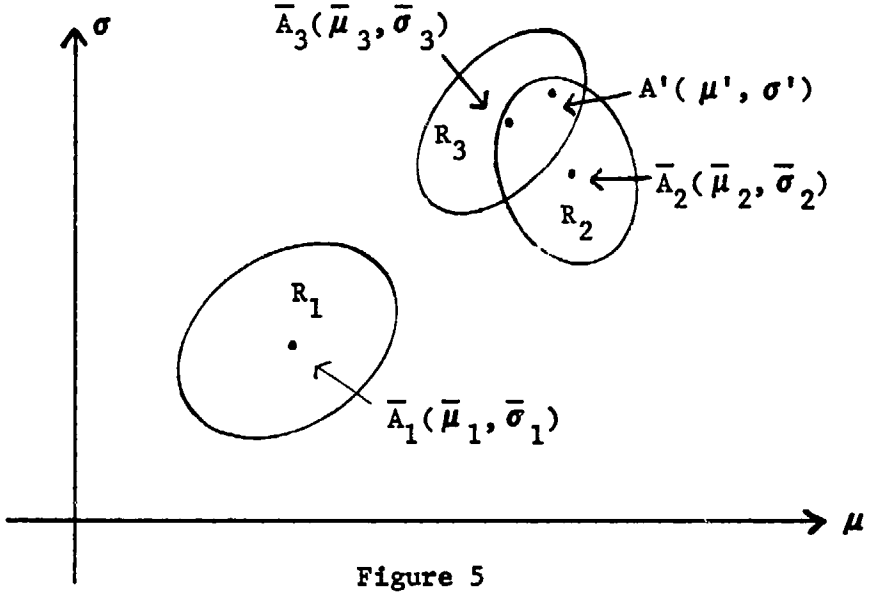

Figure 5

Maximum Likelihood Points $\bar{A}_t(\bar{\mu}_t, \bar{\sigma}_t)$ and Associated Confidence Regions.

So far we have merely stated that these confidence regions exist, and are associated one-to-one with the maximum likelihood points $A_t(\bar{\mu}_t, \bar{\sigma}_t)$ in the $\mu\sigma$-plane. We are now ready, however, to deal with such questions as the following. What is a confidence region? What conditions must be satisfied by the system of confidence regions generated by a given experiment, i.e. a given set of $\{c_i\}$, in order that the system qualifies as a set of, say, 90% confidence regions for the experiment?

First, the true but generally unknown parameters, μ_o and σ_o, are constants which we are trying to estimate from our experiment, and it is meaningless to speak of probabilities that the true parameter point $A_o(\mu_o, \sigma_o)$ lies in a given region. The true values μ_o and σ_o could be determined to any desired accuracy and confidence level by a sufficiently large number of experiments. Being constants, they are not subject to any statistical distribution. Alternatively, we may if we wish think of the true parameters μ_o and σ_o as controlled by an imaginary opponent who sets them at any values desired by him, but does not inform us of the values. Again, they are not subject to any statistical distribution. Once this opponent has set the values, our task is to estimate them by experimental methods.

Once the experiment has been defined, by specifying the constants $\{c_i\}$, a set of N_v maximum likelihood points $\{(\bar{A}_t(\bar{\mu}_t, \bar{\sigma}_t)\}$ and associated confidence regions $\{R_t\}$ (by whatever confidence region method is in use at the time) are determined. There may be many millions of them in realistic experiments.

But we can conceive of the computation of the entire finite system, since the entire system is defined once the $\{c_i\}$ are given, and it is defined before we take <u>any</u> sample of the joint distribution of the random variables $\{\delta_i\}$, as discussed above, by an actual firing of N projectiles, in the case of the armor plate problem.

For any specified outcome of the experiment defined by the given set $\{c_i\}$, either a valid or a degenerate outcome in the terminology used above, and for any assumed values (trial values, etc.) μ, σ of the parameters, whether equal to the true values μ_o, σ_o or not, there is a probability of occurrence of the given outcome expressed in terms of the variables μ and σ. We can begin with Eq. (65) giving the probability density function for each

$$f_k = f(\delta_k; \mu, \sigma) = \left[p\left(\frac{c_k - \mu}{\sigma}\right)\right]^{\delta_k} \left[q\left(\frac{c_k - \mu}{\sigma}\right)\right]^{1-\delta_k}, \qquad (240)$$

and write the joint density function for the entire set $\{\delta_i\}$ in the form

$$F(\delta_1, \ldots, \delta_N; \mu, \sigma) = \prod_{k=1}^{N} f(\delta_k; \mu, \sigma), \qquad (241)$$

$$F(\delta_1, \ldots, \delta_N; \mu, \sigma) = \prod_{k=1}^{N} \left[p\left(\frac{c_k - \mu}{\sigma}\right)\right]^{\delta_k} \cdot \prod_{k=1}^{N} \left[q\left(\frac{c_k - \mu}{\sigma}\right)\right]^{1-\delta_k}. \qquad (242)$$

Now suppose a definite outcome is specified by assigning particular values $\{\delta_i^*\}$ (each 0 or 1) to the set $\{\delta_i\}$, e.g. $\delta_1 = 0$, $\delta_2 = 0$, $\delta_3 = 1$, ... The probability of occurrence of the specified outcome is then

$$G(\mu, \sigma) \equiv F(\delta_1^*, \ldots, \delta_N^*; \mu, \sigma)$$

$$= \prod_{k=1}^{N} \left[p\left(\frac{c_k - \mu}{\sigma}\right)\right]^{\delta_k^*} \prod_{k=1}^{N} \left[q\left(\frac{c_k - \mu}{\sigma}\right)\right]^{1-\delta_k^*} . \qquad (243)$$

If we replace each δ_k^* by its value, 0 or 1, and replace each c_k which is a "success" by an a_i and each c_k which is a "failure" by a b_j, we get

$$G(\mu, \sigma) = \prod_{i=1}^{n} p\left(\frac{a_i - \mu}{\sigma}\right) \prod_{j=1}^{m} q\left(\frac{b_j - \mu}{\sigma}\right) , \qquad (244)$$

which is consistent with the expression in Eq. (2). Eq. (243) or (244), then, gives the probability, in terms of the assumed values of the variables μ and σ, that the specified outcome, valid or degenerate, will occur. The sum of all these G functions, for a given pair of values of μ and σ, over all of the 2^N possible outcomes of the experiment, must be 1, since for any sample from the distribution of the set $\{\delta_k\}$, i.e. for any firing of N projectiles at the specified speeds $\{c_k\}$ in the armor plate test, one and only one of the 2^N possible outcomes must occur.

We can now explain the significance of the confidence regions $\{R_t\}$ of Fig. 5, one R_t for each valid outcome, and state the condition which they must satisfy in order to be true confidence regions at a specified confidence level. The discussion is still perfectly general in that it applies to any method of setting up a system of these regions. For definiteness, we will specialize to 90% confidence regions, but the numerical value of the confidence level is immaterial.

The condition referred to is as follows. The system of 90% confidence regions, $\{R_t\}$, must be such that, whatever values the true but unknown parameters μ_o and σ_o may have, the conditional probability is at least 0.90 that, given that the outcome of the experiment is a valid one, the true parameter point $A_o(\mu_o, \sigma_o)$ is covered by at least one region of the system of confidence regions.

We give a simple numerical illustration in terms of the situation represented in Fig. 5, where there are only three valid outcomes, and then we phrase the condition more formally in terms of the $G(\mu, \sigma)$ notation.

In Fig. 5 we consider the situation with respect to the point $A'(\mu', \sigma')$, which is to be regarded as a possible position of the true parameter point $A_o(\mu_o, \sigma_o)$, since the position of A_o is unknown. Suppose we have the following probabilities: $G_1(\mu', \sigma') = .08$, $G_2(\mu', \sigma') = .56$, $G_3(\mu', \sigma') = .16$. This means that, if the population paremeters are μ' and σ', then the probability is .08 that the result is valid outcome No. 1 and similarly for subscripts

2 and 3. Hence the probability that the outcome is a valid one is the sum of these, or .80, and the probability of a degenerate outcome is 1 - .80 or .20. Therefore, given that the outcome is a valid one, the conditional probability that it is outcome No. 1 is .08/.80 or .10, and similarly for outcomes Nos. 2 and 3 the conditional probabilities are .56/.80 or .70, and .16/.80, or .20, respectively, these conditional probabilities summing to 1 since we suppose that there are only these three valid outcomes. But the point $A'(\mu', \sigma')$ is contained in both R_2 and R_3, and the conditional probability that the outcome is No. 2 or No. 3 is .70 + .20, or .90. Hence, if the true parameter point A_o is at A', the conditional probability, given that the outcome is a valid one, that the point A_o is covered by at least one of the regions $\{R_t\}$, is .90. Thus the required condition is satisfied for the point A' by the system $\{R_t\}$. Obviously, in order for the condition to be satisfied for all admissible positions of the point $A_o(\mu_o, \sigma_o)$, all such positions would have to be covered at least once by the system $\{R_t\}$, and this is not the case in the simplified Fig. 5.

This example can be looked at in another way in terms of a large number of replications of the experiment defined by the constants $\{c_k\}$. Suppose the experiment is performed 1,000,000 times and that the true parameter point $A_o(\mu_o, \sigma_o)$, as before, is the same as $A'(\mu', \sigma')$. Then, because of the assumed probabilities $G_1(\mu', \sigma') = .08$, etc., outcome 1 will occur about 80,000 times, outcome 2, 560,000 times, outcome 3, 160,000 times, and one or another of the possible degenerate outcomes will occur the remaining 200,000 times. Therefore, out of

800,000 replications in which a valid outcome occurs, outcome 2 or 3 will occur 720,000 times, or in 90% of the 800,000 cases. But $A'(\mu', \sigma')$, which we assume here to be the true parameter point, is covered by both of the confidence regions R_2 and R_3, and thus is covered in 720,000 out of every 800,000 replications which result in a valid outcome, or 90%. If every admissible position of the point $A_o(\mu_o, \sigma_o)$ satisfies a similar condition, the system of confidence regions is shown to be a legitimate system at the 90% confidence level.

The following analysis is a simple generalization of the foregoing example. We now assume that the set $\{c_k\}$ has N members, so that there are 2^N possible outcomes, valid and degenerate. Let $A(\mu, \sigma)$ be any point in the $\mu\sigma$-plane which is a possible position of the true parameter point $A_o(\mu_o, \sigma_o)$, and let $G_k(\mu, \sigma)$ (see Eq. (244)) be the probability that the k-th outcome will occur, if the true parameters are μ and σ. Let

$$p_v(\mu, \sigma) \equiv \sum_k \left\{ G_k(\mu, \sigma) \,\middle|\, \text{k-th outcome is valid} \right\}, \tag{245}$$

$$p_d(\mu, \sigma) = 1 - p_v(\mu, \sigma) \equiv \sum_k \left\{ G_k(\mu, \sigma) \,\middle|\, \begin{array}{l}\text{k-th outcome is} \\ \text{degenerate}\end{array} \right\}, \tag{246}$$

$$p_c(\mu, \sigma) \equiv \sum_k \left\{ G_k(\mu, \sigma) \,\middle|\, \text{point } A(\mu, \sigma) \text{ is in } R_k \right\}, \tag{247}$$

(v for "valid", d for "degenerate", c for "covers").

Then the following condition must be satisfied.

$$[p_c(\mu, \sigma)]/[p_v(\mu, \sigma)] \geqslant 0.90. \qquad (248)$$

If a similar condition is satisfied by every admissible position of the true parameter point $A_o(\mu_o, \sigma_o)$, then the system $\{R_t\}$ is a legitimate 90% system of confidence regions. It is assumed here that, given the set $\{c_k\}$, we have not only a set $\{\bar{A}_k(\bar{\mu}_k, \bar{\sigma}_k)\}$ of maximum likelihood points, one for each valid outcome, computable by the principal program of this report, but also a system $\{R_t\}$ of 90% confidence regions. Since the discussion still applies to any method of determining confidence regions, we merely assume that the system $\{R_t\}$ exists, and have not commented, in the preceding discussion, on the method of determining the system.

We now turn to the exact or so-called small sample method, the description of which is the principal object of this appendix, for determining the system $\{R_t\}$ of confidence regions.

First we comment on the phrase "admissible positions" which has been used with regard to the true parameter point $A_o(\mu_o, \sigma_o)$. We will have only a finite set $\{R_t\}$ of confidence regions, each of finite area, and hence the set of possible parameter points A_o cannot possibly be covered by the union of the sets $\{R_t\}$ if it is of infinite area. In an actual experiment it will ordinarily not be difficult to set limits μ_{min} and μ_{max} such that the true mean μ_o must be in the interval (μ_{min}, μ_{max}). In the armor plate experiment, for instance,

the projectile speeds are always positive and we may know from the characteristics of the gun, ammunition, etc., that the speed is always less than 2500 ft./sec. In such a case we could say that μ_o must be in the interval (0, 2500). From a knowledge of the bounds on μ_o and on the magnitudes of the individual stimuli, we could then compute bounds σ_{min} and σ_{max} on the true standard deviation σ_o, σ_{min} normally being 0 and σ_{max} positive. Thus in an actual experiment we can ordinarily limit the admissible positions of the true parameter point to those in the interior of a rectangle in the $\mu\sigma$-plane, determined by the inequalities $\mu_{min} < \mu_o < \mu_{max}$, $\sigma_{min} < \sigma_o < \sigma_{max}$, and this rectangle can be covered by a finite number of confidence regions, each of finite area.

We note in passing that the same problem of covering a possibly infinite area in the $\mu\sigma$-plane exists even in the asymptotic large sample method, since in practice we always have a finite number of stimuli and therefore a finite number of possible valid outcomes, each associated with its own confidence ellipse of finite area. We do not dwell on this point here, the large sample method being discussed in Section IV, although without explicit mention of this point.

In describing the determination of the confidence regions $\{R_t\}$, one confidence region R_t (as well as one maximum likelihood point $\bar{A}_k(\bar{\mu}_k, \bar{\sigma}_k)$) for each of the N_v valid outcomes of the experiment, we will consider a numerical example which will bring out the essential simplicity of the procedure, while if on the contrary we set up a

perfectly general notation with multiple subscripts, etc., we might create a false impression that the process is obscure and complicated.

We recall that the separation of the 2^N possible outcomes of the experiment into N_v valid outcomes and N_d degenerate outcomes, where $N_v + N_d = 2^N$, is independent of the assumed values μ and σ, but depends only on whether or not the $\{a_i\}$ and $\{b_j\}$, that is, the successes and failures among the stimuli $\{c_k\}$, satisfy Eqs. (35) - (36). Consequently, whatever admissible parameter point $A(\mu, \sigma)$ we consider, we will have exactly N_v valid outcomes to take into account. Moreover, $G_k(\mu, \sigma)$, the probability that the k-th valid outcome (in some enumeration of these outcomes) will result when the parameters are μ and σ (arbitrary admissible values) will be a positive number on the open interval (0, 1), though of course very close to 0 in some cases, those in which a large number of factors in Eq. (244) are small probabilities. The sum $\sum_k G_k(\mu, \sigma)$, summed over all valid outcomes, will be $p_v(\mu, \sigma)$, by definition of the latter, Eq. (245), and therefore $\sum \{[1/p_v(\mu, \sigma)]G_k(\mu, \sigma)\}$, summed over all valid outcomes, will be 1. Note, however, that all probabilities depend on μ and σ. If $A_1(\mu_1, \sigma_1)$ and $A_2(\mu_2, \sigma_2)$ are distinct parameter points, $p_v(\mu_1, \sigma_1) \neq p_v(\mu_2, \sigma_2)$ in general, and $G_k(\mu_1, \sigma_1) \neq G_k(\mu_2, \sigma_2)$ in general for the same k.

Coming now to the numerical example referred to above, let us suppose that, for some admissible position $A_1(\mu_1, \sigma_1)$ of the parameter

point, an arbitrary and representative admissible position, $[1/p_v(\mu_1, \sigma_1)]G_k(\mu_1, \sigma_1)$ takes its largest value, .39, for k = 46, its next largest value, .26, for k = 22, and so on as listed in the table below. Thus, given that a valid outcome occurs, the conditional probabilities that outcomes numbers 46, 22, ... occur, for the assumed values μ_1, σ_1 of the parameters, are .39, .26, ...

	Cumulative sums
$[1/p_v(\mu_1, \sigma_1)]\ G_{46}(\mu_1, \sigma_1) = .39$	.39
$[1/p_v(\mu_1, \sigma_1)]\ G_{22}(\mu_1, \sigma_1) = .26$	.65
$[1/p_v(\mu_1, \sigma_1)]\ G_{77}(\mu_1, \sigma_1) = .17$	.82
$[1/p_v(\mu_1, \sigma_1)]\ G_{39}(\mu_1, \sigma_1) = .07$	.89
$[1/p_v(\mu_1, \sigma_1)]\ G_{26}(\mu_1, \sigma_1) = .02$	.91
$[1/p_v(\mu_1, \sigma_1)]\ G_{51}(\mu_1, \sigma_1) = .02$	.93
$[1/p_v(\mu_1, \sigma_1)]\ G_{41}(\mu_1, \sigma_1) = .01$	.94
$[1/p_v(\mu_1, \sigma_1)]\ G_{66}(\mu_1, \sigma_1) = .01$	.95

We list the conditional probabilities for all valid outcomes in non-increasing order of the probabilities as shown in the table. In case of ties, for example .02 for k = 26 and 51, we use the increasing order of subscripts. We compute and list the cumulative sums as shown and at the end of the table this sum would attain the value 1 as has been pointed out. In defining a set which will be denoted as S_{A_1}, however, we are interested in the table only down to the point

where the cumulative sum, including "ties for last place", first reaches or exceeds the value .90 (in the case of 90% confidence regions). In the case under consideration, we do not exclude k = 51 on the ground that the cumulative sum as listed attains the value .91 with k = 26, as there is no theoretical reason for preferring k = 26 to k = 51 or vice versa. The value .90, or any other value on the interval (0, 1) will necessarily be reached or surpassed, since the cumulative sum eventually reaches the value 1.

We now define the set S_{A_1} as the set consisting of outcomes numbers 22, 26, 39, 46, 51, and 77, the order being immaterial once the makeup of the set is established. This is a set of outcomes, not of points or of probabilities. There exists a similar set S_A for every admissible position of the parameter point $A(\mu, \sigma)$, and the method of determining S_A is simple and clear in principle from the example given, although naturally it would be an enormous computing job in practice.

Also, we note that the number of admissible positions of $A(\mu, \sigma)$, ranging over the interior of a rectangle in the $\mu\sigma$-plane, is uncountably infinite. Hence we could not, even in principle, determine S_A for every admissible position of $A(\mu, \sigma)$. If we wished to program the method for a computer, we would have to approximate the interior of the rectangle by a finite grid of small mesh size, or something similar.

We can now define the point sets in the $\mu\sigma$-plane constituting the 90% confidence regions $\{R_t\}$, one for each of the N_v valid outcomes. They are defined as follows.

$$R_t = \bigcup_A \left\{ A(\mu, \sigma) \,\middle|\, S_A \text{ contains the t-th valid outcome} \right\} . \quad (249)$$

Here the symbol $\bigcup$ represents the set theoretic union, each R_t in general being a closed domain in the plane.

To show that we have defined a legitimate system of 90% confidence regions, we suppose that the true parameter point $A_o(\mu_o, \sigma_o)$ is the point $A_1(\mu_1, \sigma_1)$ of the current numerical example, and show that, given that the outcome of the experiment is a valid outcome, the probability is at least .90 that the true parameter point, $A_1(\mu_1, \sigma_1)$, is covered by the confidence region R_t corresponding to the outcome which occurred. We recall that A_1 is an arbitrary representative admissible parameter point and so, if it passes the test, every admissible parameter point $A(\mu, \sigma)$ will have done so.

Suppose that $A_1(\mu_1, \sigma_1)$ is the true parameter point, and that the outcome is a valid one. The table of probabilities for this example (page 132) shows that, with probability .93, the outcome of the experiment will be one of the following: outcome 22, 26, 39, 46, 51 or 77. But R_{22} or confidence region 22 contains $A_1(\mu_1, \sigma_1)$, by Eq. (249), since S_{A_1} contains outcome 22 as has been stated. Similarly, the point A_1 is contained in R_{26}, R_{39}, ..., R_{77}. Hence in 93% of all cases in which $A_1(\mu_1, \sigma_1)$ is the true parameter point and in which the outcome is valid, the parameter point A_1 is covered by the

pertinent confidence region R_t. To put it another way, for every 1,000,000 such cases (true parameter point A_1 and valid outcome), there will be 390,000 cases in which outcome 46 is the result, 260,000 cases of outcome 22, ..., 20,000 cases of outcome 51, for a total of 930,000 cases, and in each of these 930,000 cases the parameter point A_1 is covered by the pertinent confidence region R_t.

Hence the required test is passed by the representative admissible parameter point $A_1(\mu_1, \sigma_1)$, and therefore by all such admissible points, and it has been shown that a legitimate system of 90% confidence regions has been defined. The 90% confidence level was taken only as an example, and similar reasoning would apply to 95% or 50% confidence regions or those at any other confidence level.

We wish now to show that these confidence regions are arbitrarily small for a sufficiently large number of stimuli, by showing that the sets S_A as defined on page 133, which determine the confidence regions R_t by Eq. (249), consist of outcomes whose maximum likelihood points $\bar{A}_k(\bar{\mu}_k, \bar{\sigma}_k)$ are arbitrarily close to the assumed parameter point $A(\mu, \sigma)$, for a given confidence level such as 90%.

A heuristic proof has been worked out, indicating that these confidence regions are arbitrarily small for a sufficiently large number of stimuli, by showing that the sets S_A as defined on page 133, which determine the confidence regions R_t by Eq. (249), consist of outcomes whose maximum likelihood points $\bar{A}_k(\bar{\mu}_k, \bar{\sigma}_k)$ are arbitrarily close to the assumed parameter point $A(\mu, \sigma)$, for a given confidence level such as 90%.

We remark that this property of small confidence regions $\{R_t\}$ for large values of N is not a formal requirement of the system of confidence regions. The formal requirement is embodied in Eq. (249), for 90% confidence regions. But it is a natural and desirable property, and one which is possessed by the asymptotic large sample theory. An experimenter conducting an armor plate test might well ask himself, "Why should I fire a large number of projectiles, and use a large number of specimens of the plate, unless I thereby increase the accuracy of my knowledge of the characteristics of the plate?"

The proof referred to is not completely general or rigorous, in that only a subset of the set of all valid outcomes is considered. Moreover, the details are rather lengthy. Hence we merely state the result here, after describing the subset of valid outcomes which is used and the general nature of the proof.

In the proof, a population mean μ is assumed, and the stimuli $\{c_k\}$ are spaced at equal subintervals in the interval (μ_{min}, μ_{max}). The exact spacing is not specified in advance, and the principal object of the proof is to determine how fine a spacing is necessary in order to achieve a condition which will be described shortly regarding the probability content of subsets of the outcomes.

An arbitrarily small positive number ϵ is to be specified (we can think of the value of ϵ as being under the control of an imaginary opponent who is trying to break our proof down), and a key point of the proof consists of showing that, however small ϵ may be, it is possible to take the uniform spacing of the stimuli so fine that 90%

of the probability content of all valid outcomes considered in the proof (for 90% confidence limits) will be concentrated in the subset which has its maximum likelihood estimates $\bar{\mu}$ in the interval $(\mu - \epsilon, \mu + \epsilon)$.

The subset of the set of all possible outcomes which we consider in this heuristic proof is the set of those of the form FF ... FFSFSS ... SS, where the length of the string of consecutive failures is not necessarily the same as the length of the string of consecutive successes, since we may be much closer to one end than to the other of the interval (μ_{min}, μ_{max}). Outcomes of this form have the interlacing required by Eq. (35), so that they are valid outcomes. But this minimal interlacing is of small significance if N, the number of stimuli, is large, so that for practical purposes we can say that, for any given outcome of this set, we have failures below a certain stimulus level, say 1025 ft./sec. in the armor plate experiment, and successes above the same level.

It is intuitively clear that, for an outcome of the form FF .... FFSFSS .... SS, the maximum likelihood estimator $\bar{\mu}$ of the point $\bar{A}(\bar{\mu}, \bar{\sigma})$ will occur at approximately the stimulus level of the interlaced S and F; for in that case the factors of the expression $G(\bar{\mu}, \bar{\sigma})$ (see Eq. (244)) will consist almost entirely of factors of the form $p[(a_i - \bar{\mu})/\bar{\sigma}]$ with $a_i > \bar{\mu}$ and $q[(b_j - \bar{\mu})/\bar{\sigma}]$ with $b < \bar{\mu}$, both types of factor rapidly approaching the value 1 as $a_i - \bar{\mu}$ or $\bar{\mu} - b_j$ becomes large compared with $\bar{\sigma}$. If the isolated S of the sequence occurs for c_k = 1096 ft./sec. and the isolated F for c_{k+1} = 1097, we can assume that $\bar{\mu}$ for this outcome is approximately 1096.5.

The object is to show that N can be taken sufficiently large so that the interval $(\mu - \epsilon, \mu + \epsilon)$ contains at least 90% of the probability content of our subset of the set of all valid outcomes, for 90% confidence limits. It will be convenient to divide the interval $(\mu, \mu + \epsilon)$ into an integral number, L, of equal subintervals, and to place one of the $\{c_k\}$ at the center of each subinterval. Thus we have the situation shown in Fig. 6, in which several of the $\{c_k\}$ near $\mu + \epsilon$ are shown, and the S's and F's near $\mu + \epsilon$ for three of the outcomes are shown, the isolated S in the j-th outcome being at c_{k+1}, etc. By what was said above, the maximum likelihood estimates $\bar{\mu}$ for outcomes j-1 and j are approximately $\mu + \epsilon$ and $\mu + \epsilon + (\epsilon/L)$ respectively, ϵ/L being the distance between successive stimuli.

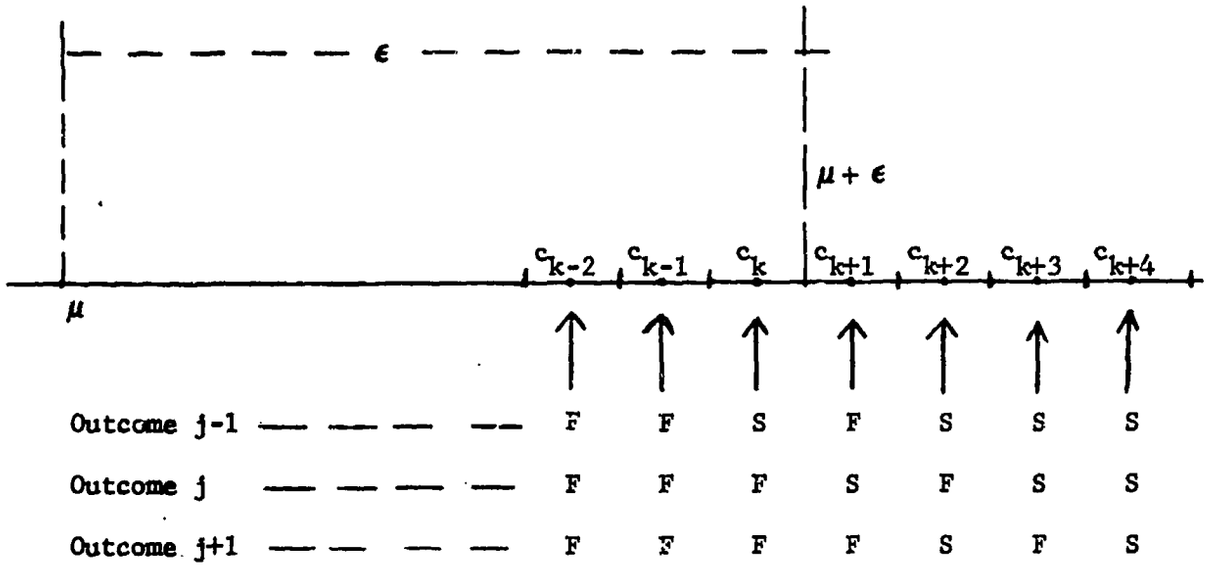

Figure 6

The mathematical details are rather lengthy and we do not give them here, but we state the result. If the integer L, the number of subintervals into which $(\mu, \mu + \epsilon)$ is divided, is so large that

$$L \geqslant \frac{9}{1 - [q(\epsilon/\sigma)/p(\epsilon/\sigma)]} , \qquad (250)$$

where p(t) is the probability integral, Eqs. (10), (12), $q(t) = 1 - p(t)$, and σ is the value assumed for the population standard deviation, then the sum of the probabilities of the outcomes whose maximum likelihood estimates $\bar{\mu}$ are in the interval $(\mu - \epsilon, \mu + \epsilon)$ is more than 90% of the sum of the probabilities of all the outcomes in the set under consideration, as described on page 137. L is very large, as expected, if ϵ is small compared with σ, for in this case q is slightly less and p slightly greater than 1/2, so that the denominator on the right-hand side is positive but very small.

Heuristically, it appears very probable that the property, which we have demonstrated for a chosen subset of the set of all valid outcomes, carries over to the entire set. This is the following property. Given a positive constant ϵ, however small, it is possible to take such a large number of stimuli that the maximum likelihood estimators $\{\bar{\mu}_k\}$ for the set S_A, as in the table on page 132, are all within a distance ϵ of μ, where $A(\mu, \sigma)$ is the assumed position of the true parameter point. Since this has the effect of making the sets $\{S_A\}$ small, page 133, it also makes the confidence regions $\{R_t\}$ small,

Eq. (249). It is true that, in addition to other respects in which the foregoing proof fails to be perfectly general and rigorous, it works with the maximum likelihood estimates $\{\bar{\mu}_k\}$ but not with $\{\bar{\sigma}_k\}$. The $\{\bar{\sigma}_k\}$ are probably all very small for our particular subset of outcomes of the form FF .... FFSFSS .... SS, and do not vary over a known range as the estimators $\{\bar{\mu}_k\}$ do. But this proof, it is felt, does make a significant contribution to the intuitive conviction which most statisticians will already have in this kind of situation, to the effect that large amounts of data, or large numbers of stimuli in the experiments with which we are concerned here, do have the effect of producing small confidence regions.

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Necessary and sufficient conditions are obtained for the existence of the maximum likelihood estimates (MLE) of the parameters of a normal distribution for quantal responses. It is shown that whenever the MLE estimates exist they are unique. A modified Newton-Raphson procedure is given which will converge globally to the MLE estimates. These results are new and directly applicable to an armor plate penetration problem or any other types of experiments based on quantal responses which fall under a normal distribution.

A computer program is described which includes as output a set of plotted confidence ellipses centered about the MLE. Various examples and the corresponding computer outputs are given.

Probit analysis and confidence regions for small samples are discussed in separate appendices.

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