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THE DETERMINATION OF STATISTICALLY BASED DESIGN LIMITS ASSOCIATED WITH ENGINEERING MODELS

(LWBR Development Program)

FEBRUARY 1980

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BETTIS ATOMIC POWER LABORATORY
WEST MIFFLIN, PENNSYLVANIA

Operated for the U. S. Department of Energy by
WESTINGHOUSE ELECTRIC CORPORATION

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H. Ginsburg

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NOTICE

FOREWORD

The Shippingport Atomic Power Station located in Shippingport, Pennsylvania was the first large-scale, central-station nuclear power plant in the United States and the first plant of such size in the world operated solely to produce electric power. This program was started in 1953 to confirm the practical application of nuclear power for large-scale electric power generation. It has provided much of the technology being used for design and operation of the commercial, central-station nuclear power plants now in use.

Subsequent to development and successful operation of the Pressurized Water Reactor in the DOE-owned reactor plant at the Shippingport Atomic Power Station, the Atomic Energy Commission in 1965 undertook a research and development program to design and build a Light Water Breeder Reactor core for operation in the Shippingport Station.

The objective of the Light Water Breeder Reactor (LWBR) program has been to develop a technology that would significantly improve the utilization of the nation's nuclear fuel resources employing the well-established water reactor technology. To achieve this objective, work has been directed toward analysis, design, component tests, and fabrication of a water-cooled, thorium oxide fuel cycle breeder reactor for installation and operation at the Shippingport Station. The LWBR core started operation in the Shippingport Station in the Fall of 1977 and is expected to be operated for about 3 to 4 years. At the end of this period, the core will be removed and the spent fuel shipped to the Naval Reactors Expended Core Facility for a detailed examination to verify core performance including an evaluation of breeding characteristics.

In 1976, with fabrication of the Shippingport LWBR core nearing completion, the Energy Research and Development Administration established the Advanced Water Breeder Applications (AWBA) program to develop and disseminate technical information which would assist U.S. industry in evaluating the LWBR concept for commercial-scale applications. The program will explore some of the problems that would be faced by industry in adapting technology confirmed in the LWBR program. Information to be developed includes concepts for commercial-scale prebreeder cores which would produce uranium-233 for light water breeder cores while producing electric power, improvements for breeder cores based on the technology developed to fabricate and operate the Shippingport LWBR core, and other information and technology to aid in evaluating commercial-scale application of the LWBR concept.

All three development programs (Pressurized Water Reactor, Light Water Breeder Reactor, and Advanced Water Breeder Applications) have been administered by the Division of Naval Reactors with the goal of developing practical improvements in the utilization of nuclear fuel resources for generation of electric energy using water cooled nuclear reactors.

Technical information developed under the Shippingport, LWBR, and AWBA programs has been and will continue to be published in technical memoranda, one of which is this present report.

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In various engineering disciplines, a great deal of effort has gone into the development of realistic mechanistic models of varying degrees of complexity for relating the behavior of phenomena with many independent variables. Computer programs using the methods of regression analysis have been successfully employed to obtain "best estimates" of the coefficients in these models from an available data base. Once the "best fit" functions have been obtained, engineers are faced with the challenging problem of determining design factors which are objective and reflect quantitatively specified risks. Unfortunately, texts which deal with statistical regression analysis have ignored this important area of application. Furthermore, even journal articles which have dealt with fitting a simple first-order model in a single independent variable do not reflect the recently improved methodology available for setting limits. This report provides a usable reference of methods and procedures for the construction of both one-sided and two sided γ/P statistical tolerance limits for design application to both linear and nonlinear models in any number of variables.

THE DETERMINATION OF STATISTICALLY BASED DESIGN LIMITS ASSOCIATED WITH ENGINEERING MODELS

H. Ginsburg

I. BACKGROUND

An age-old problem which has plagued engineers is that of determining design limits for a response variable which is expressed as a function of one or more independent or carrier variables. For those applications where no agreed-upon or mechanistic model exists, the development of best-estimate relationships or empirical mathematical models derived from experimental data is and will continue to be a challenging art. For applications where the functional form of the model exists, good computer programs are available for estimating the coefficients in the model from a data base. Practially all computer installations have programs, usually based upon the method of Least Squares, for obtaining "best estimates" of coefficients in linear and nonlinear models. However, once the "best fit" function has been obtained, the engineer is confronted with the task of using the information in the data base in the determination of design limits.

Over the years, a number of procedures have evolved in various engineering disciplines for obtaining design limits. These include: a) backing off two or three sample standard deviations from the "best fit" curve; b) invoking some rule-of-thumb which is believed to be conservative such as a factor of 2 on stress or 20 on cycles, as described in Reference (1); and c) using the extremes of the confidence intervals on each fitted parameter which are provided in the computer output. Perhaps one of the most common procedures is that of forming an envelope which contains all of the points in the existing data base. Although these and other methods are employed because of their intuitive appeal to their users, they all suffer from the fact that quantitative assessments of the risks associated with these procedures are not available. In addition, there are other problems with these methods. For example, with the envelope approach, a single most discrepant point in the data base could govern the entire design procedure. Furthermore, as additional data are collected and improved estimates of the parameters in the model are obtained, the design limits based upon enveloping the combined data base must move further and further away from the "best estimate curve."

Perhaps some of the ad-hoc procedures described above are outgrowths of situations in the early stages of development where adequate data bases are not available to the engineer and engineering judgment must therefore prevail. It is fair to state that these procedures continue to be used when valid data bases are available because objective procedures for setting design limits with quantitatively specified risks are not available in the literature. Therefore, the purpose of this report is to provide a usable reference for the development of methods and procedures for the construction of both one-sided and two-sided γ/P statistical tolerance limits for design application to both linear and nonlinear models in any number of variables.

II. STATISTICAL INTERVALS

Based upon the information contained in a random sample from some population, statistical methods provide tools for projecting or inferring characteristics of interest of the remaining values in the entire population. In addition to providing "best estimates" (single numbers) of a characteristic of interest, one may construct an interval for the unknown value of the characteristic. The end-points of these constructed intervals are known as statistical limits. Associated with any type of statistical interval constructed on the basis of sample data is a confidence coefficient. Simply stated, the confidence coefficient reflects the relative frequency of similarly constructed statistical intervals which are indeed true--i.e., contain the correct value of the unknown characteristic of interest. For a given sample of data, therefore, an interval with a 99% confidence coefficient will be wider than the corresponding one with a confidence coefficient of 95%.

Three types of statistical intervals constructed on the basis of sample data which find wide usage are called confidence intervals, prediction intervals, and statistical tolerance intervals. A simple numerical example will be presented to illustrate the interpretation of these intervals. The details of the methodology will be presented later in this report for those aspects which pertain to design limits.

Suppose one were sampling from a Normal distribution with unknown mean η and unknown standard deviation σ. To be specific, suppose a random sample of five observations were obtained whose values were 114.16, 84.94, 94.06, 119.61, and 93.33. Based upon these sample data, $\hat{\eta}$ = 101.22 and $\hat{\sigma}$ = 14.868.

In general, confidence intervals refer to population constants or parameters, or a function of these unknown parameters. For example, one may construct a confidence interval for a population mean, the slope of a line, or for the model itself. Our view here is that a fitted engineering model is an estimate of the locus of true means of all possible values of the response or dependent variable expressed as a function of independent or carrier variables. For the simple numerical example described, a lower one-sided 95% confidence limit on η is $101.22 - 2.132(14.868)/\sqrt{5} = 87.04$. Thus, with 95% confidence, we assert that the unknown mean η of the entire Normal population from which the random sample of five observations came has a value greater than 87.04. If a confidence coefficient of 99% were selected, the resulting limit would be calculated to be 76.31. For applications where both low and high values of the parameter are of technical interest, the two-sided 95% confidence interval on η would be calculated to be 101.22 ± 2.776 (14.868)/ $\sqrt{5}$ or (82.76 < η < 119.68). The corresponding 99% confidence interval turns out to be (70.61 < η < 131.83). All of the above statements refer to the unknown population parameter η and are based upon the information contained in the sample of five observations. The confidence intervals do not pertain to individual values in the population.

Prediction intervals pertain to some characteristic of interest in a future sample of data from the population. That is, on the basis of a given sample one might want to construct a prediction interval for a future sample of size m which will contain all m observations, at least r of the m observations, the average of these m observations, etc. The type of prediction interval most often used in curve-fitting problems, as discussed in References (2) and (3), for example, are for a single future observation. For the simple numerical example under consideration, a lower one-sided 95% prediction limit for the next single observation is calculated to be 101.22 - 2.335(14.868) = 66.50. The corresponding 99% prediction limit turns out to be 40.19. A two-sided 95% prediction interval for a single future observation would be calculated as 101.22 ± 3.041(14.868) or (56.01, 146.43). The corresponding 99% prediction interval is (26.24, 176.20).

Statistical tolerance intervals pertain to a specified proportion of individual values in the entire population. For example, based upon a given sample of data, one may want to construct an interval which contains at least 99% of the entire population of values of the response variable. For the simple numerical example, a lower one-sided 95/95 statistical tolerance limit is calculated as 101.22 - 4.202(14.868) = 38.74 whereas the lower one-sided 95/99 statistical tolerance limit turns out to be 15.86. That is, with 95% confidence, we assert that at least 99% of the entire Normal population from which this random sample came has individual values which exceed 15.86. A two-sided 95/95 statistical tolerance interval is calculated as 101.22 ± 5.079(14.868) = (25.71, 176.73), and a two-sided 95/99 statistical tolerance interval is (2.59, 199.85).

All of the above sample calculations are summarized in Table 1. Since the smallest observation in the sample was 84.94 and the largest was 119.61, with an average of 101.22, some might view the constructed limits as being ultra-conservative. However, the reader should keep in mind that strong statements are being made on the basis of only five observations. The intervals become narrower with increasing size of the data base, but the return is not linear.

Since the description of statistical tolerance limits appears to correspond to the engineering objective in setting design limits, this report will deal with their construction. In any given application, technical interest may center on only a lower limit or only an upper limit or both lower and upper limits. Therefore, the construction of both one-sided and two-sided statistical tolerance limits will be discussed.

III. INTRODUCTION

Suppose that there exists some mechanistic model with a general representation of $\eta = f(\underline{X};\underline{\beta})$, where $\underline{X}$ represents a vector of independent or carrier variables and $\underline{\beta}$ represents a vector of parameters. Then let any observation or measured response to this system be $Y_i = \eta_i + \epsilon_i$, where ϵ_i represents the random variability associated with the response. If the set of ϵ_i have a common unknown variance σ^2, then standard methods of Least Squares are used to obtain estimates of $\underline{\beta}$ on the basis of a sample of data. That is, the "best fit curve" is obtained through minimizing the sum of squares of deviations between the observations and the fitted function. Several excellent computer programs are contained in Reference (4) and other commercial packages, as well as the various computer manufacturer's users groups such as IBM SHARE, Control Data's VIM, Digital Equipment's DECUS, etc. These programs not only provide estimates of $\underline{\beta}$ and σ^2, but they provide other useful statistics for assessing the fit.

TABLE 1
Statistical Intervals

A. Confidence limits on η, the population mean:

1) 95% lower limit
87.04

2) 99% lower limit
76.31

3) Two-sided 95% confidence interval
82.76 — 119.00

4) Two-sided 99% confidence interval
70.61 — 131.83

B. Prediction limits for single future observation from population:

1) 95% lower limit
66.50

2) 99% lower limit
40.19

3) Two-sided 95% prediction interval
56.01 — 146.43

4) Two-sided 99% prediction interval
26.24 — 176.20

C. Statistical tolerance limits for proportion of individuals in entire population:

1) 95/95 lower limit
38.74

2) 95/99 lower limit
15.86

3) Two-sided 95/95 statistical tolerance limits
25.71 — 176.73

4) Two sided-95/99 statistical tolerance limits
2.59 — 199.85

As previously mentioned, η represents the locus of true means of the reference population of responses corresponding to various combinations of the carrier variables, $\underline{X}$. The Least Squares fit provides $\hat{\eta}$, an estimate of the locus of population means. However, for design applications, one is not concerned with the mean but with either lower or upper percentiles of the distribution, depending upon whether low or high values of the dependent variable represent limiting system conditions. The statistical method for determining bounds on percentiles of a distribution involves the construction of statistical tolerance limits.

IV. ONE-SIDED STATISTICAL TOLERANCE LIMITS FOR GAUSSIAN ERRORS

In order to describe the nature of statistical tolerance limits, we begin with the case of a simple population where the carrier variables are absent. Suppose that Y is Normally distributed with mean η and variance σ^2 (or standard deviation σ). If these population parameters are known, then it is a simple matter to determine any percentile of interest. For example, 95% of the population will be less than $\eta + 1.645\sigma$, the 95th percentile of the Normal distribution, or 95% of the population will exceed $\eta - 1.645\sigma$, the 5th percentile. However, when these population parameters are not known but are estimated from a random sample, clearly one cannot state that 95% of the population is less than $\hat{\eta} + 1.645\hat{\sigma}$, since these sample estimates are random variables which may be greater than or less than the corresponding true population parameters. However, one may determine a factor K such that one may assert with confidence coefficient γ that <u>at least</u> a proportion P of the entire Normal population is less than $\hat{\eta} + K\hat{\sigma}$. As one would intuitively expect, the magnitude of K is dependent upon the confidence coefficient γ, the required proportion of the propulation P, and the amount of information upon which the sample estimates of the population parameters were obtained. That is, one would expect the magnitude of K to increase with increasing γ and P, and decrease with increasing sample size. Indeed, K is a function of γ, P, n, and f, where n is the sample size upon which $\hat{\eta}$ is based, and f is the number of degrees of freedom associated with the estimate of σ. For the case described, f = n-1.

For the problem described above, tables of K-factors are available in texts and handbooks and are very easy to use. These tables are indexed by γ, P, and n, since f = n-1. The K-factors for the simple numerical example previously presented were obtained from such tables. However, for curve-fitting problems where $\hat{\eta}$ depends upon some function of the independent or carrier variables X_i, these standard tables of K-factors are no longer valid. For example, if the fitted function were $\hat{\eta} = b_0+b_1X_1+b_2X_2+...+b_rX_r$ and the data base consisted of n observations, then since r+1 b's are estimated from the data base, the degrees of freedom associated with $\hat{\sigma}$ are n-r-1. Furthermore, the n data points were distributed throughout the r-dimensional factor space, and the question arises with regard to the number of observations which are associated with $\hat{\eta}$ corresponding to any point in this factor space. Wallis introduced the concept of the "effective number of observations" or effective sample size at any point in the factor space, Reference (5), and we denote this by n*. The definition and interpretation of n* will be provided in the next section of this report. Thus, for curve-fitting problems, the magnitude of K depends upon the magnitudes of γ, P, n*, and f. Since n* and f are uncoupled, one cannot use the standard tables of K-factors. We will show that the values of K may be readily calculated for models of varying degrees of complexity.

V. DETERMINATION OF n*

To illustrate the concept of n*, the effective number of observations, consider the problem of fitting a straight line by the method of Least Squares. The fitted function $\hat{\eta} = b_0+b_1X$ and an estimate of the variance, $\hat{\sigma}^2$, are obtained from a sample of n pairs of points (X_i, Y_i). Corresponding to any specified value of X (say, $X = X_k$) the best estimate of the line (or, the estimate of the mean of all possible Y_k corresponding to $X = X_k$) is simply $\hat{\eta}_k = b_0+b_1X_k$. Since $\hat{\eta}$ is a function of X, the variance of $\hat{\eta}$ is also a function of X. It can be easily demonstrated that the estimated variance

of $\hat{\eta}_k$ is $\hat{\sigma}^2 \left[\frac{1}{n} + \frac{(X_k-\bar{X})^2}{\sum_{i=1}^{n}(X_i-\bar{X})^2}\right]$, where $\bar{X}$ is the arithmetic average of the X_i used to fit the line (e.g., see Reference (2)). Note that this quantity takes on its minimum value at $X_k = \bar{X}$ (the Least Squares line passes through the centroid of the data base $(\bar{X}, \bar{Y})$) and increases as one moves away from $\bar{X}$. Then n* at $X = X_k$ is defined as $\left[\frac{1}{n} + \frac{(X_k-\bar{X})^2}{\sum_i (X_i-\bar{X})^2}\right]^{-1}$. In effect, one is stating that for any value of X, the mean value of all the corresponding Y's is determined as precisely from the fitted line as if n* observations had been made at this value of X. Note that at $X_k = \bar{X}$, n* = n, and the magnitude of n* decreases as X_k departs from $\bar{X}$. Reference (5) states that "the effective number of observations for a certain statistic is that which, when divided into the variance of an observation, gives the variance of the statistic".

Since the fitted line was determined from n points in the data base through estimating the Y-intercept and slope, b_o and b_1, the degrees of freedom associated with $\hat{\sigma}^2$ are n-2. Furthermore, since n* varies with X_k whereas f = n-2, one cannot use the existing tabular values of K-factors in determining a one-sided γ/P statistical tolerance limit for straight-line models.

Rewriting the relevant aspects of the above discussion in matrix notation facilitates generalizing the description of n* to more complex models. Let **x** be the nx2 matrix $\mathbf{x} = \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_n \end{bmatrix}$, let the column vector $\underline{b}$ be $\underline{b} = \begin{pmatrix} b_o \\ b_1 \end{pmatrix}$, and the point X_k be $\underline{X}_k = \begin{pmatrix} 1 \\ X_k \end{pmatrix}$. The corresponding transposes of **x**, $\underline{b}$, and $\underline{X}_k$ are denoted by $\mathbf{x}^T$, $\underline{b}^T$, and $\underline{X}_k^T$, respectively. The inverse of a square matrix is denoted by the exponent -1. Then for some point $\underline{X}_k^T$, the corresponding value of the fitted line is $\hat{\eta}_k = \underline{X}_k^T b = \underline{b}^T \underline{X}_k$. The estimate of the variance of $\hat{\eta}_k$ is $\hat{\sigma}^2 \left[\underline{X}_k^T (\mathbf{X}^T\mathbf{X})^{-1}\underline{X}_k\right]$. $\left(\text{That is, } \frac{1}{n} + \frac{(X_k-\bar{X})^2}{\sum_i (X_i - \bar{X})^2}\right.$ may be denoted in matrix notation as $\left.\underline{X}_k^T (\mathbf{X}^T\mathbf{X})^{-1}\underline{X}_k\right)$. Therefore n* is the reciprocal of $\underline{X}_k^T (\mathbf{X}^T\mathbf{X})^{-1} \underline{X}_k$.

Now consider the extension of the above to the Least Squares fit of $\hat{\eta} = b_o + b_1X_1 + b_2X_2 + \ldots + b_rX_r$. For this case of r carrier variables, the corresponding representation is:

$$\mathbf{X} = \begin{bmatrix} 1 & X_{11} & X_{12} & \cdots & X_{1r} \\ 1 & X_{21} & X_{22} & \cdots & X_{2r} \\ \cdot & \cdot & & & \cdot \\ \cdot & \cdot & & & \cdot \\ \cdot & \cdot & & & \cdot \\ 1 & X_{n1} & X_{n2} & \cdots & X_{nr} \end{bmatrix}, \quad \underline{b} = \begin{bmatrix} b_o \\ b_1 \\ b_2 \\ \cdot \\ \cdot \\ b_r \end{bmatrix}, \text{ and } \underline{X}_k = \begin{bmatrix} 1 \\ X_{k1} \\ X_{k2} \\ \cdot \\ \cdot \\ X_{kr} \end{bmatrix}.$$

At the point $\underline{X}_k^T$, the fitted value of the function is

$\hat{\eta}_k = \underline{X}_k' b = \underline{b}^T\underline{X}_k$. The estimate of the variance of

$\hat{\eta}_k$ is $\hat{\sigma}^2\left(X_k^T (X^TX)^{-1}\underline{X}_k\right)$. Therefore, $n^* = \left[\underline{X}_k^T (X^TX)^{-1}\underline{X}_k\right]^{-1}$.

Although this representation covers polynominals in multidimensional space, the matrix representation is that obtained for the simple case of a straight line. Since the n observations were used to estimate $b_0, b_1, \ldots, b_r$ (i.e., r+1 coefficients) the number of degrees of freedom associated with $\hat{\sigma}^2$ is n-(r+1) or f = n-r-1.

All of the preceding discussion holds true for polynominal models of arbitrary order in any number of dimensions. All such models are referred to as linear models in Statistics since the coefficients to be solved for enter the model linearly. In solving for the coefficients which minimize the sum of squares of deviations between the observations and the fitted function, one solves a set of simultaneous linear equations. Letting $\underline{Y}$ represent the vector of n observations, the set of simultaneous linear equations to be solved may be represented as $X^T X \, \underline{b} = X^T \underline{Y}$. The solution vector is thus $\underline{b} = (X^T X)^{-1} X^T \underline{Y}$. The fact that the estimated variance of $\underline{b}$ is $(X^T X)^{-1} \hat{\sigma}^2$ was incorporated in obtaining the estimated variance of $\hat{\eta}$, and thus in obtaining n*.

Any model which cannot be placed in the above formulation is referred to as a nonlinear model. In the minimization of the sum of squares of deviations between the observations and the fitted nonlinear function (i.e., in setting the partial derivatives of the sum of squares with respect to each of the coefficients equal to zero) the resulting set of simultaneous equations to be solved are not linear in the coefficients. Thus, some type of iterative procedure is required for their solution.

If $\eta = f(\underline{X};\underline{\beta})$, where $\underline{X}$ represents the set of carrier variables and $\underline{\beta}$ represents the set of unknown parameters to be estimated from the data, the variance of $\hat{\eta}$ may be approximated, through a Taylor Series expansion ("propagation of error"), as

$$\mathrm{Var}\,(\hat{\eta}) \simeq \sum_j \left(\frac{\partial \eta}{\partial b_j}\right)^2 \mathrm{Var}\,(b_j) + 2 \sum_{\substack{j \\ j<\ell}} \sum_{\ell} \left(\frac{\partial \hat{\eta}}{\partial b_j}\right) \left(\frac{\partial \hat{\eta}}{\partial b_\ell}\right) \mathrm{cov}(b_j, b_\ell),$$

where $cov(b_j, b_\ell)$ is the covariance between b_j and b_ℓ. For linear models, the expression is exact and the partial derivatives involve only the known X's, not the b's. Thus, $n^* = \left(\underline{X}_k^T (X^T X)^{-1} \underline{X}_k\right)^{-1}$. For nonlinear models, however, the partial derivatives involve the b's. Nevertheless, for nonlinear models one can define a vector $\underline{P}_k$ and the matrix P such that

$$n^* = \left(\underline{P}_k^T (P^T P)^{-1} \underline{P}_k\right)^{-1} .$$

Reference (6) is a widely-used computer program for fitting nonlinear models and uses a Taylor Series expansion of the model in the iteration on parameter estimates for minimizing the sum of squares function. In addition to providing $\hat{\sigma}$ and the coefficients in $\hat{\eta}$, this program prints out a matrix labeled PTP INVERSE which is the analogue of $(X^T X)^{-1}$ for linear models. Some degree of approximation is introduced into this linearization, and as always, the validity of the resulting tolerance limit is dependent upon the correctness of the assumed functional form of the model as well as the assumed error structure.

VI. DEVELOPMENT OF K-FACTORS

Suppose that Y is Normally distributed with mean η and variance σ^2. From a random sample of size n, $\hat{\eta}$ and $\hat{\sigma}$ can be calculated. $\hat{\eta}$ is Normally distributed about η with variance σ^2/n^*, and $\hat{\sigma}^2$ is based upon f degrees of freedom and is independently distributed as $\chi^2(f)$. σ^2/f, where $\chi^2(f)$ denotes a Chi-Square variable with f degrees of freedom. Then an upper (lower) one-sided γ/P statistical tolerance limit will be of the form $\hat{\eta} + K\hat{\sigma}$ ($\hat{\eta} - K\hat{\sigma}$), where the magnitude of K is a function of γ, P, n*, and f.

$$\Pr\left[\Pr\left(Y < \hat{\eta} + K\hat{\sigma}\right) \geq P\right] = \gamma. \qquad (1)$$

$$\Pr\left[\left\{\frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{\hat{\eta}+K\hat{\sigma}} \exp\left(\frac{-(Y-\eta)^2}{2\sigma^2}\right) dY\right\} \geq P\right] = \gamma. \qquad (2)$$

Define Z_p such that $\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{Z_p} \exp\left(\frac{-X^2}{2}\right) dX = P.$

$$\text{Then, } \Pr\left[\frac{(\hat{\eta}+K\hat{\sigma}) - \hat{\eta}}{\sigma} \geq Z_p\right] = \gamma . \quad (3)$$

After some algebraic manipulation, one can express equation (3) as

$$\Pr\left[\frac{\frac{\hat{\eta}-\eta}{\sigma/\sqrt{n^*}} - \sqrt{n^*}\, Z_p}{\hat{\sigma}/\sigma} \geq \sqrt{n^*}K\right] = \gamma . \quad (4)$$

Let $\delta' = -\sqrt{n^*}\, Z_p$. Then since $\frac{\hat{\eta}-\eta}{\sigma/\sqrt{n^*}}$ is distributed as a standardized Normal variable and $\hat{\sigma}/\sigma$ is distributed as $(X^2(f)/f)^{1/2}$, equation (4) is a noncentral t(f) with noncentrality parameter δ'. That is,

$$\Pr\left[(\text{noncentral } t(f) \text{ with noncentrality parameter } \delta' = -\sqrt{n^*}\, Z_p) \geq -\sqrt{n^*}K\right] = \gamma . \quad (5)$$

An equivalent, and more convenient form of the equation is

$$\Pr\left[(\text{noncentral } t(f) \text{ with noncentrality parameter } \delta = \sqrt{n^*}\, Z_p) \leq \sqrt{n^*}\, K\right] = \gamma . \quad (6)$$

Therefore, in order to solve for the required K for a one-sided Normal γ/P statistical tolerance limit, define the noncentrality parameter as $\delta = \sqrt{n^*}\, Z_p$ and find the 100(γ)th pecentile of the noncentral t(f). The required K, then, is equal to this value of t(f) divided by the square root of n*. Although this is conceptually very straightforward, one needs the percentiles of the noncentral t(f) with the particular noncentrality parameter of $\delta = \sqrt{n^*}\, Z_p$. Even when tables of the cumulative noncentral t(f) are available, interpolation is often required. For example, in Reference (7), values are provided for P = 0.935 and P = 0.960, but not for P = 0.95.

Furthermore, these tables are based upon $\delta = \sqrt{f+1}\ Z_p$. For curve-fitting problems, n* will not equal f+1.

Reference (8) provides methodology for obtaining approximate percentiles of the noncentral t(f). Some simplification to that formulation was introduced in light of our intended end use in obtaining K-factors for one-sided statistical tolerance limits for γ and P greater than 0.5. Thus, the approximate percentiles may be obtained simply by solving for the larger root of a quadratic equation of the form $at^2 + bt + c = 0$, where

$$a = \left[E(X(f)/\sqrt{f})\right]^2 - \left[E(X(f) - \sqrt{X^2_{1-\gamma}(f)}\right]^2/f,$$

$$b = -2\ E(X(f)/\sqrt{f})\ \sqrt{n^*}\ Z_p, \text{ and}$$

$$c = n^*\ Z_p^2 - Z_\gamma^2\ .$$

In the above, n*, f, and Z_p have been previously defined, Z_γ is the 100(γ)th percentile of the standardized Normal distribution, and $X^2_{1-\gamma}$ (f) is the 100(1-γ)th percentile of the Chi-Square distribution with f degrees of freedom. The only quantity which is not known or available in standard tables is $E(X(f)/\sqrt{f})$, the mean of the Chi distribution with f degrees of freedom divided by $\sqrt{f}$. This quantity is well approximated by

$$1 - \frac{1}{4f} + \frac{1}{32f^2} + \frac{5}{128f^3} - \frac{21}{2048f^4}\ .$$

Thus, the solution for t_γ (f) is easily obtained on a computer as $t_\gamma(f) = \frac{-b + \sqrt{b^2 - 4ac}}{2a}$.

To check on the validity of this procedure, the K-factors were calculated for combinations of γ and P commonly used at Bettis and compared with tabular values. These results are presented in Table 2. Note that the calculated K-factors are within a fraction of a percent of the tabular values. The effect on the tail percentiles of the distribution is even smaller than that. Although Reference (8) also provides an alternative more precise method for obtaining percentiles of the noncentral t(f), the added complexity of that approach is not felt to be justified in light of the intrinsic approximateness of the Gaussian error model for "real-world" applications. The restriction of $f = n^*-1$ was imposed in Table 2 since this is the only case for which tabular values are available. However, there is nothing in the development of the applicability of the noncentral t(f) for calculating K-factors which requires any linkage between f and n^* or which requires that n^* be an integer.

VII. NUMERICAL EXAMPLES FOR ONE-SIDED LIMITS

Consider the data given on page 8 of Reference (2) and presented in Appendix A, where the fitted line was $\hat{\eta} = 13.6230 - 0.0798287X$. Twenty-five observations were taken over the range $28.1 \leq X \leq 76.7$, $\bar{X} = 52.60$

$\sum_{i=1}^{25} (X_i-\bar{X})^2 = 7154.42$, and $\hat{\sigma} = 0.89012$ based upon 23 degrees of freedom.

Suppose one wanted to construct a one-sided lower 95/99 statistical tolerance limit for Y corresponding to X = 70. For $X_k = 70$,

$$n^* = \left[\frac{1}{n} + \frac{(X_k-\bar{X})^2}{\sum_i (X_i-\bar{X})^2}\right]^{-1} = \left[\frac{1}{25} + \frac{(70-52.6)^2}{7154.42}\right]^{-1} = 12.15.$$

For $\gamma = 0.95$ and $P = 0.99$, one finds in standard tables $Z_{0.95} = 1.645$, $Z_{0.99} = 2.326$, and

$\chi^2_{0.05}(23) = 13.092$. K is calculated to be 3.261. Thus $\hat{\eta} - K\hat{\sigma} = 8.035 -$

$3.261(0.89012) = 5.13$. Thus, one may assert with 95% confidence that at least 99% of the entire Normal population is greater than 5.13 when X = 70. A systematic examination of the individual deviations about the fitted function did not cast doubt upon the underlying assumption of Normality of the errors.

Table 2

Calculated vs. Tabular K-Factors

γ	P	n*	f	Calculated K	Tabular K
0.90	0.90	5	4	2.745	2.742
0.95	0.95	5	4	4.190	4.202
0.95	0.99	5	4	5.731	5.741
0.90	0.90	10	9	2.065	2.065
0.95	0.95	10	9	2.905	2.911
0.95	0.99	10	9	3.976	3.981
0.90	0.90	15	14	1.867	1.866
0.95	0.95	15	14	2.562	2.566
0.95	0.99	15	14	3.516	3.520
0.90	0.90	20	19	1.765	1.765
0.95	0.95	20	19	2.393	2.396
0.95	0.99	20	19	3.292	3.295
0.90	0.90	30	29	1.657	1.657
0.95	0.95	30	29	2.218	2.220
0.95	0.99	30	29	3.062	3.064
0.90	0.90	50	49	1.560	1.560
0.95	0.95	50	49	2.064	2.065
0.95	0.99	50	49	2.861	2.863

To illustrate the methodology for more complex linear models, consider the inclusion of another independent variable as was done on page 116 of Reference (2) and presented in Appendix B. For this example, $28.1 \leq X_1 \leq 76.7$ and $11 \leq X_2 \leq 23$. The data base consisted of twenty-five observations and the fitted model was $\hat{\eta} = 9.12689 - 0.072393X_1 + 0.202815X_2$. Suppose one wanted the lower 95/99 statistical tolerance limit corresponding to $X_1 = 70$ and $X_2 = 22$. The fitted value of the function is $\hat{\eta}_k = 8.521$ and $\hat{\sigma} = 0.66157$ based upon 22 degrees of freedom. In order to determine n^*, one needs $(X^TX)^{-1}$, as previously described. Most existing multiple regression computer programs provide this either as a standard or optional part of the output. For this example, $n^* = \underline{X}_k^T(X^TX)^{-1}\underline{X}_k^{-1} = 9.10$. The systematic examination of the deviations about the fitted plane did not cast doubt on the underlying assumption of Normality of the errors. Thus, with $Z_{0.95} = 1.645$, $Z_{0.99} = 2.326$, and $\chi^2_{0.05}(22) = 12.338$ from standard tables, K was calculated to be 3.331. Therefore, the lower one-sided 95/99 statistical tolerance limit corresponding to $X_1 = 70$ and $X_2 = 22$ is 8.521 - 3.331(0.66157) or 6.32.

The calculation of n^* for polynominal models involves matrix multiplication and is, therefore, more cumbersome than that associated with a straight line. The calculation of n^* above was easily performed using a hand-held calculator. In general, however, matrix multiplication may be simply performed on any computer.

To illustrate the calculation of a one-sided statistical tolerance limit associated with a nonlinear model, a numerical example was selected from page 276 of Reference (2) and presented in Appendix C. Forty-four observations were taken over the range $8 \leq X \leq 42$ and the theoretical model was $\eta = \beta_1 + (0.49 - \beta_1)e^{-\beta_2(X-8)}$. The fitted model turned out to be $\hat{\eta} = 0.39014 + (0.49 - 0.39014)e^{-0.10163(X-8)}$ and $\hat{\sigma} = 0.010913$ based upon 42 degrees of freedom. The computer output also contained

$$(P^TP)^{-1} = \begin{pmatrix} 0.213723 & 0.502515 \\ 0.502515 & 1.498844 \end{pmatrix}.$$

Now,

$$\frac{\partial \hat{\eta}}{\partial b_1} = 1 - e^{-0.10163(X-8)} \text{ and } \frac{\partial \hat{\eta}}{\partial b_2} = -(0.49-0.39014)(X-8)e^{-0.10163(X-8)}.$$

For example, corresponding to X = 20, $\hat{\eta}_k = 0.4196$, $\frac{\partial \hat{\eta}}{\partial b_1} = 0.70464$, and $\frac{\partial \hat{\eta}}{\partial b_2} = -0.35394$, and

$$n^* = \left[(0.70464 \ -0.35394) \begin{pmatrix} 0.213723 & 0.502515 \\ 0.502515 & 1.498844 \end{pmatrix} \begin{pmatrix} 0.70464 \\ -0.35394 \end{pmatrix} \right]^{-1}$$

$$= (0.043228)^{-1} = 23.13$$

For a one-sided lower 95/99 statistical tolerance limit corresponding to X = 20, one uses the tabular values of $Z_{0.95} = 1.645$, $Z_{0.99} = 2.326$ and $\chi^2_{0.05}(42) = 28.144$, and the resulting calculated value of K is 2.966. Therefore, $\hat{\eta} - K\hat{\sigma} = 0.4196 - 2.966\ (0.010913) = 0.387$.

One-sided lower 95% confidence and prediction limits are also given in Appendixes A, B, and C for purposes of comparison.

VIII. TWO-SIDED STATISTICAL TOLERANCE LIMITS FOR GAUSSIAN ERRORS

For certain applications, both high and low values of the response variable are limiting, and for problems of this type, two-sided design limits are required. Two-sided γ/P statistical tolerance limits are of the form $\hat{\eta} \pm K\hat{\sigma}$, where K is again a function of γ, P, n, and f. In constructing a two-sided γ/P statistical tolerance interval, one asserts with confidence coefficient γ that a least a proportion of P of the entire reference Normal population is contained between $\eta - K\hat{\sigma}$ and $\hat{\eta} + K\hat{\sigma}$.

$$\Pr\left[\Pr(\hat{\eta} - K\hat{\sigma} \leq Y \leq \hat{\eta} + K\hat{\sigma}) \geq P\right] = \gamma. \qquad (7)$$

$$\Pr\left[\left\{\frac{1}{\sqrt{2\pi}\sigma} \int_{\hat{\eta}-K\hat{\sigma}}^{\hat{\eta}+K\hat{\sigma}} \exp\left(\frac{-(Y-\eta)^2}{2\sigma^2}\right) dY\right\} \geq P\right] = \gamma. \qquad (8)$$

Unfortunately, unlike the one-sided case previously discussed, there is no simple exact solution for K in equation (8). An approximate solution was proposed in Reference (9). Let r be such that

$$\frac{1}{\sqrt{2\pi}} \int_{\frac{1}{\sqrt{n}}-r}^{\frac{1}{\sqrt{n}}+r} \exp\left(\frac{-X^2}{2}\right) dX = P, \text{ and let } u = \sqrt{f/X^2_{1-\gamma}(f)}. \text{ Then, } K = ru.$$

Tables of K-factors for two-sided tolerance intervals, indexed by γ, P, and n for f = n-1, were published in Reference (10) and in many texts and handbooks since then. To handle cases where n and f are uncoupled, extensive tabulations of r(n,P) and u(f, γ) were published in Reference (11).

Reference (12) provided improved approximations to K over those in Reference (11), particularly when $f \gg n^2$. For two-sided limits, define $Z_{\frac{1+\alpha}{2}}$ such that

$$\frac{1}{\sqrt{2\pi}} \int_{-Z_{\frac{1+\alpha}{2}}}^{Z_{\frac{1+\alpha}{2}}} \exp\left(\frac{-X^2}{2}\right) dX = \alpha \text{ , and recall that } X^2_{1-\alpha}(f) \text{ is the}$$

100(1-α)th percentile of the Chi-square distribution with f degrees of freedom.

For, $f \leq n^2 \left(1+1/Z^2_{\frac{1+\gamma}{2}}\right)$,

$$K = Z_{\frac{1+P}{2}} \left[\frac{(1+1/n)f}{X^2_{1-\gamma}(f)} \left\{ 1 + \frac{f-2 - X^2_{1-\gamma}(f)}{2(n+1)^2} \right\} \right]^{1/2} . \qquad (9)$$

For $f > n^2 (1 + 1/Z^2_{\frac{1+\gamma}{2}})$,

let, $$V = 1 + \frac{Z^2_{\frac{1+\gamma}{2}}}{n} + \frac{(3-Z^2_{\frac{1+P}{2}}) \; Z^4_{\frac{1+\gamma}{2}}}{6 \; n^2} .$$

Then,

$$K = Z_{\frac{1+P}{2}} \left[V \left\{ 1+nV(1+1/Z^2_{\frac{1+\gamma}{2}})/2f \right\} \right]^{1/2} . \qquad (10)$$

Note that the value of K is given in terms of well tabulated functions such as the standardized Normal and the Chi-square.

To illustrate the effectiveness of these formulas for K, the following information was abstracted from Reference (12). For this example, the left-hand side of equation (8) was evaluated for $\gamma = 0.95$, $P = 0.95$, $n = 13$, and varying values of f using the approximation given in Reference (9), equation (9), and equation (10). That is, with a target value of $\gamma = 0.95$, the actual confidence coefficients, to the number of places given, were calculated on the basis of the three alternate procedures of Reference (9), equation (9), and equation (10).

f	Reference (9)	Equation (9)	Equation (10)
2	0.9501	0.9501	0.8749
4	0.9499	0.9503	0.9210
12	0.9485	0.9510	0.9431
48	0.9384	0.9526	0.9396
240	0.895	0.956	0.947
1500	0.8190	0.980	0.9513
∞	0.6827	1.000	0.9503

For n = 13 and $\gamma = 0.95$, $n^2(1+1/Z^2_{0.975}) = 213$. Therefore, the underlined values in the above table would have been obtained using the guidelines suggested for equations (9) and (10). Note the degradation in effectiveness of the Wald-Wolfowitz approximation exhibited above when $f \gg n^2$, as demonstrated by Howe. However, the approximation is quite good for the commonly used application where f = n-1.

Since in the theoretical development of K-factors for two-sided statistical tolerance intervals one again assumed that $\hat{\eta}$ is Normally distributed about η with variance σ^2/n while $\hat{\sigma}^2$ is based upon f degrees of freedom and is independently distributed as $\chi^2(f)\sigma^2/f$, there is no implied coupling between n and f. Therefore, for the construction of two-sided statistical tolerance intervals for curve-fitting problems, one should calculate the K-factors by substituting n* for n in either equation (9) or (10). (Note: n* was previously defined in the discussion of one-sided statistical tolerance limits.)

IX. NUMERICAL EXAMPLES FOR TWO-SIDED LIMITS

Two-sided 95/99 statistical tolerance limits are presented for the models and data bases from Reference (2) used in the one-sided case. Since for each of these three examples $f < n^{*2}(1+1/Z^2_{0.975})$, equation (9) will be used to calculate the K-factors.

For the first example which dealt with a straight line, $\hat{\sigma} = 0.89012$ and $f = 23$. Corresponding to $X = 70$, $\hat{\eta} = 8.035$ and $n^* = 12.15$. Substituting in equation (9) with $Z_{0.995} = 2.576$ and $X^2_{0.05}(23) = 13.092$, one obtains $K=3.592$ such that $\hat{\eta} \pm K\hat{\sigma} = 8.035 \pm 3.592\ (0.89102) = (4.84,\ 11.23)$. Therefore, corresponding to X = 70, we assert with 95% confidence that at least 99% of the parent Normal population is contained within the interval (4.84, 11.23).

For the second example which dealt with fitting a plane, $\hat{\sigma} = 0.66157$ and $f = 22$. Corresponding to $X_1 = 70$ and $X_2 = 22$, $\hat{\eta} = 8.521$ and $n^* = 9.10$. Using $Z_{0.995} = 2.576$ and $X^2_{0.05}\ (22) = 12.338$, the value of K was calculated to be 3.691. Thus $8.521 \pm\ 3.691\ (0.66157)$ leads to (6.08, 10.96).

Finally, for the nonlinear model, $\hat{\sigma} = 0.010913$ and $f = 42$. Corresponding to $X = 20$, $\hat{\eta} = 0.4196$ and $n^* = 23.13$. Using $Z_{0.995} = 2.576$ and $X^2_{0.05}(42) = 28.144$, the value of K is 3.230. Therefore, $0.4196 \pm 3.230\ (0.010913)$ or (0.384, 0.455) is the resulting approximate 95/99 statistical tolerance interval.

Two-sided 95% confidence and prediction limits are also given in Appendixes A, B, and C for purposes of comparison.

X. SUMMARY

Excellent standard computer programs are widely available for data reduction in obtaining "best fit curves" for engineering models of varying complexity. In order to provide design limits with a quantitative basis, this report described the use of one-sided and two-sided γ/P statistical tolerance limits for design application. For purposes of illustration, γ was set at 0.95 and P was set at 0.99. In application, however, the magnitudes of each of these quantities may be set on a case basis. The details for the calculations of these limits, along with the underlying assumptions, are also described.

Since the topic of this report is design limits, some important topics concerning model development are not discussed. Any good text such as Reference (2) covers both the formal and informal statistical methods of lack-of-fit tests, tests for non-Normality, residual analysis, etc.

Furthermore, whether the model is considered a simplified empirical graduation over a region of interest or is viewed as a mechanistic model, the implications of the model should be critically examined both inside and outside the range of the available data base. Finally, before any model is used in design application, predictions should be made based upon the model and independent data should be collected for model verification. (If it is known that this cannot be done, a subsample of the existing data base should be set aside for this purpose and not be used in fitting the coefficients.)

One topic which was intentionally avoided in this report is the subject of simultaneous tolerance intervals, the construction of tolerance limits at a number of different points in the factor space based upon the same data base. Experience shows that most design engineers want a single adjustment to the "best fit curve", be it an additive or a multiplicative factor, usually calculated at a critical or limiting combination of the independent variables. The methodology described here is consistent with that approach to design limits.

Finally, the details described in this report may give the reader the impression that these procedures are cumbersome to invoke. However, since practically all engineering models are now fit using a computer, the procedures may be readily incorporated into existing programs as has been done in our Laboratory for some of the programs in our Statistics Package. In fact, good approximations to the referenced probability distributions are available so that table look-up is no longer required.

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Appendix A

X	Y	$\hat{\eta}$	$e = Y - \hat{\eta}$
35.3	10.98	10.81	0.17
29.7	11.13	11.25	-0.12
30.8	12.51	11.17	1.34
58.8	8.40	8.93	-0.53
61.4	9.27	8.72	0.55
71.3	8.73	7.93	0.80
74.4	6.36	7.68	-1.32
76.7	8.50	7.50	1.00
70.7	7.82	7.98	-0.16
57.5	9.14	9.03	0.11
46.4	8.24	9.92	-1.68
28.9	12.19	11.32	0.87
28.1	11.88	11.38	0.50
39.1	9.57	10.50	-0.93
46.8	10.94	9.89	1.05
48.5	9.58	9.75	-0.17
59.3	10.09	8.89	1.20
70.0	8.11	8.04	0.07
70.0	6.83	8.04	-1.21
74.5	8.88	7.68	1.20
72.1	7.68	7.87	-0.19
58.1	8.47	8.98	-0.51
44.6	8.86	10.06	-1.20
33.4	10.36	10.96	-0.60
28.6	11.08	11.34	-0.26

$\hat{\eta} = 13.6230 - 0.0798287X$, $\hat{\sigma} = 0.89012$, $f = 23$

Appendix A (continued)

At $X_k = 70$, $\hat{\eta}_k = 13.6230 - 0.0798287(70) = 8.035$

$$s^2(\hat{\eta}_k) = s^2_{Y\bullet X}\left[\frac{1}{n} + \frac{(X_k-\bar{X})^2}{\sum_i (X_i-\bar{X})^2}\right] = (0.89012)^2\left[\frac{1}{25} + \frac{(70 - 52.6)^2}{7154.42}\right] = 0.065208$$

$s(\hat{\eta}_k) = 0.2554$, $t^{(23)}_{0.95} = 1.714$, $t^{(23)}_{0.975} = 2.069$

$$s^2(Y_k) = s^2_{Y\bullet X}\left[1 + \frac{1}{n} + \frac{(X_k-\bar{X})^2}{\sum_i (X_i-\bar{X})^2}\right] = 0.857530, \quad S(Y_k) = 0.9260$$

A) One-sided lower 95% confidence limit for mean $\eta_{(70)}$:

$$\hat{\eta}_k - t^{(23)}_{0.95} \bullet s(\hat{\eta}_k) = 8.035 - 1.714\ (0.2554) = 7.597$$

$$\text{Conf}\ (\eta_{(70)} > 7.60) = 95\%$$

B) Two-sided 95% confidence interval for mean $\eta_{(70)}$:

$$\hat{\eta}_k \pm t^{(23)}_{0.975} \bullet s(\hat{\eta}_k) = 8.035 \pm 2.069\ (0.2554) = 8.035 \pm 0.528$$

$$\text{Conf}\ (7.51 < \eta_{(70)} < 8.56) = 95\%$$

C) One-sided lower 95% Prediction limit for $Y_{(70)}$:

$$Y_k - t^{(23)}_{0.95} \bullet s(Y_k) = 8.035 - 1.714\ (0.9260) = 6.448$$

With 95% confidence, $Y_{(70)}$ will exceed 6.45

D) Two-sided 95% Prediction interval for $Y_{(70)}$:

$$Y_k \pm t^{(23)}_{0.975} \bullet s(Y_k) = 8.035 \pm 2.069\ (0.9260) = 8.035 \pm 1.916$$

With 95% confidence, $Y_{(70)}$ will be contained within (6.12, 9.95)

Appendix B

X_1	X_2	Y	$\hat{\eta}$	$e = Y - \hat{\eta}$
35.3	20	10.98	10.63	0.35
29.7	20	11.13	11.03	0.10
30.8	23	12.51	11.56	0.95
58.8	20	8.40	8.93	-0.53
61.4	21	9.27	8.94	0.33
71.3	22	8.73	8.43	0.30
74.4	11	6.36	5.97	0.39
76.7	23	8.50	8.24	0.26
70.7	11	7.82	8.27	-0.45
57.5	20	9.14	9.02	0.12
46.4	20	8.24	9.82	-1.58
28.9	21	12.19	11.29	0.90
28.1	21	11.88	11.35	0.53
39.1	19	9.57	10.15	-0.58
46.8	23	10.94	10.40	0.54
48.5	20	9.58	9.67	-0.09
59.3	22	10.09	9.30	0.79
70.0	22	8.11	8.52	-0.41
70.0	11	6.83	6.29	0.54
74.5	23	8.88	8.40	0.48
72.1	20	7.68	7.96	-0.28
58.1	21	8.47	9.18	-0.71
44.6	20	8.86	9.96	-1.10
33.4	20	10.36	10.77	-0.41
28.6	22	11.08	11.52	-0.44

$$\hat{\eta} = 9.12689 - 0.072393X_1 + 0.202815X_2, \quad \hat{\sigma} = 0.66157, \quad f = 22$$

At $X_1 = 70$ and $X_2 = 22$, $\hat{\eta} = 9.12689 - 0.072393(70) + 0.202815(22) = 8.521$

$$s^2(\hat{\eta}) = (0.66157)^2 \left[\frac{1}{25} + (17.4 \quad 1.76) \begin{pmatrix} 1.462068E\text{-}4 & 1.754669E\text{-}4 \\ 1.754669E\text{-}4 & 4.785985E\text{-}3 \end{pmatrix} \begin{pmatrix} 17.4 \\ 1.76 \end{pmatrix}\right]$$

$$= (0.66157)^2 \quad (0.04 + 0.069838) = 0.048072, \quad s(\hat{\eta}) = 0.2193$$

$$s^2(Y_k) = 0.485741, \quad s(Y_k) = 0.697, \quad t^{(22)}_{0.95} = 1.717, \quad t^{(22)}_{0.975} = 2.074$$

A) One-sided lower 95% confidence limit for mean $\eta_{(70,22)}$:

$$\hat{\eta}_k - t^{(22)}_{(0.95)} \bullet s(\hat{\eta}_k) = 8.521 - 1.717\ (0.2193) = 8.144$$

$$\text{Conf}\ (\eta_{(70,22)} > 8.14) = 95\%$$

B) Two-sided 95% confidence interval for mean $\eta_{(70,22)}$:

$$\hat{\eta}_k \pm t^{(22)}_{0.975} \bullet s(\hat{\eta}_k) = 8.521 \pm 2.074\ (0.2193) = 8.521 \pm 0.4548$$

$$\text{Conf}\ (8.07 < \eta_{(70,22)} < 8.98) = 95\%$$

C) One-sided lower 95% Prediction limit for $Y_{(70,22)}$:

$$Y_k - t^{(22)}_{0.95} \bullet s(Y_k) = 8.521 - 1.717\ (0.697) = 7.324$$

With 95% confidence, $Y_{(70,22)}$ will exceed 7.32

D) Two-sided 95% Prediction interval for $Y_{(70,22)}$:

$$Y_k \pm t^{(22)}_{0.975} \bullet s(Y_k) = 8.521 \pm 2.074\ (0.697) = 8.521 \pm 1.446$$

With 95% confidence, $Y_{(70,22)}$ will be contained within (7.08, 9.97)

Appendix C

X	Y	$\hat{\eta}$	$e = Y - \hat{\eta}$
8	0.49	0.490	0.000
8	0.49	0.490	0.000
10	0.48	0.472	0.008
10	0.47	0.472	-0.002
10	0.48	0.472	0.008
10	0.47	0.472	-0.002
12	0.46	0.457	0.003
12	0.46	0.457	0.003
12	0.45	0.457	-0.007
12	0.43	0.457	-0.027
14	0.45	0.444	0.006
14	0.43	0.444	-0.014
14	0.43	0.444	-0.014
16	0.44	0.434	0.006
16	0.43	0.434	-0.004
16	0.43	0.434	-0.004
18	0.46	0.426	0.034
18	0.45	0.426	0.024
20	0.42	0.420	0.000
20	0.42	0.420	0.000
20	0.43	0.420	0.010
22	0.41	0.414	-0.004
22	0.41	0.414	-0.004
22	0.40	0.414	-0.014
24	0.42	0.410	0.010
24	0.40	0.410	-0.010
24	0.40	0.410	-0.010
26	0.41	0.406	0.004
26	0.40	0.406	-0.006
26	0.41	0.406	0.004
28	0.41	0.403	0.007
28	0.40	0.403	-0.003
30	0.40	0.401	-0.001
30	0.40	0.401	-0.001
30	0.38	0.401	-0.021
32	0.41	0.399	0.011

Appendix C (continued)

X	Y	$\hat{\eta}$	$e = Y - \hat{\eta}$
32	0.40	0.399	0.001
34	0.40	0.397	0.003
36	0.41	0.396	0.014
36	0.38	0.396	-0.016
38	0.40	0.395	0.005
38	0.40	0.395	0.005
40	0.39	0.394	-0.004
42	0.39	0.393	-0.003

$$\hat{\eta} = 0.39014 + (0.49 - 0.39014)e^{-0.10163(X-8)}$$

$\hat{\sigma} = 0.010913$, $f = 42$

At $X_k = 20$, $\hat{\eta}_k = 0.39014 + (0.49 - 0.39014)e^{-0.10163(20-8)} = 0.4196$

$$s^2(\hat{\eta}_k) = (0.010913)^2 \left[(0.70464 - 0.35394)\begin{pmatrix}0.213723 & 0.502515\\ 0.502515 & 1.498844\end{pmatrix}\begin{pmatrix}0.70464\\ -0.35394\end{pmatrix}\right]$$

$$= (0.01913)^2\ (0.043228) = 5.1482E\text{-}6, \quad s(\hat{\eta}_k) = 2.269E\text{-}3$$

$$s^2(Y_k) - 1.2424E\text{-}4, \quad s(Y_k)\ 1.115E\text{-}2, \quad t_{0.95}^{(42)} = 1.683, \quad t_{0.975}^{(42)} = 2.019$$

A) One-sided lower 95% confidence limit for mean $\eta_{(20)}$:

$$\hat{\eta}_k - t_{0.95}^{(42)} \bullet s(\hat{\eta}_k) = 0.4196 - 1.683\ (2.269E\text{-}3) = 0.4158$$

$$\text{Conf}\ (\eta_{(20)} > 0.416) = 95\%$$

B) Two-sided 95% confidence interval for mean $\eta_{(20)}$:

$$\hat{\eta}_k \pm t_{0.975}^{(42)} \bullet s(\hat{\eta}_k) = 0.4196 \pm 2.019\ (2.269E\text{-}3) = 0.4196 \pm 4.581E\text{-}3$$

$$\text{Conf}\ (0.415 < \eta_{(20)} < 0.424) = 95\%$$

C) One-sided lower 95% Prediction limit for $Y_{(20)}$:

$$Y_k - t_{0.95}^{(42)} \bullet s(Y_k) = 0.4196 - 1.683\ (1.115E\text{-}2) = 0.4008$$

With 95% confidence, $Y_{(20)}$ will exceed 0.401

D) Two-sided 95% Prediction interval for $Y_{(20)}$:

$$Y_k \pm t_{0.975}^{(42)} \bullet s(Y_k) = 0.4196 \pm 2.019\ (1.115E\text{-}2) = 0.4196 \pm 0.0225$$

With 95% confidence, $Y_{(20)}$ will be contained within (0.397, 0.442)

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