

Graduate Lectures and Problems in Quality
Control and Engineering Statistics:
Theory and Methods

To Accompany

Statistical Quality Assurance Methods for Engineers

by

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Chapter 1

Measurement and Statistics

V&J §2.2 presents an introduction to the topic of measurement and the relevance of the subject of statistics to the measurement enterprise. This chapter expands somewhat on the topics presented in V&J and raises some additional issues.

Note that V&J equation (2.1) and the discussion on page 19 of V&J are central to the role of statistics in describing measurements in engineering and quality assurance. Much of Stat 531 concerns “process variation.” The discussion on and around page 19 points out that variation in measurements from a process will include both components of “real” process variation *and* measurement variation.

1.1 Theory for Range-Based Estimation of Variances

Suppose that X_1, X_2, \dots, X_n are iid Normal (μ, σ^2) random variables and let

$$\begin{aligned} R &= \max X_i - \min X_i \\ &= \max(X_i - \mu) - \min(X_i - \mu) \\ &= \sigma \left(\max \left(\frac{X_i - \mu}{\sigma} \right) - \min \left(\frac{X_i - \mu}{\sigma} \right) \right) \\ &= \sigma (\max Z_i - \min Z_i) \end{aligned}$$

where $Z_i = (X_i - \mu)/\sigma$. Then Z_1, Z_2, \dots, Z_n are iid standard normal random variables. So for purposes of studying the distribution of the range of iid normal variables, it suffices to study the standard normal case. (One can derive “general σ ” facts from the “ $\sigma = 1$ ” facts by multiplying by σ .)

Consider first the matter of the finding the mean of the range of n iid standard normal variables, Z_1, \dots, Z_n . Let

$$U = \min Z_i, \quad V = \max Z_i \quad \text{and} \quad W = V - U .$$

Then

$$EW = EV - EU$$

and

$$-EU = -E \min Z_i = E(-\min Z_i) = E \max(-Z_i) ,$$

where the n variables $-Z_1, -Z_2, \dots, -Z_n$ are iid standard normal. Thus

$$EW = EV - EU = 2EV .$$

Then, (as is standard in the theory of order statistics) note that

$$V \leq t \Leftrightarrow \text{all } n \text{ values } Z_i \text{ are } \leq t .$$

So with Φ the standard normal cdf,

$$P[V \leq t] = \Phi^n(t)$$

and thus a pdf for V is

$$f(v) = n\phi(v)\Phi^{n-1}(v) .$$

So

$$EV = \int_{-\infty}^{\infty} v (n\phi(v)\Phi^{n-1}(v)) dv ,$$

and the evaluation of this integral becomes a (very small) problem in numerical analysis. The value of this integral clearly depends upon n . It is standard to invent a constant (whose dependence upon n we will display explicitly)

$$d_2(n) \doteq EW = 2EV$$

that is tabled in Table A.1 of V&J. With this notation, clearly

$$ER = \sigma d_2(n) ,$$

(and the range-based formulas in Section 2.2 of V&J are based on this simple fact).

To find more properties of W (and hence R) requires appeal to a well-known order statistics result giving the joint density of two order statistics. The joint density of U and V is

$$f(u, v) = \begin{cases} n(n-1)\phi(u)\phi(v) (\Phi(v) - \Phi(u))^{n-2} & \text{for } v > u \\ 0 & \text{otherwise .} \end{cases}$$

A transformation then easily shows that the joint density of U and $W = V - U$ is

$$g(u, w) = \begin{cases} n(n-1)\phi(u)\phi(u+w) (\Phi(u+w) - \Phi(u))^{n-2} & \text{for } w > 0 \\ 0 & \text{otherwise .} \end{cases}$$

Then, for example, the cdf of W is

$$P[W \leq t] = \int_0^t \int_{-\infty}^{\infty} g(u, w) du dw ,$$

and the mean of W^2 is

$$EW^2 = \int_0^{\infty} \int_{-\infty}^{\infty} w^2 g(u, w) du dw .$$

Note that upon computing EW and EW^2 , one can compute both the variance of W

$$\text{Var } W = EW^2 - (EW)^2$$

and the standard deviation of W , $\sqrt{\text{Var } W}$. It is common to give this standard deviation the name $d_3(n)$ (where we continue to make the dependence on n explicit and again this constant is tabled in Table A.1 of V&J). Clearly, having computed $d_3(n) \doteq \sqrt{\text{Var } W}$, one then has

$$\sqrt{\text{Var } R} = \sigma d_3(n) .$$

1.2 Theory for Sample-Variance-Based Estimation of Variances

Continue to suppose that X_1, X_2, \dots, X_n are iid Normal (μ, σ^2) random variables and take

$$s^2 \doteq \frac{1}{n-1} \sum_{i=1}^n (X_i - \bar{X})^2 .$$

Standard probability theory says that

$$\frac{(n-1)s^2}{\sigma^2} \sim \chi_{n-1}^2 .$$

Now if $U \sim \chi_{\nu}^2$ it is the case that $EU = \nu$ and $\text{Var } U = 2\nu$. It is thus immediate that

$$Es^2 = E\left(\frac{\sigma^2}{n-1}\right) \left(\frac{(n-1)s^2}{\sigma^2}\right) = \left(\frac{\sigma^2}{n-1}\right) E\left(\frac{(n-1)s^2}{\sigma^2}\right) = \sigma^2$$

and

$$\text{Var } s^2 = \text{Var} \left(\left(\frac{\sigma^2}{n-1}\right) \left(\frac{(n-1)s^2}{\sigma^2}\right) \right) = \left(\frac{\sigma^2}{n-1}\right)^2 \text{Var} \left(\frac{(n-1)s^2}{\sigma^2}\right) = \frac{2\sigma^4}{n-1}$$

so that

$$\sqrt{\text{Var } s^2} = \sigma^2 \sqrt{\frac{2}{n-1}} .$$

Knowing that $(n-1)s^2/\sigma^2 \sim \chi_{n-1}^2$ also makes it easy enough to develop properties of $s = \sqrt{s^2}$. For example, if

$$f(x) = \begin{cases} \frac{1}{2^{(n-1)/2}\Gamma(\frac{n-1}{2})} x^{(\frac{n-1}{2})-1} \exp\left(-\frac{x}{2}\right) & \text{for } x > 0 \\ 0 & \text{otherwise} \end{cases}$$

is the χ_{n-1}^2 probability density, then

$$Es = E\sqrt{\frac{\sigma^2}{n-1}}\sqrt{\frac{(n-1)s^2}{\sigma^2}} = \frac{\sigma}{\sqrt{n-1}} \int_0^\infty \sqrt{x}f(x)dx = \sigma c_4(n),$$

for

$$c_4(n) \doteq \frac{\int_0^\infty \sqrt{x}f(x)dx}{\sqrt{n-1}}$$

another constant (depending upon n) tabled in Table A.1 of V&J. Further, the standard deviation of s is

$$\sqrt{\text{Var } s} = \sqrt{Es^2 - (Es)^2} = \sqrt{\sigma^2 - (\sigma c_4(n))^2} = \sigma\sqrt{1 - c_4^2(n)} = \sigma c_5(n)$$

for

$$c_5(n) \doteq \sqrt{1 - c_4^2(n)}$$

yet another constant tabled in Table A.1.

The fact that sums of independent χ^2 random variables are again χ^2 (with degrees of freedom equal to the sum of the component degrees of freedom) and the kinds of relationships in this section provide means of combining various kinds of sample variances to get “pooled” estimators of variances (and variance components) and finding the means and variances of these estimators. For example, if one pools in the usual way the sample variances from r normal samples of size m to get a single pooled sample variance, s_{pooled}^2 , $r(m-1)s_{\text{pooled}}^2/\sigma^2$ is χ^2 with degrees of freedom $\nu = r(m-1)$. That is, all of the above can be applied by thinking of s_{pooled}^2 as a sample variance based on a sample of size “ n ” = $r(m-1) + 1$.

1.3 Sample Variances and Gage R&R

The methods of gage R&R analysis presented in V&J §2.2.2 are based on ranges (and the facts in §1.1 above). They are presented in V&J not because of their efficiency, but because of their computational simplicity. Better (and analogous) methods can be based on the facts in §1.2 above. For example, under the two-way random effects model (2.4) of V&J, if one pools $I \times J$ “cell” sample variances s_{ij}^2 to get s_{pooled}^2 , all of the previous paragraph applies and gives methods of estimating the repeatability variance component σ^2 (or the repeatability standard deviation σ) and calculating means and variances of estimators based on s_{pooled}^2 .

Or, consider the problem of estimating $\sigma_{\text{reproducibility}}$ defined in display (2.5) of V&J. With \bar{y}_{ij} as defined on page 24 of V&J, note that for fixed i , the J random variables $\bar{y}_{ij} - \alpha_i$ have the same sample variance as the J random variables \bar{y}_{ij} , namely

$$s_i^2 \doteq \frac{1}{J-1} \sum_j (\bar{y}_{ij} - \bar{y}_{i.})^2 .$$

But for fixed i the J random variables $\bar{y}_{ij} - \alpha_i$ are iid normal with mean μ and variance $\sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2/m$, so that

$$E s_i^2 = \sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2/m .$$

So

$$\frac{1}{I} \sum_i s_i^2$$

is a plausible estimator of $\sigma_\beta^2 + \sigma_{\alpha\beta}^2 + \sigma^2/m$. Hence

$$\frac{1}{I} \sum_i s_i^2 - \frac{s_{\text{pooled}}^2}{m} ,$$

or better yet

$$\max \left(0, \frac{1}{I} \sum_i s_i^2 - \frac{s_{\text{pooled}}^2}{m} \right) \quad (1.1)$$

is a plausible estimator of $\sigma_{\text{reproducibility}}^2$.

1.4 ANOVA and Gage R&R

Under the two-way random effects model (2.4) of V&J, with balanced data, it is well-known that the ANOVA mean squares

$$\begin{aligned} MSE &= \frac{1}{IJ(m-1)} \sum_{i,j,k} (y_{ijk} - \bar{y}_{..})^2 , \\ MSAB &= \frac{m}{(I-1)(J-1)} \sum_{i,j} (\bar{y}_{ij} - \bar{y}_{i.} - \bar{y}_{.j} + \bar{y}_{..})^2 , \\ MSA &= \frac{mJ}{I-1} \sum_i (\bar{y}_{i.} - \bar{y}_{..})^2 , \quad \text{and} \\ MSB &= \frac{mI}{J-1} \sum_j (\bar{y}_{.j} - \bar{y}_{..})^2 , \end{aligned}$$

are independent random variables, that

$$\begin{aligned} EMSE &= \sigma^2 , \\ EMSAB &= \sigma^2 + m\sigma_{\alpha\beta}^2 , \\ EMSA &= \sigma^2 + m\sigma_{\alpha\beta}^2 + mJ\sigma_\alpha^2 , \quad \text{and} \\ EMSB &= \sigma^2 + m\sigma_{\alpha\beta}^2 + mI\sigma_\beta^2 , \end{aligned}$$

Table 1.1: Two-way Balanced Data Random Effects Analysis ANOVA Table
ANOVA Table

Source	<i>SS</i>	<i>df</i>	<i>MS</i>	<i>EMS</i>
Parts	<i>SSA</i>	$I - 1$	<i>MSA</i>	$\sigma^2 + m\sigma_{\alpha\beta}^2 + mJ\sigma_{\alpha}^2$
Operators	<i>SSB</i>	$J - 1$	<i>MSB</i>	$\sigma^2 + m\sigma_{\alpha\beta}^2 + mI\sigma_{\beta}^2$
Parts×Operators	<i>SSAB</i>	$(I - 1)(J - 1)$	<i>MSAB</i>	$\sigma^2 + m\sigma_{\alpha\beta}^2$
Error	<i>SSE</i>	$(m - 1)IJ$	<i>MSE</i>	σ^2
Total	<i>SSTot</i>	$mIJ - 1$		

and that the quantities

$$\frac{(m - 1)IJMSE}{EMSE}, \quad \frac{(I - 1)(J - 1)MSAB}{EMSAB}, \quad \frac{(I - 1)MSA}{EMSA} \quad \text{and} \quad \frac{(J - 1)MSB}{EMSB}$$

are χ^2 random variables with respective degrees of freedom

$$(m - 1)IJ, (I - 1)(J - 1), (I - 1) \text{ and } (J - 1) .$$

These facts about sums of squares and mean squares for the two-way random effects model are often summarized in the usual (two-way random effects model) ANOVA table, Table 1.1. (The sums of squares are simply the mean squares multiplied by the degrees of freedom. More on the interpretation of such tables can be found in places like §8-4 of V.)

As a matter of fact, the ANOVA error mean square is exactly s_{pooled}^2 from §1.3 above. Further, the expected mean squares suggest ways of producing sensible estimators of other parametric functions of interest in gage R&R contexts (see V&J page 27 in this regard). For example, note that

$$\sigma_{\text{reproducibility}}^2 = \frac{1}{mI}EMSB + \frac{1}{m}\left(1 - \frac{1}{I}\right)EMSAB - \frac{1}{m}EMSE ,$$

which suggests the ANOVA-based estimator

$$\hat{\sigma}_{\text{reproducibility}}^2 = \max\left(0, \frac{1}{mI}MSB + \frac{1}{m}\left(1 - \frac{1}{I}\right)MSAB - \frac{1}{m}MSE\right) . \quad (1.2)$$

What may or may not be well known is that this estimator (1.2) is exactly the estimator of $\sigma_{\text{reproducibility}}^2$ in display (1.1).

Since many common estimators of quantities of interest in gage R&R studies are functions of mean squares, it is useful to have at least some crude standard errors for them. These can be derived from “delta method”/“propagation of error”/Taylor series argument provided in the appendix to these notes. For example, if MS_i $i = 1, \dots, k$ are independent random variables, $(\nu_i MS_i / EMS_i)$ with a $\chi_{\nu_i}^2$ distribution, consider a function of k real variables $f(x_1, \dots, x_k)$ and the random variable

$$U = f(MS_1, MS_2, \dots, MS_k) .$$

Propagation of error arguments produce the approximation

$$\text{Var } U \approx \sum_{i=1}^k \left(\left. \frac{\partial f}{\partial x_i} \right|_{EMS_1, EMS_2, \dots, EMS_k} \right)^2 \text{Var } MS_i = \sum_{i=1}^k \left(\left. \frac{\partial f}{\partial x_i} \right|_{EMS_1, EMS_2, \dots, EMS_k} \right)^2 \frac{2(EMS_i)^2}{\nu_i},$$

and upon substituting mean squares for their expected values, one has a standard error for U , namely

$$\sqrt{\widehat{\text{Var}} U} = \sqrt{2 \sum_{i=1}^k \left(\left. \frac{\partial f}{\partial x_i} \right|_{MS_1, MS_2, \dots, MS_k} \right)^2 \frac{(MS_i)^2}{\nu_i}}. \quad (1.3)$$

In the special case where the function of the mean squares of interest is linear in them, say

$$U = \sum_{i=1}^k c_i MS_i,$$

the standard error specializes to

$$\sqrt{\widehat{\text{Var}} U} = \sqrt{2 \sum_{i=1}^k \frac{c_i^2 (MS_i)^2}{\nu_i}},$$

which provides at least a crude method of producing standard errors for $\hat{\sigma}_{\text{reproducibility}}^2$ and $\hat{\sigma}_{\text{overall}}^2$. Such standard errors are useful in giving some indication of the precision with which the quantities of interest in a gage R&R study have been estimated.

1.5 Confidence Intervals for Gage R&R Studies

The parametric functions of interest in gage R&R studies (indeed in all random effects analyses) are functions of variance components, or equivalently, functions of expected mean squares. It is thus possible to apply theory for estimating such quantities to the problem of assessing precision of estimation in a gage study. As a first (and very crude) example of this, note that taking the point of view of §1.4 above, where $U = f(MS_1, MS_2, \dots, MS_k)$ is a sensible point estimator of an interesting function of the variance components and $\sqrt{\widehat{\text{Var}} U}$ is the standard error (1.3), simple approximate two-sided 95% confidence limits can be made as

$$U \pm 1.96 \sqrt{\widehat{\text{Var}} U}.$$

These limits have the virtue of being amenable to “hand” calculation from the ANOVA sums of squares, but they are not likely to be reliable (in terms of holding their nominal/asymptotic coverage probability) for I, J or m small.

Linear models experts have done substantial research aimed at finding reliable confidence interval formulas for important functions of expected mean

squares. For example, the book *Confidence Intervals on Variance Components* by Burdick and Graybill gives results (on the so-called “modified large sample method”) that can be used to make confidence intervals on various important functions of variance components. The following is some material taken from Sections 3.2 and 3.3 of the Burdick and Graybill book.

Suppose that MS_1, MS_2, \dots, MS_k are k independent mean squares. (The MS_i are of the form SS_i/ν_i , where $SS_i/EMS_i = \nu_i MS_i/EMS_i$ has a $\chi^2_{\nu_i}$ distribution.) For $1 \leq p < k$ and positive constants c_1, c_2, \dots, c_k suppose that the quantity

$$\theta = c_1 EMS_1 + \dots + c_p EMS_p - c_{p+1} EMS_{p+1} - \dots - c_k EMS_k \quad (1.4)$$

is of interest. Let

$$\hat{\theta} = c_1 MS_1 + \dots + c_p MS_p - c_{p+1} MS_{p+1} - \dots - c_k MS_k .$$

Approximate confidence limits on θ in display (1.4) are of the form

$$L = \hat{\theta} - \sqrt{V_L} \quad \text{and/or} \quad U = \hat{\theta} + \sqrt{V_U} ,$$

for V_L and V_U defined below.

Let $F_{\alpha:df_1,df_2}$ be the upper α point of the F distribution with df_1 and df_2 degrees of freedom. (It is then the case that $F_{\alpha:df_1,df_2} = (F_{1-\alpha:df_2,df_1})^{-1}$.) Also, let $\chi^2_{\alpha:df}$ be the upper α point of the χ^2_{df} distribution. With this notation

$$V_L = \sum_{i=1}^p c_i^2 MS_i^2 G_i^2 + \sum_{i=p+1}^k c_i^2 MS_i^2 H_i^2 + \sum_{i=1}^p \sum_{j=p+1}^k c_i c_j MS_i MS_j G_{ij} + \sum_{i=1}^{p-1} \sum_{j>i}^p c_i c_j MS_i MS_j G_{ij}^* ,$$

for

$$G_i = 1 - \frac{\nu_i}{\chi^2_{\alpha:\nu_i}} ,$$

$$H_i = \frac{\nu_i}{\chi^2_{1-\alpha:\nu_i}} - 1 ,$$

$$G_{ij} = \frac{(F_{\alpha:\nu_i,\nu_j} - 1)^2 - G_i^2 F_{\alpha:\nu_i,\nu_j}^2 - H_j^2}{F_{\alpha:\nu_i,\nu_j}} ,$$

and

$$G_{ij}^* = \begin{cases} 0 & \text{if } p = 1 \\ \frac{1}{p-1} \left(\left(1 - \frac{\nu_i + \nu_j}{\chi_{\alpha:\nu_i+\nu_j}} \right)^2 \frac{(\nu_i + \nu_j)^2}{\nu_i \nu_j} - \frac{G_i^2 \nu_i}{\nu_j} - \frac{G_j^2 \nu_j}{\nu_i} \right) & \text{otherwise .} \end{cases}$$

On the other hand,

$$V_U = \sum_{i=1}^p c_i^2 MS_i^2 H_i^2 + \sum_{i=p+1}^k c_i^2 MS_i^2 G_i^2 + \sum_{i=1}^p \sum_{j=p+1}^k c_i c_j MS_i MS_j H_{ij} + \sum_{i=p+1}^{k-1} \sum_{j>i}^k c_i c_j MS_i MS_j H_{ij}^* ,$$

for G_i and H_i as defined above, and

$$H_{ij} = \frac{(1 - F_{1-\alpha:\nu_i,\nu_j})^2 - H_i^2 F_{1-\alpha:\nu_i,\nu_j}^2 - G_j^2}{F_{1-\alpha:\nu_i,\nu_j}},$$

and

$$H_{ij}^* = \begin{cases} 0 & \text{if } k = p + 1 \\ \frac{1}{k - p - 1} \left(\left(1 - \frac{\nu_i + \nu_j}{\chi_{\alpha:\nu_i+\nu_j}^2} \right)^2 \frac{(\nu_i + \nu_j)^2}{\nu_i \nu_j} - \frac{G_i^2 \nu_i}{\nu_j} - \frac{G_j^2 \nu_j}{\nu_i} \right) & \text{otherwise.} \end{cases}$$

One uses (L, ∞) or $(-\infty, U)$ for confidence level $(1 - \alpha)$ and the interval (L, U) for confidence level $(1 - 2\alpha)$. (Using these formulas for “hand” calculation is (obviously) no picnic. The C program written by Brandon Paris (available off the Stat 531 Web page) makes these calculations painless.)

A problem similar to the estimation of quantity (1.4) is that of estimating

$$\theta = c_1 EMS_1 + \cdots + c_p EMS_p \quad (1.5)$$

for $p \geq 1$ and positive constants c_1, c_2, \dots, c_p . In this case let

$$\hat{\theta} = c_1 MS_1 + \cdots + c_p MS_p,$$

and continue the G_i and H_i notation from above. Then approximate confidence limits on θ given in display (1.5) are of the form

$$L = \hat{\theta} - \sqrt{\sum_{i=1}^p c_i^2 MS_i^2 G_i^2} \quad \text{and/or} \quad U = \hat{\theta} + \sqrt{\sum_{i=1}^p c_i^2 MS_i^2 H_i^2}.$$

One uses (L, ∞) or $(-\infty, U)$ for confidence level $(1 - \alpha)$ and the interval (L, U) for confidence level $(1 - 2\alpha)$.

The Fortran program written by Andy Chiang (available off the Stat 531 Web page) applies Burdick and Graybill-like material and the standard errors (1.3) to the estimation of many parametric functions of relevance in gage R&R studies.

Chiang’s 2000 Ph.D. dissertation work (to appear in *Technometrics* in August 2001) has provided an entirely different method of interval estimation of functions of variance components that is a uniform improvement over the “modified large sample” methods presented by Burdick and Graybill. His approach is related to “improper Bayes” methods with so called “Jeffreys priors.” Andy has provided software for implementing his methods that, as time permits, will be posted on the Stat 531 Web page. He can be contacted (for preprints of his work) at stackl@nus.edu.sg at the National University of Singapore.

1.6 Calibration and Regression Analysis

The estimation of standard deviations and variance components is a contribution of the subject of statistics to the quantification of measurement system *precision*. The subject also has contributions to make in the matter of improving measurement *accuracy*. Calibration is the business of bringing a local measurement system in line with a standard measurement system. One takes measurements y with a gage or system of interest on test items with “known” values x (available because they were previously measured using a “gold standard” measurement device). The data collected are then used to create a conversion scheme for translating local measurements to approximate gold standard measurements, thereby hopefully improving local accuracy. In this short section we note that usual regression methodology has implications in this kind of enterprise.

The usual polynomial regression model says that n observed random values y_i are related to fixed values x_i via

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \cdots + \beta_k x_i^k + \varepsilon_i \quad (1.6)$$

for iid Normal $(0, \sigma^2)$ random variables ε_i . The parameters β and σ are the usual objects of inference in this model. In the calibration context with x a gold standard value, σ quantifies precision for the local measurement system. Often (at least over a limited range of x) 1) a low order polynomial does a good job of describing the observed x - y relationship between local and gold standard measurements and 2) the usual (least squares) fitted relationship

$$\hat{y} = g(x) = b_0 + b_1 x + b_2 x^2 + \cdots + b_k x^k$$

has an inverse $g^{-1}(y)$. When such is the case, given a measurement y_{n+1} from the local measurement system, it is plausible to estimate that a corresponding measurement from the gold standard system would be $\hat{x}_{n+1} = g^{-1}(y_{n+1})$. A reasonable question is then “How good is this estimate?”. That is, the matter of confidence interval estimation of x_{n+1} is important.

One general method for producing such confidence sets for x_{n+1} is based on the usual “prediction interval” methodology associated with the model (1.6). That is, for a given x , it is standard (see, e.g. §9-2 of V or §9.2.4 of V&J#2) to produce a prediction interval of the form

$$\hat{y} \pm t \sqrt{s^2 + (\text{std error}(\hat{y}))^2}$$

for an additional corresponding y . And those intervals have the property that for all choices of $x, \sigma, \beta_0, \beta_1, \beta_2, \dots, \beta_k$

$$\begin{aligned} &P_{x, \sigma, \beta_0, \beta_1, \beta_2, \dots, \beta_k} [y \text{ is in the prediction interval at } x] \\ &= \text{desired confidence level} \\ &= 1 - P[\text{a } t_{n-k-1} \text{ random variable exceeds } |t|] . \end{aligned}$$

But rewording only slightly, the event

“ y is in the prediction interval at x ”

is the same as the event

“ x produces a prediction interval including y .”

So a confidence set for x_{n+1} based on the observed value y_{n+1} is

$$\{x \mid \text{the prediction interval corresponding to } x \text{ includes } y_{n+1}\}. \quad (1.7)$$

Conceptually, one simply makes prediction limits around the fitted relationship $\hat{y} = g(x) = b_0 + bx + b_2x^2 + \dots + b_kx^k$ and then upon observing a new y sees what x 's are consistent with that observation. This produces a confidence set with the desired confidence level.

The only real difficulties with the above general prescription are 1) the lack of simple explicit formulas and 2) the fact that when σ is large (so that the regression \sqrt{MSE} tends to be large) or the fitted relationship is very nonlinear, the method can produce (completely rational but) unpleasant-looking confidence sets. The first “problem” is really of limited consequence in a time when standard statistical software will automatically produce plots of prediction limits associated with low order regressions. And the second matter is really inherent in the problem.

For the (simplest) linear version of this “inverse prediction” problem, there is an approximate confidence method in common use that doesn't have the deficiencies of the method (1.7). It is derived from a Taylor series argument and has its own problems, but is nevertheless worth recording here for completeness sake. That is, under the $k = 1$ version of the model (1.6), commonly used approximate confidence limits for x_{n+1} are (for $\hat{x}_{n+1} = (y_{n+1} - b_0)/b_1$ and \bar{x} the sample mean of the gold standard measurements from the calibration experiment)

$$\hat{x}_{n+1} \pm t \frac{\sqrt{MSE}}{|b_1|} \sqrt{1 + \frac{1}{n} + \frac{(\hat{x}_{n+1} - \bar{x})^2}{\sum_{i=1}^n (x_i - \bar{x})^2}}.$$

1.7 Crude Gaging and Statistics

All real-world measurement is “to the nearest something.” Often one may ignore this fact, treat measured values as if they were “exact” and experience no real difficulty when using standard statistical methods (that are really based on an assumption that data are exact). However, sometimes in industrial applications gaging is “crude” enough that standard (e.g. “normal theory”) formulas give nonsensical results. This section briefly considers what can be done to appropriately model and draw inferences from crudely gaged data. The assumption throughout is that what are available are integer data, obtained by coding raw observations via

$$\text{integer observation} = \frac{\text{raw observation} - \text{some reference value}}{\text{smallest unit of measurement}}.$$

(the “*smallest unit of measurement*” is “the nearest something” above).

1.7.1 Distributions of Sample Means and Ranges from Integer Observations

To begin with something simple, note first that in situations where only a few different coded values are ever observed, rather than trying to model observations with some continuous distribution (like a normal one) it may well make sense to simply employ a discrete pmf, say f , to describe any single measurement. In fact, suppose that a single (crudely gaged) observation Y has a pmf $f(y)$ such that

$$f(y) = 0 \quad \text{unless } y = 1, 2, \dots, M .$$

Then if Y_1, Y_2, \dots, Y_n are iid with this marginal discrete distribution, one can easily approximate the distribution of a function of these variables via simulation (using common statistical packages). And for two of the most common statistics used in QC settings (the sample mean and range) one can even work out exact probability distributions using computationally feasible and very elementary methods.

To find the probability distribution of \bar{Y} in this context, one can build up the probability distributions of sums of iid Y_i 's recursively by “adding probabilities on diagonals in two-way joint probability tables.” For example the $n = 2$ distribution of \bar{Y} can be obtained by making out a two-way table of joint probabilities for Y_1 and Y_2 and adding on diagonals to get probabilities for $Y_1 + Y_2$. Then making a two-way table of joint probabilities for $(Y_1 + Y_2)$ and Y_3 one can add on diagonals and find a joint distribution for $Y_1 + Y_2 + Y_3$. Or noting that the distribution of $Y_3 + Y_4$ is the same as that for $Y_1 + Y_2$, it is possible to make a two-way table of joint probabilities for $(Y_1 + Y_2)$ and $(Y_3 + Y_4)$, add on diagonals and find the distribution of $Y_1 + Y_2 + Y_3 + Y_4$. And so on. (Clearly, after finding the distribution for a sum, one simply divides possible values by n to get the corresponding distribution of \bar{Y} .)

To find the probability distribution of $R = \max Y_i - \min Y_i$ (for Y_i 's as above) a feasible computational scheme is as follows. Let

$$S_{kj} = \begin{cases} \sum_{x=k}^j f(x) = P[k \leq Y \leq j] & \text{if } k \leq j \\ 0 & \text{otherwise} \end{cases}$$

and compute and store these for $1 \leq k, j \leq M$. Then define

$$M_{kj} = P[\min Y_i = k \text{ and } \max Y_i = j] .$$

Now the event $\{\min Y_i = k \text{ and } \max Y_i = j\}$ is the event $\{\text{all observations are between } k \text{ and } j \text{ inclusive}\}$ less the event $\{\text{the minimum is greater than } k \text{ or the maximum is less than } j\}$. Thus, it is straightforward to see that

$$M_{kj} = (S_{kj})^n - (S_{k+1,j})^n - (S_{k,j-1})^n + (S_{k+1,j-1})^n$$

and one may compute and store these values. Finally, note that

$$P[R = r] = \sum_{k=1}^{M-r} M_{k,k+r} .$$

These “algorithms” are good for any distribution f on the integers $1, 2, \dots, M$. Karen (Jensen) Hulting’s “DIST” program (available off the Stat 531 Web page) automates the calculations of the distributions of \bar{Y} and R for certain f ’s related to “integer rounding of normal observations.” (More on this rounding idea directly.)

1.7.2 Estimation Based on Integer-Rounded Normal Data

The problem of drawing inferences from crudely gaged data is one that has a history of at least 100 years (if one takes a view that crude gaging essentially “rounds” “exact” values). Sheppard in the late 1800’s noted that if one rounds a continuous variable to integers, the variability in the distribution is typically increased. He thus suggested not using the sample standard deviation (s) of rounded values but instead employing what is known as Sheppard’s correction to arrive at

$$\sqrt{\frac{(n-1)s^2}{n} - \frac{1}{12}} \tag{1.8}$$

as a suitable estimate of “standard deviation” for integer-rounded data.

The notion of “interval-censoring” of fundamentally continuous observations provides a natural framework for the application of modern statistical theory to the analysis of crudely gaged data. For univariate X with continuous cdf $F(x|\boldsymbol{\theta})$ depending upon some (possibly vector) parameter $\boldsymbol{\theta}$, consider X^* derived from X by rounding to the nearest integer. Then the pmf of X^* is, say,

$$g(x^*|\boldsymbol{\theta}) \doteq \begin{cases} F(x^* + .5|\boldsymbol{\theta}) - F(x^* - .5|\boldsymbol{\theta}) & \text{for } x^* \text{ an integer} \\ 0 & \text{otherwise .} \end{cases}$$

Rather than doing inference based on the unobservable variables X_1, X_2, \dots, X_n that are iid $F(x|\boldsymbol{\theta})$, one might consider inference based on $X_1^*, X_2^*, \dots, X_n^*$ that are iid with pmf $g(x^*|\boldsymbol{\theta})$.

The normal version of this scenario (the integer-rounded normal data model) makes use of

$$g(x^*|\mu, \sigma) \doteq \begin{cases} \Phi\left(\frac{x^* + .5 - \mu}{\sigma}\right) - \Phi\left(\frac{x^* - .5 - \mu}{\sigma}\right) & \text{for } x^* \text{ an integer} \\ 0 & \text{otherwise ,} \end{cases}$$

and the balance of this section will consider the use of this specific important model. So suppose that $X_1^*, X_2^*, \dots, X_n^*$ are iid integer-valued random observations (generated from underlying normal observations by rounding). For an observed vector of integers $(x_1^*, x_2^*, \dots, x_n^*)$ it is useful to consider the so-called

“likelihood function” that treats the (joint) probability assigned to the vector $(x_1^*, x_2^*, \dots, x_n^*)$ as a function of the parameters,

$$L(\mu, \sigma) \doteq \prod_i g(x_i^* | \mu, \sigma) = \prod_i \left(\Phi \left(\frac{x_i^* + .5 - \mu}{\sigma} \right) - \Phi \left(\frac{x_i^* - .5 - \mu}{\sigma} \right) \right) .$$

The log of this function of μ and σ is (naturally enough) called the loglikelihood and will be denoted as

$$\mathcal{L}(\mu, \sigma) \doteq \ln L(\mu, \sigma) .$$

A sensible estimator of the parameter vector (μ, σ) is “the point $(\hat{\mu}, \hat{\sigma})$ maximizing the loglikelihood.” This prescription for estimation is only partially complete, depending upon the nature of the sample $x_1^*, x_2^*, \dots, x_n^*$. There are three cases to consider, namely:

1. When the sample range of $x_1^*, x_2^*, \dots, x_n^*$ is at least 2, $\mathcal{L}(\mu, \sigma)$ is well-behaved (nice and “mound-shaped”) and numerical maximization or just looking at contour plots will quickly allow one to maximize the loglikelihood. (It is worth noting that in this circumstance, usually $\hat{\sigma}$ is close to the “Sheppard corrected” value in display (1.8).)
2. When the sample range of $x_1^*, x_2^*, \dots, x_n^*$ is 1, strictly speaking $\mathcal{L}(\mu, \sigma)$ fails to achieve a maximum. However, with

$$m \doteq \#[x_i^* = \min x_i^*] ,$$

(μ, σ) pairs with σ small and

$$\mu \approx \min x_i^* + .5 - \sigma \Phi^{-1} \left(\frac{m}{n} \right)$$

will have

$$\mathcal{L}(\mu, \sigma) \approx \sup_{\mu, \sigma} \mathcal{L}(\mu, \sigma) = m \ln m + (n - m) \ln(n - m) - n \ln n .$$

That is, in this case one ought to “estimate” that σ is small and the relationship between μ and σ is such that a fraction m/n of the underlying normal distribution is to the left of $\min x_i^* + .5$, while a fraction $1 - m/n$ is to the right.

3. When the sample range of $x_1^*, x_2^*, \dots, x_n^*$ is 0, strictly speaking $\mathcal{L}(\mu, \sigma)$ fails to achieve a maximum. However,

$$\sup_{\mu, \sigma} \mathcal{L}(\mu, \sigma) = 0$$

and for any $\mu \in (x_1^* - .5, x_1^* + .5)$, $\mathcal{L}(\mu, \sigma) \rightarrow 0$ as $\sigma \rightarrow 0$. That is, in this case one ought to “estimate” that σ is small and $\mu \in (x_1^* - .5, x_1^* + .5)$.

Beyond the making of point estimates, the loglikelihood function can provide approximate confidence sets for the parameters μ and/or σ . Standard “large sample” statistical theory says that (for large n and $\chi_{\alpha;\nu}^2$ the upper α point of the χ_{ν}^2 distribution):

1. An approximate $(1 - \alpha)$ level confidence set for the parameter vector (μ, σ) is

$$\{(\mu, \sigma) | \mathcal{L}(\mu, \sigma) > \sup_{\mu, \sigma} \mathcal{L}(\mu, \sigma) - \frac{1}{2} \chi_{\alpha;2}^2\}. \quad (1.9)$$

2. An approximate $(1 - \alpha)$ level confidence set for the parameter μ is

$$\{\mu | \sup_{\sigma} \mathcal{L}(\mu, \sigma) > \sup_{\mu, \sigma} \mathcal{L}(\mu, \sigma) - \frac{1}{2} \chi_{\alpha;1}^2\}. \quad (1.10)$$

3. An approximate $(1 - \alpha)$ level confidence set for the parameter σ is

$$\{\sigma | \sup_{\mu} \mathcal{L}(\mu, \sigma) > \sup_{\mu, \sigma} \mathcal{L}(\mu, \sigma) - \frac{1}{2} \chi_{\alpha;1}^2\}. \quad (1.11)$$

Several comments and a fuller discussion are in order regarding these confidence sets. In the first place, Karen (Jensen) Hulting’s CONEST program (available off the Stat 531 Web page) is useful in finding $\sup_{\mu, \sigma} \mathcal{L}(\mu, \sigma)$ and producing rough contour plots of the (joint) sets for (μ, σ) in display (1.9). Second, it is common to call the function of μ defined by

$$\mathcal{L}^*(\mu) = \sup_{\sigma} \mathcal{L}(\mu, \sigma)$$

the “profile loglikelihood” function for μ and the function of σ

$$\mathcal{L}^{**}(\sigma) = \sup_{\mu} \mathcal{L}(\mu, \sigma)$$

the “profile loglikelihood” function for σ . Note that display (1.10) then says that the confidence set should consist of those μ ’s for which the profile loglikelihood is not too much smaller than the maximum achievable. And something entirely analogous holds for the sets in (1.11). Johnson Lee (in 2001 Ph.D. dissertation work) has carefully studied these confidence interval estimation problems and determined that some modification of methods (1.10) and (1.11) is necessary in order to provide guaranteed coverage probabilities for small sample sizes. (It is also very important to realize that contrary to naive expectations, not even a large sample size will make the usual t -intervals for μ and χ^2 -intervals for σ hold their nominal confidence levels in the event that σ is small, i.e. that the rounding or crudeness of the gaging is important. Ignoring the rounding when it is important can produce actual confidence levels near 0 for methods with large nominal confidence levels.)

Table 1.2: Δ for 0-Range Samples Based on Very Small n

n	α		
	.05	.10	.20
2	3.084	1.547	.785
3	.776	.562	
4	.517		

Intervals for a Normal Mean Based on Integer-Rounded Data

Specifically regarding the sets for μ in display (1.10), Lee (in work to appear in the *Journal of Quality Technology*) has shown that one must replace the value $\chi_{\alpha;1}^2$ with something larger in order to get small n actual confidence levels not too far from nominal for “most” (μ, σ) . In fact, the choice

$$c(n, \alpha) = n \ln \left(\frac{t_{\frac{\alpha}{2};(n-1)}^2}{n-1} + 1 \right)$$

(for $t_{\frac{\alpha}{2};(n-1)}$ the upper $\frac{\alpha}{2}$ point of the t distribution with $\nu = n - 1$ degrees of freedom) is appropriate.

After replacing $\chi_{\alpha;1}^2$ with $c(n, \alpha)$ in display (1.10) there remains the numerical analysis problem of actually finding the interval prescribed by the display. The nature of the numerical analysis required depends upon the sample range encountered in the crudely gaged data. Provided the range is at least 2, $\mathcal{L}^*(\mu)$ is well-behaved (continuous and “mound-shaped”) and even simple trial and error with Karen (Jensen) Hulting’s CONEST program will quickly produce the necessary interval. When the range is 0 or 1, $\mathcal{L}^*(\mu)$ has respectively 2 or 1 discontinuities and the numerical analysis is a bit trickier. Lee has recorded the results of the numerical analysis for small sample sizes and $\alpha = .05, .10$ and $.20$ (confidence levels respectively 95%, 90% and 80%).

When a sample of size n produces range 0 with, say, all observations equal to x^* , the intuition that one ought to estimate $\mu \in (x^* - .5, x^* + .5)$ is sound unless n is very small. If n and α are as recorded in Table 1.2 then display (1.10) (modified by the use of $c(n, \alpha)$ in place of $\chi_{\alpha;1}^2$) leads to the interval $(x^* - \Delta, x^* + \Delta)$. (Otherwise it leads to $(x^* - .5, x^* + .5)$ for these α .)

In the case that a sample of size n produces range 1 with, say, all observations x^* or $x^* + 1$, the interval prescribed by display (1.10) (with $c(n, \alpha)$ used in place of $\chi_{\alpha;1}^2$) can be thought of as having the form $(x^* + .5 - \Delta_L, x^* + .5 + \Delta_U)$ where Δ_L and Δ_U depend upon

$$n_{x^*} = \#[\text{observations } x^*] \quad \text{and} \quad n_{x^*+1} = \#[\text{observations } x^* + 1]. \quad (1.12)$$

When $n_{x^*} \geq n_{x^*+1}$, it is the case that $\Delta_L \geq \Delta_U$. And when $n_{x^*} \leq n_{x^*+1}$, correspondingly $\Delta_L \leq \Delta_U$. Let

$$m = \max\{n_{x^*}, n_{x^*+1}\} \quad (1.13)$$

Table 1.3: (Δ_1, Δ_2) for Range 1 Samples Based on Small n

n	m	α		
		.05	.10	.20
2	1	(6.147, 6.147)	(3.053, 3.053)	(1.485, 1.485)
3	2	(1.552, 1.219)	(1.104, 0.771)	(0.765, 0.433)
4	3	(1.025, 0.526)	(0.082, 0.323)	(0.639, 0.149)
	2	(0.880, 0.880)	(0.646, 0.646)	(0.441, 0.441)
5	4	(0.853, 0.257)	(0.721, 0.132)	(0.592, 0.024)
	3	(0.748, 0.548)	(0.592, 0.339)	(0.443, 0.248)
6	5	(0.772, 0.116)	(0.673, 0.032)	(0.569, 0.000)
	4	(0.680, 0.349)	(0.562, 0.235)	(0.444, 0.126)
	3	(0.543, 0.543)	(0.420, 0.420)	(0.299, 0.299)
7	6	(0.726, 0.035)	(0.645, 0.000)	(0.556, 0.000)
	5	(0.640, 0.218)	(0.545, 0.130)	(0.446, 0.046)
	4	(0.534, 0.393)	(0.432, 0.293)	(0.329, 0.193)
8	7	(0.698, 0.000)	(0.626, 0.000)	(0.547, 0.000)
	6	(0.616, 0.129)	(0.534, 0.058)	(0.446, 0.000)
	5	(0.527, 0.281)	(0.439, 0.197)	(0.347, 0.113)
	4	(0.416, 0.416)	(0.327, 0.327)	(0.236, 0.236)
9	8	(0.677, 0.000)	(0.613, 0.000)	(0.541, 0.000)
	7	(0.599, 0.065)	(0.526, 0.010)	(0.448, 0.000)
	6	(0.521, 0.196)	(0.443, 0.124)	(0.361, 0.054)
	5	(0.429, 0.321)	(0.350, 0.242)	(0.267, 0.163)
10	9	(0.662, 0.000)	(0.604, 0.000)	(0.537, 0.000)
	8	(0.587, 0.020)	(0.521, 0.000)	(0.450, 0.000)
	7	(0.515, 0.129)	(0.446, 0.069)	(0.371, 0.012)
	6	(0.437, 0.242)	(0.365, 0.174)	(0.289, 0.105)
	5	(0.346, 0.346)	(0.275, 0.275)	(0.200, 0.200)

and correspondingly take

$$\Delta_1 = \max\{\Delta_L, \Delta_U\} \text{ and } \Delta_2 = \min\{\Delta_L, \Delta_U\} .$$

Table 1.3 then gives values for Δ_1 and Δ_2 for $n \leq 10$ and $\alpha = .05, .10$ and $.2$.

Intervals for a Normal Standard Deviation Based on Integer-Rounded Data

Specifically regarding the sets for σ in display (1.11), Lee found that in order to get small n actual confidence levels not too far from nominal, one must not only replace the value $\chi_{\alpha;1}^2$ with something larger, but must make an additional adjustment for samples with ranges 0 and 1.

Consider first replacing $\chi_{\alpha;1}^2$ in display (1.11) with a (larger) value $d(n, \alpha)$ given in Table 1.4. Lee found that for those (μ, σ) with moderate to large σ ,

Table 1.4: $d(n, \alpha)$ for Use in Estimating σ

n	α	
	.05	.10
2	10.47	7.71
3	7.26	5.23
4	6.15	4.39
5	5.58	3.97
6	5.24	3.71
7	5.01	3.54
8	4.84	3.42
9	4.72	3.33
10	4.62	3.26
15	4.34	3.06
20	4.21	2.97
30	4.08	2.88
∞	3.84	2.71

making this $d(n, \alpha)$ for $\chi_{\alpha;1}^2$ substitution is enough to produce an actual confidence level approximating the nominal one. However, even this modification is not adequate to produce an acceptable coverage probability for (μ, σ) with small σ .

For samples with range 0 or 1, formula (1.11) prescribes intervals of the form $(0, U)$. And reasoning that when σ is small, samples will typically have range 0 or 1, Lee was able to find (larger) replacements for the limit U prescribed by (1.11) so that the resulting estimation method has actual confidence level not much below the nominal level for any (μ, σ) (with σ large or small).

That is if a 0-range sample is observed, estimate σ by

$$(0, \Lambda_0)$$

where Λ_0 is taken from Table 1.5. If a range 1 sample is observed consisting, say, of values x^* and $x^* + 1$, and n_{x^*}, n_{x^*+1} and m are as in displays (1.12) and (1.13), estimate σ using

$$(0, \Lambda_{1,m})$$

where $\Lambda_{1,m}$ is taken from Table 1.6.

The use of these values Λ_0 for range 0 samples, and $\Lambda_{1,m}$ for range 1 samples, and the values $d(n, \alpha)$ in place of $\chi_{\alpha;1}^2$ in display (1.11) finally produces a reliable method of confidence interval estimation for σ when normal data are integer-rounded.

Table 1.5: Λ_0 for Use in Estimating σ
 α

n	.05	.10
2	5.635	2.807
3	1.325	0.916
4	0.822	0.653
5	0.666	0.558
6	0.586	0.502
7	0.533	0.464
8	0.495	0.435
9	0.466	0.413
10	0.443	0.396
11	0.425	0.381
12	0.409	0.369
13	0.396	0.358
14	0.384	0.349
15	0.374	0.341

Table 1.6: $\Lambda_{1,m}$ for Use in Estimating σ (m in Parentheses)

n	α					
	.05			.10		
2	16.914(1)			8.439(1)		
3	3.535(2)			2.462(2)		
4	1.699(3)	2.034(2)		1.303(3)	1.571(2)	
5	1.143(4)	1.516(3)		0.921(4)	1.231(3)	
6	0.897(5)	1.153(4)	1.285(3)	0.752(5)	0.960(4)	1.054(3)
7	0.768(6)	0.944(5)	1.106(4)	0.660(6)	0.800(5)	0.949(4)
8	0.687(7)	0.819(6)	0.952(5)	0.599(7)	0.707(6)	0.825(5)
	1.009(4)			0.880(4)		
9	0.629(8)	0.736(7)	0.837(6)	0.555(8)	0.644(7)	0.726(6)
	0.941(5)			0.831(5)		
10	0.585(9)	0.677(8)	0.747(7)	0.520(9)	0.597(8)	0.654(7)
	0.851(6)	0.890(5)		0.753(6)	0.793(5)	
11	0.550(10)	0.630(9)	0.690(8)	0.493(10)	0.560(9)	0.609(8)
	0.775(7)	0.851(6)		0.685(7)	0.763(6)	
12	0.522(11)	0.593(10)	0.646(9)	0.470(11)	0.531(10)	0.573(9)
	0.708(8)	0.789(7)	0.818(6)	0.626(8)	0.707(7)	0.738(6)
13	0.499(12)	0.563(11)	0.610(10)	0.452(12)	0.506(11)	0.544(10)
	0.658(9)	0.733(8)	0.791(7)	0.587(9)	0.655(8)	0.716(7)
14	0.479(13)	0.537(12)	0.580(11)	0.436(13)	0.485(12)	0.520(11)
	0.622(10)	0.681(9)	0.745(8)	0.558(10)	0.607(9)	0.674(8)
	0.768(7)			0.698(7)		
15	0.463(14)	0.515(13)	0.555(12)	0.422(14)	0.468(13)	0.499(12)
	0.593(11)	0.639(10)	0.701(9)	0.534(11)	0.574(10)	0.632(9)
	0.748(8)			0.682(8)		