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Uncertainty Analysis of Instrument Calibration and Application

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Symbols

$\mathbf{A}, \mathbf{B}$	$K \times K$ matrix
a_{mn}, b_{mn}	mnth elements of matrices $\mathbf{A}$ and $\mathbf{B}$
B	bias error
b	offset voltage of angle of attack sensor
$\mathbf{C}$	$M_{\mathbf{c}} \times L$ coefficient matrix
$\mathbf{c}$, c_m	$M_{\mathbf{c}} \times 1$ parameter vector with elements c_m
$\widehat{\mathbf{c}}, \widehat{c}_m$	$M_{\mathbf{c}} \times 1$ estimated parameter vector with elements $\widehat{c}_m$
$\widehat{\mathbf{c}}_{\mathbf{G}}$	globally estimated parameter vector
$\widehat{\mathbf{c}}_{\mathbf{R}_n}$	$M_{\mathbf{c}} \times 1$ estimated parameter vector of nth replication
$\cos\boldsymbol{\theta}$	$K \times 1$ vector formed by element-by-element cosine evaluation of $K \times 1$ vector $\boldsymbol{\theta}$
D	experimental design, a subset of $\Im$
$\mathbf{D}_{\mathbf{NK}}$	$NK \times NK$ block-diagonal matrix
d_i	distance
$\mathbf{e(c,Z)}$	$K \times 1$ vector function of $\mathbf{c}$ and $\mathbf{Z}$
$\mathbf{e}_{\mathbf{M}}, \mathbf{e}_{\mathbf{X}}$	error vectors
$\widehat{\mathbf{e}}, \widehat{\mathbf{e}}_{\mathbf{v}}$	$K \times 1$ residual vectors
$\widehat{\mathbf{e}}_n$	$K \times 1$ residual vector at nth replication
$\bar{\mathbf{e}}_{\mathbf{k}}$	averaged residual vector
$\bar{e}_k$	element of $\bar{\mathbf{e}}_{\mathbf{k}}$
F	ratio of variances
$\mathbf{F}_{\mathbf{c}}$	$K \times M_{\mathbf{c}}$ derivative matrix of $\mathbf{f(c,Z)}$ with respect to $\mathbf{c}$
$\mathbf{F}_{\mathbf{cc}}$	$M_{\mathbf{c}} \times M_{\mathbf{c}} \times K$ array
$\mathbf{F}_{\mathbf{cK}}$	$K \times M_{\mathbf{c}}$ derivative matrix of $\mathbf{f(c,Z_K)}$ with respect to $\mathbf{c}$
$F_{i,j}(\alpha)$	α percentile value of F-distribution with i, j degrees of freedom
$\mathbf{f(c,Z)}$	$K \times 1$ vector function of $\mathbf{c}$ and $\mathbf{Z}$
$f(\mathbf{c}, \mathbf{z})$	real-value multivariate function of $\mathbf{c}$ and $\mathbf{z}$
$\mathbf{f}_{\mathbf{c_m}}$	mth column of $\mathbf{F}_{\mathbf{c}}$
$\mathbf{f}_{\mathbf{c}}(\mathbf{c},\mathbf{z})$	$M_c \times 1$ gradient vector of $f(\mathbf{c}, \mathbf{z})$ with respect to $\mathbf{c}$
$\mathbf{f}_{\mathbf{cc}_{ij}}$	ijth column vector of length K contained in array $\mathbf{F}_{\mathbf{cc}}$
$\mathbf{f}_{\mathbf{cc}_{ij\,k}}$	kth element of vector $\mathbf{f}_{\mathbf{cc}_{ij}}$
$\mathbf{f}_{\mathbf{z}}(\mathbf{c}, \mathbf{z_k})$	$1 \times K$ gradient vector of f with respect to $\mathbf{z}$
$\delta\mathbf{f}_{\mathbf{z}}$	error vector

δf_{zk}	element of error vector $\delta \mathbf{f_z}$
$\mathbf{G}$	$K \times L$ matrix of $g_j(\mathbf{c}_{\bullet j}, \mathbf{z})$ functions
$\mathbf{G_H}$	$NK \times NK$ matrix
$\mathbf{g}(\mathbf{C}, \mathbf{z})$	$1 \times L$ row vector of scalar-value functions of $\mathbf{C}$ and $\mathbf{z}$
$g_j(\mathbf{c}_{\bullet j}, \mathbf{z})$	jth element of $\mathbf{g}(\mathbf{C}, \mathbf{z})$
$\mathbf{H}$	$K \times NK$ replication matrix containing N copies of $K \times K$ identity matrix $\mathbf{I_K}$
$\mathbf{H_E}$	$M_\mathbf{c} \times M_\mathbf{c}$ matrix
$\mathbf{h}(\mathbf{c}, \mathbf{Z})$	$1 \times M_\mathbf{c}$ vector gradient of S_{SQ} with respect to $\mathbf{c}$
$h_{E_{ij}}$	ijth element of $\mathbf{H_E}$
$\mathbf{I}$	identity matrix
$\mathbf{I_K}$	$K \times K$ identity matrix
$\mathbf{I_W}$	diagonal matrix of ones and zeros
$\Im$	subset of input space $\Re^{M_\mathbf{z}}$
i, j, k, m, n	integer indices
J	normalized average predicted output variance over set $\Im$
K	number of calibration observations
L	dimension of multivariate function
M	order of multivariate polynomial or integer
$M_\mathbf{c}$	length of parameter vector $\mathbf{c}$
$M_\mathbf{z}$	length of extended input vector $\mathbf{z}$
N	number of replications or integer
N_I	number of input variables
$\mathbf{P}$	nonsingular matrix
$\mathbf{P}_m$	orthonormal matrix
$\mathbf{P}_{r_m}, \mathbf{P}_{s_m}$	submatrices of $\mathbf{P}_m$
$\mathbf{p}_m$	mth row of $\mathbf{R}^{-1}$
$\mathbf{Q}$	$M_\mathbf{z} \times M_\mathbf{z}$ weighted moment matrix
$\mathbf{Q_c}$	$M_\mathbf{c} \times M_\mathbf{c}$ nonlinear moment matrix
$\mathbf{Q}_m$	$N \times N$ matrix
q_m	quadratic form
$\mathbf{R}$	$M_\mathbf{c} \times M_\mathbf{c}$ Jacobian matrix of S_{SQ} with respect to $\mathbf{c}$
$\mathbf{R}_r$	$N \times N$ matrix
$\mathbf{R}_{r_m}$	submatrix of $\mathbf{R_r}$ of rank r_m

$\Re$	set of real numbers
$\Re^M$	M-dimensional space over set of real numbers
r	rank
$r_{\mathbf{A}}$	rank of matrix $\mathbf{A}$
r_m	rank of matrix $\mathbf{Q}_m$
S	sensitivity of AOA sensor
S_E, S_Y	standard errors of regression
S_M	standard error due to measurement uncertainty after replication
S_{SE}	total residual sum of squares
S_{SG_m}	total residual sum of squares of N replications with parameter substitution
$S_{SG_{m,n}}$	residual sum of squares of nth replication with parameter substitution
S_{SM}	sum of squares due to measurement uncertainty after replication
S_{SQ}	inner product to be minimized by least-squares estimation of parameter vector
S_{SR}	total residual sum of squares of N replications
S_{SR_n}	residual sum of squares of nth replication
S_{SW}	quadratic form
S_{SX}	sum of squares due to bias uncertainty after replication
S_X	standard error due to bias uncertainty after replication
$\mathbf{sin}\ \boldsymbol{\theta}$	$K \times 1$ vector formed by element-by-element sine evaluation of $K \times 1$ vector $\boldsymbol{\theta}$
T_{CM}, T_{XM}	variance ratio
t	ratio
$t_k(\alpha)$	t-distribution with k degrees of freedom at confidence level α
$\mathbf{U}$	symmetric positive definite matrix
V	variance error
$\mathbf{v}$	transformed output or observation vector
$\mathbf{W}, \mathbf{W}_K$	matrix, subscript K denotes dimension
$\mathbf{W}_{\mathbf{F}}, \mathbf{W}_{\mathbf{F}_K}$	matrix, subscript K denotes dimension
$\mathbf{x}$	$1 \times N$ input vector
x	applied scalar input
$\hat{\mathbf{x}}$	estimated applied scalar input
$\mathbf{x}_k$	kth applied $1 \times N$ input vector of experimental design
$\mathbf{Y}$	$K \times L$ matrix of observed output vectors $\mathbf{y_k}$.
$\mathbf{y}$	$K \times 1$ calibration observation vector

y	observed scalar output
y_k	kth observed scalar output
$\mathbf{y}_{k\cdot}$	kth observed output vector
y_0	new observation for input $\mathbf{z_0}$ after calibration
$y_x(\widehat{x}_0)$	partial derivative of output y with respect to input x
$\widehat{y}(\mathbf{z})$	predicted scalar output for input vector $\mathbf{z}$
$\widehat{y}_0$	predicted value of new observation y_0
$\mathbf{Z}$	$K \times M_{\mathbf{z}}$ general design matrix
$\mathbf{Z_K}$	$K \times M_{\mathbf{z}}$ submatrix of $NK \times M_{\mathbf{z}}$ replicated design matrix $\mathbf{Z_{NK}}$
$\mathbf{Z_{NK}}$	$NK \times M_{\mathbf{z}}$ replicated design matrix
$\mathbf{z}$, $\mathbf{z(x)}$	$M_{\mathbf{z}} \times 1$ extended input vector obtained from input $\mathbf{x}$
z	element of extended input vector $\mathbf{z}$
$\mathbf{z}_k$	$1 \times M_{\mathbf{z}}$ extended input vector from kth row of design matrix $\mathbf{Z}$
$\mathbf{z}_0$	new extended input vector after calibration
α	angle of attack or confidence level; ratio
β	variable
Γ	matrix
$\boldsymbol{\gamma}$	transformed coefficient vector
$\boldsymbol{\gamma}(\mathbf{Z})$	$K \times 1$ vector of modeling errors
$\gamma(\mathbf{z})$	modeling error
$\mathbf{E_V}, \mathbf{E_E}$	$K \times L$ matrix of measurement uncertainty vectors $\boldsymbol{\epsilon}_{\mathbf{v}k\cdot}$ and $\boldsymbol{\epsilon}_{\mathbf{E}k\cdot}$
$\boldsymbol{\epsilon}_{\mathbf{E}}$	$K \times 1$ measurement error vector
ϵ_E	scalar measurement uncertainty
$\boldsymbol{\epsilon}_{\mathbf{E_n}}$	$K \times 1$ measurement error vector at nth replication
$\boldsymbol{\epsilon}_{\mathbf{v}}$	transformed $K \times 1$ measurement error vector
$\boldsymbol{\epsilon}_{\mathbf{x}_k}$	uncertainty vector of kth applied input $\mathbf{x}_k$
$\boldsymbol{\epsilon}_0$	uncertainty of new measurement
$\boldsymbol{\zeta}_{\mathbf{w}}$	transformed vector
$\boldsymbol{\eta}$	$K \times 1$ vector of angle of attack sensor outputs
η	angle of attack sensor output
Λ	diagonal matrix of eigenvalues
λ	element of Λ
$\boldsymbol{\mu}_{\mathbf{v}}$	expected value of vector $\mathbf{v}$

$\boldsymbol{\xi}$	$N \times 1$ vector
$\boldsymbol{\xi}_m$	$r_m \times 1$ subvector of $\boldsymbol{\xi}$
ρ_{ij}	ijth element of inverse moment matrix $\mathbf{Q}^{-1}$
$\rho_{\hat{y}}(\mathbf{z})$	quadratic form
$\boldsymbol{\Sigma}_{\mathbf{e}}$, $\boldsymbol{\Sigma}_{\mathbf{y}}$,...	covariance matrix of vector denoted by subscript
$\boldsymbol{\Sigma}_{\mathbf{z_{ij}}}$	covariance matrix of input vectors $\mathbf{z}_i$ and $\mathbf{z}_j$
σ_E	standard deviation of measurement error
σ_{ij}	covariance of ith and jth output measurements
$\sigma_{\mathbf{v}_{ij}}$	ijth element of measurement uncertainty covariance matrix $\boldsymbol{\Sigma}_{\mathbf{E}}$
σ_Y	variance coefficient of $\boldsymbol{\Sigma}_{\mathbf{Y}}$
$\sigma_y^2(\mathbf{z})$	variance function of variable y
σ_0	standard deviation of new measurement
$\boldsymbol{\phi}$	misalignment angle of angle of attack sensor
$\chi_{\boldsymbol{\alpha}}$	α percentile value of chi-square distribution
Ω	volume integral of input subspace $\Im$
$\boldsymbol{\Omega}_{\mathbf{F}}, \boldsymbol{\Omega}_{\mathbf{FK}}, \boldsymbol{\Omega}_{\mathbf{K}}$	$K \times K$ matrix
$\mathbf{0}_{\mathrm{K}}$	$K \times K$ matrix of zeros

General notation:

$\mathbf{c}_{m\bullet}$	mth row of matrix $\mathbf{C}$
$\mathbf{c}_{\bullet n}$	nth column of matrix $\mathbf{C}$
$\mathcal{E}$	expected value operator
$\mathbf{P}^{-\mathbf{T}}$	$= [\mathbf{P}^{-1}]^{\mathbf{T}}$
$^{\mathbf{T}}$	matrix transpose
$\mathrm{tr}(\mathbf{A})$	trace of matrix $\mathbf{A}$
δ	uncertainty operator
$^{-}$	average value
$\hat{}$	predicted value or least-squares estimate of associated variable
$\circ$	element-by-element multiplication of equally dimensioned matrices
$\otimes$	inner product of vector with columns of three-dimensional array

Bold capital letters represent matrices

Bold integer subscript denotes dimension of matrix

Bold lower case letters represent vectors

Bold $\mathbf{0}$ or $\mathbf{1}$ denotes a vector of zeros or ones, respectively

Italic upper and lower case letters represent scalars

Lower case subscripts represent indices: a_k denotes vector element; a_{mn} denotes matrix element; $\mathbf{z}_k$ denotes kth vector of sequence of vectors

Subscript 0 represents new measurement

1. Summary

In 1993, a detailed uncertainty analysis of the six-component strain-gauge balance was undertaken for the first time in wind tunnel tests at the Langley Research Center to provide confidence and prediction intervals of the outputs as functions of the measurands instead of using a general root-mean-square error quantity per component as a percentage of full-scale output. The success of this effort, published in 1994 as AIAA-94-2589, has demonstrated the need for similar analyses of the other wind tunnel instrumentation in use at Langley.

The present publication develops and documents a generalized set of mathematical tools needed for thorough statistical analyses of instrument calibration and application. A comprehensive unified treatment directed toward wind tunnel instrument calibration was not found in the literature.

2. Introduction

Aerospace research requires measurement of basic physical properties such as aerodynamic forces and moments; strain; skin friction force; model attitude, including pitch, roll, and yaw angles; translational position; temperature; pressure; mass-flow rate; and other properties. The aerospace industry now requires that experimental aerodynamic data be furnished with uncertainties specified at a statistical confidence level, typically 95 percent. This requirement, in turn, imposes the need to quantify the uncertainty of each basic physical measurement at the transducer and instrument level in the test facility as a function of the corresponding property value at the specified confidence level.

A standard method for treatment of measurement uncertainty in gas turbine engine performance testing was developed by Abernethy et al. (ref. 1). Based on National Bureau of Standards handbooks, Abernethy separated elementary measurement errors into two components: precision error, which is a zero-mean random error due to measurement scatter, and bias error, which is systematic and repeatable although unpredictable. The uncertainty of a final computed parameter is determined by propagation of individual measurement uncertainties through the functional expressions which define the parameter, usually by means of multivariable Taylor's series expansions. The final total uncertainty equals the root-sum-square of the propagated bias and precision uncertainties.

Abernethy's techniques were extended and formalized into an American National Standard (ref. 2). Coleman and Steele (ref. 3) provide a detailed academic development of the standardized uncertainty analysis specified in reference 2 that includes statistical concepts, experimental design, the effects of replication, and confidence intervals. Reference 3 also provides practical details for application of the standard to engineering practice. It introduces the concepts of generalized uncertainty analysis for the conceptual validation of a proposed experiment and detailed uncertainty analysis for processing experimental results of a completed experiment. The useful concept of "fossilized bias uncertainty" resulting from the acceptance of calibration data is introduced.

An international standard for wind tunnel data uncertainty analysis has been developed by an AGARD working group (ref. 4), which provides a standardized approach for estimating precision and bias limits, for error propagation computation, and for determining confidence intervals of the computed results in the wind tunnel testing context. Batill (ref. 5) has applied AGARD techniques to the data reduction problem at the National Transonic Facility.

The present publication extends the analysis of instrument calibration uncertainty presently addressed in the uncertainty analysis literature. Specifically, correlated measurement precision error, calibration standard uncertainties, and correlated calibration standard bias uncertainties are considered. The effects of mathematical modeling error on calibration bias uncertainty

are quantified. Statistical tests for detection of modeling error and calibration standard error through the use of replication are developed. The effects of experimental design on precision and bias uncertainties are also investigated.

Measurement uncertainties of individual measurements during calibration and experimental testing have usually been considered to be statistically independent to facilitate computations. The extensive use of multichannel multiplexed data acquisition systems with common amplifiers and analog-to-digital converters introduces correlated measurement uncertainties which may be significant. This publication allows rigorous treatment of correlated measurement uncertainties whose covariance matrix is known.

During calibration, the uncertainties of the calibration standard are generally neglected by assuming that their level is at least 1 order of magnitude less than that of the instrument being calibrated. Often calibration standards must be used which do not satisfy this assumption. In addition for calibration, the common use of stacked deadweight loadings for load cell, strain-gauge balance, and skin friction balance introduces significant correlated uncertainties that can magnify the resultant instrument calibration uncertainty several fold. Similar effects can occur during calibration of any instrument with a similar "standard instrument" such as a load cell or skin friction balance. This publication develops the rigorous statistical techniques for computation of calibration standard covariances and their inclusion in calculation of overall instrument confidence intervals. These techniques have been applied to calibration uncertainty analysis of the six-component strain-gauge balance as described in reference 6.

Precision errors are traditionally viewed as zero-mean random variables whose uncertainties can be reduced without limit by replication as shown by the central limit theorem (ref. 7). However, the presence of systematic bias errors during calibration can lead to unrealistically low computed standard errors when very large calibration experimental designs are used. The large number of degrees of freedom can inadvertently reduce the portion of the standard error due to bias uncertainty if correlation effects are neglected.

Other specific work is in progress that applies this analysis to important wind tunnel instruments, including invariable transducers such as load cells and skin friction balances, and multivariable transducers, including the strain-gauge balance and inertial model attitude sensors. Other systems should be analyzed in the future.

3. Instrument Modeling and Calibration Experimental Design

Instruments are routinely calibrated by means of analytical models through the use of multivariate regression analysis to estimate calibration parameter. To quantify statistical confidence levels of measurements obtained by a calibrated instrument, the uncertainty of predicted outputs must be estimated as a function of the input value through the use of the analytic model.

3.1. General Multivariate Process

A formal mathematical representation of a multivariate (multiple-input)–single-output static process, including stochastic components, is presented to describe the steady-state input–output relationship for an instrument. The analysis does not include transient effects.

Let $\Re^{M_c}$ and $\Re^{M_z}$ denote M_c and M_z dimensional Euclidean spaces, respectively, where $\Re$ is the set of real numbers. Consider a real-valued multivariate function f of $M_z \times 1$ input vector $\mathbf{z} \in \Re^{M_z}$, and $M_c \times 1$ parameter vector $\mathbf{c} \in \Re^{M_c}$. Function f maps the Cartesian product of spaces $\Re^{M_c}$ and $\Re^{M_z}$ into the set of real numbers $\Re$; thus,

$$f : \Re^{M_c} \times \Re^{M_z} \Rightarrow \Re \tag{1}$$

The notation $f(\mathbf{c}, \mathbf{z})$ denotes the output value of the function, an analytic model of a physical process dependent upon stochastic input vector $\mathbf{z}$ and deterministic parameter vector $\mathbf{c}$.

The observed output y of the process is generally a measured voltage whose uncertainty δy depends upon both the uncertainty of the applied input $\delta\mathbf{z}$ and the uncertainty of the stochastic process measurement ϵ_E, a zero-mean random variable which is independent of $\delta\mathbf{z}$. Thus the observed output is

$$y = f(\mathbf{c}, \mathbf{z}+\delta\mathbf{z}) + \epsilon_E \tag{2}$$

where stochastic input vector $\mathbf{z}$ has been replaced by the sum of deterministic vector $\mathbf{z}$ plus stochastic input uncertainty vector $\delta\mathbf{z}$. The purpose of calibration is to estimate parameter vector $\mathbf{c}$ based upon multiple observations of output y corresponding to a set of selected inputs specified by an *experimental design*.

3.2. Single-Input–Single-Output Process

An example of a single-input–single-output process model in terms of a nonlinear polynomial using inner-product notation is presented. Let x denote a known applied input to an instrument; let y denote the corresponding observed output, in electrical units, for example; and let ϵ_E denote the measurement error, which is assumed to be a zero-mean random variable with standard deviation σ. Often the measurement process can be accurately modeled by an Mth degree polynomial of the form

$$y = c_0 + c_1 x + c_2 x^2 + \ldots + c_M x^M + \epsilon_E \tag{3}$$

which is seen to be a special case of equation (2). Arranging the polynomial coefficients into $(M+1) \times 1$ vector $\mathbf{c}$ gives

$$\mathbf{c} = [c_0 \; c_1 \ldots \; c_M]^{\mathbf{T}} \tag{4}$$

Define an $(M+1) \times 1$ input vector $\mathbf{z}$, denoted the *extended input vector*, containing the first M powers of x as

$$\mathbf{z}(x) = [1 \; x \; x^2 \ldots \; x^M]^{\mathbf{T}} \tag{5}$$

The functional notation $\mathbf{z}(x)$ is used in the subsequent development only when needed for clarity. Equation (3) can then be expressed in inner-product form as

$$y = \mathbf{z}^{\mathbf{T}}\mathbf{c} + \epsilon_E \tag{6}$$

Note that although the actual process input is scalar variable x, the process model function f is constructed as a multivariate linear function of the $(M+1)$th element input vector $\mathbf{z}$ which is, in turn, a nonlinear function of x.

3.3. Linear, Polynomial, and Nonlinear Multivariate Processes

More general notation suitable for representation of linear, polynomial, and general nonlinear multivariate processes is presented. Consider a multivariate process with vector $\mathbf{x}$ denoting a $1 \times N_I$ vector of input variables,

$$\mathbf{x} = [x_1 \; x_2 \; \ldots \; x_{N_I}] \tag{7}$$

The multivariate process is represented by equation (6) where y is a linear function of an $M_Z \times 1$ extended input vector $\mathbf{z}$ represented by

$$\mathbf{z} = [1 \; z_2 \; z_3 \; \ldots \; z_{M_z}]^{\mathbf{T}} \tag{8}$$

where $z_1 \equiv 1$. For a *univariate linear process*, the elements of $\mathbf{z}$, generated from input variable x, consist only of $[1 \; \mathrm{x}]^{\mathbf{T}}$. For a *univariate polynomial process*, vector $\mathbf{z}$ consists of the powers of x from degree 0 through M as shown in equation (5). For a *multivariate linear process*, vector $\mathbf{z}$ consists of the independent variables $\mathbf{z}(\mathbf{x}) = [1 \vdots \mathbf{x}]^{\mathbf{T}}$. For a *multivariate polynomial process*, vector $\mathbf{z}$ contains the powers and cross products of the elements of $\mathbf{x}$ from degree 0 through M. For example, if $N_I = 3$, then $\mathbf{x} = [x_1 \; x_2 \; x_3]$; if $M = 2$, then $M_{\mathbf{z}} = 10$; and $\mathbf{z}(\mathbf{x})$ is given by

$$\mathbf{z}(\mathbf{x}) = \begin{bmatrix} 1 & x_1 & x_2 & x_3 & x_1^2 & x_1x_2 & x_1x_3 & x_2^2 & x_2x_3 & x_3^2 \end{bmatrix}^{\mathbf{T}} \tag{9}$$

For a multivariate polynomial process of power M, the length of $\mathbf{z}$ is equal to

$$M_{\mathbf{z}} = \frac{(N_I + M)!}{N_I!M!} \tag{10}$$

For example, for a six-component strain-gauge balance modeled by a second-degree multivariate polynomial where $N_I = 6$ and $M = 2$, the length $M_{\mathbf{z}}$ of vector $\mathbf{z}$ equals 28; that is, $\mathbf{z}$ contains 28 terms. Finally, for a *general nonlinear multivariate process*, $\mathbf{z}$ is identical to input vector $\mathbf{x}$.

3.4. Calibration Experimental Design

The *experimental design* for instrument calibration consists of a set of input values applied by using calibrated input standards for which the instrument outputs are observed. The calibration data set is used to estimate the parameters of the mathematical model. Notation for representation of the experimental design and a figure of merit are introduced.

To estimate parameter vector $\mathbf{c}$ during calibration, output y is observed for K values of applied input vector $\mathbf{z}$ contained in a representative subset $\Im$ of input space $\Re^{M_z}$. Subset $\Im$ is selected to cover the anticipated operating envelope of the instrument. The experimental design, $\mathrm{D} \subset \Im$, is ideally chosen to minimize the variance of estimated process output $\widehat{\mathbf{y}}$ averaged over $\Im$, with parameter vector $\widehat{\mathbf{c}}$ obtained by least-squares estimation. Box and Draper (ref. 8) define a design figure of merit J as the average predicted output variance over set $\Im$, normalized by the number of calibration points K and measurement variance σ^2 to remove the effects due to the number of points in design D, and measurement noise. Thus,

$$J = \frac{K \int_{\Im} \sigma_{\hat{y}}^2(\mathbf{z}) \, d\mathbf{x}}{\sigma_E^2 \int_{\Im} d\mathbf{x}} \tag{11}$$

where $\sigma_{\hat{y}}^2(\mathbf{z})$ is the predicted output variance function defined later.

After determination of subset $\mathrm{D} \subset \Im$, construct $K \times M_z$ *design matrix* $\mathbf{Z}$ from the elements $\mathbf{x}_k \in \mathrm{D}$, where the kth row of $\mathbf{Z}$ equals the kth extended input vector $\mathbf{z}(\mathbf{x}_k)$ for $k = 1 \ldots K$ as follows:

$$\mathbf{Z} = \begin{bmatrix} \mathbf{z}(\mathbf{x}_1)^{\mathbf{T}} \\ \mathbf{z}(\mathbf{x}_2)^{\mathbf{T}} \\ \vdots \\ \mathbf{z}(\mathbf{x}_K)^{\mathbf{T}} \end{bmatrix} \tag{12}$$

Arrange the corresponding observed output values and measurement errors into observation vector $\mathbf{y}$ and measurement error vector $\boldsymbol{\epsilon}_{\mathbf{E}}$, respectively, each having dimension of $K \times 1$ as

$$\mathbf{y} = [y_1 \; y_2 \; \ldots \; y_K]^{\mathbf{T}} \tag{13}$$

and

$$\boldsymbol{\epsilon}_{\mathbf{E}} = [\epsilon_{E_1} \; \epsilon_{E_2} \; \ldots \; \epsilon_{E_K}]^{\mathbf{T}} \tag{14}$$

where measurement error vector $\boldsymbol{\epsilon}_{\mathbf{E}}$ has zero mean and $K \times K$ covariance matrix $\boldsymbol{\Sigma}_{\mathbf{E}}$. For linear and polynomial models, equation (6) is extended to a matrix form for K observations with the help of equations (4) and (12) through (14) as

$$\mathbf{y} = \mathbf{Z}\mathbf{c} + \boldsymbol{\epsilon}_{\mathbf{E}} \tag{15}$$

4. Generalized Linear Multivariate Regression Analysis

Multivariate linear regression techniques are developed (ref. 9) for least-squares estimation of coefficient vector $\mathbf{c}$ in equation (15), denoted by $\widehat{\mathbf{c}}$, where the measurement errors are correlated. Techniques are also provided for determination of confidence intervals for $\widehat{\mathbf{c}}$ and for confidence and prediction intervals for new measurements based on the calibrated value of $\widehat{\mathbf{c}}$. Measurement error covariance matrix $\boldsymbol{\Sigma}_{\mathbf{E}}$ is assumed to be symmetric, positive definite, and expressible in the form

$$\boldsymbol{\Sigma}_{\mathbf{E}} = \sigma_E^2 \mathbf{U} \tag{16}$$

where $K \times K$ matrix $\mathbf{U}$ is a known symmetric positive definite matrix and σ^2 is a scalar to be estimated. If the K calibration observations are uncorrelated, then covariance matrix $\boldsymbol{\Sigma}_{\mathbf{E}}$ is diagonal. Otherwise a linear transformation must be applied to output vector $\mathbf{y}$ to diagonalize $\boldsymbol{\Sigma}_{\mathbf{E}}$, which decorrelates the observations. If measurement error vector $\boldsymbol{\epsilon}_{\mathbf{E}}$ is normally distributed, the decorrelated observations are independent, a necessary condition for computation of confidence intervals using chi-square and t-distributions (ref. 7). Detailed proofs of the following results are given in the appendix.

4.1. Decorrelation of Covariance Matrix

A coordinate transformation is applied to observation $\mathbf{y}$ which diagonalizes measurement covariance matrix $\mathbf{\Sigma_E}$. Because matrix $\mathbf{U}$ is symmetric and positive definite, a nonsingular matrix $\mathbf{P}$ exists such that $\mathbf{U}$ can be decomposed into the matrix product as follows:

$$\mathbf{U} = \mathbf{P}\mathbf{P}^{\mathbf{T}} \tag{17}$$

Define transformed observation vector $\mathbf{v}$ as

$$\mathbf{v} = \mathbf{P}^{-1}\mathbf{y} \tag{18}$$

Equation (15) can now be transformed through a change of coordinates into the following:

$$\mathbf{v} = \mathbf{P}^{-1}\mathbf{Z}\mathbf{c} + \boldsymbol{\epsilon}_{\mathbf{v}} \tag{19}$$

where $\boldsymbol{\epsilon}_{\mathbf{v}} = \mathbf{P}^{-1}\boldsymbol{\epsilon}_{\mathbf{E}}$. The covariance matrix of $\mathbf{v}$ is given by

$$\mathbf{\Sigma}_{\mathbf{v}} = \mathbf{P}^{-1}\mathbf{\Sigma}_{\mathbf{E}}\mathbf{P}^{-\mathbf{T}} = \sigma_E^2\mathbf{I} \tag{20}$$

where $\mathbf{P}^{-\mathbf{T}} \equiv (\mathbf{P}^{-1})^{\mathbf{T}}$; thereby, the elements of $\mathbf{v}$ are confirmed as uncorrelated (ref. 9).

4.2. Least-Squares Estimation of Process Parameters

The least-squares estimate of coefficient vector $\mathbf{c}$, denoted by $\widehat{\mathbf{c}}$, is obtained by minimizing the following inner product with respect to $\mathbf{c}$:

$$\begin{aligned} S_{SQ} &= (\mathbf{v} - \mathbf{P}^{-1}\mathbf{Z}\mathbf{c})^{\mathbf{T}}(\mathbf{v} - \mathbf{P}^{-1}\mathbf{Z}\mathbf{c}) \\ &= (\mathbf{y} - \mathbf{Z}\mathbf{c})^{\mathbf{T}}\mathbf{U}^{-1}(\mathbf{y} - \mathbf{Z}\mathbf{c}) \end{aligned} \tag{21}$$

Note that S_{SQ} equals the residual sum of squares of the multivariate regression on vector $\mathbf{v}$ and that the regression is equivalent to least-squares estimation of $\mathbf{c}$ on vector $\mathbf{y}$, weighted by the inverse of measurement uncertainty covariance matrix $\mathbf{\Sigma_E}$. Define $M_{\mathbf{z}} \times M_{\mathbf{z}}$ weighted moment matrix $\mathbf{Q}$ as

$$\mathbf{Q} \equiv \mathbf{Z}^{\mathbf{T}}\mathbf{U}^{-1}\mathbf{Z} \tag{22}$$

The least-squares estimated coefficient vector $\widehat{\mathbf{c}}$ is obtained as

$$\widehat{\mathbf{c}} = \mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{U}^{-1}\mathbf{y} \tag{23}$$

The expected value of $\widehat{\mathbf{c}}$ equals $\mathbf{c}$ and its covariance matrix is given by

$$\mathbf{\Sigma}_{\widehat{\mathbf{c}}} = \sigma_E^2\mathbf{Q}^{-1} \tag{24}$$

Define $K \times 1$ predicted output vector $\widehat{\mathbf{v}} = \mathbf{P}^{-1}\mathbf{Z}\widehat{\mathbf{c}}$, and define $K \times 1$ residual vector $\widehat{\mathbf{e}}_{\mathbf{v}}$ by

$$\widehat{\mathbf{e}}_{\mathbf{v}} \equiv \mathbf{v} - \widehat{\mathbf{v}} = \mathbf{W}_{\mathbf{K}}\mathbf{e}_{\mathbf{v}} \tag{25}$$

where $K \times K$ matrix $\mathbf{W}_{\mathbf{K}}$ is defined as

$$\mathbf{W}_{\mathbf{K}} \equiv \mathbf{I}_{\mathbf{K}} - \mathbf{\Omega}_{\mathbf{K}} \tag{26}$$

$\mathbf{I}_{\mathbf{K}}$ is the $K \times K$ identity matrix, and $\mathbf{\Omega}_{\mathbf{K}}$ is defined as

$$\mathbf{\Omega}_{\mathbf{K}} \equiv (\mathbf{P}^{-1}\mathbf{Z})\mathbf{Q}^{-1}(\mathbf{P}^{-1}\mathbf{Z})^{\mathbf{T}} \tag{27}$$

Note that $\mathbf{\Omega}_{\mathbf{K}}$ is symmetric. Residual vector $\widehat{\mathbf{e}}_{\mathbf{v}}$ has zero expected value and covariance matrix

$$\mathbf{\Sigma}_{\widehat{\mathbf{e}}_v} = \sigma_E^2 \mathbf{W}_{\mathbf{K}} \tag{28}$$

The residual sum of squares S_{SE}, obtained by minimization of equation (21), is defined as

$$S_{SE} \equiv \widehat{\mathbf{e}}_{\mathbf{v}}^{\mathbf{T}}\widehat{\mathbf{e}}_{\mathbf{v}} = \boldsymbol{\epsilon}_{\mathbf{v}}^{\mathbf{T}}\mathbf{W}_{\mathbf{K}}\boldsymbol{\epsilon}_{\mathbf{v}} \tag{29}$$

The *standard error* of the regression, defined as

$$S_E \equiv \left(\frac{S_{SE}}{K - M_{\mathbf{z}}}\right)^{1/2} \tag{30}$$

has expected value $\mathcal{E}[S_E] = \sigma_E$ and is thus an unbiased estimate of σ_E.

5. Confidence and Prediction Intervals

The confidence interval for a statistical variate, such as the estimated parameter vector or the predicted process output, is a closed interval within which the variate is computed to lie at a specified probability or confidence level. See references 7 and 10 for detailed definitions.

5.1. Confidence Intervals of Estimated Parameters

If error vector $\boldsymbol{\epsilon}_{\mathrm{v}}$ is normally distributed, then S_{SE}/σ_E^2 is chi-square distributed with $K - M_{\mathbf{z}}$ degrees of freedom. It follows that a confidence ellipsoid for estimated coefficient vector $\widehat{\mathbf{c}}$ at confidence level $1 - \alpha$ is given by the following inequality:

$$(\mathbf{c} - \widehat{\mathbf{c}})^{\mathbf{T}}\mathbf{Q}(\mathbf{c} - \widehat{\mathbf{c}}) \leq M_{\mathbf{z}} S_E^2 F_{M_{\mathbf{z}}, K - M_{\mathbf{z}}}(\alpha) \tag{31}$$

where $F_{i,j}(\alpha)$ is the α level of the F-distribution with i, j degrees of freedom (ref. 7). The length and direction of the semiaxes of the ellipsoid are determined from the eigenvalues and eigenvectors, respectively, of matrix $\mathbf{Q}$.

5.2. Calibration Confidence Intervals of Predicted Process Output

The *calibration confidence interval* is the closed interval within which a predicted process output is computed to lie based on the calibration uncertainty. Let $\widehat{y}(\mathbf{z})$ denote the predicted scalar output for arbitrary input vector $\mathbf{z}$ based on estimated parameter vector $\widehat{\mathbf{c}}$; that is

$$\widehat{y}(\mathbf{z}) = \mathbf{z}^{\mathbf{T}}\widehat{\mathbf{c}} \tag{32}$$

The expected value of $\widehat{y}(\mathbf{z})$ equals $\mathbf{z}^{\mathbf{T}}\mathbf{c}$ and its variance is given by the following quadratic form:

$$\sigma^2_{\widehat{y}}(\mathbf{z}) = \sigma^2_E\ \mathbf{z}^{\mathbf{T}}\mathbf{Q}^{-1}\mathbf{z} \tag{33}$$

Equation (33) equals the variance of the calibration based on estimated parameter vector $\widehat{\mathbf{c}}$. Matrix $\mathbf{Q}$, dependent only upon the experimental design $\mathbf{Z}$ and covariance matrix $\mathbf{\Sigma_v}$, is fixed after calibration. Hence, the calibration uncertainty becomes a fixed deterministic function of applied input vector $\mathbf{z}$. If $\boldsymbol{\epsilon}_{\mathrm{v}}$ is normally distributed, a confidence interval at level α for predicted value $\widehat{y}(\mathbf{z})$ is specified by the following inequality:

$$|y - \widehat{y}| \leq (\mathbf{z}^{\mathbf{T}}\mathbf{Q}^{-1}\mathbf{z})^{1/2} S_E\, t_{K-M_{\mathbf{z}}}\left(\frac{\alpha}{2}\right) \tag{34}$$

where $t_k(\alpha)$ is the α-percentile value of the two-tailed t-distribution with k degrees of freedom (ref. 9).

5.3. Prediction Interval of New Measurement

The *prediction interval* is the closed interval within which the predicted process output is computed to lie due to both calibration uncertainty and the uncertainty of a single new measurement. After calibration, let y_0 denote a new observation of the response of the instrument to input $\mathbf{z_0}$, with uncertainty ϵ_0 and standard deviation σ_0 that is independent of calibration measurement error vector $\boldsymbol{\epsilon}_{\mathbf{v}}$. The observed value y_0 is given by

$$y_0 = \mathbf{z}_0^{\mathbf{T}}\mathbf{c} + \epsilon_0 \tag{35}$$

The predicted value of the new observed y_0 obtained from equation (32), that is, the calibration curve, is given by

$$\widehat{y}_0 = \mathbf{z}_0^{\mathbf{T}}\widehat{\mathbf{c}} \tag{36}$$

The prediction error $\delta\widehat{y}_0$, defined as the difference between the observed and the predicted observations, is given by

$$\delta\widehat{y}_0 \equiv y_0 - \widehat{y}_0 = \mathbf{z}_0^{\mathbf{T}}(\mathbf{c} - \widehat{\mathbf{c}}) + \epsilon_0 \tag{37}$$

and has zero mean and variance

$$\sigma^2_{\widehat{y}_0}(\mathbf{z}_0) = \sigma_0^2 + \sigma_E^2\mathbf{z}_0^{\mathbf{T}}\mathbf{Q}^{-1}\mathbf{z}_0 \tag{38}$$

The *prediction interval* at confidence level α is specified for $\widehat{y}_0$ as follows:

$$|y - \widehat{y}_0| \leq \left(\frac{\sigma_0^2}{\sigma_E^2} + \mathbf{z}_0^{\mathbf{T}} \mathbf{Q}^{-1} \mathbf{z}_0 \right)^{1/2} S_E \, t_{K-M_z} \left(\frac{\alpha}{2} \right) \tag{39}$$

This inequality represents the uncertainty of a single measurement after calibration. Note that prediction error $\delta\widehat{y}_0$ is composed of two components: the uncertainty of the new measurement whose variance is σ_0^2 and the calibration uncertainty whose variance, given by equation (33), is a deterministic function of applied input $\mathbf{z}_0$. The uncertainty of the new measurement is a precision error which can be reduced by replicated measurements, whereas the calibration uncertainty is a fossilized bias error (ref. 3) dependent upon x_0 that, after calibration, does not decrease with replication.

6. Computation of Inferred Input With Confidence and Prediction Intervals

During instrument application an unknown input x_0 is applied, and output y_0 is observed. The desire is to infer input x_0 from observation y_0 by inverting the calibration equation (eq. (36)) rewritten as

$$y_0 = \mathbf{z}^{\mathbf{T}}(x_0)\widehat{\mathbf{c}} \tag{40}$$

Solve equation (40) for x and denote the solution by $\widehat{x}_0$, the estimated inferred input. Whenever $\mathbf{z}(x)$ is nonlinear, solution of equation (40) may require an iterative computational technique. Calibration confidence intervals and prediction intervals of inferred input $\widehat{x}_0$ are obtained by dividing equations (34) and (39) by $y_x(\widehat{x})$ and $y_x(\widehat{x}_0)$, respectively, where

$$y_x(\widehat{x}) = \frac{\partial \mathbf{z}^{\mathbf{T}}(\widehat{x})}{\partial x} \, \widehat{\mathbf{c}} \tag{41}$$

Then the calibration confidence interval of the inferred input, obtained from equation (34), is given by

$$|x - \widehat{x}| \leq \frac{\left[\mathbf{z}^{\mathbf{T}}(\widehat{x})\mathbf{Q}^{-1}\mathbf{z}(\widehat{x})\right]^{1/2} S_E \, t_{K-M_z}(\alpha/2)}{y_x(\widehat{x})} \tag{42}$$

Similarly, the prediction interval of the inferred input, obtained from equation (39), is given by

$$|x - \widehat{x}_0| \leq \frac{\left[\sigma_0^2/\sigma^2 + \mathbf{z}_0^{\mathbf{T}}(\widehat{x}_0)\mathbf{Q}^{-1}\mathbf{z}_0(\widehat{x}_0)\right]^{1/2} S_E \, t_{K-M_z}(\alpha/2)}{y_x(\widehat{x}_0)} \tag{43}$$

7. Calibration Uncertainty Caused by Combined Input Errors and Measurement Errors

In general, overall calibration uncertainty arises from input calibration standard uncertainties as well as from output measurement uncertainty. The previously developed analyses are extended to accommodate uncertainty in applied input $\mathbf{x}$ as well as measurement uncertainty $\boldsymbol{\epsilon}_E$. Consider the combined effects during calibration of the uncertainty of the kth applied input vector $\mathbf{x}_k$,

denoted by $\boldsymbol{\epsilon}_{xk}$, and the corresponding measurement uncertainty $\boldsymbol{\epsilon}_{Ek}$. The uncertainty of the kth extended input vector $\mathbf{z}_k$, denoted by $M_\mathbf{z} \times 1$ vector $\delta\mathbf{z}_k$, is obtained as

$$\delta\mathbf{z}_k = \mathbf{z}(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}k}) - \mathbf{z}(\mathbf{x}_k) \tag{44}$$

Vector $\delta\mathbf{z}_k$ has zero expected value and $M_\mathbf{z} \times M_\mathbf{z}$ covariance matrix $\boldsymbol{\Sigma}_{\mathbf{z}_{kk}}$; the uncertainties of the elements of $\mathbf{z}_k$ may be correlated. In addition, every pair of input vectors $\mathbf{z}_i$ and $\mathbf{z}_j$ may be correlated with covariance matrix $\boldsymbol{\Sigma}_{\mathbf{z}_{ij}}$. Design matrix $\mathbf{Z}$, defined in equation (12), then has $K \times M_\mathbf{z}$ uncertainty matrix $\delta\mathbf{Z}$ constructed as follows:

$$\delta\mathbf{Z} \equiv \begin{bmatrix} \delta\mathbf{z}_1^\mathbf{T} \\ \delta\mathbf{z}_2^\mathbf{T} \\ \vdots \\ \delta\mathbf{z}_K^\mathbf{T} \end{bmatrix} \tag{45}$$

which has expected value $\mathbf{0}$, where $\mathbf{0}$ is a $K \times M_\mathbf{z}$ matrix of zeros. Each element of input uncertainty matrix $\delta\mathbf{Z}$ is assumed to be independent of measurement error vector $\boldsymbol{\epsilon}_\mathbf{E}$ defined in equation (14).

The observed output vector $\mathbf{y}$ corresponding to the actual input matrix $\mathbf{Z} + \delta\mathbf{Z}$ is given by

$$\mathbf{y} = (\mathbf{Z} + \delta\mathbf{Z})\mathbf{c} + \boldsymbol{\epsilon}_\mathbf{E} \tag{46}$$

and the combined output error vector, denoted by $\delta\mathbf{y}$, is given by

$$\delta\mathbf{y} \equiv \mathbf{y} - \mathbf{Z}\mathbf{c} = \delta\mathbf{Z}\mathbf{c} + \boldsymbol{\epsilon}_\mathbf{E} \tag{47}$$

which has expected value $\mathbf{0}$. The $K \times K$ covariance matrix of combined output error vector $\delta\mathbf{y}$, denoted by $\boldsymbol{\Sigma}_\mathbf{y}$, is computed element-by-element with the following equation (eq. (48)) for $i = 1$ to K and $j = i$ to K. Because $\delta\mathbf{Z}$ and $\boldsymbol{\epsilon}_\mathbf{E}$ are independent, the covariance between elements $\delta\mathbf{y}_i$ and $\delta\mathbf{y}_j$ of $\delta\mathbf{y}$ is obtained as

$$\begin{aligned} \text{cov}\,(\delta\mathbf{y}_i, \delta\mathbf{y}_j) &= \mathcal{E}\left[\mathbf{c}^\mathbf{T}\delta z_i \delta z_j \mathbf{c}\right] + \mathcal{E}[\boldsymbol{\epsilon}_i \boldsymbol{\epsilon}_j] \\ &= \mathbf{c}^\mathbf{T}\boldsymbol{\Sigma}_{z_{ij}}\mathbf{c} + \sigma_{ij} \end{aligned} \tag{48}$$

where σ_{ij} is the ijth element of measurement uncertainty covariance matrix $\boldsymbol{\Sigma}_\mathbf{E}$.

Rewrite equation (47) to express observed output vector $\mathbf{y}$ in the form of equation (15) as

$$\mathbf{y} = \mathbf{Z}\mathbf{c} + \delta\mathbf{y} \tag{49}$$

where $\mathbf{y}$ has expected value $\mathbf{Zc}$. Least-squares estimation of coefficient vector $\mathbf{c}$ proceeds as before, after replacing vector $\boldsymbol{\epsilon}_{\mathbf{v}}$ by $\delta\mathbf{y}$ and matrix $\boldsymbol{\Sigma}_{\mathbf{v}}$ by $\boldsymbol{\Sigma}_{\mathbf{Y}}$, respectively, in equations (16) through (39). An analysis of variance for replicated calibrations of a multi-input–single-output sensor presented in the subsequent development provides a test of significance for the presence of calibration bias error due to loading uncertainty.

8. Effects of Process Modeling Error

Models of instrument steady-state input–output relationships are typically approximate empirical relationships such as multivariate polynomials. The effects of modeling error and experimental design on calibration uncertainty are quantified, based on generalized multivariate linear regression analysis. Calibration standard uncertainty is neglected.

8.1. Uncertainty Analysis of Modeling Error

Let process $f(\mathbf{c},\mathbf{z})$ be modeled as a linear function of an extended input vector $\mathbf{z}$ according to $f(\mathbf{c},\mathbf{z}) = \mathbf{z}\,\mathbf{c}$, whereas the actual functional relationship is given by

$$y(\mathbf{z}) = f(\mathbf{c},\mathbf{z}) = \mathbf{z}\mathbf{c} + \gamma(\mathbf{z}) \tag{50}$$

where $\gamma(\mathbf{z})$ represents the modeling error. However, the system is calibrated by using experimental design matrix $\mathbf{Z}$ based on the linear model of equation (6). During calibration the kth observation is given by

$$y_k = \mathbf{z}_k\mathbf{c} + \gamma(\mathbf{z}_k) + \epsilon_{\mathbf{E}_k} \tag{51}$$

which is extended over K observations into matrix form as

$$\mathbf{y} = \mathbf{Zc} + \boldsymbol{\gamma}(\mathbf{Z}) + \boldsymbol{\epsilon}_{\mathbf{E}} \tag{52}$$

where $\boldsymbol{\gamma}(\mathbf{Z})$ is the $K \times 1$ vector of modeling errors. Coefficient vector $\widehat{\mathbf{c}}$ is estimated by means of equation (23); the expected value of $\widehat{\mathbf{c}}$, biased by the modeling error, is given by

$$\mathcal{E}(\widehat{\mathbf{c}}) = \mathbf{c} + \mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{U}^{-1}\boldsymbol{\gamma}(\mathbf{Z}) \tag{53}$$

Predicted calibration output vector $\widehat{\mathbf{y}}$ is obtained by using equation (32). Then the expected value of $\widehat{\mathbf{y}}$ is given by

$$\mathcal{E}(\widehat{\mathbf{y}}) = \mathbf{Zc} + \mathbf{ZQ}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{U}^{-1}\boldsymbol{\gamma}(\mathbf{Z}) \tag{54}$$

where the second term represents the predicted output bias error due to modeling error. Residual vector $\widehat{\mathbf{e}}_{\mathbf{v}}$, defined in equation (25), is found to be

$$\widehat{\mathbf{e}}_{\mathbf{v}} = \mathbf{W}_{\mathbf{K}}[\mathbf{P}^{-1}\boldsymbol{\gamma}(\mathbf{Z}) + \boldsymbol{\epsilon}_{\mathbf{v}}] \tag{55}$$

and from this the expected value of $\widehat{\mathbf{e}}_{\mathbf{v}}$ is

$$\mathcal{E}[\widehat{\mathbf{e}}_{\mathbf{v}}] = \mathbf{W_K P^{-1} \gamma(Z)} \tag{56}$$

The covariance matrix of $\widehat{\mathbf{e}}_{\mathbf{v}}$ is given by

$$\mathbf{\Sigma}_{\hat{\mathbf{e}}_v} = \sigma_E^2 \mathbf{W_K} \tag{57}$$

The expected value of weighted error sum of squares S_{SE} given in equation (29) equals the following:

$$\mathcal{E}[S_{SE}] = (K - M_{\mathbf{Z}})\sigma_E^2 + \boldsymbol{\gamma}^{\mathbf{T}}(\mathbf{Z})\mathbf{P}^{-\mathbf{T}}\mathbf{W_K P^{-1}}\boldsymbol{\gamma}(\mathbf{Z}) \tag{58}$$

It is seen that S_E, given in equation (30), becomes a biased estimate of σ whenever modeling error $\boldsymbol{\gamma}(\mathbf{Z})$ is nonzero.

The variance function (ref. 8) of predicted output $\widehat{y}$ is computed by using the above results as is now shown. For arbitrary vector $\mathbf{z}$, the predicted output is given by equation (32). The corresponding actual output function value y without measurement uncertainty, shown in equation (50), is given by

$$y(\mathbf{z}) = \mathbf{zc} + \gamma(\mathbf{z}) \tag{59}$$

The corresponding predicted output error $\delta\widehat{y}$ is then

$$\begin{aligned} \delta\widehat{y}(\mathbf{z}) &= y(\mathbf{z}) - \widehat{y}(\mathbf{z}) \\ &= \gamma(\mathbf{z}) - \mathbf{zQ^{-1}Z^T\,U^{-1}}[\boldsymbol{\gamma}(\mathbf{Z}) + \boldsymbol{\epsilon}_{\mathbf{E}}] \end{aligned} \tag{60}$$

To find the variance function of $\widehat{y}$, take the expected value of the square of equation (60) and after some algebraic manipulation, the following result is obtained:

$$\sigma_{\widehat{y}}^2(\mathbf{z}) = \sigma_E^2 \mathbf{z^T Q^{-1} z} + [\gamma(\mathbf{z}) - \mathbf{z\,Q^{-1}Z^TU^{-1}}\boldsymbol{\gamma}(\mathbf{Z})]^2 \tag{61}$$

The first right-hand term of equation (61), identical to the predicted output variance function of the model previously given in equation (33), represents the portion of the bias uncertainty of the predicted output due to calibration measurement uncertainty. The second right-hand term of equation (61) represents the portion of the bias uncertainty of the predicted output due to modeling error.

8.2. Design Figure of Merit

Design figure of merit J defined in equation (11) is obtained by integrating equation (61) over input subspace $\Im$. It allows examination of the effects of the experimental design on predicted output error due to precision uncertainty and bias uncertainty. As in reference 8, figure of merit J is separated into variance error term V and bias error term B:

$$J = V + B \tag{62}$$

The precision uncertainty portion of J obtained from the first right-hand term of equation (61) equals

$$V = \frac{K}{\Omega} \int_{\Im} \mathbf{z}^{\mathbf{T}} \mathbf{Q}^{-1} \mathbf{z} \; d\mathbf{x} \tag{63}$$

Similarly, the bias uncertainty portion of J obtained from the second right-hand term of equation (61) equals

$$B = \frac{K}{\sigma_E^2 \Omega} \int_{\Im} [\gamma(\mathbf{z}) - \mathbf{z}\mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\boldsymbol{\gamma}(\mathbf{Z})]^2 \; d\mathbf{x} \tag{64}$$

where Ω is the volume integral of subspace $\Im$ given by

$$\Omega = \int_{\Im} d\mathbf{x} \tag{65}$$

8.3. Effects of Experimental Design on Figure of Merit

The effects of the experimental design on calibration uncertainty due to measurement uncertainty and on calibration error due to modeling error are quantified by means of figure of merit J. Simultaneous minimization of V and B imposes conflicting requirements on selection of experimental design D. Equation (63) indicates that precision uncertainty V tends to decrease as the vector length magnification of matrix $\mathbf{Q}$ increases. The vector length magnification of $\mathbf{Q}$ tends to increase as the distance of the design points from the origin increases, generally to the boundary of volume $\Im$. On the other hand, reference 8 demonstrates that bias uncertainty B tends to be minimized by uniform placement of test points throughout space $\Im$. Hence, the accepted practice of uniformly spacing test points from zero input, to full scale input, and back to zero can reduce calibration uncertainty caused by improperly modeled phenomena such as nonlinearity and hysteresis.

A number of well-known methods exist for detection of modeling errors. Examination of residual error plots often discloses the presence of systematic errors in addition to random measurement errors (refs. 7 and 10). Residual normal probability plots (ref. 10) indicate the presence of nonnormally distributed errors which are likely to be systematic. The process of detecting modeling error may indicate the functional extension required for model improvement. On the other hand, polynomial models should be limited to the minimum order needed to avoid fitting data to random noise (ref. 10).

9. Uncertainty Analysis of Nonlinear Instrument Calibration

The previously developed generalized linear regression analysis of instrument calibration, with calibration standard uncertainty, is extended to include general multivariable-input–single-output nonlinear processes.

9.1. Combined Input and Measurement Uncertainties

Consider a process modeled by nonlinear function $y = f(\mathbf{c}, \mathbf{z})$ defined in equation (2). Output uncertainty δy can be approximated as the sum of the differential of $f(\mathbf{c}, \mathbf{z})$ with respect to $\mathbf{z}$ and measurement uncertainty ϵ_E as follows:

$$\delta y = f(\mathbf{c}, \mathbf{z} + \delta\mathbf{z}) - f(\mathbf{c}, \mathbf{z}) + \epsilon_E = \left[\frac{\partial f(\mathbf{c}, \mathbf{z})}{\partial \mathbf{z}}\right] \delta\mathbf{z} + \epsilon_E \tag{66}$$

During calibration, K observations are acquired in accordance with $K \times M_{\mathbf{z}}$ design matrix $\mathbf{Z}$ defined in equation (12). The uncertainty δy_k of the kth observation y_k is given by

$$\delta y_k = \left[\frac{\partial f(\mathbf{c}, \mathbf{z}_k)}{\partial \mathbf{z}}\right] \delta\mathbf{z}_k + \epsilon_{E_k} = \mathbf{f}_{\mathbf{z}}(\mathbf{c}, \mathbf{z}_k)\delta\mathbf{z}_k + \epsilon_{E_k} \tag{67}$$

where $1 \times K$ gradient vector $\mathbf{f}_{\mathbf{z}}(\mathbf{c}, \mathbf{z}_k) \equiv [\partial f(\mathbf{c}, \mathbf{z}_k)/\partial \mathbf{z}]$. Note that δy_k is normally distributed if both $\delta\mathbf{z}_k$ and ϵ_{E_k} are normally distributed. The actual value of the kth observation is given by

$$y_k = f(\mathbf{c}, \mathbf{z}_k) + \delta y_k \tag{68}$$

Let $\mathbf{f}(\mathbf{c}, \mathbf{Z})$ denote the $K \times 1$ vector function which is obtained by evaluating function $f(\mathbf{c}, \mathbf{z})$ for each of the K rows of $\mathbf{Z}$. Also, let $\mathbf{y}$ and $\delta\mathbf{y}$ denote the corresponding $K \times 1$ vectors of observed outputs and output uncertainties obtained by evaluating equations (67) and (68) for $k = 1$ to K, respectively. Then $\mathbf{y}$ is given by

$$\mathbf{y} = \mathbf{f}(\mathbf{c}, \mathbf{Z}) + \delta\mathbf{y} \tag{69}$$

The $K \times K$ covariance matrix of $\delta\mathbf{y}$, denoted by $\mathbf{\Sigma_Y}$, is obtained element by element with equation (67) as follows:

$$\mathbf{\Sigma}_{\mathbf{Y}_{ij}} = \mathbf{f}_{\mathbf{z}}(\mathbf{c}, \mathbf{z}_i)\mathbf{\Sigma}_{\mathbf{z}_{ij}}\mathbf{f}_{\mathbf{z}}^{\mathbf{T}}(\mathbf{c}, \mathbf{z}_j) + \sigma_{ij} \tag{70}$$

where $\mathbf{\Sigma}_{\mathbf{z}_{ij}}$ is the covariance matrix of the ith and jth input vectors $\mathbf{z}_i$ and $\mathbf{z}_j$, σ_{ij} is the covariance of the ith and jth voltage measurements, and i and j range from 1 to K. If $\mathbf{\Sigma_Y}$ is symmetric and positive definite, then it can be expressed in the form of equation (16) as

$$\mathbf{\Sigma_Y} = \sigma_Y^2 \mathbf{U} \tag{71}$$

where $K \times K$ matrix $\mathbf{U}$ is known and can be decomposed into the product $\mathbf{U} = \mathbf{P}\mathbf{P}^{\mathbf{T}}$ as shown in equation (17). Output vector $\mathbf{y}$ is transformed into vector $\mathbf{v}$ by equation (18), that is, $\mathbf{v} = \mathbf{P}^{-1}\mathbf{y}$. Equation (69) then becomes

$$\mathbf{v} = \mathbf{P}^{-1}\mathbf{f}(\mathbf{c}, \mathbf{Z}) + \delta\mathbf{v} \tag{72}$$

where $\delta\mathbf{v} = \mathbf{P}^{-1}\delta\mathbf{y}$. The expected value of $\mathbf{v}$ is

$$\mathcal{E}[\mathbf{v}] = \mathbf{P}^{-1}\mathbf{f}(\mathbf{c}, \mathbf{Z}) \tag{73}$$

The covariance matrix of $\delta\mathbf{v}$ is given by

$$\mathbf{\Sigma}_{\mathbf{v}} = \sigma_{\mathrm{Y}}^2 \mathbf{I} \tag{74}$$

Therefore the elements of $\delta\mathbf{v}$ are uncorrelated and $\delta\mathbf{v}$ is normally distributed whenever $\delta\mathbf{y}$ is normally distributed.

9.2. Least-Squares Estimation of Process Parameters

The least-squares estimate of parameter vector $\mathbf{c}$, denoted by $\widehat{\mathbf{c}}$, is obtained by minimizing the error sum of squares S_{SQ}, given by the following quadratic form, with respect to $\mathbf{c}$:

$$S_{SQ} = [\mathbf{v} - \mathbf{P}^{-1}\mathbf{f}(\mathbf{c}, \mathbf{Z})]^{\mathrm{T}}[\mathbf{v} - \mathbf{P}^{-1}\mathbf{f}(\mathbf{c}, \mathbf{Z})] = [\mathbf{y} - \mathbf{f}(\mathbf{c}, \mathbf{Z})]^{\mathrm{T}}\mathbf{U}^{-1}[\mathbf{y} - \mathbf{f}(\mathbf{c}, \mathbf{Z})] \tag{75}$$

To minimize S_{SQ}, compute the gradient of equation (75) with respect to $\mathbf{c}$ and set the resulting set of M_{c} equations equal to zero and expressed in vector form as

$$\mathbf{h} \equiv \frac{1}{2}\frac{\partial S_{SQ}}{\partial \mathbf{c}} = [\mathbf{v} - \mathbf{P}^{-1}\mathbf{f}(\mathbf{c}, \mathbf{Z})]^{\mathrm{T}}\mathbf{P}^{-1}\mathbf{F}_{\mathrm{c}} = \mathbf{0} \tag{76}$$

where $\mathbf{h}$ is a function of independent arguments $\mathbf{v}$, $\mathbf{c}$, and $\mathbf{Z}$; the dimension of $\mathbf{h}$ is $1 \times M_{\mathrm{c}}$ and of vector $[\mathbf{v} - \mathbf{P}^{-1}\mathbf{f}(\mathbf{c}, \mathbf{Z})]$ is $K \times 1$; and $K \times M_{\mathrm{c}}$ matrix $\mathbf{F}_{\mathrm{c}}$ is defined as

$$\mathbf{F}_{\mathrm{c}}(\mathbf{c}, \mathbf{Z}) \equiv \frac{\partial \mathbf{f}(\mathbf{c}, \mathbf{Z})}{\partial \mathbf{c}} \tag{77}$$

Equation (76) can be solved for $\widehat{\mathbf{c}}$ by means of a Newton-Raphson iteration or a similar method, provided that the symmetric $M_{\mathrm{c}} \times M_{\mathrm{c}}$ Jacobian matrix of S_{SQ} with respect to $\mathbf{c}$, denoted by $\mathbf{R}$, is nonsingular in some region about $\widehat{\mathbf{c}}$ and $\mathbf{Z}$; that is

$$\mathbf{R} \equiv \frac{\partial^2 S_{SQ}}{\partial \mathbf{c}^2} = \frac{\partial \mathbf{h}}{\partial \mathbf{c}} \tag{78}$$

9.3. Uncertainty of Estimated Process Parameters

The uncertainty $\delta\widehat{\mathbf{c}}$ of stochastic vector $\widehat{\mathbf{c}}$ is obtained in terms of combined output uncertainty $\delta\mathbf{v}$ from the differential of equation (76) as follows:

$$\left[\frac{\partial \mathbf{h}}{\partial \mathbf{v}}\right]^{\mathrm{T}} \delta\mathbf{v} + \mathbf{R}\delta\widehat{\mathbf{c}} = \mathbf{0} \tag{79}$$

where $K \times M_{\mathrm{c}}$ matrix $[\partial\mathbf{h}/\partial\mathbf{v}]$ equals

$$\left[\frac{\partial \mathbf{h}}{\partial \mathbf{v}}\right] = \mathbf{P}^{-\mathrm{T}}\mathbf{F}_{\mathrm{c}} \tag{80}$$

Matrix $\mathbf{R}$ is shown in the appendix to be

$$\mathbf{R} = \left[\frac{\partial \mathbf{h}}{\partial \mathbf{c}}\right] = \mathbf{F}_{\mathrm{c}}^{\mathrm{T}}\mathbf{U}^{-1}\mathbf{F}_{\mathrm{c}} + \mathbf{H}_{\mathrm{E}} \tag{81}$$

where the ijth element of $M_c \times M_c$ matrix $\mathbf{H_E}$ is given by

$$h_{E_{ij}} = [\mathbf{v} - \mathbf{P}^{-1}\mathbf{f}(\mathbf{c}, \mathbf{Z})]^{\mathbf{T}}\mathbf{P}^{-1}\mathbf{f}_{\mathbf{cc}_{ij}} \tag{82}$$

where $K \times 1$ vector $\mathbf{f}_{\mathbf{cc}_{ij}}$ is the ijth column of $M_c \times M_c \times K$ array $\mathbf{F}_{\mathbf{cc}}$ defined by

$$\mathbf{F}_{\mathbf{cc}} = \frac{\partial \mathbf{F}_{\mathbf{c}}^{\mathbf{T}}(\mathbf{c}, \mathbf{Z})}{\partial \mathbf{c}} = \frac{\partial^2 \mathbf{f}(\mathbf{c}, \mathbf{Z})}{\partial \mathbf{c}^2} \tag{83}$$

and $1 \leq i, j \leq M_c$. It is seen that the $K \times 1$ vector expression $[\mathbf{v} - \mathbf{P}^{-1}\mathbf{f}(\widehat{\mathbf{c}}, \mathbf{Z})]$ contained in equation (82) equals the vector of residuals denoted by $\widehat{\mathbf{e}}_{\mathbf{v}}$. Then if the norm of $\widehat{\mathbf{e}}_{\mathbf{v}}$ is sufficiently small, matrix $\mathbf{H_E}$ can be neglected in equation (81) to yield the following approximation:

$$\mathbf{R} \approx \mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{U}^{-1}\mathbf{F}_{\mathbf{c}} \tag{84}$$

From equations (77) to (80), the uncertainty of estimated parameter vector $\widehat{\mathbf{c}}$ equals

$$\delta\widehat{\mathbf{c}} = -\left[\frac{\partial \mathbf{h}}{\partial \mathbf{c}}\right]^{-1}\left[\frac{\partial \mathbf{h}}{\partial \mathbf{v}}\right]^{\mathbf{T}}\delta\mathbf{v} = -\mathbf{R}^{-1}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\delta\mathbf{v} \tag{85}$$

From equation (85), calibration parameter uncertainty $\delta\widehat{\mathbf{c}}$ has zero mean, it is normally distributed whenever $\delta\mathbf{y}$ is normally distributed, and its covariance matrix is given by

$$\mathbf{\Sigma}_{\hat{\mathbf{c}}} = \sigma_Y^2\,\mathbf{Q}_{\mathbf{c}}^{-1} \tag{86}$$

where

$$\mathbf{Q}_{\mathbf{c}} \equiv \left[\mathbf{R}^{-1}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{U}^{-1}\mathbf{F}_{\mathbf{c}}\mathbf{R}^{-1}\right]^{-1} \tag{87}$$

If approximation (84) holds and if the rank of $K \times M_c$ matrix $\mathbf{F}_{\mathbf{c}}$ equals M_c, then matrix $\mathbf{R}$ is nonsingular and matrix $\mathbf{Q}_{\mathbf{c}}$ is approximated by

$$\mathbf{Q}_{\mathbf{c}} \approx \mathbf{R} \tag{88}$$

9.4. Residual Sum of Squares and Standard Error of Regression

Let $\widehat{\mathbf{v}}$ denote the predicted calibration output vector corresponding to design matrix $\mathbf{Z}$ and estimated parameter vector $\widehat{\mathbf{c}}$, where

$$\widehat{\mathbf{v}} \equiv \mathbf{P}^{-1}\mathbf{f}(\widehat{\mathbf{c}}, \mathbf{Z}) \tag{89}$$

The vector of residuals $\widehat{\mathbf{e}}_{\mathbf{v}}$ is defined as follows:

$$\widehat{\mathbf{e}}_{\mathbf{v}} \equiv \mathbf{v} - \widehat{\mathbf{v}} = \mathbf{P}^{-1}[\mathbf{f}(\mathbf{c}, \mathbf{Z}) - \mathbf{f}(\widehat{\mathbf{c}}, \mathbf{Z})] + \delta\mathbf{v} \tag{90}$$

which is represented in differential form as

$$\widehat{\mathbf{e}}_{\mathbf{v}} \equiv \mathbf{P}^{-1}\mathbf{F}_{\mathbf{c}}(\widehat{\mathbf{c}}, \mathbf{Z})\delta\widehat{\mathbf{c}} + \delta\mathbf{v} = (\mathbf{I}_{\mathbf{K}} - \mathbf{\Omega}_{\mathbf{F}})\delta\mathbf{v} \tag{91}$$

where $K \times K$ matrix $\mathbf{\Omega}_{\mathbf{F}}$ is

$$\mathbf{\Omega}_{\mathbf{F}} \equiv (\mathbf{P}^{-1}\mathbf{F}_{\mathbf{c}})\mathbf{R}^{-1}(\mathbf{P}^{-1}\mathbf{F}_{\mathbf{c}})^{\mathbf{T}} \tag{92}$$

The expected value of $\widehat{\mathbf{e}}_{\mathbf{v}}$ equals zero, and the covariance matrix is given by

$$\mathbf{\Sigma}_{\widehat{\mathbf{e}}_v} = \sigma_Y^2(\mathbf{I}_{\mathbf{K}} - \mathbf{\Omega}_{\mathbf{F}}) \tag{93}$$

An unbiased estimate of σ_Y^2 is now obtained. The residual sum of squares is defined as

$$S_{SE} \equiv \widehat{\mathbf{e}}_{\mathbf{v}}^{\mathbf{T}}\widehat{\mathbf{e}}_{\mathbf{v}} = \delta\mathbf{v}^{\mathbf{T}}(\mathbf{I}_{\mathbf{K}} - \mathbf{\Omega}_{\mathbf{F}})\delta\mathbf{v} \tag{94}$$

As shown in the appendix, S_{SE}/σ_Y^2 is chi-square distributed with $K - M_{\mathbf{c}}$ degrees of freedom, and the expected value of S_{SE} is

$$\mathcal{E}(S_{SE}) = (K - M_{\mathbf{c}})\sigma_Y^2 \tag{95}$$

Therefore an unbiased estimate of σ_Y is given by standard error S_Y, which is defined as

$$S_Y \equiv \left(\frac{S_{SE}}{K - M_{\mathbf{c}}}\right)^{1/2} \tag{96}$$

A confidence interval for σ_Y at confidence level α is given by

$$\frac{(K - M_{\mathbf{c}})^{1/2}S_Y}{\chi_{(1+\alpha)/2}} \leq \sigma_Y \leq \frac{(K - M_{\mathbf{c}})^{1/2}S_Y}{\chi_{(1-\alpha)/2}} \tag{97}$$

where χ_α is the α-percentile value of the chi-square distribution with $K - M_{\mathbf{c}}$ degrees of freedom.

9.5. Confidence and Prediction Intervals of Predicted Output

The confidence ellipsoid for estimated calibration parameter vector $\widehat{\mathbf{c}}$ is defined by the following inequality:

$$(\mathbf{c} - \widehat{\mathbf{c}})^{\mathbf{T}}\mathbf{Q}_{\mathbf{C}}(\mathbf{c} - \widehat{\mathbf{c}}) \leq M_{\mathbf{c}}S_Y^2 F_{M_{\mathbf{c}},K-M_{\mathbf{c}}}(\alpha) \tag{98}$$

where $F_{M_{\mathbf{c}},K-M_{\mathbf{c}}}(\alpha)$ is the α-percentile value of the F-distribution with $M_{\mathbf{c}}, K - M_{\mathbf{c}}$ degrees of freedom.

After calibration, consider $\mathbf{z}_0$ as an arbitrary deterministic input. The corresponding predicted value $\widehat{y}_0 = f(\widehat{\mathbf{c}}, \mathbf{z}_0)$ is computed by using calibration parameter vector $\widehat{\mathbf{c}}$. The

uncertainty $\delta\widehat{y}$ of $\widehat{y}$ due to *calibration uncertainty alone* is obtained from the differential of equation (2) as

$$\begin{aligned}\delta\widehat{y}_0 &= y_0 - \widehat{y}_0 = f(\mathbf{c}, \mathbf{z}_0) - f(\widehat{\mathbf{c}}, \mathbf{z}_0) \\ &= \mathbf{f}_{\mathrm{c}}^{\mathbf{T}}(\widehat{\mathbf{c}}, \mathbf{z}_0)\delta\mathbf{c} = \mathbf{f}_{\mathrm{c}}^{\mathbf{T}}(\widehat{\mathbf{c}}, \mathbf{z}_0)\mathbf{R}^{-1}\mathbf{F}_{\mathbf{C}}^{\mathbf{T}}\mathbf{P}^{-1}\delta\mathbf{v}\end{aligned} \tag{99}$$

where $M_{\mathrm{c}} \times 1$ gradient vector $\mathbf{f}_{\mathrm{c}}(\mathbf{c}, \mathbf{z})$ is defined as

$$\mathbf{f}_{\mathrm{c}}(\mathbf{c}, \mathbf{z}) \equiv \frac{\partial f(\mathbf{c}, \mathbf{z})}{\partial \mathbf{c}} \tag{100}$$

The variance of predicted value $\widehat{y}(\mathbf{z}_0)$, termed the output *variance function* (ref. 8), is given by the following quadratic form:

$$\sigma_{\hat{y}}^2(\mathbf{z}_0) = \sigma_Y^2 \left[\mathbf{f}_{\mathrm{c}}^{\mathbf{T}}(\widehat{\mathbf{c}}, \mathbf{z}_0)\mathbf{Q}_{\mathbf{C}}^{-1}\mathbf{f}_{\mathrm{c}}(\widehat{\mathbf{c}}, \mathbf{z}_0)\right]^{1/2} \tag{101}$$

From equation (67) we can see that if uncertainty $\delta\mathbf{v}$ is normally distributed, $\delta\widehat{y}_0/\sigma_{\hat{y}}$ is normally distributed with zero mean and unit variance. Since S_Y^2/σ_Y^2 is chi-square distributed with $K - M_{\mathrm{c}}$ degrees of freedom, a confidence interval at level α is given for $\widehat{y}$ as

$$|\widehat{y}_0 - f(\widehat{\mathbf{c}}, \mathbf{z}_0)| \leq \left[\mathbf{f}_{\mathrm{c}}^{\mathbf{T}}(\widehat{\mathbf{c}}, \mathbf{z}_0)\mathbf{Q}_{\mathbf{C}}^{-1}\mathbf{f}_{\mathrm{c}}(\widehat{\mathbf{c}}, \mathbf{z}_0)\right]^{1/2} t_\alpha S_Y \tag{102}$$

where t_α is the tail of Student's t-distribution at confidence level α with $K - M_{\mathrm{c}}$ degrees of freedom. Inequality (102) defines the *calibration confidence interval.*

Let a single new measurement y_0 be made after calibration by using an instrument for which the variance of a single measurement equals σ_0^2. With the use of equation (101), the variance of the single new measurement is

$$\sigma_{y_0}^2(\mathbf{z}_0) = \sigma_Y^2\rho_{\hat{y}}^2(\mathbf{z}_0) + \sigma_0^2 = \sigma_Y^2\left[\rho_{\hat{y}}^2(\mathbf{z}_0) + \frac{\sigma_0^2}{\sigma_Y^2}\right] \tag{103}$$

where quadratic form $\rho_{\hat{y}}^2$ is defined as follows:

$$\rho_{\hat{y}}^2(\mathbf{z}_0) \equiv \mathbf{f}_{\mathrm{c}}^{\mathbf{T}}(\widehat{\mathbf{c}}, \mathbf{z}_0)\mathbf{Q}_{\mathbf{C}}^{-1}\mathbf{f}_{\mathrm{c}}(\widehat{\mathbf{c}}, \mathbf{z}_0) \tag{104}$$

The confidence interval at level α of new measurement y_0 is given by

$$|y_0 - f(\widehat{\mathbf{c}}, \mathbf{z}_0)| \leq \left[\rho_{\hat{y}}^2(\mathbf{z}_0) + \frac{\sigma_0^2}{\sigma_Y^2}\right]^{1/2} t_\alpha S_Y \tag{105}$$

which is termed the *prediction interval.*

An analysis of variance for N replicated calibrations of a nonlinear multi-input–single-output sensor is obtained in the appendix which provides a test of significance for the presence of calibration bias error due to loading uncertainty. In addition, equations are provided for

computation of matrix R, given by equation (81), in terms of the $K \times K$ covariance matrices of a single replication.

10. Multivariate Multiple-Output Analysis

The preceding analysis is now extended to a multi-input–multi-output instrument such as a six-component strain-gauge balance. Although the notation becomes cumbersome, the extended computational procedure simply iterates the previous multi-input–single-output technique for each process output element.

Consider an L-valued process $\mathbf{g}$ represented by a $1 \times L$ row vector of scalar functions of an $M_{\mathrm{c}} \times 1$ parameter vector $\mathbf{c}_{\cdot j}$ and $\mathbf{z}$, each of the form of mapping equation (1). Let $g_j(\mathbf{c}_{\cdot j}, \mathbf{z})$ denote the jth function, where j ranges from 1 to L, where g_j is dependent upon the corresponding $M_{\mathrm{c}} \times 1$ parameter vector $\mathbf{c}_{\cdot j}$ and $1 \times M_{\mathrm{z}}$ input vector $\mathbf{z}$ which is common over all values of j. Arrange the coefficient vectors L into $M_{\mathrm{c}} \times L$ coefficient matrix $\mathbf{C}$ as

$$\mathbf{C} = \left[c_{\cdot 1} \mid c_{\cdot 2} \mid \cdots \mid \mathbf{c}_{\cdot L} \right] \tag{106}$$

As usual, K observations are made during calibration in accordance with design matrix $\mathbf{Z}$. For the kth observation let $\mathbf{g}$, $\mathbf{y}_{k\cdot}$, and $\boldsymbol{\epsilon}_{\mathbf{v}k\cdot}$ denote $1 \times L$ vectors of functions g_j, observed outputs, and measurement errors, respectively, where

$$\mathbf{g}(\mathbf{C}, \mathbf{z}_k) = [g_1(\mathbf{c}_{\cdot 1}, \mathbf{z}_k) \; g_2(\mathbf{c}_{\cdot 2}, \mathbf{z}_k) \; \ldots \; g_L(\mathbf{c}_{\cdot L}, \mathbf{z}_k)] \tag{107}$$

$$\mathbf{y}_{k\cdot} = [y_{k,1} \; y_{k,2} \; \ldots \; y_{k,L}] \tag{108}$$

$$\boldsymbol{\epsilon}_{\mathbf{v}k\cdot} = [\epsilon_{vk,1} \; \epsilon_{vk,2} \; \ldots \; \epsilon_{vk,L}] \tag{109}$$

respectively, where $\boldsymbol{\epsilon}_{\mathbf{v}k\cdot}$ has zero mean and $\mathbf{z}_k^{\mathrm{T}}$ denotes the corresponding $1 \times M_{\mathrm{z}}$ input vector defined in equation (12) as the kth row of design matrix $\mathbf{Z}$. Then the functional relationship for the kth observation is obtained by extension of equation (2) to L space as follows:

$$\begin{aligned} \mathbf{y}_{k\cdot} &= \mathbf{g}(\mathbf{C}, \mathbf{z}_k + \delta\mathbf{z}_k) + \boldsymbol{\epsilon}_{\mathbf{v}k\cdot} \\ &= \mathbf{g}(\mathbf{C}, \mathbf{z}_k) + \delta\mathbf{y}_{k\cdot} \end{aligned} \tag{110}$$

where uncertainty $\delta\mathbf{y}_{k\cdot}$ is given by

$$\begin{aligned} \delta\mathbf{y}_{k\cdot} &= \mathbf{g}(\mathbf{C}, \mathbf{z}_k + \delta\mathbf{z}) - \mathbf{g}(\mathbf{C}, \mathbf{z}_k) + \boldsymbol{\epsilon}_{\mathbf{v}k\cdot} \\ &= \delta\mathbf{z}_k^{\mathrm{T}} \left[\frac{\partial \mathbf{g}(\mathbf{C}, \mathbf{z}_k)}{\partial \mathbf{z}} \right] + \boldsymbol{\epsilon}_{\mathbf{v}k\cdot} \end{aligned} \tag{111}$$

Note that matrix $[\partial \mathbf{g}(\mathbf{C}, \mathbf{z}_z)/\partial \mathbf{z}]$ has dimension $M_\mathbf{z} \times L$. Vector equation (110) is then extended to a $K \times L$ matrix equation as shown by the following equations:

$$\begin{aligned} \mathbf{Y} &= \mathbf{G}(\mathbf{C}, \mathbf{Z}+\delta\mathbf{Z}) + \mathbf{E}_\mathbf{V} \\ &= \mathbf{G}(\mathbf{C}, \mathbf{Z}) + \delta\mathbf{Y} \end{aligned} \tag{112}$$

$$\mathbf{G}(\mathbf{C}, \mathbf{Z}) = \begin{bmatrix} \mathbf{g}(\mathbf{C}, \mathbf{z}_1) \\ \mathbf{g}(\mathbf{C}, \mathbf{z}_2) \\ \vdots \\ \mathbf{g}(\mathbf{C}, \mathbf{z}_K) \end{bmatrix} \tag{113}$$

$$\mathbf{Y} = \begin{bmatrix} \mathbf{y}_{1\bullet} \\ \mathbf{y}_{2\bullet} \\ \vdots \\ \mathbf{y}_{K\bullet} \end{bmatrix} \tag{114}$$

$$\mathbf{E}_\mathbf{v} = \begin{bmatrix} \boldsymbol{\epsilon}_{\mathbf{v}1\bullet} \\ \boldsymbol{\epsilon}_{\mathbf{v}2\bullet} \\ \vdots \\ \boldsymbol{\epsilon}_{\mathbf{v}K\bullet} \end{bmatrix} = [\boldsymbol{\epsilon}_{\mathbf{v}\bullet 1}, \boldsymbol{\epsilon}_{\mathbf{v}\bullet 2}, \boldsymbol{\epsilon}_{\mathbf{v}\bullet L}] \tag{115}$$

Note that $K \times 1$ vectors $\boldsymbol{\epsilon}_{\mathbf{v}\bullet 1}$, ..., $\boldsymbol{\epsilon}_{\mathbf{v}\bullet L}$ denote columns 1, ..., L of matrix $\mathbf{E}_\mathbf{v}$. Also $K \times L$ matrix $\delta\mathbf{Y}$ is obtained by extension of equation (111) as

$$\delta\mathbf{Y} = \begin{bmatrix} \delta\mathbf{y}_{1\bullet} \\ \delta\mathbf{y}_{2\bullet} \\ \vdots \\ \delta\mathbf{y}_{K\bullet} \end{bmatrix} + \mathbf{E}_\mathbf{v} \tag{116}$$

Let $\boldsymbol{\Sigma}_{\mathbf{V}m,m}$ denote the $K \times K$ covariance matrix of error vector $\boldsymbol{\epsilon}_{\mathbf{V}\bullet m}$, and $\boldsymbol{\Sigma}_{\mathbf{Y}m,m}$ denote the $K \times K$ covariance matrix of column m of matrix $\delta\mathbf{Y}$, which is computed element by element by using equation (48) with m ranging from 1 to L and f replaced by g_m. Furthermore, define S_{SQ_m} as in equation (75) with f replaced by g_m for each of the L elements of $\mathbf{g}$. The least-squares estimated coefficient matrix, denoted by $\widehat{\mathbf{C}}$, is computed column by column by solving equation (76) to

minimize S_{SQ_m} for $m = 1, ..., L$, with $\widehat{\mathbf{c}}_{\bullet m}$ the mth column of $\widehat{\mathbf{C}}$. The covariance matrix and confidence ellipsoid for $\widehat{\mathbf{c}}_{\bullet m}$ are computed as before with equations (86) and (98), respectively.

After calibration, the predicted output matrix $\widehat{\mathbf{y}}$ for arbitrary input $\mathbf{z}$ using estimated coefficient matrix $\widehat{\mathbf{C}}$ is given by $\widehat{\mathbf{y}} = \mathbf{g}(\widehat{\mathbf{C}}, \mathbf{z})$. The uncertainty $\delta\widehat{\mathbf{y}}$ due to calibration uncertainty alone equals

$$\delta\widehat{\mathbf{y}} = \mathbf{g}(\mathbf{C}, \mathbf{z}) - \widehat{\mathbf{g}}(\mathbf{C}, \mathbf{z}) \tag{117}$$

The calibration confidence interval for $\delta\widehat{\mathbf{y}}$ is obtained element by element by equation (102). Similarly, the prediction interval of a new measurement is obtained element by element by equation (105). This analysis is illustrated by an example of a two-input–two-output linear process given in the subsequent development.

11. Uncertainties of Inferred Inputs From Inverse Process Function

An instrument is normally employed to infer the value of an input $\mathbf{x}$ based on the corresponding observed output $\mathbf{y}$ by means of the process model $f(\mathbf{c}, \mathbf{z})$ for the single output case, or $\mathbf{g}(\mathbf{C}, \mathbf{z})$ for the L-dimensional case, following calibration. Calibration confidence intervals and prediction intervals of the estimated process input are obtained.

Let $\mathbf{g}$ denote both cases in the following discussion. Input $\mathbf{z}$ can be computed if inverse function $\mathbf{g}^{-1}$ exists. A necessary and sufficient condition for the existence of $\mathbf{g}^{-1}$ is that function $\mathbf{g}$ be *bijective*, that is, a one-to-one onto mapping from $\Re^{M_z}$ to $\Re^L$. If $M_z = L$, $\mathbf{g}$ is continuous and differentiable and if for observed output vector $\mathbf{y}_0$, an input vector $\mathbf{z}_0$ exists such that $\mathbf{y}_0 = \mathbf{g}(\mathbf{C}, \mathbf{z}_0)$, then a necessary condition (ref. 11) for the existence of the inverse function $\mathbf{g}^{-1}$ is that $L \times L$ matrix $\partial\mathbf{g}/\partial\mathbf{z}$ be nonsingular in a region about $\mathbf{z}_0$. Indeed, the inverse function may be obtained by solving the following system of ordinary differential equations obtained from equation (111):

$$d\mathbf{z}^{\mathbf{T}} = d\mathbf{y} \left[\frac{\partial\mathbf{g}(\mathbf{C}, \mathbf{z})}{\partial\mathbf{z}}\right]^{-1} \tag{118}$$

Whenever a closed-form inverse function is unavailable, given observed output $\mathbf{y}_0$, the corresponding predicted input value $\widehat{\mathbf{z}}_0$ is computed iteratively from the relation $\mathbf{y}_0 = \mathbf{g}(\mathbf{C}, \widehat{\mathbf{z}}_0)$ by means of Newton-Raphson iteration or a similar method.

If input $\mathbf{z}_0$ were known, the uncertainty $\delta\widehat{\mathbf{y}}$ of the corresponding predicted output would be given by equation (117). However, since predicted input $\mathbf{z}_0$ is inferred from known output $\mathbf{y}_0$, the uncertainty $\delta\widehat{\mathbf{y}}_0$ is obtained from equation (118) as

$$\delta\widehat{\mathbf{z}}_0^{\mathbf{T}} = \delta\widehat{\mathbf{y}}_0 \left[\frac{\partial\mathbf{g}(\mathbf{C}, \widehat{\mathbf{z}}_0)}{\partial\mathbf{z}}\right]^{-1} \tag{119}$$

where $\partial\mathbf{g}/\partial\mathbf{z}$ must be nonsingular and $\delta\widehat{\mathbf{y}}_0$ is estimated by equation (117) with $\mathbf{z}_0$ replaced by $\widehat{\mathbf{z}}_0$. Confidence and prediction intervals for $\widehat{\mathbf{z}}_0$ are then obtained from those computed for $\widehat{\mathbf{y}}_0$ with equations (102) and (105) followed by transformation (eq. (119)).

12. Replicated Calibration

A statistical technique for detection and estimation of bias errors due to either modeling error or calibration standard error is now developed, which requires multiple replications of

the calibration experiment. The use of replicated calibrations over an extended time period is important for the following reasons:

1. To obtain adequate statistical sampling over time
2. To test for nonstationarity and drift
3. To test for bias uncertainty
4. To estimate bias and precision uncertainties

The variance of averaged random errors is known to decrease as $1/N$ over N replications, whereas that of bias errors, which are repeatable, does not decrease with replication. Tests for the existence of significant bias uncertainty by analysis of variance are based on this fact. The bias test, derived for a general multivariate nonlinear process in the appendix, computes the sum of squares S_{SX} of the set of K residuals averaged over N replications. The mean value of S_{SX} is an estimate of the variance due to bias uncertainty. The mean value, denoted by S_M, of the difference S_{SM} between the sum of squares S_{SE} of the global set of NK residuals and S_{SX} is an estimate of the variance due to measurement error. The variance ratio NS_X/S_M provides a test of significance for the presence of bias errors. A similar analysis allows detection of drift of any estimated parameter during replication. Details are given in the appendix.

12.1. Computation of Replicated Design Matrix

A replication matrix is defined which provides convenient computational notation for replicated calibration experimental designs. Consider a single-output sensor modeled by an (M_z-1)th degree polynomial. The sensor is typically calibrated by using K standard loadings applied in a predefined order, say zero to full scale and back in $(K-1)$ equal increments, represented by $K \times M_z$ experimental design matrix $\mathbf{Z_K}$. The calibration is replicated N times, described by $N_K \times M_z$ design matrix $\mathbf{Z_{NK}}$, where

$$\mathbf{Z_{NK}} = \begin{bmatrix} \mathbf{Z_K} \\ \mathbf{Z_K} \\ \vdots \\ \mathbf{Z_K} \end{bmatrix} = \mathbf{H^T Z_K} \tag{120}$$

and where $K \times NK$ replication matrix $\mathbf{H}$ equals

$$\mathbf{H} \equiv [\mathbf{I_K} \quad \mathbf{I_K} \quad \ldots \quad \mathbf{I_K}] \tag{121}$$

12.2. Replicated Moment Matrix for Linear Single-Output Process

Moment matrix $\mathbf{Q}$ is computed for a replicated experimental design for calibration of a linear single-output instrument with uncorrelated measurement uncertainties. Use of replication matrix $\mathbf{H}$ permits computation of $\mathbf{Q}$ in terms of the single-replication $K \times M_z$ experimental design matrix $\mathbf{Z_K}$. Assume that the calibration standard uncertainties are fixed unknown bias errors modeled as a zero-mean normally distributed random variable and that design matrix $\mathbf{Z_K}$ has $K \times K$ covariance matrix $\sigma^2\mathbf{I_K}$. Because complete design $\mathbf{Z_{NK}}$ contains N replications of design $\mathbf{Z_K}$, the N subsets of K loadings are correlated with the $NK \times NK$ covariance matrix $\mathbf{\Sigma_z}$ of design $\mathbf{Z_{NK}}$ given by

$$\mathbf{\Sigma_z} = \sigma_x^2 \mathbf{H^T H} = \sigma_x^2 \begin{bmatrix} \mathbf{I_K} & \mathbf{I_K} & \dots & \mathbf{I_K} \\ \mathbf{I_K} & \mathbf{I_K} & \dots & \mathbf{I_K} \\ \vdots & \vdots & \dots & \vdots \\ \mathbf{I_K} & \mathbf{I_K} & \dots & \mathbf{I_K} \end{bmatrix} \tag{122}$$

Assume also that sensor output measurements are uncorrelated with covariance matrix

$$\mathbf{\Sigma_E} = \sigma_E^2 \begin{bmatrix} \mathbf{I_K} & \mathbf{0_K} & \dots & \mathbf{0_K} \\ \mathbf{0_K} & \mathbf{I_K} & \dots & \mathbf{0_K} \\ \vdots & \vdots & \dots & \vdots \\ \mathbf{0_K} & \mathbf{0_K} & \dots & \mathbf{I_K} \end{bmatrix} = \sigma_E^2 \mathbf{I_{NK}} \tag{123}$$

Then combined input covariance

$$\mathbf{\Sigma_Y} = \sigma_x^2 \mathbf{U_{NK}}$$

where

$$\mathbf{U_{NK}} = \mathbf{I_{NK}} + \alpha \mathbf{H^T H} = \begin{bmatrix} (\alpha+1)\mathbf{I_K} & \mathbf{I_K} & \dots & \mathbf{I_K} \\ \mathbf{I_K} & (\alpha+1)\mathbf{I_K} & \dots & \mathbf{I_K} \\ \vdots & \vdots & \dots & \vdots \\ \mathbf{I_K} & \mathbf{I_K} & \dots & (\alpha+1)\mathbf{I_K} \end{bmatrix} \tag{124}$$

and

$$\alpha = \frac{\sigma_x^2}{\sigma_E^2} \tag{125}$$

It is readily shown that

$$\mathbf{U_{NK}^{-1}} = \mathbf{I_{NK}} - \beta \mathbf{H^T H} = \beta \begin{bmatrix} (1-\beta)/\beta \mathbf{I_K} & -\mathbf{I_K} & \dots & -\mathbf{I_K} \\ -\mathbf{I_K} & (1-\beta)/\beta \mathbf{I_K} & \dots & -\mathbf{I_K} \\ \vdots & \vdots & \dots & \vdots \\ -\mathbf{I_K} & -\mathbf{I_K} & \dots & (1-\beta)/\beta \mathbf{I_K} \end{bmatrix} \tag{126}$$

where

$$\beta = \frac{\alpha}{N\alpha + 1} \tag{127}$$

As shown in the appendix, the $M_z \times M_z$ generalized moment matrix $\mathbf{Q_{NK}} = \mathbf{Z_{NK}^T U_{NK}^{-1} Z_{NK}}$ is given by

$$\mathbf{Q_{NK}} = \frac{\sigma_E^2}{(\sigma_E^2/N) + \sigma_x^2}\, \mathbf{Z_K^T Z_K} \tag{128}$$

The portion of the calibration uncertainty due to calibration standard uncertainty, represented by σ_x^2 in the denominator of equation (128), does not decrease with replication. On the other hand, the portion of the calibration uncertainty due to measurement uncertainty, represented by σ_E^2 in the denominator of equation (128), decreases as $N^{-1/2}$ with replication. Note that equation (128) permits more efficient computation of uncertainties for an $NK \times M_z$ replicated experimental design in terms of nonreplicated $K \times M_z$ design matrix $\mathbf{Z_K}$ because computational storage requirements are reduced by a factor of N.

12.3. Replicated Moment Matrix for General Single-Output Process

The technique developed in the previous section for computation of moment matrix $\mathbf{Q}$ for a replicated experimental design is extended to a general nonlinear single-output instrument with correlated measurement uncertainties. Consider a general multi-input–single-output process calibrated by using experimental design $\mathbf{Z_K}$ replicated N times. The $K \times 1$ output uncertainty vector of a single replication, denoted by $\delta\mathbf{y_K}$, is given by expanding equation (67) for $k = 1, \ldots, K$. Then for N replications, $NK \times 1$ output uncertainty vector $\delta\mathbf{y_{NK}}$ is given by

$$\delta\mathbf{y_{NK}} = \mathbf{H^T}\delta\mathbf{f_z} + \boldsymbol{\epsilon_E} \tag{129}$$

where $K \times 1$ gradient vector $\delta\mathbf{f_z}$, defined in the appendix, has $K \times K$ covariance matrix $\boldsymbol{\Sigma}_{\mathbf{f_{ZK}}} = \sigma_x^2\mathbf{U}_{\mathbf{f_{ZK}}}$ and $NK \times 1$ measurement uncertainty vector $\boldsymbol{\epsilon_E}$ has $NK \times NK$ covariance matrix $\boldsymbol{\Sigma_E} = \sigma_E^2\mathbf{U}_{\mathbf{E_{NK}}}$, all defined in the appendix. The measurement uncertainty is assumed uncorrelated between replications and the $K \times K$ measurement covariance matrix of each replication is assumed to be $\boldsymbol{\Sigma}_{\mathbf{E_K}} = \sigma_E^2\mathbf{U}_{\mathbf{E_K}}$. From equation (129),

$$\boldsymbol{\Sigma}_{\mathbf{Y_{NK}}} = \boldsymbol{\Sigma_E} + \boldsymbol{\Sigma}_{\mathbf{f_{ZNK}}} = \sigma_E^2\mathbf{U}_{\mathbf{E_{NK}}} + \sigma_x^2\mathbf{U}_{\mathbf{f_{ZNK}}} = \sigma_E^2\mathbf{U}_{\mathbf{Y_{NK}}} \tag{130}$$

where $NK \times NK$ covariance matrix $\boldsymbol{\Sigma}_{\mathbf{f_{ZNK}}}$ is given by

$$\boldsymbol{\Sigma}_{\mathbf{f_{ZNK}}} = \sigma_x^2\mathbf{U}_{\mathbf{f_{ZNK}}} = \sigma_x^2\mathbf{H^T}\mathbf{U}_{\mathbf{f_{ZK}}}\mathbf{H} \tag{131}$$

From equation (131), $\mathbf{U}_{\mathbf{Y_{NK}}}$ can be written as

$$\mathbf{U}_{\mathbf{Y_{NK}}} = \mathbf{U}_{\mathbf{E_{NK}}} + \alpha\mathbf{U}_{\mathbf{f_{ZNK}}} \tag{132}$$

where α is defined in equation (125).

As shown in the appendix, the inverse of $NK \times NK$ matrix $\mathbf{U}_{\mathbf{Y_{NK}}}$ can be expressed in terms of $K \times K$ matrices $\mathbf{U}_{\mathbf{f_{ZK}}}$ and $\mathbf{U}_{\mathbf{E_K}}$. Define $K \times K$ matrix $\mathbf{B}$ as

$$\mathbf{B} \equiv \left[\mathbf{U}_{\mathbf{E_K}} + (N-1)\alpha \mathbf{U}_{\mathbf{f_{ZK}}}\right]^{-1} \mathbf{U}_{\mathbf{f_{ZK}}} \tag{133}$$

and $K \times K$ matrix $\mathbf{A}$ as

$$\mathbf{A} = \left(\mathbf{U}_{\mathbf{E_K}} + \alpha \mathbf{U}_{\mathbf{f_{ZK}}} \left[\mathbf{I_K} - (N-1)\mathbf{B}\right]\right)^{-1} \tag{134}$$

If the inverse matrices contained in equations (133) and (134) exist, then $M_z \times M_z$ moment matrix $\mathbf{Q_{NK}} = \mathbf{Z_{NK}^T} \mathbf{U_{Y_{NK}}^{-1}} \mathbf{Z_{NK}}$, defined in terms of $NK \times M_z$ matrix $\mathbf{Z_{NK}}$, and $NK \times NK$ matrix $\mathbf{U_{Y_{NK}}}$, can be computed in terms of $K \times M_z$ matrix $\mathbf{Z_K}$ and $K \times K$ matrices $\mathbf{I_K}$, $\mathbf{B}$, and $\mathbf{A}$ as

$$\mathbf{Q_{NK}} = N \mathbf{Z_K^T} [\mathbf{I_K} - (N-1)\mathbf{B}] \mathbf{A} \, \mathbf{Z_K} \tag{135}$$

12.4. Analysis of Variance for Estimation of Bias and Precision Uncertainties

A test of significance for bias uncertainty due to calibration standard error or modeling error and an estimate of the corresponding standard error are obtained by analysis of variance techniques, as shown in detail in the appendix. Assume as null hypothesis that the calibration bias error is zero; then matrix $\mathbf{U_{NK}}$ equals $\mathbf{I_{NK}}$ in equation (124). By using equation (27), $NK \times NK$ matrix $\mathbf{\Omega_{NK}}$ becomes

$$\mathbf{\Omega_{NK}} = \mathbf{Z_{NK}} \mathbf{Q_{NK}^{-1}} \mathbf{Z_{NK}^T} = \frac{1}{N} \mathbf{H^T} \mathbf{\Omega_K} \mathbf{H} \tag{136}$$

where the $K \times K$ matrix $\mathbf{\Omega_K}$ is defined as

$$\mathbf{\Omega_K} \equiv \mathbf{Z_K} (\mathbf{Z_K^T} \mathbf{Z_K})^{-1} \mathbf{Z_K^T} \tag{137}$$

The $NK \times 1$ residual vector $\widehat{\mathrm{e}}$ has zero expected value and $NK \times NK$ covariance matrix $\sigma^2 \mathbf{W_{NK}}$, given in equation (26) as

$$\mathbf{W_{NK}} = \mathbf{I_{NK}} - \mathbf{\Omega_{NK}} \tag{138}$$

As shown in the appendix, the residual vector $\widehat{\mathrm{e}}$ can be expressed as

$$\widehat{\mathrm{e}} = \mathbf{W_{NK}} \epsilon_{\mathbf{E}} \tag{139}$$

where $NK \times 1$ error vector $\epsilon_{\mathbf{E}}$ is normally distributed with covariance matrix $\sigma^2 \mathbf{I_{NK}}$. Let $\widehat{\epsilon}_{\mathbf{n}}$ denote the $K \times 1$ residual vector at the nth replication, which has zero expected value and covariance matrix $\sigma^2 \mathbf{W_K}$, given in equation (26) as

$$\mathbf{W_K} = \mathbf{I_K} - \mathbf{\Omega_K} \tag{140}$$

Thus, $\widehat{\mathbf{e}}$ is partitioned into N, $(K \times 1)$ subvectors

$$\widehat{\mathbf{e}}^{\mathbf{T}} = \left[\widehat{\mathbf{e}}_1^{\mathbf{T}}\ \widehat{\mathbf{e}}_2^{\mathbf{T}}\ \ldots\ \widehat{\mathbf{e}}_N^{\mathbf{T}}\right]^{\mathbf{T}} \tag{141}$$

Let $\bar{\mathbf{e}}_{\mathbf{K}}$ denote the mean value of residual vector $\widehat{\mathbf{e}}_n$ averaged over N replications; that is,

$$\bar{\mathbf{e}}_{\mathbf{K}} = \frac{1}{N}\sum_{n=1}^{N}\widehat{\mathbf{e}}_n = \frac{1}{N}\mathbf{H}\widehat{\mathbf{e}} = \frac{1}{N}\mathbf{H}\mathbf{W}_{\mathbf{NK}}\boldsymbol{\epsilon}_{\mathbf{E}} \tag{142}$$

The total residual sum of squares can be partitioned as follows:

$$S_{SE} \equiv \widehat{\mathbf{e}}^{\mathbf{T}}\widehat{\mathbf{e}} = \sum_{n=1}^{N}\widehat{\mathbf{e}}_n^{\mathbf{T}}\widehat{\mathbf{e}}_n = N\bar{\mathbf{e}}_{\mathbf{K}}^{\mathbf{T}}\bar{\mathbf{e}}_{\mathbf{K}} + \sum_{n=1}^{N}(\widehat{\mathbf{e}}_n - \bar{\mathbf{e}}_{\mathbf{K}})^{\mathbf{T}}(\widehat{\mathbf{e}}_n - \bar{\mathbf{e}}_{\mathbf{K}}) \tag{143}$$

As shown previously, S_{SE}/σ^2 is chi-square distributed with $NK - M_{\mathbf{z}}$ degrees of freedom, and the standard error of the regression given by

$$S_E = \left(\frac{S_{SE}}{NK - M_{\mathbf{z}}}\right)^{1/2} \tag{144}$$

is an unbiased estimate of σ. Define the first right-hand term of equation (143) as the sum of squares due to bias uncertainty, which can be expressed as

$$S_{SX} \equiv N\sum_{k=1}^{K}\bar{e}_k^2 = N\bar{\mathbf{e}}_{\mathbf{K}}^{\mathbf{T}}\bar{\mathbf{e}}_{\mathbf{K}} = \frac{1}{N}\boldsymbol{\epsilon}_{\mathbf{E}}^{\mathbf{T}}\mathbf{W}_{\mathbf{NK}}\mathbf{G}_{\mathbf{H}}\mathbf{W}_{\mathbf{NK}}\boldsymbol{\epsilon}_{\mathbf{E}} \tag{145}$$

where $\mathbf{G}_{\mathbf{H}} \equiv (1/N)\mathbf{H}^{\mathbf{T}}\mathbf{H}$ is defined in the appendix and $\bar{e}_k$ is the kth element of $\bar{\mathbf{e}}_{\mathbf{K}}$. It can be shown that S_{SX}/σ^2 is chi-square distributed with $K - M_{\mathbf{z}}$ degrees of freedom. Variable S_X, defined as

$$S_X \equiv \left(\frac{S_{SX}}{K - M_{\mathbf{z}}}\right)^{1/2} \tag{146}$$

is interpreted as the standard error due to bias uncertainty. Define the second right-hand term of equation (143) as the sum of squares due to measurement uncertainty as follows:

$$S_{SM} \equiv \sum_{n=1}^{N}(\widehat{\mathbf{e}}_n - \bar{\mathbf{e}}_{\mathbf{K}})^{\mathbf{T}}(\widehat{\mathbf{e}}_n - \bar{\mathbf{e}}_{\mathbf{K}}) = \boldsymbol{\epsilon}_{\mathbf{E}}^{\mathbf{T}}\mathbf{W}_{\mathbf{NK}}(\mathbf{I}_{\mathbf{NK}} - \mathbf{G}_{\mathbf{H}})\mathbf{W}_{\mathbf{NK}}\boldsymbol{\epsilon}_{\mathbf{E}} \tag{147}$$

It can be shown that S_{SM}/σ^2 is chi-square distributed with $NK - K$ degrees of freedom; the mean value

$$S_M = \left(\frac{S_{SM}}{NK - K} \right)^{1/2} \tag{148}$$

is interpreted as the standard error due to measurement uncertainty. Chi-square variates S_X^2/σ_E^2 and S_M^2/σ_E^2 can be shown to be independent. Hence, the ratio S_X^2/S_M^2 is F-distributed with $K - M_{\mathbf{z}}$, $NK - K$ degrees of freedom; the test of significance for bias error is as follows:

$$F \equiv \frac{S_X^2}{S_M^2} > F_{K-M_{\mathbf{z}},NK-K}(\alpha) \tag{149}$$

If inequality (149) is satisfied, then the null hypothesis is rejected; this indicates the existence of bias error at confidence level α. The analysis of variance is summarized in table 1.

Table 1. Analysis of Variance of Residual Sum of Squares

Source of variation	Degrees of freedom	Sum of squares	Root-mean-square
Bias uncertainty	$K - M_{\mathbf{z}}$	S_{SX}	S_X
Measurement uncertainty	$NK - K$	S_{SM}	S_M
Residual sum of squares	$NK - M_{\mathbf{z}}$	$S_{SE} = S_{SX} + S_{SM}$	S_E

12.5. Stationarity Test of Estimated Parameters

A test for stationarity of an element $\widehat{c}_m$ contained in estimated parameter vector $\widehat{\mathbf{c}}$ over N replicated calibrations is developed in the appendix. For example, significant variation of the intercept or slope during replicated calibrations may be detected.

Let $\widehat{\mathbf{c}}$ denote the parameter vector estimated globally over N sets of K-point calibrations. Let $\widehat{\mathbf{c}}_{\mathbf{R}_n}$ denote the parameter vector estimated over the K-point data set obtained during the nth replication and S_{SR_n} equal the corresponding residual sum of squares for $n = 1, \ldots, N$. Define

$$S_{SR} = \sum_{n=1}^{N} S_{SR_n} \tag{150}$$

It is shown that S_{SR}/σ_E^2 is chi-square distributed with $N(K - M_{\mathbf{z}})$ degrees of freedom.

To test for stationarity of parameter c_m, replace the mth element of $\widehat{\mathbf{c}}_{\mathbf{R_n}}$ by $\widehat{c}_m \in \widehat{\mathbf{c}}$, and compute the resulting error sum of squares, denoted by $S_{SG_{m,n}}$, for $n = 1, \ldots, N$. Compute the sum

$$S_{SG_m} = \sum_{n=1}^{N} S_{SG_{m,n}} \tag{151}$$

It is shown that $(S_{SG_m} - S_{SR})/\sigma^2$ is chi-square distributed with $N - 1$ degrees of freedom. Therefore, the ratio $[(S_{SG_m} - S_{SR})/(N-1)]/\{S_{SR}/[N(K - M_{\mathbf{z}})]\}$ is F-distributed with $N - 1$,

$N(K - M_{\mathbf{z}})$ degrees of freedom. The test of significance for nonstationarity of parameter $\widehat{c}_m$ is then as follows:

$$T_{\widehat{c}_m} = \frac{(S_{SG_m} - S_{SR})/(N-1)}{S_{SR}/[N(K - M_{\mathbf{z}})]} > F_{N-1,N(K-M_{\mathbf{z}})}(\alpha) \tag{152}$$

13. Examples

13.1. Calibration of Single-Input–Single-Output Nonlinear Sensor

Consider an inertial angle-of-attack sensor which senses the projection of the gravitational force onto the aircraft model axis. At zero roll, the angle of attack sensor is accurately modeled by the following equation:

$$\eta = f(\mathbf{c}, \alpha) = S \sin\,(\alpha - \phi) + b \tag{153}$$

where the scalar α, the angle of attack in radians, is the independent variable $\mathbf{z}$; the 3×1 parameter vector is given by $\mathbf{c} = [b\ S\ \phi]^{\mathrm{T}}$, where b = Offset in V, S = Sensitivity in V/g, ϕ = Misalignment angle in radians, and η is the sensor output in V. For this example input vector $\mathbf{z}$ equals applied angle α and δz denotes the uncertainty of α during calibration.

Calibration design matrix $\mathbf{Z}$ has dimension $K \times 1$. Equation (153) is extended to K dimensions as follows:

$$\boldsymbol{\eta} = \mathbf{f}(\mathbf{c}, \mathbf{Z}) = S\ \mathbf{sin}\ (\mathbf{z} - \phi\mathbf{1}) + b\mathbf{1} \tag{154}$$

where $\boldsymbol{\eta}$ denotes the $K \times 1$ angle of attack sensor output vector, $\mathbf{z}$ denotes the single column of design matrix $\mathbf{Z}$, $\mathbf{sin}$ denotes the $K \times 1$ vector obtained following element-by-element sine function evaluation of the elements of $(\mathbf{z} - \phi\mathbf{1})$, and $\mathbf{1}$ denotes a $K \times 1$ vector of ones.

Let δz denote the calibration angle uncertainty, and let ϵ_E denote the uncertainty of the sensor voltage measurement with variance σ_E^2. Then the observed output y is given by

$$y = f(\mathbf{c}, \alpha + \delta z) + \epsilon_E = S \sin\,(\alpha + \delta z - \phi) + b + \epsilon_E \tag{155}$$

Output uncertainty δy is obtained with equations (66) and (153)

$$\delta y = S \cos\,(z - \phi)\delta z + \epsilon_E \tag{156}$$

Equation (156) is extended to K dimensions as follows:

$$\delta\mathbf{y} = S\ \mathbf{cos}\ (\mathbf{z} - \phi\mathbf{1})\ \circ \delta\mathbf{z} + \boldsymbol{\epsilon}_{\mathbf{E}} \tag{157}$$

where $\mathbf{cos}$ denotes the $K \times 1$ vector obtained following element-by-element cosine function evaluation of the vector $\mathbf{z} - \phi\mathbf{1}$, $\circ$ denotes element-by-element multiplication of equally dimensioned matrices, and $\delta\mathbf{y}$, $\delta\mathbf{z}$, and $\epsilon_{\mathbf{E}}$ denote $K \times 1$ vectors of uncertainties δ_η, $\delta\alpha$, and ϵ_E, respectively.

The observed calibration output vector, including measurement uncertainty and calibration input uncertainty, is thus extended to K dimensions with the use of equation (153) to the following equation:

$$\mathbf{y} = \boldsymbol{\eta} + \delta\mathbf{y} = S\ \mathbf{sin}\ (\mathbf{z} - \phi\mathbf{1}) + b\,\mathbf{1} + \delta\mathbf{y} \tag{158}$$

It can be shown that the $K \times K$ covariance matrix of $\mathbf{y}$ is given by

$$\boldsymbol{\Sigma}_{\mathbf{Y}} = \text{cov}\ (\delta\mathbf{y}) = S^2[\mathbf{cos}\ (\mathbf{z} - \phi\mathbf{1})\ \mathbf{cos}\ (\mathbf{z} - \phi\mathbf{1})^{\mathbf{T}}] \circ \boldsymbol{\Sigma}_{\mathbf{Z}} + \boldsymbol{\Sigma}_{\mathbf{E}} \tag{159}$$

where $\boldsymbol{\Sigma}_{\mathbf{Z}}$ and $\boldsymbol{\Sigma}_{\mathbf{E}}$ are the covariance matrices of $\delta\mathbf{z}$ and $\boldsymbol{\epsilon}_{\mathbf{E}}$, respectively. It is seen that $\boldsymbol{\Sigma}_{\mathbf{Y}}$ and $\mathbf{U}$ given by equation (71) are symmetric and positive definite.

The least-squares estimate of parameter vector $\mathbf{c}$ is obtained by minimization of the following quadratic form given in equation (75):

$$S_{SQ} = [\mathbf{y} - b\mathbf{1} - S\ \mathbf{sin}\ (\mathbf{z} - \phi\mathbf{1})]^{\mathbf{T}}\mathbf{U}_{\mathbf{Y}}^{-1}[\mathbf{y} - b\mathbf{1} - S\ \mathbf{sin}\ (\mathbf{z} - \phi\mathbf{1})] \tag{160}$$

The $K \times 3$ Jacobian matrix of $\mathbf{f}(\mathbf{c}, \mathbf{Z})$ is found to be the following:

$$\mathbf{F}_{\mathbf{c}}(\mathbf{c}, \mathbf{z}) = [\mathbf{1} \,\vdots\, \mathbf{sin}\ (\mathbf{z} - \phi\mathbf{1}) \,\vdots\, -S\ \mathbf{cos}\,(\mathbf{z} - \phi\mathbf{1})] \tag{161}$$

The least-squares estimated coefficient vector $\widehat{\mathbf{c}}$ is obtained by solving the following 1×3 system of nonlinear equations:

$$\begin{aligned} \mathbf{h}(\mathbf{c}, \mathbf{Z}) &= [\mathbf{y} - b\mathbf{1} - S\ \mathbf{sin}\ (\mathbf{z} - \phi\mathbf{1})]^{\mathbf{T}}\mathbf{U}^{-1}[\mathbf{F}_{\mathbf{c}}(\mathbf{c}, \mathbf{Z})] \\ &= \mathbf{e}(\mathbf{c}, \mathbf{Z})^{\mathbf{T}}\mathbf{U}^{-1}[\mathbf{F}_{\mathbf{c}}(\mathbf{c}, \mathbf{Z})] = \mathbf{0} \end{aligned} \tag{162}$$

where $\mathbf{e}(\mathbf{c}, \mathbf{Z}) = [\mathbf{y} - b\mathbf{1} - S\ \mathbf{sin}\ (\mathbf{z} - \phi\mathbf{1})]$. The standard error of the regression is given by

$$S_Y = \left\{ \frac{[\mathbf{y} - \widehat{b}\mathbf{1} - \widehat{S}\ \mathbf{sin}\ (\mathbf{z} - \widehat{\phi}\mathbf{1})]^{\mathbf{T}}\mathbf{U}^{-1}[\mathbf{y} - \widehat{b}\mathbf{1} - \widehat{S}\ \mathbf{sin}\ (\mathbf{z} - \widehat{\phi}\mathbf{1})]}{K - 3} \right\}^{1/2} \tag{163}$$

which provides an unbiased estimate of σ_E.

From equation (161), equation (162) may be partitioned as follows:

$$\mathbf{h}(\mathbf{c}, \mathbf{Z}) = [\mathbf{e}^{\mathbf{T}}(\mathbf{c}, \mathbf{Z})\mathbf{U}^{-1}\mathbf{1} \,\vdots\, \mathbf{e}^{\mathbf{T}}(\mathbf{c}, \mathbf{Z})\mathbf{U}^{-1}\ \mathbf{sin}\ (\mathbf{z} - \phi\mathbf{1}) \,\vdots\, -S\mathbf{e}^{\mathbf{T}}(\mathbf{c}, \mathbf{Z})\mathbf{U}^{-1}\ \mathbf{cos}\ (\mathbf{z} - \phi\mathbf{1})] \tag{164}$$

Then matrix $\mathbf{R} = [\partial\mathbf{h}(\mathbf{c}, \mathbf{Z})/\partial\mathbf{c}]$, given in equation (81), is found to be

$$\mathbf{R} = \mathbf{F}_{\mathbf{c}}^{\mathbf{T}}(\mathbf{c}, \mathbf{Z})\mathbf{U}^{-1}\mathbf{F}_{\mathbf{c}}(\mathbf{c}, \mathbf{Z}) + \mathbf{H}_{\mathbf{E}} \tag{165}$$

where

$$\mathbf{H_E} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -\mathbf{e^T}(\mathbf{c},\mathbf{Z})\mathbf{U}^{-1}\mathbf{cos}\ (\mathbf{z}-\phi\mathbf{1}) \\ 0 & -\mathbf{e^T}(\mathbf{c},\mathbf{Z})\mathbf{U}^{-1}\mathbf{cos}\ (\mathbf{z}-\phi\mathbf{1}) & Se^{\mathbf{T}}(\mathbf{c},\mathbf{Z})\mathbf{U}^{-1}\mathbf{sin}(\mathbf{z}-\phi\mathbf{1}) \end{bmatrix} \tag{166}$$

The covariance matrix of $\widehat{\mathbf{c}}$, denoted by $\mathbf{\Sigma_c} = \sigma_Y^2\mathbf{Q_c^{-1}}$ can now be computed with equation (86). The three-dimensional confidence ellipsoid for $\widehat{\mathbf{c}}$ is given by equation (98); calibration confidence intervals and prediction intervals for predicted output voltages are given by equations (102) and (105), respectively.

Following calibration, confidence intervals and prediction intervals for inferred input angles, given observed angle of attack sensor output voltages are now obtained. For this system, a unique inverse function of $f(\mathbf{c},\alpha)$ exists for values of α in the interval $[-\pi/2,\pi/2]$, given by

$$\widehat{\alpha} = \arcsin\left(\frac{\eta-\widehat{b}}{\widehat{S}}\right) - \widehat{\phi} \tag{167}$$

Confidence and prediction intervals for α are obtained by dividing equations (102) and (105), respectively, by the gradient of $f(\mathbf{c},\alpha)$ with respect to α, where

$$\frac{\partial f(\mathbf{c},\alpha)}{\partial\alpha} = S\ \cos\ (\alpha-\phi) \tag{168}$$

The desired 95 percent calibration confidence interval for angle α is then

$$|\alpha - \widehat{\alpha}(\widehat{\mathbf{c}})| \leq \frac{t_{K-3}(0.95)S_Y\rho_{\hat{y}}(\alpha)}{\widehat{S}\ \cos\ (\alpha+\widehat{\phi})} \tag{169}$$

where $\rho_{\hat{y}}(\mathbf{z})$ is defined in equation (104). Similarly, the 95 percent prediction interval for new measurement α_0 is obtained as

$$|\alpha_0 - \widehat{\alpha}_0(\widehat{\mathbf{c}})| \leq \frac{t_{K-3}(0.95)S_Y\left[\rho_y^2(\alpha_0)+\sigma_0^2/\sigma_Y^2\right]^{1/2}}{\widehat{S}\ \cos\ (\alpha_0+\widehat{\phi})} \tag{170}$$

where $\widehat{\alpha}_0(\widehat{\mathbf{c}})$ denotes the predicted value of new measurement α_0 inferred from measured output y_0 by means of equation (167).

13.2. Two-Input–Two-Output Linear Instrument

Consider a two-input–two-output linear process—for example, a two-component strain-gauge balance—with 1×2 input vector $\mathbf{x} = [x_1\ x_2]$, 3×1 extended input vector $\mathbf{z}^{\mathrm{T}} = [1\ x_1\ x_2]$, 2×1 output vector $\mathbf{y} = [y_1\ y_2]$, and measurement error vector $\boldsymbol{\epsilon}_{\mathbf{E}} = [\epsilon_1\ \epsilon_2]$. Coefficient matrix $\mathbf{C}$ is given by

$$\mathbf{C} = [\mathbf{c}_{\bullet 1} \mid \mathbf{c}_{\bullet 2}] = \begin{bmatrix} c_{01} & c_{02} \\ c_{11} & c_{12} \\ c_{21} & c_{22} \end{bmatrix} \tag{171}$$

where $\mathbf{c}_{\bullet \mathbf{n}} = [c_{0n}\ c_{1n}\ c_{2n}]^{\mathrm{T}}$ for $n = 1, 2$.

For a single observation, the output is given by $\mathbf{y} = \mathbf{z}^{\mathbf{T}}\mathbf{C} + \boldsymbol{\epsilon}_{\mathbf{E}}$. During calibration, K calibration input vectors are applied, represented by the following $K \times 3$ design matrix $\mathbf{Z}$:

$$\mathbf{Z} = \begin{bmatrix} 1 & x_{11} & x_{12} \\ 1 & x_{21} & x_{22} \\ \vdots & \vdots & \vdots \\ 1 & x_{K1} & x_{K2} \end{bmatrix} \tag{172}$$

Measurement uncertainty is represented by $K \times 2$ measurement error matrix $\mathbf{E}_{\mathbf{E}}$, where

$$\mathbf{E}_{\mathbf{E}} = [\boldsymbol{\epsilon}_{\mathbf{E}\bullet 1} \boldsymbol{\epsilon}_{\mathbf{E}\bullet 2}] = \begin{bmatrix} \epsilon_{11} & \epsilon_{12} \\ \epsilon_{21} & \epsilon_{22} \\ \vdots & \vdots \\ \epsilon_{K1} & \epsilon_{K2} \end{bmatrix} \tag{173}$$

The $K \times K$ covariance matrix for error vectors $\boldsymbol{\epsilon}_{\mathbf{E}\bullet m}$ and $\boldsymbol{\epsilon}_{\mathbf{E}\bullet n}$, for m and $n = 1$ and 2, respectively, is denoted by $\boldsymbol{\Sigma}_{\mathbf{E}_{mn}}$.

For K calibration measurements, the $K \times N$ output matrix $\mathbf{Y}$ is given by

$$\mathbf{Y} = (\mathbf{Z} + \delta\mathbf{Z})\mathbf{C} + \mathbf{E}_{\mathbf{E}} \tag{174}$$

where $K \times M_{\mathbf{z}}$ input error matrix $\delta\mathbf{Z}$ is given by

$$\delta\mathbf{Z} = [\mathbf{0}\ \delta\mathbf{x}_{\bullet 1} \delta\mathbf{x}_{\bullet 2}] = \begin{bmatrix} 0 & \delta x_{11} & \delta x_{12} \\ 0 & \delta x_{21} & \delta x_{22} \\ \vdots & \vdots & \vdots \\ 0 & \delta x_{K1} & \delta x_{K2} \end{bmatrix} \tag{175}$$

The 2×2 covariance matrix of input error vectors $\delta\mathbf{x}_{\bullet \mathbf{i}}$ and $\delta\mathbf{x}_{\bullet \mathbf{j}}$ is denoted by $\boldsymbol{\Sigma}_{\mathbf{x}_{\mathrm{ij}}}$.

$$\boldsymbol{\Sigma}_{\mathbf{x}_{ij}} = \begin{bmatrix} \sigma_{X_{ij,11}} & \sigma_{X_{ij,12}} \\ \sigma_{X_{ij,12}} & \sigma_{X_{ij,22}} \end{bmatrix} \tag{176}$$

Let input vector $\mathbf{x}$ be random with zero-mean uncertainty $\boldsymbol{\epsilon}_{\mathbf{x}} = [\boldsymbol{\epsilon}_{\mathbf{x}_1}\ \boldsymbol{\epsilon}_{\mathbf{x}_2}]$. Then extended input vector $\mathbf{z}$T has uncertainty $\boldsymbol{\epsilon}_{\mathbf{z}}^{\mathbf{T}} = [0\ \epsilon_{x_1}\ \epsilon_{x_2}]$; $K \times 3$ design matrix $\mathbf{Z}$ has uncertainty matrix $\mathbf{E}_{\mathbf{Z}}$, whose rows $\boldsymbol{\epsilon}_{\mathbf{Z}_i}$ and $\boldsymbol{\epsilon}_{\mathbf{Z}_j}$ have 3×3 covariance matrix $\boldsymbol{\Sigma}_{\mathbf{Z}_{ij}}$, where

$$\boldsymbol{\Sigma}_{\mathbf{Z}_{ij}} = \mathcal{E}\left[\boldsymbol{\epsilon}_{\mathbf{Z}_i}\ \boldsymbol{\epsilon}_{\mathbf{Z}_j}^{\mathbf{T}}\right] \begin{bmatrix} 0 & 0 & 0 \\ 0 & \sigma_{X_{ij,11}} & \sigma_{X_{ij,12}} \\ 0 & \sigma_{X_{ij,12}} & \sigma_{X_{ij,22}} \end{bmatrix} \tag{177}$$

Consider process outputs y_1 and y_2 separately; subscripts are omitted in the following computations. The total error vector $\boldsymbol{\epsilon}_{\mathbf{Y}}$, expressed as $\boldsymbol{\epsilon}_{\mathbf{Y}} = \mathbf{E}_{\mathbf{Z}}\mathbf{c} + \boldsymbol{\epsilon}_{\mathbf{E}}$, expands into

$$\boldsymbol{\epsilon}_{\mathbf{Y}} = \begin{bmatrix} \epsilon_{x_{11}}c_1 + \epsilon_{x_{12}}c_2 + \epsilon_1 \\ \epsilon_{x_{21}}c_1 + \epsilon_{x_{22}}c_2 + \epsilon_2 \\ \vdots \\ \epsilon_{x_{K1}}c_1 + \epsilon_{x_{K2}}c_2 + \epsilon_K \end{bmatrix} \tag{178}$$

The covariance between elements ϵ_{y_i} and ϵ_{y_j} of total error vector $\epsilon_{\mathbf{y}}$ is given by

$$\text{cov}\ (\epsilon_{y_i}, \epsilon_{y_j}) = \mathbf{c}^{\mathbf{T}}\boldsymbol{\Sigma}_{\mathbf{Z_{ij}}}\mathbf{c} + \sigma_{ij} = c_1^2\sigma_{X_{ij,11}} + c_1c_2\sigma_{X_{ij,12}} + c_2^2\sigma_{X_{ij,22}} + \sigma_{ij} \tag{179}$$

The confidence interval at level $1 - \alpha$ for estimated coefficient vector $\widehat{\mathbf{c}}$ is expressed as a three-dimensional ellipsoid as

$$(\mathbf{c} - \widehat{\mathbf{c}})^{\mathbf{T}}\mathbf{Q}(\mathbf{c} - \widehat{\mathbf{c}}) \leq 3S^2F_{3,K-3}(\alpha) \tag{180}$$

The ellipsoid can be characterized as follows: Since $\mathbf{Q}$ is symmetric, it is unitarily similar to a real diagonal matrix Λ; in particular $\mathbf{Q} = \mathbf{P}^{\mathbf{T}}\Lambda\mathbf{P}$, where Λ consists of the eigenvalues of $\mathbf{Q}$ and $\mathbf{P}$ is unitary; that is, $\mathbf{P}\mathbf{P}^{\mathbf{T}} = \mathbf{I}$. Matrix $\mathbf{P}$ consists of the set of orthonormal eigenvectors of $\mathbf{Q}$. Apply the transformation $\boldsymbol{\gamma} = \mathbf{P}\mathbf{c}$ to coefficient vector $\mathbf{c}$. The confidence ellipsoid then simplifies to the form

$$\boldsymbol{\gamma}^{\mathbf{T}}\Lambda\boldsymbol{\gamma} = \lambda_1(\gamma_1 - \widehat{\gamma}_1)^2 + \lambda_2(\gamma_2 - \widehat{\gamma}_2)^2 + \lambda_3(\gamma_3 - \widehat{\gamma}_3)^2 \leq 3S^2F_{3,K-3}(\alpha) \tag{181}$$

Let λ denote the ith eigenvalue of $\mathbf{Q}$. It is readily seen that the ith vertex of the ellipsoid is located at distance

$$d_i = \sqrt{\frac{3S^2F_{3,K-3}(\alpha)}{\lambda_i}} \tag{182}$$

from point $\widehat{\mathbf{c}}$ in the direction of the corresponding eigenvector, that is, the ith column of $\mathbf{P}$.

The uncertainty of the regression function, which is dependent upon extended input vector $\mathbf{z}$, is expressed by the calibration confidence interval at level of inequality (34):

$$\begin{aligned} |y - \widehat{y}| &\leq (\mathbf{z}^{\mathbf{T}}\mathbf{Q}^{-1}\mathbf{z})^{1/2} St_{K-3}(\alpha) \\ &\leq (\rho_{11} + 2\rho_{12}x_1 + 2\rho_{13}x_2 + \rho_{22}x_1^2 + 2\rho_{23}x_1x_2 + \rho_{33}x_2^2)^{1/2} St_{K-3}(\alpha) \end{aligned} \tag{183}$$

where ρ_{ij} is the ijth element of $\mathbf{Q}^{-1}$.

After calibration, apply input $\mathbf{z}_0$ and make a single new measurement, where the measurement uncertainty is ϵ_0. The prediction interval for output $\widehat{y}_0$ is obtained as follows with equation (39):

$$\begin{aligned} |y - \widehat{y}_0| &\leq \left(\frac{\sigma_0^2}{\sigma^2} + \mathbf{z}_0^{\mathbf{T}}\mathbf{Q}^{-1}\mathbf{z}_0 \right)^{1/2} St_{K-3}(\alpha) \\ &= \left(\frac{\sigma_0^2}{\sigma^2} + \rho_{11} + 2\rho_{12}x_1 + 2\rho_{13}x_2 + \rho_{22}x_1^2 + 2\rho_{23}x_1x_2 + \rho_{33}x_2^2 \right)^{1/2} St_{K-3}(\alpha) \end{aligned} \tag{184}$$

Confidence and prediction intervals for inferred inputs are obtained as follows: let 1×2 vector $\delta\mathbf{y} = [\delta y_1 \ \delta y_2]$ denote the simultaneous two-dimensional calibration confidence interval or prediction interval defined in equations (183) and (184) that corresponds to observed output vector $\mathbf{y}_0$. Let $\delta\mathbf{x}$ denote the uncertainty (calibration confidence interval or prediction interval) of inferred input vector $\mathbf{x}_0$ corresponding to observed output $\mathbf{y}_0$. Then $\delta\mathbf{x}$ is given by

$$\delta\mathbf{x}_0 = \delta\mathbf{y}_0 \widehat{\mathbf{C}}_{12}^{-1} \tag{185}$$

where

$$\widehat{\mathbf{C}}_{12} = \begin{bmatrix} \widehat{c}_{11} & \widehat{c}_{12} \\ \widehat{c}_{21} & \widehat{c}_{22} \end{bmatrix} \tag{186}$$

14. Concluding Remarks

A generalized statistical treatment of uncertainty analysis for instrument calibration and application has been developed. Techniques for propagation of measurement uncertainties through experimental data reduction equations and for presentation of final engineering test data results, which are well-established in the literature, have not been presented. Instead, the emphasis has been on rigorous development of the correct statistical treatment of correlated measurement uncertainties, correlated calibration standard uncertainties, nonlinear mathematical instrument models, and replicated calibrations, for which only heuristic approaches had been available. Correlated bias errors may produce significant magnification of the uncertainties of the calibration standard.

The effects of mathematical modeling error upon bias uncertainties have been quantified. A design figure of merit has been established to assess the effects of experimental design on both precision and bias uncertainties during calibration. Generally, predicted output variance due to precision errors is minimized by calibrating only at zero and full-scale loads, whereas predicted output variance due to modeling error is minimized by uniformly spacing test points throughout the operating envelope of the instrument.

Calibration confidence intervals and prediction intervals of a new measurement, for both the predicted output and the inferred input, are obtained as functions of the applied load. Previously, instrument uncertainties were typically specified as constant error bands or as a fixed percentage of the full-scale input.

Replicated calibration is necessary to obtain adequate statistical sampling, to test for nonstationarity, and to test for significant bias uncertainty. Analyses of variance of the regression residual sum of squares have been applied to obtain individual estimated values of the standard error due to bias uncertainty and the standard error due to precision uncertainty.

Additional associated uncertainty analyses are in progress which apply the results of this document to the force sensor modeled by a linear function, the strain-gauge balance modeled by a second-degree multivariate polynomial, and the inertial model attitude sensor in pitch and roll modeled by a nonlinear coordinate transformation. The techniques have also been applied to calibration of a skin friction balance modeled by a quadratic polynomial.

Appendix

Mathematical Derivations

A1. Preliminaries

A1.1. Extended Least-Squares Analysis. Let the instrument calibration data input-output relationship be expressed in matrix form as follows:

$$\mathbf{y} = \mathbf{Z}\mathbf{c} + \boldsymbol{\epsilon}_{\mathbf{E}} \tag{187}$$

where $\mathbf{Z}$ is the $K \times M_z$ calibration design matrix, $\mathbf{c}$ is the $M_z \times 1$ parameter vector, $\mathbf{y}$ is the $K \times 1$ output observation vector, and $\boldsymbol{\epsilon}_{\mathbf{E}}$ is the $K \times 1$ random measurement error vector with zero mean and $K \times K$ covariance matrix $\boldsymbol{\Sigma}_{\mathbf{E}}$. It is assumed that $\boldsymbol{\Sigma}_{\mathbf{E}}$ can be expressed as

$$\boldsymbol{\Sigma}_{\mathbf{E}} = \sigma_E^2 \mathbf{U} \tag{188}$$

where $K \times K$ matrix $\mathbf{U}$ is symmetric and positive definite and measurement variance σ_E^2 is to be determined. Then $\mathbf{U}$ can be decomposed into the matrix product

$$\mathbf{U} = \mathbf{P}\mathbf{P}^{\mathbf{T}} \tag{189}$$

where $K \times K$ matrix $\mathbf{P}$ is a nonsingular lower triangular matrix (ref. 12). For notational convenience let $\mathbf{P}^{-\mathbf{T}} \equiv [\mathbf{P}^{-1}]^{\mathbf{T}}$.

A1.2. Lemmas and Theorems.

The following simple propositions, used frequently in the development, are proven for later use. A matrix is said to be diagonalizable if it is similar to a diagonal matrix.

Lemma 1. $\mathbf{U}^{-1} = \mathbf{P}^{-\mathbf{T}}\mathbf{P}^{-1}$

Proof:

$$\begin{aligned} \mathbf{U}(\mathbf{P}^{-\mathbf{T}}\mathbf{P}^{-1}) &= \mathbf{P}\mathbf{P}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\mathbf{P}^{-1} \\ &= \mathbf{P}(\mathbf{P}^{-1}\mathbf{P})^{\mathbf{T}}\mathbf{P}^{-1} = \mathbf{P}\mathbf{P}^{-1} = \mathbf{I}_{\mathbf{K}} \end{aligned} \tag{190}$$

where $\mathbf{I}_{\mathbf{K}}$ is the $K \times K$ identity matrix.

QED

Lemma 2. Matrix $\mathbf{A}$ is idempotent if and only if it is diagonalizable and its eigenvalues are either 0 or 1.

Proof of Sufficiency: By hypothesis $\mathbf{A}^2 = \mathbf{A}$. It is well-known from linear algebra (ref. 12) that the eigenvalues of $\mathbf{A}$ must satisfy the scalar equation $\lambda^2 = \lambda$, from which it follows that $\lambda = 0$ or $\lambda = 1$. In reference 11, $\mathbf{A}$ is shown to be diagonalizable.

QED Sufficiency

Proof of Necessity: By hypothesis the eigenvalues of $\mathbf{A}$ are either 0 or 1. Since $\mathbf{A}$ is diagonalizable a nonsingular matrix Γ exists such that $\mathbf{A} = \Gamma\ \mathbf{I_A}\Gamma^{-1}$ and $\mathbf{I_A}$ is a diagonal matrix of zeros and ones. It is clear that $\mathbf{I_A}\mathbf{I_A} = \mathbf{I_A}$. Therefore, $\mathbf{AA} = \mathbf{A}$.

QED Necessity

Lemma 3. If matrices $\mathbf{A}$ and $\mathbf{B}$ have dimension $N \times M$ and $M \times N$, respectively, then $\mathrm{tr}\,(\mathbf{AB}) = \mathrm{tr}\,(\mathbf{BA})$.

Proof:

$$\begin{aligned}\mathrm{tr}\,(\mathbf{AB}) &= \sum_{n=1}^{N} (\mathbf{AB})_{m} = \sum_{n=1}^{N}\sum_{m=1}^{M} a_{nm}b_{mn} \\ &= \sum_{m=1}^{M}\sum_{n=1}^{N} b_{mn}a_{nm} = \sum_{m=1}^{M} (\mathbf{BA})_{mm} = \mathrm{tr}\,(\mathbf{BA})\end{aligned} \tag{191}$$

QED

Lemma 4. If square matrix $\mathbf{A}$ is diagonalizable, then $\mathrm{tr}\,(\mathbf{A}) = \mathrm{tr}\,(\Lambda)$, where Λ is the diagonal matrix of eigenvalues of $\mathbf{A}$.

Proof: By hypothesis there exists nonsingular matrix Γ such that $\mathbf{A}= \Gamma\Lambda\Gamma^{-1}$ (ref. 12). By using Lemma 3,

$$\mathrm{tr}\,(\mathbf{A}) = \mathrm{tr}\,(\Gamma\Lambda\Gamma^{-1}) = \mathrm{tr}\,(\Gamma^{-1}\Gamma\Lambda) = \mathrm{tr}\,(\Lambda) \tag{192}$$

QED

Lemma 5. For $N \times N$ matrices $\mathbf{A}$ and $\mathbf{B}$, $\mathrm{tr}\,(\mathbf{A} + \mathbf{B}) = \mathrm{tr}\,(\mathbf{A}) + \mathrm{tr}\,(\mathbf{B})$.

Proof:

$$\begin{aligned}\mathrm{tr}\,(\mathbf{A} + \mathbf{B}) &= \sum_{n=1}^{N}(a_{nn} + b_{nn}) = \sum_{n=1}^{N} a_{nn} + \sum_{n=1}^{N} b_{nn} \\ &= \mathrm{tr}\,(\mathbf{A}) + \mathrm{tr}\,(\mathbf{B})\end{aligned} \tag{193}$$

QED

Lemma 6. If matrix $\mathbf{A}$ is idempotent, then $\mathrm{rank}\,(\mathbf{A}) = \mathrm{tr}\,(\mathbf{A})$.

Proof: By Lemma 2, $\mathbf{A}$ is diagonalizable and its eigenvalues are either 0 or 1. Then, by Lemma 4, $\mathrm{tr}(\mathbf{A}) = \mathrm{tr}(\Lambda)$, where Λ is the diagonal matrix of eigenvalues. Hence, $\mathrm{rank}(\mathbf{A}) = \mathrm{tr}(\mathbf{A})$.

QED

Lemma 7. If $K \times K$ matrix $\mathbf{A}$ is idempotent, then $\mathbf{I_K} - \mathbf{A}$ is idempotent with rank $K - r_A$, where $r_A = \mathrm{rank}(\mathbf{A})$.

Proof:

$$(\mathbf{I_K} - \mathbf{A})(\mathbf{I_K} - \mathbf{A}) = \mathbf{I_K} - 2\mathbf{A} + \mathbf{AA} = \mathbf{I_K} - \mathbf{A}$$

By Lemmas 5 and 6, rank $(\mathbf{I_K} - \mathbf{A}) = K - r_A$.

QED

Theorem 1. Let $S_{SW} = \boldsymbol{\epsilon}^{\mathbf{T}}\mathbf{W}\boldsymbol{\epsilon}$ where $1 \times N$ vector $\boldsymbol{\epsilon}$ is normally distributed with covariance matrix $\boldsymbol{\Sigma}_E = \boldsymbol{\sigma}_E^2\mathbf{I_N}$ and $\mathbf{W}$ is an $N \times N$ symmetric matrix with rank r. Then S_{SW}/σ_E^2 is chi-square distributed with r degrees of freedom and expected value r if and only if $\mathbf{W}$ is idempotent.

Proof of Necessity: Since $\mathbf{W}$ is idempotent, by Lemma 2 its eigenvalues are either 0 or 1. Hence, there exists an $N \times N$ matrix Γ such that

$$\mathbf{W} = \Gamma^{\mathrm{T}}\mathbf{I_W}\Gamma \tag{194}$$

where $\Gamma^{\mathbf{T}}\Gamma = \mathbf{I_N}$, and $\mathbf{I_W}$ is diagonal with r ones and $N - r$ zeros. Note that $\mathbf{I_W} = \mathbf{I_W}\mathbf{I_W}$. Let $\boldsymbol{\zeta}_{\mathbf{W}} = \mathbf{I_W}\Gamma\boldsymbol{\epsilon}$. Then

$$\boldsymbol{\zeta}_{\mathbf{W}}^{\mathbf{T}}\boldsymbol{\zeta}_{\mathbf{W}} = \boldsymbol{\epsilon}^{\mathbf{T}}\Gamma^{\mathbf{T}}\mathbf{I_W}\Gamma\boldsymbol{\epsilon} = \boldsymbol{\epsilon}^{\mathbf{T}}\mathbf{W}\boldsymbol{\epsilon} = S_{SW} \tag{195}$$

Moreover,

$$\begin{aligned}\boldsymbol{\Sigma}_{\zeta_{\mathbf{W}}} &= \mathcal{E}\left[\boldsymbol{\zeta}_{\mathbf{W}}\boldsymbol{\zeta}_{\mathbf{W}}^{\mathbf{T}}\right] = \mathbf{I_W}\Gamma\boldsymbol{\Sigma}_{\mathbf{E}}\Gamma^{\mathbf{T}}\mathbf{I_W} \\ &= \sigma_E^2\mathbf{I_W}\Gamma\Gamma^{\mathbf{T}}\mathbf{I_W} = \sigma_E^2\mathbf{I_W}\end{aligned} \tag{196}$$

Therefore, $\boldsymbol{\zeta}_{\mathbf{W}}/\sigma_E$ is normally distributed with covariance matrix $\mathbf{I_W}$. Thus, S_{SW}/σ_E^2 equals the sum of squares of r independent unit variance normal variates, and therefore S_{SW}/σ_E^2 is chi-square distributed with r degrees of freedom (ref. 7). The expected value of S_{SW} is obtained by using Lemma 3 and equations (195) and (196) to yield

$$\begin{aligned}\mathcal{E}[S_{SW}] &= \mathcal{E}\left[\mathrm{tr}\left(\boldsymbol{\zeta}_{\mathbf{W}}^{\mathbf{T}}\boldsymbol{\zeta}_{\mathbf{W}}\right)\right] = \mathcal{E}\left[\mathrm{tr}\left(\boldsymbol{\zeta}_{\mathbf{W}}\boldsymbol{\zeta}_{\mathbf{W}}^{\mathbf{T}}\right)\right] \\ &= \mathrm{tr}\left(\boldsymbol{\Sigma}_{\zeta_{\mathbf{W}}}\right) = \sigma^2\,\mathrm{tr}\left(\mathbf{I_W}\right) = \sigma^2 r\end{aligned} \tag{197}$$

QED Necessity

Proof of Sufficiency: By hypothesis S_{SW}/σ_E^2 is chi-square distributed with r degrees of freedom and, hence, equals the sum of squares of r independent zero-mean, unit-variance normal variates. Symmetric matrix $\mathbf{W}$ can be written as

$$\mathbf{W} = \Gamma^{\mathbf{T}} \Lambda_{\mathbf{W}} \Gamma \tag{198}$$

where $N \times N$ diagonal matrix $\Lambda_{\mathbf{W}}$ contains r nonzero elements since $\mathbf{W}$ has rank r. Define $\boldsymbol{\zeta}_{\mathbf{W}} \equiv \Lambda_{\mathbf{W}}^{1/2} \Gamma \boldsymbol{\epsilon}$, where the elements of diagonal matrix $\Lambda_{\mathbf{W}}^{1/2}$ equal the square roots of the corresponding elements of $\Lambda_{\mathbf{W}}$. Note that $\boldsymbol{\zeta}_{\mathbf{W}}$ contains r nonzero elements. Then

$$\boldsymbol{\zeta}_{\mathbf{W}}^{\mathbf{T}} \boldsymbol{\zeta}_{\mathbf{W}} = \boldsymbol{\epsilon}^{\mathbf{T}} \Gamma^{\mathbf{T}} \Lambda_{\mathrm{W}} \Gamma \boldsymbol{\epsilon} = \boldsymbol{\epsilon}^{\mathbf{T}} \mathbf{W} \boldsymbol{\epsilon} = S_{SW} \tag{199}$$

But

$$\boldsymbol{\Sigma}_{\zeta_{\mathbf{W}}} = \mathcal{E}[\boldsymbol{\zeta}_{\mathbf{W}} \boldsymbol{\zeta}_{\mathbf{W}}^{\mathbf{T}}] = \Lambda_{\mathbf{W}}^{1/2} \Gamma \boldsymbol{\Sigma}_{\mathbf{E}} \Gamma^{\mathbf{T}} \Lambda_{\mathbf{W}}^{1/2} = \sigma_E^2 \Lambda_{\mathbf{W}}^{1/2} \Gamma \Gamma^{\mathbf{T}} \Lambda_{\mathbf{W}}^{1/2} = \sigma_E^2 \Lambda_{\mathbf{W}} \tag{200}$$

If any nonzero element of $\Lambda_{\mathbf{W}}$ does not equal 1, the hypothesis that S_{SW}/σ_E^2 equals the sum of squares of r independent unit-variance normal variates is contradicted. Hence, diagonal matrix $\Lambda_{\mathbf{W}}$ contains only ones and zeros, and by Lemma 2, $\mathbf{W}$ is idempotent.

QED Sufficiency

Theorem 2 (ref. 10). Let $\boldsymbol{\epsilon}^{\mathbf{T}} \boldsymbol{\epsilon} = \boldsymbol{\Sigma}\, q_m$, for $1 \leq m \leq M$, where $1 \times N$ random vector $\boldsymbol{\epsilon}$ is normally distributed with covariance matrix $\mathbf{I_N}$, $q_m = \boldsymbol{\epsilon}^{\mathbf{T}} \mathbf{Q}_m \boldsymbol{\epsilon}$, and nonnegative indefinite $N \times N$ matrix $\mathbf{Q}_m$ is symmetric with rank r_m. Then the variables q_m are independent chi-square distributed random variables if and only if $\sum r_m = N$, for $1 \leq m \leq M$.

Proof of Necessity: By Theorem 1, $\boldsymbol{\epsilon}^{\mathbf{T}} \boldsymbol{\epsilon}$ is chi-square distributed. Also, by hypothesis

$$\boldsymbol{\epsilon}^{\mathbf{T}} \boldsymbol{\epsilon} = \sum_{m=1}^{M} \boldsymbol{\epsilon}^{\mathbf{T}} \mathbf{Q}_m \boldsymbol{\epsilon} = \sum_{m=1}^{M} q_m \tag{201}$$

where $\mathbf{Q}_m$ has rank r_m and

$$\sum_{m=1}^{M} r_m = N \tag{202}$$

Since $\mathbf{Q}_m$ is symmetric and nonnegative indefinite with rank r_m, it can be expressed in the form

$$\mathbf{Q}_m = \mathbf{P}_m^{\mathbf{T}} \Lambda_m \mathbf{P}_m \tag{203}$$

where $\mathbf{P}_m$ is orthonormal and Λ_m is diagonal, containing r_m positive elements and $(N - r_m)$ zero elements on the diagonal. After rearranging its elements, matrix $\mathbf{Q}_m$ can be written in partitioned form as

$$\mathbf{Q}_m = \left[\mathbf{P}_{\mathbf{r}_m}^{\mathbf{T}} \;\vdots\; \mathbf{P}_{\mathbf{s}_m}^{\mathbf{T}}\right] \left[\begin{array}{c|c} \Lambda_{\mathbf{r}_m} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array}\right] \left[\begin{array}{c} \mathbf{P}_{\mathbf{r}_m} \\ \hline \mathbf{P}_{\mathbf{s}_m} \end{array}\right] = \mathbf{P}_{\mathbf{r}_m}^{\mathbf{T}} \Lambda_{\mathbf{r}_m} \mathbf{P}_{\mathbf{r}_m} \tag{204}$$

where $N \times N$ matrix $\mathbf{P}_m^{\mathbf{T}} = [\mathbf{P}_{\mathbf{r}_m}^{\mathbf{T}} \;\vdots\; \mathbf{P}_{\mathbf{s}_m}^{\mathbf{T}}]$, $\mathbf{P}_{\mathbf{r}_m}$ has dimension $r_m \times N$, $\mathbf{P}_{\mathbf{s}_m}$ has dimension $(N - r_m) \times N$, and $\Lambda_{\mathbf{r}_m}$ has dimension $r_m \times r_m$. Define $r_m \times N$ matrix $\mathbf{R}_{\mathbf{r}_m}$ as

$$\mathbf{R}_{\mathbf{r}_m} \equiv \Lambda_{\mathbf{r}_m}^{1/2} \mathbf{P}_{\mathbf{r}_m} \tag{205}$$

It is seen that $\mathbf{R}_{\mathbf{r}_m}$ has rank r_m and that $\mathbf{R}_{\mathbf{r}_m}^{\mathbf{T}} \mathbf{P}_{\mathbf{r}_m} = \mathbf{Q}_m$. Also define $r_m \times 1$ vector $\boldsymbol{\xi}_m$ as

$$\boldsymbol{\xi}_m \equiv \mathbf{R}_{\mathbf{r}_m} \mathbf{x} \tag{206}$$

where $\mathbf{x}$ is an arbitrary $N \times 1$ normally distributed random vector with covariance matrix $\mathbf{I_N}$. Then, inner product $q_m = \boldsymbol{\xi}_m^{\mathbf{T}} \boldsymbol{\xi}_m = \mathbf{x}^{\mathbf{T}} \mathbf{Q}_m \mathbf{x}$ forms $N \times N$ matrix $\mathbf{R}_r$ from the set of M matrices $\mathbf{R}_{r_m}$ as

$$\mathbf{R}_r = \begin{bmatrix} \mathbf{R}_{r_1} \\ \vdots \\ \mathbf{R}_{r_M} \end{bmatrix} \tag{207}$$

It follows from equation (202) that $\mathbf{R}_r$ has rank N and is therefore nonsingular. Construct $N \times 1$ vector $\boldsymbol{\xi}$ from subvectors $\boldsymbol{\xi}_1, ..., \boldsymbol{\xi}_M$ defined in equation (206) as

$$\boldsymbol{\xi} = \begin{bmatrix} \boldsymbol{\xi}_1 \\ \vdots \\ \boldsymbol{\xi}_M \end{bmatrix} = \mathbf{R}_r \mathbf{x} \tag{208}$$

It follows that

$$\mathbf{x}^{\mathbf{T}} \mathbf{x} = \sum_{m=1}^{M} \mathbf{x}^{\mathbf{T}} \mathbf{Q}_m \mathbf{x} = \sum_{m=1}^{M} \boldsymbol{\xi}_m^{\mathbf{T}} \boldsymbol{\xi}_m = \boldsymbol{\xi}^{\mathbf{T}} \boldsymbol{\xi} = \mathbf{x}^{\mathbf{T}} \mathbf{R}_r^{\mathbf{T}} \mathbf{R}_r \mathbf{x} \tag{209}$$

Since equation (209) holds for arbitrary vector $\mathbf{x}$, it follows that $\mathbf{R}_r^{\mathbf{T}} \mathbf{R}_r = \mathbf{I_N} = \mathbf{R}_r \mathbf{R}_r^{\mathbf{T}}$ and, hence, $\mathbf{R}_r$ is orthonormal. The covariance matrix of $\boldsymbol{\xi}$ is found to be

$$\boldsymbol{\Sigma}_{\xi} = \mathcal{E}\left[\boldsymbol{\xi}\boldsymbol{\xi}^{\mathbf{T}}\right] = \mathbf{R}_r \, \mathcal{E}\left[\mathbf{x}\mathbf{x}^{\mathbf{T}}\right] \mathbf{R}_r^{\mathbf{T}} = \mathbf{R}_r \mathbf{R}_r^{\mathbf{T}} = \mathbf{I_N} \tag{210}$$

Therefore, the covariance matrix of $\boldsymbol{\xi}_m$ equals $\mathbf{I_m}$. It then follows from Theorem 1 that random variable $q_m = \boldsymbol{\xi}_m^{\mathbf{T}} \boldsymbol{\xi}_m$ is chi-square distributed with r_m degrees of freedom. Moreover, since $\mathbf{R}_r$ is orthonormal, the set of random variables q_m is mutually independent.

QED Necessity

Proof of Sufficiency: Construct matrix $\mathbf{R}_r$ and vector $\boldsymbol{\xi}$ as before. By hypothesis, the elements $\boldsymbol{\xi}_m$ are mutually independent with chi-square distributed inner products; thus, covariance matrix $\boldsymbol{\Sigma}_\xi$ contains $r = \boldsymbol{\Sigma} r_m$ ones on the diagonal and zeros elsewhere. Since $\mathbf{x}^\mathbf{T}\mathbf{x}$ is chi-square distributed with N degrees of freedom, it follows from equation (209) that $\boldsymbol{\xi}^\mathbf{T}\boldsymbol{\xi}$ is likewise distributed. Hence, rank $\boldsymbol{\Sigma}_\xi$ equals N and $N = r$.

QED Sufficiency

A1.3. Linear Least-Squares Estimation.

From equation (187), note that the expected value of $\mathbf{y}$ is given by

$$\mathcal{E}[\mathbf{y}] = \mathbf{Zc} \tag{211}$$

Define $K \times 1$ transformed observation vector $\mathbf{v}$ as

$$\mathbf{v} \equiv \mathbf{P}^{-1}\mathbf{y} \tag{212}$$

Equation (187) now becomes

$$\mathbf{v} = \mathbf{P}^{-1}\mathbf{Zc} + \mathbf{P}^{-1}\boldsymbol{\epsilon}_\mathbf{E} = \mathbf{P}^{-1}\mathbf{Zc} + \boldsymbol{\epsilon}_\mathbf{v} \tag{213}$$

where $K \times 1$ vector $\boldsymbol{\epsilon}_\mathbf{v} \equiv \mathbf{P}^{-1}\boldsymbol{\epsilon}_\mathbf{E}$. Immediately the expected value of $\mathbf{v}$ is

$$\boldsymbol{\mu}_\mathbf{v} \equiv \mathcal{E}[\mathbf{v}] = \mathbf{P}^{-1}\mathbf{Zc} \tag{214}$$

Then the $K \times K$ covariance matrix of $\mathbf{v}$ (which equals the covariance matrix of $\boldsymbol{\epsilon}_\mathbf{v}$ as well), denoted by $\boldsymbol{\Sigma}_\mathbf{v}$, is obtained with the help of equations (188) and (189) as

$$\begin{aligned}\boldsymbol{\Sigma}_\mathbf{v} &\equiv \mathcal{E}[(\mathbf{v} - \boldsymbol{\mu}_\mathbf{v})(\mathbf{v} - \boldsymbol{\mu}_\mathbf{v})^\mathbf{T}] = \mathbf{P}^{-1}\mathcal{E}[\boldsymbol{\epsilon}_\mathbf{E}\boldsymbol{\epsilon}_\mathbf{E}^\mathbf{T}]\mathbf{P}^{-\mathbf{T}} \\ &= \mathbf{P}^{-1}\boldsymbol{\Sigma}_\mathbf{E}\mathbf{P}^{-\mathbf{T}} = \sigma_E^2\mathbf{P}^{-1}\mathbf{P}\mathbf{P}^\mathbf{T}\mathbf{P}^{-\mathbf{T}} = \sigma_E^2\mathbf{I}_\mathbf{K}\end{aligned} \tag{215}$$

Thus the elements of $\mathbf{v}$ and of $\boldsymbol{\epsilon}_\mathbf{v}$ are uncorrelated.

Based on transformed output observation vector $\mathbf{v}$, the desire is to estimate the value of parameter vector $\mathbf{c}$, denoted by $\widehat{\mathbf{c}}$, which minimizes the sum of squares S_{SQ} given by the following inner product:

$$S_{SQ} = (\mathbf{v} - \boldsymbol{\mu}_\mathbf{v})^\mathbf{T}(\mathbf{v} - \boldsymbol{\mu}_\mathbf{V}) = (\mathbf{v} - \mathbf{P}^{-1}\mathbf{Zc})^\mathbf{T}(\mathbf{v} - \mathbf{P}^{-1}\mathbf{Zc}) \tag{216}$$

Note that equation (216) may be rewritten as

$$S_{SQ} = (\mathbf{y} - \mathbf{Zc})^\mathbf{T}\mathbf{P}^{-\mathbf{T}}\mathbf{P}^{-1}(\mathbf{y} - \mathbf{Zc}) = (\mathbf{y} - \mathbf{Zc})^\mathbf{T}\mathbf{U}^{-1}(\mathbf{y} - \mathbf{Zc}) \tag{217}$$

It is well-known (ref. 7) that the least-squares value $\widehat{\mathbf{c}}$ which minimizes equation (216) is obtained as follows:

$$\begin{aligned}\widehat{\mathbf{c}} &= [(\mathbf{P}^{-1}\mathbf{Z})^{\mathbf{T}}(\mathbf{P}^{-1}\mathbf{Z})]^{-1}(\mathbf{P}^{-1}\mathbf{Z})^{\mathbf{T}}\mathbf{v} = (\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\mathbf{P}^{-1}\mathbf{Z})^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\mathbf{v} \\ &= (\mathbf{Z}^{\mathbf{T}}\mathbf{U}^{-1}\mathbf{Z})^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\mathbf{v} = \mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\mathbf{v}\end{aligned} \tag{218}$$

where $M_{\mathbf{z}} \times M_{\mathbf{z}}$ generalized moment matrix $\mathbf{Q}$ of the experimental design is defined as

$$\mathbf{Q} \equiv \mathbf{Z}^{\mathbf{T}}\mathbf{U}^{-1}\mathbf{Z} \tag{219}$$

It is to be noted that $\mathbf{Q}^{\mathbf{T}} = \mathbf{Q}$. With the help of equations (213), (214), and (218) the expected value of $\widehat{\mathbf{c}}$ is found to be an unbiased estimate of $\mathbf{c}$ as follows:

$$\begin{aligned}\mathcal{E}[\widehat{\mathbf{c}}] &= \mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\ \mathcal{E}[\mathbf{v}] = \mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{U}^{-1}\mathbf{Z}\mathbf{c} \\ &= \mathbf{Q}^{-1}\mathbf{Q}\mathbf{c} = \mathbf{c}\end{aligned} \tag{220}$$

The covariance matrix of $\widehat{\mathbf{c}}$ is found by first combining equations (213) and (218) to obtain

$$\begin{aligned}\widehat{\mathbf{c}} - \mathbf{c} &= \mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}(\mathbf{P}^{-1}\mathbf{Z}\mathbf{c} + \boldsymbol{\epsilon}_{\mathbf{v}}) - \mathbf{c} = \mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{U}^{-1}\mathbf{Z}\mathbf{c} + \mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\boldsymbol{\epsilon}_{\mathbf{v}} - \mathbf{c} \\ &= \mathbf{Q}^{-1}\mathbf{Q}\mathbf{c} + \mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\boldsymbol{\epsilon}_{\mathbf{v}} - \mathbf{c} = \mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\boldsymbol{\epsilon}_{\mathbf{v}}\end{aligned} \tag{221}$$

It is seen that $\widehat{\mathbf{c}} - \mathbf{c}$ is normally distributed since $\boldsymbol{\epsilon}_{\mathbf{v}}$ is normally distributed. From equations (219) and (221) it follows that $M_{\mathbf{z}} \times M_{\mathbf{z}}$ covariance matrix $\boldsymbol{\Sigma}_{\widehat{\mathbf{c}}}$ is given by

$$\begin{aligned}\boldsymbol{\Sigma}_{\widehat{\mathbf{c}}} &= \mathcal{E}\left[(\widehat{\mathbf{c}} - \mathbf{c})(\widehat{\mathbf{c}} - \mathbf{c})^{\mathbf{T}}\right] = \mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\ \mathcal{E}[\boldsymbol{\epsilon}_{\mathbf{v}}\boldsymbol{\epsilon}_{\mathbf{v}}^{\mathbf{T}}] = \mathbf{P}^{-1}\mathbf{Z}\mathbf{Q}^{-1} \\ &= \sigma_E^2\mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{U}^{-1}\mathbf{Z}\mathbf{Q}^{-1} = \sigma_E^2\mathbf{Q}^{-1}\mathbf{Q}\mathbf{Q}^{-1} = \sigma_E^2\mathbf{Q}^{-1}\end{aligned} \tag{222}$$

Define $K \times 1$ predicted output vector $\widehat{\mathbf{v}}$ by

$$\widehat{\mathbf{v}} \equiv \mathbf{P}^{-1}\mathbf{Z}\widehat{\mathbf{c}} \tag{223}$$

and define $K \times 1$ residual vector $\widehat{\mathbf{e}}_{\mathbf{v}} \equiv \mathbf{v} - \widehat{\mathbf{v}}$. Using equations (213), (218), and (223) yields

$$\begin{aligned}\widehat{\mathbf{e}}_{\mathbf{v}} &= \mathbf{v} - \widehat{\mathbf{v}} = \mathbf{v} - \mathbf{P}^{-1}\mathbf{Z}\mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\mathbf{v} \\ &= \left(\mathbf{I}_{\mathbf{K}} - \mathbf{P}^{-1}\mathbf{Z}\mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\right)(\mathbf{P}^{-1}\mathbf{Z}\mathbf{c} + \boldsymbol{\epsilon}_{\mathbf{v}}) \\ &= \left(\mathbf{I}_{\mathbf{K}} - \mathbf{P}^{-1}\mathbf{Z}\mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\right)\boldsymbol{\epsilon}_{\mathbf{v}} = \mathbf{W}_{\mathbf{K}}\boldsymbol{\epsilon}_{\mathbf{v}}\end{aligned} \tag{224}$$

where $K \times K$ matrix $\mathbf{W}_{\mathbf{K}}$ is defined as

$$\mathbf{W}_{\mathbf{K}} \equiv \mathbf{I}_{\mathbf{K}} - \boldsymbol{\Omega}_{\mathbf{K}} \tag{225}$$

and $K \times K$ matrix $\boldsymbol{\Omega}_{\mathbf{K}}$ is defined as

$$\mathbf{\Omega_K} \equiv (\mathbf{P}^{-1}\mathbf{Z})\mathbf{Q}^{-1}(\mathbf{P}^{-1}\mathbf{Z})^{\mathbf{T}} \tag{226}$$

An integer subscript will be appended as needed to distinguish the dimension of matrices $\mathbf{U}$, $\mathbf{W}$, $\mathbf{\Omega}$, $\mathbf{Z}$, $\mathbf{Q}$, and $\mathbf{I}$ for nonreplicated and replicated experimental designs.

It is seen that $\mathbf{\Omega_K}$ is both symmetric and idempotent as follows:

$$\begin{aligned}\mathbf{\Omega_K}\mathbf{\Omega_K} &= \left[\mathbf{P}^{-1}\mathbf{Z}\mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\right]\left[\mathbf{P}^{-1}\mathbf{Z}\mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\right] \\ &= \mathbf{P}^{-1}\mathbf{Z}\mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{U}^{-1}\mathbf{Z}\mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}} \\ &= \mathbf{P}^{-1}\mathbf{Z}\mathbf{Q}^{-1}\mathbf{Q}\mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}} = \mathbf{P}^{-1}\mathbf{Z}\mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}} = \mathbf{\Omega_K}\end{aligned} \tag{227}$$

Also, using Lemmas 3, 4, and 6,

$$\begin{aligned}\text{rank}\,(\mathbf{\Omega_K}) &= \text{tr}\,(\mathbf{P}^{-1}\mathbf{Z}\mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}) = \text{tr}\,\left(\mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\mathbf{P}^{-1}\mathbf{Z}\right) \\ &= \text{tr}\,(\mathbf{Q}^{-1}\mathbf{Q}) = M_Z\end{aligned} \tag{228}$$

Then by Lemma 7, $\mathbf{W_K}$ is idempotent with rank $K - M_{\mathbf{z}}$.

It is seen that $\widehat{\mathbf{e}}_{\mathbf{v}}$ is normally distributed. From equation (224), the expected value of $\widehat{\mathbf{e}}_{\mathbf{v}}$ is zero. The covariance matrix of $\widehat{\mathbf{e}}_{\mathbf{v}}$ then is found by using equations (215) and (224) as follows:

$$\begin{aligned}\mathbf{\Sigma}_{\widehat{\epsilon_{\mathbf{v}}}} &= \mathcal{E}\left[\widehat{\mathbf{e}}_{\mathbf{v}}\widehat{\mathbf{e}}_{\mathbf{v}}^{\mathbf{T}}\right] = \mathbf{W_K}\ \mathcal{E}\left[\epsilon_{\mathbf{v}}\epsilon_{\mathbf{v}}^{\mathbf{T}}\right]\mathbf{W_K^T} \\ &= \sigma_E^2\mathbf{W_K}\mathbf{W_K^T} = \sigma_E^2\mathbf{W_K}\end{aligned} \tag{229}$$

The $M_{\mathbf{z}} \times K$ covariance matrix of $\widehat{\mathbf{c}}$ and $\widehat{\mathbf{e}}_{\mathbf{v}}$ is shown to be zero (ref. 7), and with the help of equation (215),

$$\begin{aligned}\text{cov}\ (\widehat{\mathbf{c}}, \widehat{\mathbf{e}}_{\mathbf{v}}) &= \mathcal{E}\left[(\widehat{\mathbf{c}} - \mathbf{c})\widehat{\mathbf{e}}_{\mathbf{v}}^{\mathbf{T}}\right] = \mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\ \mathcal{E}\left[\epsilon_{\mathbf{v}}\epsilon_{\mathbf{v}}^{\mathbf{T}}\right]\left(\mathbf{I_K} - \mathbf{P}^{-1}\mathbf{Z}\mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\right) \\ &= \sigma_E^2\left(\mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}} - \mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\right) = \mathbf{0}\end{aligned} \tag{230}$$

Thus $\widehat{\mathbf{c}}$ and $\widehat{\mathbf{e}}_{\mathbf{v}}$ are uncorrelated and independent.

The residual sum of squares S_{SE}, defined as the sum of squares of the elements of residual vector $\widehat{\mathbf{e}}_{\mathbf{v}}$, is obtained with the help of equation (224) as

$$S_{SE} \equiv \widehat{\mathbf{e}}_{\mathbf{v}}^{\mathbf{T}}\widehat{\mathbf{e}}_{\mathbf{v}} = \epsilon_{\mathbf{v}}^{\mathbf{T}}\mathbf{W_K^T}\mathbf{W_K}\epsilon_{\mathbf{v}} = \epsilon_{\mathbf{v}}^{\mathbf{T}}\mathbf{W_K}\epsilon_{\mathbf{v}} \tag{231}$$

$$\mathcal{E}[S_{SE}] = \sigma_E^2(K - M_{\mathbf{z}}) \tag{232}$$

From equation (228) and Theorem 1, S_{SE}/σ_E^2 is chi-square distributed with $K - M_{\mathbf{z}}$ degrees of freedom and expected value $K - M_{\mathbf{z}}$.

Therefore S_E, denoted the *standard error*, is defined as

$$S_E \equiv \left(\frac{S_{SE}}{K - M_{\mathbf{z}}} \right)^{1/2} \tag{233}$$

Note that S_E is an unbiased estimate of σ_E.

A confidence ellipsoid for $\widehat{\mathbf{c}}$ is now obtained. Evaluate the quadratic form

$$S_{SC} = (\mathbf{c} - \widehat{\mathbf{c}})^{\mathbf{T}} \mathbf{Q} (\mathbf{c} - \widehat{\mathbf{c}})$$

with equation (221) to yield

$$S_{SC} = (\mathbf{c} - \widehat{\mathbf{c}})^{\mathbf{T}} \mathbf{Q} (\mathbf{c} - \widehat{\mathbf{c}}) = \boldsymbol{\epsilon}_{\mathbf{v}}^{\mathbf{T}} \mathbf{P}^{-1} \mathbf{Z} \mathbf{Q}^{-1} \mathbf{Z}^{\mathbf{T}} \mathbf{P}^{-\mathbf{T}} \boldsymbol{\epsilon}_{\mathbf{v}} = \boldsymbol{\epsilon}_{\mathbf{v}}^{\mathbf{T}} \boldsymbol{\Omega}_{\mathbf{K}} \boldsymbol{\epsilon}_{\mathbf{v}} \tag{234}$$

Recall that $K \times K$ matrix $\boldsymbol{\Omega}_{\mathbf{K}}$ was shown by equation (228) to be idempotent with rank $M_{\mathbf{z}}$. Then by Theorem 1, it follows that S_{SC}/σ_E^2 is chi-square distributed with $M_{\mathbf{z}}$ degrees of freedom and expected value $M_{\mathbf{z}}$. Since $\widehat{\mathbf{c}} - \mathbf{c}$ and $\widehat{\mathbf{e}}_{\mathbf{v}}$ are independent, S_{SC} and S_{SQ} are independent. Hence, the ratio $F = [S_{SC}/(\sigma_E^2 M_{\mathbf{z}})]/\{S_{SE}/[\sigma_E^2 (K - M_{\mathbf{z}})]\}$ is F-distributed with $M_{\mathbf{z}}, K - M_{\mathbf{z}}$ degrees of freedom (ref. 6). Therefore, a confidence interval for $\widehat{\mathbf{c}}$ at level α is given by the following inequality:

$$(\mathbf{c} - \widehat{\mathbf{c}})^{\mathbf{T}} \mathbf{Q} (\mathbf{c} - \widehat{\mathbf{c}}) \leq M_{\mathbf{z}} S_E^2 F_{M_{\mathbf{z}}, K - M_{\mathbf{z}}}(\alpha) \tag{235}$$

where $F_{i,j}(\alpha)$ is the $1 - \alpha$ tail of the F-distribution with i, j degrees of freedom and S_E is defined in equation (233). The quadratic form of equation (235) defines an ellipsoid in $M_{\mathbf{z}}$ dimensional hyperspace termed the *confidence ellipsoid*.

Given $M_{\mathbf{z}} \times 1$ input vector $\mathbf{z}$, the corresponding predicted scalar output $\widehat{y}$ is given by

$$\widehat{y}(\mathbf{z}) = \mathbf{z}^{\mathbf{T}} \widehat{\mathbf{c}} \tag{236}$$

From equation (220), the expected value of $\widehat{y}(\mathbf{z})$ equals $\mathbf{z}^{\mathbf{T}} \mathbf{c}$. With equations (222) and (236), the variance of $\widehat{y}(\mathbf{z})$ is obtained as follows:

$$\begin{aligned} \sigma_{\widehat{y}}^2(\mathbf{z}) &\equiv \mathcal{E}(\{\widehat{y}(\mathbf{z}) - \mathcal{E}[\widehat{y}(\mathbf{z})]\}^2) = \mathcal{E}\{[\mathbf{z}^{\mathbf{T}}(\mathbf{c} - \widehat{\mathbf{c}})]^2\} \\ &= \mathcal{E}[\mathbf{z}^{\mathbf{T}}(\mathbf{c} - \widehat{\mathbf{c}})(\mathbf{c} - \widehat{\mathbf{c}})^{\mathbf{T}} \mathbf{z}] = \mathbf{z}^{\mathbf{T}} \mathcal{E}[(\mathbf{c} - \widehat{\mathbf{c}})(\mathbf{c} - \widehat{\mathbf{c}})^{\mathbf{T}}] \mathbf{z} \\ &= \mathbf{z}^{\mathbf{T}} \boldsymbol{\Sigma}_{\widehat{\mathbf{c}}} \mathbf{z} = \sigma_E^2 \mathbf{z}^{\mathbf{T}} \mathbf{Q}^{-1} \mathbf{z} \end{aligned} \tag{237}$$

Then the normally distributed variate $\delta\widehat{y}(\mathbf{z}) / \left[\sigma_E (\mathbf{z}^{\mathbf{T}} \mathbf{Q}^{-1} \mathbf{z})^{1/2}\right]$ has zero mean and unit variance, where $\delta\widehat{y} = y - \widehat{y}$. Recall that S_{SE}^2/σ_E^2 is chi-square distributed with $K - M_{\mathbf{z}}$ degrees of freedom. Then the ratio t defined as follows has Student's t-distribution with $K - M_{\mathbf{z}}$ degrees of freedom (ref. 7):

$$t = \frac{\delta\widehat{y}(\mathbf{z}) / \left[\sigma_E (\mathbf{z}^{\mathbf{T}} \mathbf{Q}^{-1} \mathbf{z})^{1/2}\right]}{S_{SE} / \left[\sigma_E (K - M_{\mathbf{z}})^{1/2}\right]} \tag{238}$$

Combine equations (233), (237), and (238) to obtain the calibration output confidence interval defined by the following inequality:

$$|y - \widehat{y}| \leq (\mathbf{z}^{\mathbf{T}}\mathbf{Q}^{-1}\mathbf{z})^{1/2} S_E \, t_{K-M_{\mathbf{z}}}(\alpha/2) \tag{239}$$

where $t_n(\alpha)$ is the α-percentile of the two-tailed t-distribution with n degrees of freedom.

A2. Effects of Process Modeling Error

Consider a process $f(\mathbf{c}, \mathbf{z})$ modeled as a linear function of extended input vector $\mathbf{z}$

$$f(\mathbf{c}, \mathbf{z}) = \mathbf{z}\mathbf{c} \tag{240}$$

whereas the actual functional relationship is

$$f(\mathbf{c}, \mathbf{z}) = \mathbf{z}\mathbf{c} + \gamma(\mathbf{z}) \tag{241}$$

where $\gamma(\mathbf{z})$ is the modeling error. Let the system be calibrated with calibration design $\mathbf{Z}$ in accordance with equation (187) based on the linear model in equation (240). The observed calibration output is then

$$\mathbf{y} = \mathbf{Z}\mathbf{c} + \boldsymbol{\gamma}(\mathbf{Z}) + \boldsymbol{\epsilon}_{\mathbf{E}} \tag{242}$$

where $\boldsymbol{\gamma}(\mathbf{Z})$ denotes the $K \times 1$ vector of modeling errors

$$\boldsymbol{\gamma}(\mathbf{z}) = \begin{bmatrix} \gamma(\mathbf{z}_1) \\ \vdots \\ \gamma(\mathbf{z}_K) \end{bmatrix} \tag{243}$$

Estimated coefficient vector $\widehat{\mathbf{c}}$ is obtained from equations (218) and (242) as follows:

$$\begin{aligned} \widehat{\mathbf{c}} &= \mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{U}^{-1}\mathbf{y} = \mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{U}^{-1}\left[\mathbf{Z}\mathbf{c} + \boldsymbol{\gamma}(\mathbf{Z}) + \boldsymbol{\epsilon}_{\mathbf{E}}\right] \\ &= \mathbf{c} + \mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{U}^{-1}[\boldsymbol{\gamma}(\mathbf{Z}) + \boldsymbol{\epsilon}_{\mathbf{E}}] \end{aligned} \tag{244}$$

The expected value of $\widehat{\mathbf{c}}$ is seen to be

$$\mathcal{E}[\widehat{\mathbf{c}}] = \mathbf{c} + \mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{U}^{-1}\boldsymbol{\gamma}(\mathbf{Z}) \tag{245}$$

Predicted output vector $\widehat{\mathbf{y}}$ becomes

$$\widehat{\mathbf{y}} = \mathbf{Z}\widehat{\mathbf{c}} = \mathbf{Z}\mathbf{c} + \mathbf{Z}\mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{U}^{-1}[\boldsymbol{\gamma}(\mathbf{Z}) + \boldsymbol{\epsilon}_{\mathbf{E}}] \tag{246}$$

It follows from equation (246) that the expected value of predicted output vector $\widehat{\mathbf{y}}$ is given by

$$\mathcal{E}[\widehat{\mathbf{y}}] = \mathbf{Zc} + \mathbf{ZQ}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{U}^{-1}\boldsymbol{\gamma}(\mathbf{Z}) \tag{247}$$

Combine equations (242) and (246) with (225) to obtain residual vector $\widehat{\mathbf{e}}_{\mathbf{v}}$ as

$$\begin{aligned}\widehat{\mathbf{e}}_{\mathbf{v}} \equiv \mathbf{v} - \widehat{\mathbf{v}} = \mathbf{P}^{-1}(\mathbf{y} - \widehat{\mathbf{y}}) &= \mathbf{P}^{-1}\left(\mathbf{I}_{\mathbf{K}} - \mathbf{ZQ}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\mathbf{P}^{-1}\right)[\boldsymbol{\gamma}(\mathbf{Z}) + \boldsymbol{\epsilon}_{\mathbf{E}}] \\ &= \left(\mathbf{I}_{\mathbf{K}} - \mathbf{P}^{-1}\mathbf{ZQ}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\right)[\mathbf{P}^{-1}\boldsymbol{\gamma}(\mathbf{Z}) + \boldsymbol{\epsilon}_{\mathbf{v}}] = \mathbf{W}_{\mathbf{K}}[\mathbf{P}^{-1}\boldsymbol{\gamma}(\mathbf{Z}) + \boldsymbol{\epsilon}_{\mathbf{v}}]\end{aligned} \tag{248}$$

The expected value of $\widehat{\mathbf{e}}_{\mathbf{v}}$ is seen to be

$$\mathcal{E}[\widehat{\mathbf{e}}_{\mathbf{v}}] = \mathbf{W}_{\mathbf{K}}\mathbf{P}^{-1}\boldsymbol{\gamma}(\mathbf{Z}) \tag{249}$$

After combining equations (215), (248), and (249), the covariance matrix of $\widehat{\mathbf{e}}_{\mathbf{v}}$ is found to be

$$\boldsymbol{\Sigma}_{\widehat{\mathbf{e}}_{\mathbf{v}}} \equiv \mathcal{E}\left\{[\widehat{\mathbf{e}}_{\mathbf{v}} - \mathcal{E}(\widehat{\mathbf{e}}_{\mathbf{v}})][\widehat{\mathbf{e}}_{\mathbf{v}} - \mathcal{E}(\widehat{\mathbf{e}}_{\mathbf{v}})]^{\mathbf{T}}\right\} = \sigma_E^2\mathbf{W}_{\mathbf{K}} \tag{250}$$

Since $\mathbf{W}_{\mathbf{K}}$ is idempotent, the residual sum of squares is obtained from equation (248) as follows:

$$S_{SE} \equiv \widehat{\mathbf{e}}_{\mathbf{v}}^{\mathbf{T}}\widehat{\mathbf{e}}_{\mathbf{v}} = [\mathbf{P}^{-1}\boldsymbol{\gamma}(\mathbf{Z}) + \boldsymbol{\epsilon}_{\mathbf{v}}]^{\mathbf{T}}\mathbf{W}_{\mathbf{K}}[\mathbf{P}^{-1}\boldsymbol{\gamma}(\mathbf{Z}) + \boldsymbol{\epsilon}_{\mathbf{v}}] \tag{251}$$

Because $\mathbf{W}_{\mathbf{K}}$ has rank $K - M_{\mathbf{z}}$, the expected value of S_{SE} is

$$\mathcal{E}[S_{SE}] = (K - M_{\mathbf{z}})\sigma_E^2 + \boldsymbol{\gamma}(\mathbf{Z})^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\mathbf{W}_{\mathbf{K}}\mathbf{P}^{-1}\boldsymbol{\gamma}(\mathbf{Z}) \tag{252}$$

Note that $S_E = [S_{SE}/(K - M_{\mathbf{z}})]^{1/2}$ is no longer an unbiased estimate of σ when modeling error $\gamma(\mathbf{z})$ is nonzero.

Consider arbitrary input vector $\mathbf{z}$. The corresponding output y, obtained with equation (241), is

$$y = f(\mathbf{c}, \mathbf{z}) = \mathbf{zc} + \gamma(\mathbf{z}) \tag{253}$$

The predicted output is $\widehat{y} = \mathbf{z}\widehat{\mathbf{c}}$. Prediction error δy is then

$$\delta y \equiv y - \widehat{y} = \gamma(\mathbf{z}) - \mathbf{ZQ}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{U}^{-1}[\boldsymbol{\gamma}(\mathbf{Z}) + \boldsymbol{\epsilon}_{\mathbf{E}}] \tag{254}$$

The expected mean-square prediction error is obtained from equation (254) as

$$\sigma_{\widehat{y}}^2(\mathbf{z}) = \mathcal{E}[\delta\widehat{y}^2] = [\gamma(\mathbf{z}) - \mathbf{z}\,\mathbf{Q}^{-1}\mathbf{Z}^{\mathbf{T}}\mathbf{U}^{-1}\boldsymbol{\gamma}(\mathbf{Z})]^2 + \sigma_E^2\mathbf{z}^{\mathbf{T}}\mathbf{Q}^{-1}\mathbf{z} \tag{255}$$

A3. Nonlinear Least-Squares Estimation With Input Uncertainty

Let $\mathbf{c}$ denote the $M_{\mathbf{c}} \times 1$ parameter vector; $(\mathbf{z} + \delta\mathbf{z})$, the $1 \times M_{\mathbf{z}}$ stochastic input vector, where $\mathbf{z}$ is the $1 \times M_{\mathbf{z}}$ nominal input vector and $\delta\mathbf{z}$ is the $1 \times M_{\mathbf{z}}$ stochastic input uncertainty vector; ϵ_E, the measurement uncertainty, a zero-mean random variable. Then the process output is of the form

$$y = f(\mathbf{c}, \mathbf{z} + \delta\mathbf{z}) + \epsilon_E = f(\mathbf{c}, \mathbf{z}) + \delta y \tag{256}$$

The uncertainty δy_k of the kth observation is then

$$\delta y_k = \delta f_{zk} + \epsilon_{E_k} \tag{257}$$

where

$$\delta f_{zk} = \mathbf{f}_{\mathbf{z}}(\mathbf{c}, \mathbf{z}_k)\delta\mathbf{z}_k \tag{258}$$

and the $1 \times M_{\mathbf{z}}$ vector $\mathbf{f}_{\mathbf{z}}(\mathbf{c}, \mathbf{z}_k)$ is defined as

$$\mathbf{f}_{\mathbf{z}}(\mathbf{c}, \mathbf{z}_k) \equiv \left[\frac{\partial f(\mathbf{c}, \mathbf{z}_k)}{\partial \mathbf{z}}\right] \tag{259}$$

Define $K \times 1$ error vector $\delta\mathbf{f}_{\mathbf{z}}$ as

$$\delta\mathbf{f}_{\mathbf{z}} \equiv [\delta f_{z1} \ldots \delta f_{zK}]^{\mathbf{T}} \tag{260}$$

It is seen that $\delta\mathbf{f}_{\mathbf{z}}$ is given by

$$\delta\mathbf{f}_{\mathbf{z}} = \begin{bmatrix} \mathbf{f}_{\mathbf{z}}(\mathbf{c}, \mathbf{z}_1)\delta\mathbf{z}_1^{\mathbf{T}} \\ \vdots \\ \mathbf{f}_{\mathbf{z}}(\mathbf{c}, \mathbf{z}_K)\delta\mathbf{z}_K^{\mathbf{T}} \end{bmatrix} \tag{261}$$

Note that subscript $\mathbf{z}$ is appended to indicate that $\delta\mathbf{f}$ depends on the entire design matrix $\mathbf{Z}$. The $K \times K$ covariance matrix of $\delta\mathbf{f}_{\mathbf{z}}$ is given by

$$\mathbf{\Sigma}_{\mathbf{f}_{\mathbf{z}}} \equiv \mathcal{E}[\delta\mathbf{f}_{\mathbf{z}}\delta\mathbf{f}_{\mathbf{z}}^{\mathbf{T}}] \tag{262}$$

The $K \times 1$ output vector $\mathbf{y}$ is obtained by extending scalar equation (256) to the following $K \times 1$ vector equation

$$\mathbf{y} = \mathbf{f}(\mathbf{c}, \mathbf{Z}) + \delta\mathbf{y} \tag{263}$$

where $\mathbf{Z}$ is the $K \times M_{\mathbf{z}}$ design matrix, and $\delta\mathbf{y}$ is the $K \times 1$ zero-mean combined output uncertainty vector given by

$$\delta\mathbf{y} = \delta\mathbf{f}_{\mathbf{z}} + \boldsymbol{\epsilon}_{\mathbf{E}} \tag{264}$$

and $\delta\mathbf{y}$ has $K \times K$ combined output covariance matrix $\boldsymbol{\Sigma}_{\mathbf{Y}}$ which can be expressed as

$$\boldsymbol{\Sigma}_{\mathbf{Y}} = \boldsymbol{\Sigma}_{\mathbf{f}_{\mathbf{z}}} + \boldsymbol{\Sigma}_{\mathbf{E}} \tag{265}$$

The assumption is that $\boldsymbol{\Sigma}_{\mathbf{Y}}$ can be expressed in the form of equation (188), namely $\boldsymbol{\Sigma}_{\mathbf{Y}} = \sigma_Y^2\mathbf{U}$, where $\mathbf{U}$ satisfies the conditions of equation (189), with transformed $K \times 1$ output vector $\mathbf{v}$ defined in equation (213), and equation (263) becomes

$$\mathbf{v} = \mathbf{P}^{-1}\mathbf{f}(\mathbf{c}, \mathbf{Z}) + \delta\mathbf{v} \tag{266}$$

where $K \times 1$ uncertainty vector $\delta\mathbf{v} = \mathbf{P}^{-1}\delta\mathbf{y}$ and $K \times K$ matrix $\mathbf{P}$ is defined as in equation (189). The expected value of $\delta\mathbf{v}$ is zero, and the expected value of $\mathbf{v}$ is

$$\boldsymbol{\mu}_{\mathbf{v}} \equiv \mathcal{E}[\mathbf{v}] = \mathbf{P}^{-1}\mathbf{f}(\mathbf{c}, \mathbf{Z}) \tag{267}$$

The $K \times K$ covariance matrix of $\delta\mathbf{v}$, denoted by $\boldsymbol{\Sigma}_{\mathbf{v}}$, then becomes

$$\boldsymbol{\Sigma}_{\mathbf{v}} = \mathcal{E}[\delta\mathbf{v}\delta\mathbf{v}^{\mathbf{T}}] = \mathbf{P}^{-1}\,\mathcal{E}[\delta\mathbf{y}\delta\mathbf{y}^{\mathbf{T}}]\mathbf{P}^{-\mathbf{T}} = \sigma_Y^2\mathbf{P}^{-1}\mathbf{U}\mathbf{P}^{-\mathbf{T}} = \sigma_Y^2\mathbf{I}_{\mathbf{K}} \tag{268}$$

It is seen that $\delta\mathbf{v}$ is uncorrelated and normally distributed whenever $\delta\mathbf{y}$ is normally distributed. As in equation (216) define the sum of squares as

$$S_{SQ} \equiv (\mathbf{v} - \boldsymbol{\mu}_{\mathbf{v}})^{\mathbf{T}}(\mathbf{v} - \boldsymbol{\mu}_{\mathbf{v}}) = [\mathbf{v} - \mathbf{P}^{-1}\mathbf{f}(\mathbf{c}, \mathbf{Z})]^{\mathbf{T}}[\mathbf{v} - \mathbf{P}^{-1}\mathbf{f}(\mathbf{c}, \mathbf{Z})] \tag{269}$$

To minimize S_{SQ} (ref. 13) compute its gradient with respect to $\mathbf{c}$ and equate the resultant $1 \times M_c$ set of equations to zero as follows:

$$\begin{aligned}\mathbf{h} \equiv \frac{1}{2}\left(\frac{\partial S_{SQ}}{\partial \mathbf{c}}\right) &= [\mathbf{v} - \mathbf{P}^{-1}\mathbf{f}(\mathbf{c}, \mathbf{Z})]^{\mathbf{T}}\mathbf{P}^{-1}\left[\frac{\partial \mathbf{f}}{\partial \mathbf{c}}(\mathbf{c}, \mathbf{Z})\right] \\ &= [\mathbf{v} - \mathbf{P}^{-1}\mathbf{f}(\mathbf{c}, \mathbf{Z})]^{\mathbf{T}}\mathbf{P}^{-1}\mathbf{F}_{\mathbf{c}} = 0\end{aligned} \tag{270}$$

where $\mathbf{h}$ is a function of independent arguments $\mathbf{v}$, $\mathbf{c}$, and $\mathbf{Z}$ and has dimension $1 \times M_{\mathbf{c}}$, $[\mathbf{v} - \mathbf{P}^{-1}\mathbf{f}(\mathbf{c}, \mathbf{Z})]$ is $K \times 1$, $\mathbf{P}$ is $K \times K$, and $K \times M_{\mathbf{c}}$ matrix $\mathbf{F}_{\mathbf{c}}$ is defined as

$$\mathbf{F}_{\mathbf{c}} \equiv \left[\frac{\partial \mathbf{f}}{\partial \mathbf{c}}(\mathbf{c}, \mathbf{Z})\right] = \begin{bmatrix} \frac{\partial f_1(\mathbf{c},\mathbf{z}_1)}{\partial c_1} & \cdots & \frac{\partial f_1(\mathbf{c},\mathbf{z}_1)}{\partial c_{M_{\mathbf{c}}}} \\ \vdots & \cdots & \vdots \\ \frac{\partial f_K(\mathbf{c},\mathbf{z}_K)}{\partial c_1} & \cdots & \frac{\partial f_K(\mathbf{c},\mathbf{z}_K)}{\partial c_{M_c}} \end{bmatrix} \tag{271}$$

Finally $\mathbf{0}$ denotes a $1 \times M_{\mathrm{c}}$ vector of zeros. Equation (270) is solved numerically for $\widehat{\mathbf{c}}$ by Newton-Raphson iteration or similar method. Necessary conditions for the existence of a solution are now obtained.

To obtain the uncertainty of $\widehat{\mathbf{c}}$ denoted by $\delta\widehat{\mathbf{c}}$, compute the total differential of equation (270) and equate to zero as follows:

$$\delta\mathbf{h} = \delta\mathbf{v}^{\mathbf{T}} \left[\frac{\partial\mathbf{h}}{\partial\mathbf{v}}\right] + \delta\widehat{\mathbf{c}}^{\mathbf{T}}\mathbf{R} = 0 \tag{272}$$

where $K \times M_{\mathrm{c}}$ matrix $[\partial\mathbf{h}/\partial\mathbf{v}]$ is seen to equal

$$\left[\frac{\partial\mathbf{h}}{\partial\mathbf{v}}\right] = \mathbf{P}^{-1}\mathbf{F}_{\mathrm{c}} \tag{273}$$

and the $M_{\mathrm{c}} \times M_{\mathrm{c}}$ matrix $\mathbf{R}$ is defined as

$$\mathbf{R} \equiv \left[\frac{\partial\mathbf{h}}{\partial\mathbf{c}}\right] = \begin{bmatrix} \frac{\partial^2 S_{SQ}}{\partial c_1^2} & \cdots & \frac{\partial^2 S_{SQ}}{\partial c_1 \ \partial c_{M_{\mathrm{Z}}}} \\ \vdots & \cdots & \vdots \\ \frac{\partial^2 S_{SQ}}{\partial c_1 \ \partial c_{M_{\mathrm{Z}}}} & \cdots & \frac{\partial^2 S_{SQ}}{\partial c_{M_{\mathrm{Z}}}^2} \end{bmatrix} \tag{274}$$

A necessary condition for the existence of a solution to equation (270) for $\widehat{\mathbf{c}}$ and to equation (272) for $\delta\widehat{\mathbf{c}}$ is that matrix $\mathbf{R}$ be nonsingular in some open interval about $\widehat{\mathbf{c}}$ (ref. 11).

To evaluate $\mathbf{R}$ differentiate equation (270) with respect to $\mathbf{c}$ as indicated to obtain

$$\mathbf{R} = \mathbf{F}_{\mathrm{c}}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\mathbf{P}^{-1}\mathbf{F}_{\mathrm{c}} + [\mathbf{v} - \mathbf{P}^{-1}\mathbf{f}(\mathbf{c},\mathbf{Z})]^{\mathbf{T}}\mathbf{P}^{-1} \otimes \mathbf{F}_{\mathrm{cc}} = \mathbf{F}_{\mathrm{c}}^{\mathbf{T}}\mathbf{U}^{-1}\mathbf{F}_{\mathrm{c}} + \mathbf{H}_{\mathbf{E}} \tag{275}$$

where $\mathbf{H}_{\mathbf{E}}$ is defined as

$$\mathbf{H}_{\mathbf{E}} \equiv [\mathbf{v} - \mathbf{P}^{-1}\mathbf{f}(\mathbf{c},\mathbf{Z})]^{\mathbf{T}}\mathbf{P}^{-1} \otimes \mathbf{F}_{\mathrm{cc}} \tag{276}$$

The $M_{\mathrm{c}} \times M_{\mathrm{c}} \times K$ array $\mathbf{F}_{\mathrm{cc}}$ is defined as the partial derivative of $M_{\mathrm{c}} \times K$ array $\mathbf{F}_{\mathrm{c}}^{\mathbf{T}}$ with respect to vector $\mathbf{c}$; that is,

$$\mathbf{F}_{\mathrm{cc}} \equiv \left[\frac{\partial\mathbf{F}_{\mathrm{c}}^{\mathbf{T}}(\mathbf{c},\mathbf{Z})}{\partial\mathbf{c}}\right] \tag{277}$$

where the ijkth element of $\mathbf{F}_{\mathrm{cc}}(\mathbf{c},\mathbf{Z})$ equals the second partial derivative of the kth element of function $\mathbf{f}(\mathbf{c},\mathbf{Z})$ with respect to c_i and c_j as follows:

$$f_{\mathrm{cc},ijk} = \frac{\partial^2 f_k(\mathbf{c},\mathbf{z}_k)}{\partial c_i \, \partial c_j} \tag{278}$$

for $1 \leq i, j \leq M_c$, and $1 \leq k \leq K$. The $\otimes$ operator denotes formation of the inner product of $1 \times K$ row vector $[\mathbf{v} - \mathbf{P}^{-1}\mathbf{f}(\mathbf{c}, \mathbf{Z})]^{\mathbf{T}}\mathbf{P}^{-1}$ with each $K \times 1$ column of array $\mathbf{F}_{\mathbf{cc}}$. Thus the ijth element of $M_c \times M_c$ matrix $\mathbf{H_E}$ is given by

$$\mathbf{h}_{E,ij} = \left[\mathbf{v} - \mathbf{P}^{-1}\mathbf{f}(\mathbf{c}, \mathbf{Z})\right]^{\mathbf{T}} \mathbf{P}^{-1}\mathbf{F}_{\mathbf{cc},ij} = \mathbf{e}_{\mathbf{v}}^{\mathbf{T}}\mathbf{P}^{-1}\mathbf{F}_{\mathbf{cc},ij} \tag{279}$$

for $1 \leq i, j \leq M_c$, where $\mathbf{F}_{\mathbf{cc},ij}$ denotes the ijth $(K \times 1)$ column of array $\mathbf{F}_{\mathbf{cc}}$, and $\mathbf{e}_{\mathbf{v}} = \mathbf{v} - \mathbf{P}^{-1}\mathbf{f}(\mathbf{c}, \mathbf{Z})$. After least-squares estimation of vector $\widehat{\mathbf{c}}$, vector $\mathbf{e}_{\mathbf{v}}$ becomes residual vector $\widehat{\mathbf{e}}_{\mathbf{v}}$ defined subsequently. If norm $\| \widehat{\mathbf{e}}_{\mathbf{v}} \|$ is small, matrix $\mathbf{H_E}$ can be neglected in equation (275). Then $\mathbf{R}$ is closely approximated by

$$\mathbf{R} \approx \mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{U}^{-1}\mathbf{F}_{\mathbf{c}} \tag{280}$$

Note that matrix $\mathbf{R}$ has rank M_c, i.e., is nonsingular, only if rank $(\mathbf{F}_{\mathbf{c}}) = M_c$. Combine equations (272) and (273) and solve for $M_c \times 1$ uncertainty vector $\delta\widehat{\mathbf{c}}$ to yield

$$\delta\widehat{\mathbf{c}} = -\mathbf{R}^{-1}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\delta\mathbf{v} \tag{281}$$

From equation (281), $\delta\widehat{\mathbf{c}}$ has zero mean and covariance matrix as follows:

$$\begin{aligned} \mathbf{\Sigma}_{\hat{\mathbf{c}}} &= \mathbf{R}^{-1}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\mathbf{\Sigma}_{\mathbf{v}}\mathbf{P}^{-1}\mathbf{F}_{\mathbf{c}}\mathbf{R}^{-1} \\ &= \sigma_Y^2\mathbf{R}^{-1}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{U}^{-1}\mathbf{F}_{\mathbf{c}}\mathbf{R}^{-1} = \sigma_Y^2\mathbf{Q}_{\mathbf{c}}^{-1} \end{aligned} \tag{282}$$

where $M_c \times M_c$ matrix $\mathbf{Q}_{\mathbf{c}}$ equals

$$\mathbf{Q}_{\mathbf{c}} = \left[\mathbf{R}^{-1}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{U}^{-1}\mathbf{F}_{\mathbf{c}}\mathbf{R}^{-1}\right]^{-1} \tag{283}$$

Note that satisfaction of the approximation in equation (280) is a sufficient condition, but not necessary, for the existence of matrix $\mathbf{Q}_{\mathbf{c}}$. Equation (280) implies that

$$\mathbf{Q}_{\mathbf{c}} \approx \mathbf{R} \tag{284}$$

A3.1. Residual Sum of Squares.

As for calibration design matrix $\mathbf{Z}$ and estimated parameter vector $\widehat{\mathbf{c}}$, define $K \times 1$ predicted output vector $\widehat{\mathbf{v}}$ as

$$\begin{aligned} \widehat{\mathbf{v}} &= \mathbf{P}^{-1}\mathbf{f}(\widehat{\mathbf{c}}, \mathbf{Z}) = \mathbf{P}^{-1}\left[\mathbf{f}(\mathbf{c}, \mathbf{Z}) + \mathbf{F}_{\mathbf{c}}\delta\widehat{\mathbf{c}}\right] \\ &= \mathbf{P}^{-1}\left[\mathbf{f}(\widehat{\mathbf{c}}, \mathbf{Z}) - \mathbf{F}_{\mathbf{c}}\mathbf{R}^{-1}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\delta\mathbf{v}\right] = \mathbf{P}^{-1}\mathbf{f}(\mathbf{c}, \mathbf{Z}) - \mathbf{\Omega}_{\mathbf{F}}\delta\mathbf{v} \end{aligned} \tag{285}$$

where

$$\mathbf{\Omega}_{\mathbf{F}} \equiv \left(\mathbf{P}^{-1}\mathbf{F}_{\mathbf{c}}\right)\mathbf{R}^{-1}\left(\mathbf{P}^{-1}\mathbf{F}_{\mathbf{c}}\right)^{\mathbf{T}} \tag{286}$$

As before, $K \times 1$ residual vector $\widehat{\mathbf{e}}_{\mathbf{v}}$ is defined as

$$\widehat{\mathbf{e}}_{\mathbf{v}} \equiv \mathbf{v} - \widehat{\mathbf{v}} = \mathbf{P}^{-1}[\mathbf{f}(\mathbf{c}, \mathbf{Z}) - \mathbf{f}(\widehat{\mathbf{c}}, \mathbf{Z})] + \delta\mathbf{v} \tag{287}$$

Let $\delta\mathbf{f}_{\mathbf{c}} \equiv \mathbf{f}(\mathbf{c}, \mathbf{Z}) - \mathbf{f}(\widehat{\mathbf{c}}, \mathbf{Z})$, which is closely approximated by $\delta\mathbf{f}_{\mathbf{c}} = \mathbf{F}_{\mathbf{c}}(\mathbf{c}, \mathbf{Z})\delta\widehat{\mathbf{c}}$. Then equation (287) can be expressed in differential form as

$$\widehat{\mathbf{e}}_{\mathbf{v}} = \mathbf{P}^{-1}\mathbf{F}_{\mathbf{c}}(\mathbf{c}, \mathbf{Z})\delta\widehat{\mathbf{c}} + \delta\mathbf{v} \tag{288}$$

Combine equations (281), (286), and (288) to obtain

$$\widehat{\mathbf{e}}_{\mathbf{v}} = \left(\mathbf{I}_{\mathbf{K}} - \mathbf{P}^{-1}\mathbf{F}_{\mathbf{c}}\mathbf{R}^{-1}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\right)\delta\mathbf{v} = \mathbf{W}_{\mathbf{F}_K}\delta\mathbf{v} \tag{289}$$

where

$$\mathbf{W}_{\mathbf{F}_{\mathbf{K}}} \equiv \mathbf{I}_{\mathbf{K}} - \mathbf{\Omega}_{\mathbf{F}} \tag{290}$$

Subscript K, appended to denote the matrix dimension, is treated as an index. If approximation in equation (280) holds, then $\mathbf{\Omega}_{\mathbf{F}}$ is idempotent as is shown in the following equation:

$$\begin{aligned}\mathbf{\Omega}_{\mathbf{F}}\mathbf{\Omega}_{\mathbf{F}} &= \mathbf{P}^{-1}\mathbf{F}_{\mathbf{c}}\mathbf{R}^{-1}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\mathbf{P}^{-1}\mathbf{F}_{\mathbf{c}}\mathbf{R}^{-1}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}} \\ &= \mathbf{P}^{-1}\mathbf{F}_{\mathbf{c}}\mathbf{R}^{-1}\left(\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{U}^{-1}\mathbf{F}_{\mathbf{c}}\right)\mathbf{R}^{-1}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}} \\ &= \mathbf{P}^{-1}\mathbf{F}_{\mathbf{c}}\mathbf{R}^{-1}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}} = \mathbf{\Omega}_{\mathbf{F}}\end{aligned} \tag{291}$$

By using Lemmas 2, 3, and 6,

$$\begin{aligned}\text{rank}\,(\mathbf{\Omega}_{\mathbf{F}}) &= \text{tr}\,\left(\mathbf{P}^{-1}\mathbf{F}_{\mathbf{c}}\mathbf{R}^{-1}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\right) = \text{tr}\,\left(\mathbf{R}^{-1}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{P}^{-\mathbf{T}}\mathbf{P}^{-1}\mathbf{F}_{\mathbf{c}}\right) \\ &= \text{tr}\,\left(\mathbf{R}^{-1}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{U}^{-1}\mathbf{F}_{\mathbf{c}}\right) = \text{tr}\,(\mathbf{R}^{-1}\mathbf{R}) = M_{\mathbf{c}}\end{aligned} \tag{292}$$

Therefore, by Lemma 7, $\mathbf{W}_{\mathbf{F}_K}$ is idempotent with rank $K - M_{\mathbf{c}}$.

The covariance matrix of $\widehat{\mathbf{e}}_{\mathbf{v}}$ is given by

$$\mathbf{\Sigma}_{\hat{\mathbf{e}}_v} = \sigma_Y^2\mathbf{W}_{\mathbf{F}_K} \tag{293}$$

and the residual sum of squares S_{SE} is given by

$$S_{SE} = \widehat{\mathbf{e}}_{\mathbf{v}}^{\mathbf{T}}\widehat{\mathbf{e}}_{\mathbf{v}} = \delta\mathbf{v}^{\mathbf{T}}\mathbf{W}_{\mathbf{F}_K}\delta\mathbf{v} \tag{294}$$

Then by Theorem 1, S_{SE} is chi-square distributed with $K - M_{\mathbf{c}}$ degrees of freedom and with expected value

$$\mathcal{E}(S_{SE}) = (K - M_{\mathbf{c}})\sigma_Y^2 \tag{295}$$

An unbiased estimate of σ_Y is provided by standard error S_Y, where

$$S_Y = \left(\frac{S_{SE}}{K - M_c}\right)^{1/2} \tag{296}$$

A confidence interval for σ_Y at confidence level α is given by

$$\frac{(K - M_c)^{1/2} S_Y}{\chi_{(1+\alpha)/2}} \leq \sigma_Y \leq \frac{(K - M_c)^{1/2} S_Y}{\chi_{(1-\alpha)/2}} \tag{297}$$

where χ_α is the α percentile value of the chi-square distribution with $K - M_c$ degrees of freedom.

A3.2. Confidence Intervals.

A confidence ellipsoid is now obtained for $\widehat{c}$. Let

$$\begin{aligned} S_{SC} &\equiv (\mathbf{c} - \widehat{\mathbf{c}})^{\mathbf{T}} \mathbf{Q_C} (\mathbf{c} - \widehat{\mathbf{c}}) = \delta \mathbf{v}^{\mathbf{T}} \mathbf{P}^{-1} \mathbf{F}_{\mathbf{c}} \mathbf{R}^{-1} \mathbf{Q}_{\mathbf{c}} \mathbf{R}^{-1} \mathbf{F}_{\mathbf{c}}^{\mathbf{T}} \mathbf{P}^{-\mathbf{T}} \delta \mathbf{v} \\ &= \delta \mathbf{v}^{\mathbf{T}} \mathbf{P}^{-1} \mathbf{F}_{\mathbf{c}} \mathbf{R}^{-1} \mathbf{F}_{\mathbf{c}}^{\mathbf{T}} \mathbf{P}^{-\mathbf{T}} \delta \mathbf{v} = \delta \mathbf{v}^{\mathbf{T}} \mathbf{\Omega_F} \delta \mathbf{v} \end{aligned} \tag{298}$$

Because $\mathbf{\Omega_F}$ is idempotent, S_{SC}/σ_Y^2 is chi-square distributed with M_c degrees of freedom by Theorem 1. Hence, the ratio $F = [S_{SC}/\sigma_E^2 M_c]/\{S_{SE}/[\sigma_E^2(K - M_c)]\}$ is F-distributed with M_c, $K - M_c$ degrees of freedom (ref. 7). Then the confidence ellipsoid at level α for $\widehat{c}$ is defined by

$$(\mathbf{c} - \widehat{\mathbf{c}})^{\mathbf{T}} \mathbf{Q}_{\mathbf{c}} (\mathbf{c} - \widehat{\mathbf{c}}) \leq M_c S_Y^2 F_{M_c, K - M_c}(\alpha) \tag{299}$$

For arbitrary input vector $\mathbf{z}$, the corresponding predicted scalar output denoted by $\widehat{y}(\mathbf{z})$ is

$$\widehat{y}(\mathbf{z}) \equiv f(\widehat{\mathbf{c}}, \mathbf{z}) \tag{300}$$

The uncertainty of $\widehat{y}(\mathbf{z})$ due to calibration uncertainty alone is obtained with equation (281) as

$$\begin{aligned} \delta \widehat{y} &= y - \widehat{y} = f(\mathbf{c}, \mathbf{z}) - f(\widehat{\mathbf{c}}, \mathbf{z}) \\ &= \left[\frac{\partial f(\widehat{\mathbf{c}}, \mathbf{z})}{\partial \mathbf{c}}\right] \delta \widehat{\mathbf{c}} = -\mathbf{f}_{\mathbf{c}}^{\mathbf{T}}(\mathbf{c}, \mathbf{z}) \mathbf{R}^{-1} \mathbf{F}_{\mathbf{c}}^{\mathbf{T}} \mathbf{P}^{-1} \delta \mathbf{v} \end{aligned} \tag{301}$$

where $M_c \times 1$ gradient vector $\mathbf{f}_{\mathbf{c}}(\mathbf{c}, \mathbf{z})$ is defined as

$$\mathbf{f}_{\mathbf{c}}(\mathbf{c}, \mathbf{z}) = \left[\frac{\partial f(\mathbf{c}, \mathbf{z})}{\partial \mathbf{c}}\right] \tag{302}$$

It follows that $\delta \widehat{\mathbf{y}}$ is normally distributed with zero expected value. Then the expected value of $\widehat{y}(\mathbf{z})$ is

$$\mathcal{E}[\widehat{y}(\mathbf{z})] = f(\mathbf{c}, \mathbf{z}) \tag{303}$$

The variance of predicted output $\widehat{y}(\mathbf{z})$, denoted the variance function, is obtained from equation (301) as follows:

$$\begin{aligned}\sigma^2_{\widehat{y}}(\mathbf{z}) &\equiv \mathcal{E}[\delta\widehat{y}\ \delta\widehat{y}] = \mathbf{f}_c^{\mathbf{T}}(\mathbf{c},\mathbf{z})\mathbf{R}^{-1}\mathbf{F}_c^{\mathbf{T}}\mathbf{P}^{-1}\mathcal{E}[\delta\mathbf{v}\ \delta\mathbf{v}^{\mathbf{T}}]\mathbf{P}^{-\mathbf{T}}\mathbf{F}_c\mathbf{R}^{-1}\mathbf{f}_c(\mathbf{c},\mathbf{z}) \\ &= \sigma^2_{\widehat{Y}}\mathbf{f}_c^{\mathbf{T}}(\mathbf{c},\mathbf{z})\mathbf{R}^{-1}\mathbf{F}_c^{\mathbf{T}}\mathbf{U}^{-1}\mathbf{F}_c\mathbf{R}^{-1}\mathbf{f}_c(\mathbf{c},\mathbf{z}) \\ &= \sigma^2_{\widehat{Y}}\mathbf{f}_c^{\mathbf{T}}(\mathbf{c},\mathbf{z})\mathbf{Q}_{\mathbf{C}}^{-1}\mathbf{f}_c(\mathbf{c},\mathbf{z}) \end{aligned} \tag{304}$$

If the approximation in equation (280) holds, then equation (304) simplifies to

$$\sigma^2_{\widehat{y}}(\mathbf{z}) = \sigma^2_Y\mathbf{f}_c^{\mathbf{T}}(\mathbf{c},\mathbf{z})\mathbf{R}^{-1}\mathbf{f}_c(\mathbf{c},\mathbf{z}) \tag{305}$$

The normally distributed variate $\delta\widehat{y}(\mathbf{z})/\left\{\sigma_Y\left[\mathbf{f}_c^{\mathbf{T}}(\mathbf{c},\mathbf{z})\mathbf{Q}_c^{-1}\mathbf{f}_c(\mathbf{c},\mathbf{z})\right]^{1/2}\right\}$ has zero-mean and unit variance. It was shown previously that S_{SE}/σ^2_Y is chi-square distributed with $K - M_c$ degrees of freedom when the approximation in equation (280) holds. Then the ratio t defined below has Student's t-distribution with $K - M_c$ degrees of freedom.

$$t = \frac{\delta\widehat{y}(\mathbf{z})/\left\{\sigma_Y\left[\mathbf{f}_c^{\mathbf{T}}(\mathbf{c},\mathbf{z})\mathbf{Q}_{\mathbf{C}}^{-1}\mathbf{f}_c(\mathbf{c},\mathbf{z})\right]^{1/2}\right\}}{S_{SE}/\left[\sigma_Y(K - M_c)^{1/2}\right]} \tag{306}$$

Then the output prediction confidence interval at α confidence level is given by

$$|y - \widehat{y}| \leq [\mathbf{f}_c^{\mathbf{T}}(\widehat{\mathbf{c}},\mathbf{z})\mathbf{Q}_{\mathbf{C}}^{-1}\mathbf{f}_c(\widehat{\mathbf{c}},\mathbf{z})]^{1/2}S_Y t_{K-M_c}(\alpha/2) \tag{307}$$

where $t_n(\alpha)$ is the α percentile value of the two-tailed t-distribution with n degrees of freedom.

A4. Analysis of Replicated Calibrations

In the following development, subscripts **K** and **NK** are appended to matrices **I**, **Z**, **Q**, **U**, and $\mathbf{\Omega}$ to distinguish between single calibrations (K observations) and replicated calibrations (NK observations). Consider an arbitrary $K \times M_z$ experimental design matrix $\mathbf{Z_K}$ for calibration of a single- output sensor, which is replicated N times. The sets of input loading uncertainties are seen to be intercorrelated among replications. The $NK \times M_z$ replicated experimental design $\mathbf{Z_{NK}}$ is

$$\mathbf{Z_{NK}} = \begin{bmatrix}\mathbf{Z_K}\\ \mathbf{Z_K}\\ \vdots\\ \mathbf{Z_K}\end{bmatrix} = \mathbf{H}^{\mathbf{T}}\mathbf{Z_K} \tag{308}$$

where $K \times NK$ replication matrix **H** is defined as

$$\mathbf{H} \equiv [\mathbf{I_K}\quad \mathbf{I_K}\quad \ldots\quad \mathbf{I_K}] \tag{309}$$

The following properties of $\mathbf{H}$ are used in the subsequent development. The $K \times K$ matrix product $\mathbf{HH^T}$ equals

$$\mathbf{HH^T} = N\mathbf{I_K} \tag{310}$$

and $NK \times NK$ matrix product $\mathbf{H^TH}$ equals

$$\mathbf{H^TH} = \begin{bmatrix} \mathbf{I_K} & \mathbf{I_K} & \dots & \mathbf{I_K} \\ \mathbf{I_K} & \mathbf{I_K} & \dots & \mathbf{I_K} \\ \vdots & \vdots & \dots & \vdots \\ \mathbf{I_K} & \mathbf{I_K} & \dots & \mathbf{I_K} \end{bmatrix} \tag{311}$$

For any $K \times K$ matrix $\mathbf{A}$, the $NK \times NK$ matrix product $\mathbf{H^TAH}$ equals

$$\mathbf{H^TAH} = \begin{bmatrix} \mathbf{A} & \mathbf{A} & \dots & \mathbf{A} \\ \mathbf{A} & \mathbf{A} & \dots & \mathbf{A} \\ \vdots & \vdots & \dots & \vdots \\ \mathbf{A} & \mathbf{A} & \dots & \mathbf{A} \end{bmatrix} \tag{312}$$

Let $\mathbf{D_{NK}}$ be an $NK \times NK$ block diagonal matrix constructed from $K \times K$ matrix $\mathbf{A}$ as

$$\mathbf{D_{NK}} = \begin{bmatrix} \mathbf{A} & \mathbf{0_K} & \dots & \mathbf{0_K} \\ \mathbf{0_K} & \mathbf{A} & \dots & \mathbf{0_K} \\ \vdots & \vdots & \dots & \vdots \\ \mathbf{0_K} & \mathbf{0_K} & \dots & \mathbf{A} \end{bmatrix} \tag{313}$$

where $\mathbf{0_K}$ is a $K \times K$ matrix of zeros. Then it follows that

$$\mathbf{HD_{NK}H^T} = N\mathbf{A} \tag{314}$$

A4.1. Single-Input–Single-Output Process With Uncorrelated Uncertainties.

Over N replicated calibrations, let the elements of $NK \times 1$ measurement uncertainty vector $\boldsymbol{\epsilon}_\mathbf{E}$ be uncorrelated with $NK \times NK$ covariance matrix $\sigma_E^2\mathbf{I_{NK}}$, and let the unknown bias uncertainties of a single replication due to the calibration standard be uncorrelated with covariance matrix $\sigma_x^2\mathbf{I_K}$. Since the loading sequence is replicated, then

$$\begin{aligned} \text{cov}\ (z_{k_m}, z_{lm}) &= \sigma_x^2 \qquad (|k-l| = nK; n=1,\dots,N-1; m=1,\dots,M_z) \\ &= 0 \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{(Otherwise)} \end{aligned} \tag{315}$$

where z_{k_m} is the mth element of vector $\mathbf{z}_k$ and $k = 1,\dots,NK$. Thus, from equation (311), the $NK \times NK$ covariance matrix of design matrix $\mathbf{Z}$ is given by

$$\boldsymbol{\Sigma}_\mathbf{Z} = \sigma_x^2\mathbf{H^TH} \tag{316}$$

Similarly, the $NK \times NK$ measurement uncertainty covariance matrix is given by

$$\mathbf{\Sigma_E} = \sigma_E^2 \mathbf{I_{NK}} = \sigma_E^2 \begin{bmatrix} \mathbf{I_K} & \mathbf{0_K} & \dots & \mathbf{0_K} \\ \mathbf{0_K} & \mathbf{I_K} & \dots & \mathbf{0_K} \\ \vdots & \vdots & \dots & \vdots \\ \mathbf{0_K} & \mathbf{0_K} & \dots & \mathbf{I_K} \end{bmatrix} \tag{317}$$

Noting that $\sigma_E^2 > 0$ and $\sigma_x^2 \geq 0$, define combined output covariance matrix $\mathbf{\Sigma_Y}$ as

$$\mathbf{\Sigma_Y} \equiv \mathbf{\Sigma_E} + \mathbf{\Sigma_Z} = \sigma_E^2 \mathbf{I_{NK}} + \sigma_x^2 \mathbf{H^T H} = \sigma_E^2 \mathbf{U_{NK}} \tag{318}$$

where

$$\mathbf{U_{NK}} = \mathbf{I_{NK}} + \alpha \mathbf{H^T H} = \begin{bmatrix} (\alpha+1)\mathbf{I_K} & \alpha \mathbf{I_K} & \dots & \alpha \mathbf{I_K} \\ \alpha \mathbf{I_K} & (\alpha+1)\mathbf{I_K} & \dots & \alpha \mathbf{I_K} \\ \vdots & \vdots & \dots & \vdots \\ \alpha \mathbf{I_K} & \alpha \mathbf{I_K} & \dots & (\alpha+1)\mathbf{I_K} \end{bmatrix} \tag{319}$$

and

$$\alpha = \frac{\sigma_x^2}{\sigma_E^2} \tag{320}$$

It is readily shown that

$$\mathbf{U_{NK}^{-1}} = \mathbf{I_{NK}} - \beta \mathbf{H^T H} = \begin{bmatrix} (1-\beta)\mathbf{I_K} & -\beta \mathbf{I_K} & \dots & -\beta \mathbf{I_K} \\ -\beta \mathbf{I_K} & (1-\beta)\mathbf{I_K} & \dots & -\beta \mathbf{I_K} \\ \vdots & \vdots & \dots & \vdots \\ -\beta \mathbf{I_K} & -\beta \mathbf{I_K} & \dots & (1-\beta)\mathbf{I_K} \end{bmatrix} \tag{321}$$

where

$$\beta = \frac{\alpha}{N\alpha + 1} \tag{322}$$

Then $M_z \times M_z$ generalized moment matrix $\mathbf{Q_{NK}}$ is obtained with the help of equation (310) as follows:

$$\begin{aligned} \mathbf{Q_{NK}} &= \mathbf{Z_{NK}^T U_{NK}^{-1} Z_{NK}} = \mathbf{Z_K^T H (I_{NK} - \beta H^T H) H^T Z_K} \\ &= N(1 - N\beta)\mathbf{Z_K^T Z_K} \end{aligned} \tag{323}$$

Combine equations (320), (322), and (323) to yield

$$\mathbf{Q_{NK}} = \frac{\sigma_E^2}{(\sigma_E^2/N) + \sigma_x^2}\mathbf{Z_K^T Z_K} \tag{324}$$

Note from equation (324) that the portion of calibration uncertainty due to calibration standard bias errors is not reduced by replication, whereas that due to measurement errors decreases roughly as $N^{-1/2}$.

For the analysis of variance tests presented subsequently in the null hypothesis the input uncertainty is assumed to be zero. Then $\sigma_x = 0$ and matrix $\mathbf{U_{NK}}$ equals $\mathbf{I_{NK}}$; consequently, $\mathbf{P}$ equals $\mathbf{I_{NK}}$ in equation (189). For this special case, equations (308), (310), and (323) imply that

$$\mathbf{Q_{NK}} = \mathbf{Z_{NK}^T Z_{NK}} = \mathbf{Z_K^T H H^T Z_K} = N\mathbf{Z_K^T Z_K} = N\mathbf{Q_K} \tag{325}$$

From equations (226) and (325), $NK \times NK$ matrix $\mathbf{\Omega_{NK}}$ is given by

$$\mathbf{\Omega_{NK}} = \mathbf{Z_{NK} Q_{NK}^{-1} Z_{NK}^T} = \frac{1}{N}\mathbf{H^T \Omega_K H} \tag{326}$$

where $K \times K$ matrix $\mathbf{\Omega_K}$ is

$$\mathbf{\Omega_K} = \mathbf{Z_K Q_K^{-1} Z_K^T} \tag{327}$$

As shown in equations (226) and (228), $\mathbf{\Omega_K}$ and $\mathbf{\Omega_{NK}}$ are symmetric and idempotent with rank M_Z.

A4.2. General Multi-Input—Single-Output Process.

Consider a general multi-input–single-output nonlinear process calibrated by using experimental design $\mathbf{Z_K}$ replicated N times as before. The $K \times 1$ output uncertainty vector of a single replication, denoted by $\delta\mathbf{y_K}$, is given by equation (264). Then for N replications $NK \times 1$ output uncertainty vector $\delta\mathbf{y_{NK}}$ is given by

$$\delta\mathbf{y_{NK}} = \mathbf{H^T}\delta\mathbf{f_Z} + \boldsymbol{\epsilon_E} \tag{328}$$

where $K \times 1$ vector $\delta\mathbf{f_Z}$ is given by equation (261) with $K \times K$ covariance matrix $\mathbf{\Sigma_{fZ_K}} = \sigma_x^2\mathbf{U_{fZ_K}}$, given in equation (262), and where $NK \times 1$ measurement uncertainty vector $\boldsymbol{\epsilon_E}$ has $NK \times NK$ covariance matrix $\mathbf{\Sigma_E} = \sigma_E^2\mathbf{U_{E_{NK}}}$. The measurement uncertainty is assumed uncorrelated between replications and the $K \times K$ measurement covariance matrix of each replication is assumed to be $\mathbf{\Sigma_{E_K}} = \sigma_E^2\mathbf{U_{E_K}}$. Then

$$\mathbf{U_{E_{NK}}} = \begin{bmatrix} \mathbf{U_{E_K}} & \mathbf{0_K} & \dots & \mathbf{0_K} \\ \mathbf{0_K} & \mathbf{U_{E_K}} & \dots & \mathbf{0_K} \\ \vdots & \vdots & \dots & \vdots \\ \mathbf{0_K} & \mathbf{0_K} & \dots & \mathbf{U_{E_K}} \end{bmatrix} \tag{329}$$

and from equation (328),

$$\mathbf{\Sigma}_{\mathbf{Y_{NK}}} = \mathbf{\Sigma}_{\mathbf{E}} + \mathbf{\Sigma}_{\mathbf{fZ_{NK}}} = \sigma_E^2 \mathbf{U}_{\mathbf{E_{NK}}} + \sigma_x^2 \mathbf{U}_{\mathbf{fZ_{NK}}} = \sigma_E^2 \mathbf{U}_{\mathbf{Y_{NK}}} \tag{330}$$

where $NK \times NK$ covariance matrix $\mathbf{\Sigma}_{\mathbf{fZ_{NK}}}$ is given by

$$\mathbf{\Sigma}_{\mathbf{fZ_{NK}}} = \sigma_x^2 \mathbf{U}_{\mathbf{fZ_{NK}}} = \sigma_x^2 \mathbf{H}^{\mathbf{T}} \mathbf{U}_{\mathbf{fZ_K}} \mathbf{H} \tag{331}$$

From equation (330), $\mathbf{U}_{\mathbf{Y_{NK}}}$ can be expanded into

$$\mathbf{U}_{\mathbf{Y_{NK}}} = \mathbf{U}_{\mathbf{E_{NK}}} + \alpha \mathbf{U}_{\mathbf{fZ_{NK}}} = \begin{bmatrix} \mathbf{U}_{\mathbf{E_{NK}}} + \alpha \mathbf{U}_{\mathbf{fZ_K}} & \alpha \mathbf{U}_{\mathbf{fZ_K}} & \dots & \alpha \mathbf{U}_{\mathbf{fZ_K}} \\ \alpha \mathbf{U}_{\mathbf{fZ_K}} & \mathbf{U}_{\mathbf{E_K}} + \alpha \mathbf{U}_{\mathbf{fZ_K}} & \dots & \alpha \mathbf{U}_{\mathbf{fZ_K}} \\ \vdots & \vdots & \dots & \vdots \\ \alpha \mathbf{U}_{\mathbf{fZ_K}} & \alpha \mathbf{U}_{\mathbf{fZ_K}} & \dots & \mathbf{U}_{\mathbf{E_K}} + \alpha \mathbf{U}_{\mathbf{fZ_K}} \end{bmatrix} \tag{332}$$

where α is defined in equation (320).

The inverse of $NK \times NK$ matrix $\mathbf{U}_{\mathbf{Y_{NK}}}$ can be computed in terms of $K \times K$ matrices $\mathbf{U}_{\mathbf{fZ_K}}$ and $\mathbf{U}_{\mathbf{E_K}}$ as follows. Define $K \times K$ matrix $\mathbf{B}$ as

$$\mathbf{B} \equiv [\mathbf{U}_{\mathbf{E_K}} + (N-1)\alpha \mathbf{U}_{\mathbf{fZ_K}}]^{-1} \mathbf{U}_{\mathbf{fZ_K}} \tag{333}$$

and $K \times K$ matrix $\mathbf{A}$ as

$$\mathbf{A} \equiv \left\{ \mathbf{U}_{\mathbf{E_K}} + \alpha \mathbf{U}_{\mathbf{fZ_K}} [\mathbf{I_K} - (N-1)\mathbf{B}] \right\}^{-1} \tag{334}$$

If the inverse matrices of equations (333) and (334) exist, then $\mathbf{U}_{\mathbf{Y_{NK}}}^{-1}$ can be shown to be given by

$$\mathbf{U}_{\mathbf{Y_{NK}}}^{-1} = \mathbf{D_{NK}} - \mathbf{H}^{\mathbf{T}} \mathbf{BAH} = \begin{bmatrix} \mathbf{A} & -\mathbf{BA} & \dots & -\mathbf{BA} \\ -\mathbf{BA} & \mathbf{A} & \dots & -\mathbf{BA} \\ \vdots & \vdots & \dots & \vdots \\ -\mathbf{BA} & -\mathbf{BA} & \dots & \mathbf{A} \end{bmatrix} \tag{335}$$

where $NK \times NK$ block-diagonal matrix $\mathbf{D_{NK}}$ is constructed from N replications of $K \times K$ matrix $(\mathbf{A} + \mathbf{BA})$ as

$$\mathbf{D_{NK}} = \begin{bmatrix} \mathbf{A} + \mathbf{BA} & \mathbf{0_K} & \dots & \mathbf{0_K} \\ \mathbf{0_K} & \mathbf{A} + \mathbf{BA} & \dots & \mathbf{0_K} \\ \vdots & \vdots & \dots & \vdots \\ \mathbf{0_K} & \mathbf{0_K} & \dots & \mathbf{A} + \mathbf{BA} \end{bmatrix} \tag{336}$$

For the linear case $M_z \times M_z$ moment matrix $\mathbf{Q_{NK}}$ can now be computed in terms of $K \times K$ matrices as follows:

$$\mathbf{Q_{NK}} = \mathbf{Z_{NK}^T U_{Y_{NK}}^{-1} Z_{NK}} = (\mathbf{Z_K^T H})\mathbf{U_{Y_{NK}}^{-1}}(\mathbf{Z_K^T H})^{\mathbf{T}} \tag{337}$$

It can readily be seen from equations (314), (335), and (336) that

$$\mathbf{H U_{Y_{NK}}^{-1} H^T} = \mathbf{H}(\mathbf{D_{NK}} - \mathbf{H^T B A H})\mathbf{H^T} = N[\mathbf{I_K} - (N-1)\mathbf{B}]\mathbf{A} \tag{338}$$

Hence for the linear case,

$$\mathbf{Q_{NK}} = N\mathbf{Z_K^T}[\mathbf{I_K} - (N-1)\mathbf{B}]\mathbf{A}\,\mathbf{Z_K} \tag{339}$$

For the nonlinear case, a single replication of experimental design $\mathbf{Z_K}$, evaluation of equation (271) yields $K \times M_c$ matrix $\mathbf{F_{c_K}}$. Then over N replications of $\mathbf{Z_K}$, with design matrix $\mathbf{Z_{NK}}$ given by equation (308), equation (271) yields $NK \times M_c$ matrix $\mathbf{F_{c_{NK}}} = \mathbf{H^T F_{c_K}}$. If equation (275) holds, it follows from equation (338) that

$$\begin{aligned}\mathbf{R} &\approx \mathbf{F_{c_{NK}}^T U_{Y_{NK}}^{-1} F_{c_{NK}}} = \mathbf{F_{c_K}^T H U_{Y_{NK}}^{-1} H^T F_{c_K}} \\ &= N\mathbf{F_{c_K}^T}[\mathbf{I_K} - (N-1)\mathbf{B}]\mathbf{A}\mathbf{F_{c_K}}\end{aligned} \tag{340}$$

Equation (340) permits computation of confidence and prediction intervals for replicated calibration data in terms of $K \times K$ matrices; thereby, required computer storage and computational resources are reduced when N is large.

With reference to equations (188) and (189), the analysis of variance null hypothesis assumes that if matrix $\mathbf{U_{Y_{NK}}} = \mathbf{I_{NK}}$; then matrix $\mathbf{P} = \mathbf{I_{NK}}$. If equation (280) holds, then for the null hypothesis $M_c \times M_c$ matrix $\mathbf{R}$ becomes

$$\begin{aligned}\mathbf{R} &\approx \mathbf{F_{c_{NK}}^T F_{c_{NK}}} = \mathbf{F_{c_K}^T H H^T F_{c_K}} \\ &= N\mathbf{F_{c_K}^T F_{c_K}}\end{aligned} \tag{341}$$

It follows that $NK \times NK$ matrix $\mathbf{\Omega_{F_{NK}}}$, given in equation (286), is given by

$$\begin{aligned}\mathbf{\Omega_{F_{NK}}} &= \mathbf{F_{c_{NK}} R^{-1} F_{c_{NK}}^T} = \frac{1}{N}\mathbf{H^T F_{c_K}}(\mathbf{F_{c_K}^T F_{c_K}})^{-1}\mathbf{F_{c_K}^T H} \\ &= \frac{1}{N}\mathbf{H^T \Omega_{F_K} H}\end{aligned} \tag{342}$$

where $K \times K$ matrix $\mathbf{\Omega_{FK}}$ is obtained from equation (286) as

$$\mathbf{\Omega_{FK}} = \mathbf{F_{c_K}}(\mathbf{F_{c_K}^T F_{c_K}})^{-1}\mathbf{F_{c_K}^T} \tag{343}$$

As shown in equation (291), matrices $\mathbf{\Omega_{F_K}}$ and $\mathbf{\Omega_{F_{NK}}}$ are symmetric and idempotent with rank M_c.

A4.3. Analysis of Variance of Replicated Calibrations.

Analysis of variance of replicated calibrations provides tests of significance for the presence of bias uncertainty due to input loading errors or mathematical modeling errors, as well as for nonstationarity of estimated parameters. The analysis of variance is developed in this section with single-input–single-output process notation. Note that similar results are obtained for the general multi-input–single output case by replacing $\mathbf{\Omega_{NK}}$, $\mathbf{\Omega_K}$, $\mathbf{W_{NK}}$, $\mathbf{W_K}$, and M_z by $\mathbf{\Omega_{F_{NK}}}$, $\mathbf{\Omega_{F_K}}$, $\mathbf{W_{F_{NK}}}$, $\mathbf{WF_K}$, and M_c, respectively.

Let the null hypothesis (ref. 7) assume that input loading uncertainties and modeling errors are zero and that $NK \times 1$ measurement uncertainty vector $\boldsymbol{\epsilon_E}$ has $NK \times NK$ covariance matrix $\mathbf{\Sigma_E} = \sigma_E^2 \mathbf{I_{NK}}$. Then $NK \times NK$ matrices $\mathbf{U}$ and $\mathbf{P}$ are both equal to $\mathbf{I_{NK}}$ and do not appear in the following equations. Transformed output vector $\mathbf{v}$ is equal to and replaced by observed output vector $\mathbf{y}$.

The $K \times K$ matrix $\mathbf{W_K}$ is defined in equation (225) as

$$\mathbf{W_K} = \mathbf{I_K} - \mathbf{\Omega_K} \tag{344}$$

Matrix $\mathbf{W_{F_K}}$ is defined similarly in equation (290). After N replications $K \times K$ matrix $\mathbf{W_K}$ expands to $NK \times NK$ matrix $\mathbf{W_{NK}}$ given as

$$\mathbf{W_{NK}} = \mathbf{I_{NK}} - \mathbf{\Omega_{NK}} \tag{345}$$

where matrices $\mathbf{\Omega_{NK}}$ and $\mathbf{\Omega_{F_{NK}}}$ are in equations (326) and (342) and has rank M_z. Since $\mathbf{\Omega_{NK}}$ is idempotent, then by Lemma 7 matrix $\mathbf{W_{NK}}$ is idempotent with rank $NK - M_z$.

For use in the development, define $NK \times NK$ matrix $\mathbf{G_H}$ as

$$\mathbf{G_H} \equiv \frac{1}{N}\mathbf{H^T H} = \frac{1}{N}\begin{bmatrix} \mathbf{I_K} & \mathbf{I_K} & \dots & \mathbf{I_K} \\ \vdots & \vdots & \dots & \vdots \\ \mathbf{I_K} & \mathbf{I_K} & \dots & \mathbf{I_K} \end{bmatrix} \tag{346}$$

It is readily seen that $\mathbf{G_H}$ is idempotent with rank K. By Lemma 7, matrix $\mathbf{I_{NK}} - \mathbf{G_H}$ is idempotent with rank $NK - K$.

Next $\mathbf{G_H}$ is shown to be a two-sided identity of any matrix of the form $1/N\mathbf{H^T A H}$, in particular $\mathbf{\Omega_{NK}}$. Indeed, from equations (326) and (342),

$$\begin{aligned} \mathbf{G_H \Omega_{NK}} &= \frac{1}{N^2}\mathbf{H^T H H^T \Omega_K H} = \frac{1}{N}\mathbf{H^T \Omega_K H} = \mathbf{\Omega_{NK}} \\ &= \frac{1}{N^2}\mathbf{H^T \Omega_K H H^T H} = \mathbf{\Omega_{NK} G_H} \end{aligned} \tag{347}$$

From equations (345) and (347),

$$\mathbf{G_H W_{NK}} = \mathbf{W_{NK} G_H} \tag{348}$$

Therefore, $NK \times NK$ matrix product $\mathbf{W_{NK}G_H W_{NK}}$, to be used later, is idempotent. Also, it is seen that

$$\begin{aligned}\mathbf{W_{NK}G_H W_{NK}} &= (\mathbf{I_{NK}} - \mathbf{\Omega_{NK}})\mathbf{G_H}(\mathbf{I_{NK}} - \mathbf{\Omega_{NK}}) = (\mathbf{G_H} - \mathbf{\Omega_{NK}})(\mathbf{I_{NK}} - \mathbf{\Omega_{NK}}) \\ &= \mathbf{G_H} - \mathbf{\Omega_{NK}}\end{aligned} \tag{349}$$

Since $\mathbf{G_H}$ has rank K and $\mathbf{\Omega_{NK}}$ has rank M_z, it follows from Lemmas 5 and 6 and equation (349) that product $\mathbf{W_{NK}G_H W_{NK}}$ has rank $K - M_z$. Note that $K - M_z > 0$.

Estimated $M_z \times 1$ parameter vector $\widehat{\mathbf{c}}$, $NK \times 1$ predicted output vector $\widehat{\mathbf{y}}$, and $NK \times 1$ residual vector $\widehat{\mathbf{e}}$ are obtained with equations (218), (223), and (224), respectively, for a linear process, and equations (270), (285), and (289), respectively, for a nonlinear process. Recall from equation (224) that $\widehat{\mathbf{e}}$ can be expressed as

$$\widehat{\mathbf{e}} = \mathbf{W_{NK}}\boldsymbol{\epsilon}_\mathbf{E} \tag{350}$$

with zero expected value and $NK \times NK$ covariance matrix $\sigma^2\mathbf{W_{NK}}$.

Let $\widehat{\mathbf{e}}_\mathbf{n}$ denote the $K \times 1$ residual vector at the nth replication, which has zero expected value and covariance matrix $\sigma^2\mathbf{W_K}$. Then residual vector $\widehat{\mathbf{e}}$ can be partitioned into N, $K \times 1$ subvectors as shown below:

$$\widehat{\mathbf{e}}^\mathbf{T} = \begin{bmatrix}\widehat{\mathbf{e}}_1^\mathbf{T} & \widehat{\mathbf{e}}_2^\mathbf{T} & \ldots & \widehat{\mathbf{e}}_\mathbf{N}^\mathbf{T}\end{bmatrix}^\mathbf{T} \tag{351}$$

Let $\bar{\mathbf{e}}_\mathbf{K}$ denote the mean value of the set of residual vectors $\widehat{\mathbf{e}}_\mathbf{n}$ averaged over N replications; that is,

$$\bar{\mathbf{e}}_\mathbf{K} = \frac{1}{N}\sum_{n=1}^{N}\widehat{\mathbf{e}}_\mathbf{n} = \frac{1}{N}\mathbf{H}\widehat{\mathbf{e}} = \frac{1}{N}\mathbf{HW_{NK}}\boldsymbol{\epsilon}_\mathbf{E} \tag{352}$$

The residual sum of squares, denoted by S_{SE}, is defined in equation (231) as

$$S_{SE} \equiv \widehat{\mathbf{e}}^\mathbf{T}\widehat{\mathbf{e}} = \boldsymbol{\epsilon}_\mathbf{E}^\mathbf{T}\mathbf{W_{NK}}\boldsymbol{\epsilon}_\mathbf{E} \tag{353}$$

By Theorem 1, S_{SE} is chi-square distributed with $NK - M_z$ degrees of freedom; the standard error of the regression given by

$$S_E = \left(\frac{S_{SE}}{NK - M_z}\right)^{1/2} \tag{354}$$

is an unbiased estimate of σ.

Residual sum of squares S_{SE} can be partitioned into the following sum of quadratic forms:

$$S_{SE} = \widehat{\mathbf{e}}^{\mathbf{T}}\widehat{\mathbf{e}} = \widehat{\mathbf{e}}^{\mathbf{T}}\mathbf{W}_{\mathbf{NK}}\mathbf{G}_{\mathbf{H}}\mathbf{W}_{\mathbf{NK}}\widehat{\mathbf{e}} + \widehat{\mathbf{e}}^{\mathbf{T}}\left(\mathbf{I}_{\mathbf{NK}} - \mathbf{W}_{\mathbf{NK}}\mathbf{G}_{\mathbf{H}}\mathbf{W}_{\mathbf{NK}}\right)\widehat{\mathbf{e}} \tag{355}$$

By using equations (348) and (350) and the fact that $\mathbf{W}_{\mathbf{NK}}$ is idempotent, S_{SE} can be expressed as

$$S_{SE} = \boldsymbol{\epsilon}_{\mathbf{E}}^{\mathbf{T}}\mathbf{W}_{\mathbf{NK}}\mathbf{G}_{\mathbf{H}}\mathbf{W}_{\mathbf{NK}}\boldsymbol{\epsilon}_{\mathbf{E}} + \boldsymbol{\epsilon}_{\mathbf{E}}^{\mathbf{T}}\mathbf{W}_{\mathbf{NK}}\left(\mathbf{I}_{\mathbf{NK}} - \mathbf{G}_{\mathbf{H}}\right)\mathbf{W}_{\mathbf{NK}}\boldsymbol{\epsilon}_{\mathbf{E}} \tag{356}$$

Denote the first right-hand term in equation (355) by S_{SX} as follows:

$$S_{SX} \equiv \widehat{\mathbf{e}}^{\mathbf{T}}\mathbf{W}_{\mathbf{NK}}\mathbf{G}_{\mathbf{H}}\mathbf{W}_{\mathbf{NK}}\widehat{\mathbf{e}} = \boldsymbol{\epsilon}_{\mathbf{E}}^{\mathbf{T}}\mathbf{W}_{\mathbf{NK}}\mathbf{G}_{\mathbf{H}}\mathbf{W}_{\mathbf{NK}}\boldsymbol{\epsilon}_{\mathbf{E}} \tag{357}$$

which follows from equation (350) and the fact that $\mathbf{W}_{\mathbf{NK}}$ is idempotent. Then S_{SX} can be expressed as

$$S_{SX} = \boldsymbol{\epsilon}_{\mathbf{E}}^{\mathbf{T}}\mathbf{W}_{\mathbf{NK}}\mathbf{G}_{\mathbf{H}}\mathbf{W}_{\mathbf{NK}}\boldsymbol{\epsilon}_{\mathbf{E}} = N\bar{\mathbf{e}}_{\mathbf{K}}^{\mathbf{T}}\bar{\mathbf{e}}_{\mathbf{K}} \tag{358}$$

which follows from equations (350), (352), and (357). It has been shown that $\mathbf{W}_{\mathbf{NK}}\mathbf{G}_{\mathbf{H}}\mathbf{W}_{\mathbf{NK}}$ is idempotent with $K - M_{\mathbf{z}}$ degrees of freedom. Therefore, it follows from equation (358) and Theorem 1 that S_{SX}/σ_E^2 is chi-square distributed with $K - M_{\mathbf{z}}$ degrees of freedom. Define the root-mean-square value of S_{SX} as

$$S_X \equiv \left(\frac{S_{SX}}{K - M_{\mathbf{z}}}\right)^{1/2} \tag{359}$$

Variable S_X is interpreted as the standard error due to bias uncertainty.

Consider next the second right-hand term of S_{SE} in equation (355). Define S_{SM} as

$$S_{SM} \equiv \sum_{k=1}^{K}\sum_{n=1}^{N}(\widehat{e}_{n_k} - \bar{e}_k)^2 = \sum_{n=1}^{N}(\widehat{\mathbf{e}}_{\mathbf{n}} - \bar{\mathbf{e}}_{\mathbf{k}})^{\mathbf{T}}(\widehat{\mathbf{e}}_{\mathbf{n}} - \bar{\mathbf{e}}_{\mathbf{K}}) \tag{360}$$

where $\widehat{e}_{n_k}$ is the kth element of $K \times 1$ residual vector $\widehat{\mathbf{e}}_{\mathbf{n}}$, and $\bar{e}_k$ is the kth element of $K \times 1$ vector $\bar{\mathbf{e}}_{\mathbf{k}}$. Variable S_{SM} is seen to equal the sum of squares about the means of the set of N residual vectors $\widehat{\mathbf{e}}_{\mathbf{n}}$ each of dimension $K \times 1$. It follows from the definition of $\mathbf{H}$ that

$$S_{SM} = \sum_{n=1}^{N}(\widehat{\mathbf{e}}_{\mathbf{n}} - \bar{\mathbf{e}}_{\mathbf{K}})^{\mathbf{T}}(\widehat{\mathbf{e}}_{\mathbf{n}} - \bar{\mathbf{e}}_{\mathbf{K}}) = (\widehat{\mathbf{e}} - \mathbf{H}^{\mathbf{T}}\bar{\mathbf{e}}_{\mathbf{K}})^{\mathbf{T}}(\widehat{\mathbf{e}} - \mathbf{H}^{\mathbf{T}}\bar{\mathbf{e}}_{\mathbf{K}}) \tag{361}$$

Define $NK \times 1$ vector $\mathbf{e}_{\mathbf{M}}$ as follows and use equations (350) and (352) to obtain the result

$$\begin{aligned}\mathbf{e}_{\mathbf{M}} &\equiv \widehat{\mathbf{e}} - \mathbf{H}^{\mathbf{T}}\bar{\mathbf{e}}_{\mathbf{K}} = \widehat{\mathbf{e}} - \frac{1}{N}\mathbf{H}^{\mathbf{T}}\mathbf{H}\widehat{\mathbf{e}} = (\mathbf{I}_{\mathbf{NK}} - \mathbf{G}_{\mathbf{H}})\widehat{\mathbf{e}} \\ &= (\mathbf{I}_{\mathbf{NK}} - \mathbf{G}_{\mathbf{H}})\mathbf{W}_{\mathbf{NK}}\boldsymbol{\epsilon}_{\mathbf{E}}\end{aligned} \tag{362}$$

By using equations (360) to (362),

$$S_{SM} = \mathbf{e_M^T e_M} = \boldsymbol{\epsilon}_\mathbf{E}^\mathbf{T} \mathbf{W_{NK}} (\mathbf{I_{NK}} - \mathbf{G_H}) \mathbf{W_{NK}} \boldsymbol{\epsilon}_\mathbf{E} \tag{363}$$

Comparison of equations (356) and (363) shows that S_{SM} equals the second right-hand term of S_{SE}. Moreover, it is clear that matrix product

$$\mathbf{W_{NK}}(\mathbf{I_{NK}} - \mathbf{G_H})\mathbf{W_{NK}} = \mathbf{W_{NK}} - \mathbf{W_{NK}}\mathbf{G_H}\mathbf{W_{NK}}$$

is idempotent and, by Lemmas 5 and 6, has rank $NK - K$, since $\mathbf{W_{NK}}$ has rank $NK - M_\mathbf{z}$, and $\mathbf{W_{NK}}\mathbf{G_H}\mathbf{W_{NK}}$ has rank $K - M_\mathbf{z}$. By Theorem 1, S_{SM}/σ_E^2 is chi-square distributed with $NK - K$ degrees of freedom. Variable S_{SM} can be interpreted as the portion of residual sum of squares S_{SE} due to measurement uncertainty. The root-mean-square value

$$S_M = \left(\frac{S_{SM}}{NK - K} \right)^{1/2} \tag{364}$$

is interpreted as an estimate of the standard deviation σ_E of the measurement uncertainty.

It follows from Theorem 2 that S_{SX} and S_{SM} are independent. Therefore, the ratio $T_{X_M} = [S_{SX}/(K - M_\mathbf{z})]/[S_{SM}/(NK - K)]$ is F-distributed with $K - M_\mathbf{z}$, $NK - K$ degrees of freedom. The test of significance for the existence of distinct input loading biases is as follows. Assume as the null hypothesis that input loading bias error and modeling error are zero. Form the expression

$$T_{X_M} = \frac{S_{SX}/(K - M_\mathbf{z})}{S_{SM}/(NK - K)} > F_{K-M_\mathbf{z},\ NK-K}(\alpha) \tag{365}$$

If inequality (365) is satisfied, then the null hypothesis that both input loading bias error and modeling error equal zero is rejected at confidence level α.

A4.4. Stationarity Test of Estimated Parameters.

A test is developed for nonstationarity of estimated individual parameter $\widehat{c}_m \in \widehat{\mathbf{c}}$ over N replicated calibrations. Let $\widehat{\mathbf{c}}_{\mathbf{R}_n}$ denote the parameter vector estimated at the nth replication by a K-point regression, with residual sum-of-squares S_{SR_n}, for $n = 1, \ldots, N$. Define

$$S_{SR} = \sum_{n=1}^{N} \mathbf{S_{SR}}_n \tag{366}$$

Let $\widehat{\mathbf{c}}$ denote the parameter vector estimated by an NK-point global regression over the complete set of N replicated calibrations. To test for stationarity of parameter c_m replace the mth element of $\widehat{\mathbf{c}}_{\mathbf{R}_n}$ by $\widehat{c}_m \in \widehat{\mathbf{c}}$ and compute resulting the error sum-of-squares, denoted by $S_{SG_{m,n}}$ for $n = 1, \ldots, N$. Compute $S_{SG_m} = \sum S_{SG_{m,n}}$ for n = 1, ..., N. The ratio $(S_{SG_m} - S_{SR})/S_{SR}$ is subsequently shown to be F-distributed and thereby provides a test of significance for nonstationarity of the estimated value of c_m over the N replicated calibrations.

The null hypothesis assumes that calibration standard errors and modeling errors are zero and that estimated parameter vector $\widehat{\mathbf{c}}_{\mathbf{R}_n}$ is stationary over the N replications. Let $NK \times 1$ measurement error vector $\boldsymbol{\epsilon}_{\mathbf{E}}$ be partitioned among the N replications as $[\boldsymbol{\epsilon}_{\mathbf{E}_1}^{\mathbf{T}} ... \boldsymbol{\epsilon}_{\mathbf{E}_N}^{\mathbf{T}}]^{\mathbf{T}}$, where $\boldsymbol{\epsilon}_{\mathbf{E}_n}$ denotes the $K \times 1$ measurement error vector at the nth replication. Also, let $\delta\widehat{\mathbf{c}}_{\mathbf{R}_n}$ denote the uncertainty of the nth estimated parameter vector, which is obtained from equation (281) as

$$\delta\widehat{\mathbf{c}}_{\mathbf{R}_n} = -\mathbf{R}^{-1}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\boldsymbol{\epsilon}_{\mathbf{E}_n} \tag{367}$$

The uncertainty of element $\widehat{c}_{R_{m,n}} \in \widehat{\mathbf{c}}_{\mathbf{R}_n}$ is seen to be

$$\delta\widehat{c}_{R_{m,n}} = -\mathbf{p}_m^{\mathbf{T}}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\boldsymbol{\epsilon}_{\mathbf{E}_n} \tag{368}$$

where $\mathbf{p}_m^{\mathbf{T}}$ is the mth row of $\mathbf{R}^{-1}$. Similarly, the uncertainty of globally estimated parameter vector $\widehat{\mathbf{c}}_{\mathbf{G}}$ is given by

$$\delta\widehat{\mathbf{c}}_{\mathbf{G}} = -\frac{1}{N}\mathbf{R}^{-1}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{H}\boldsymbol{\epsilon}_{\mathbf{E}} \tag{369}$$

and the uncertainty of element $\widehat{c}_{G_m} \in \widehat{\mathbf{c}}_{\mathbf{G}}$ is

$$\delta\widehat{c}_{G_m} = -\frac{1}{N}\mathbf{p}_m^{\mathbf{T}}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\mathbf{H}\boldsymbol{\epsilon}_{\mathbf{E}} \tag{370}$$

The residual vector of the nth replication, denoted by $\widehat{\mathbf{e}}_{\mathbf{R}_n}$, is found by using equation (288) as

$$\widehat{\mathbf{e}}_{\mathbf{R}_n} = \mathbf{F}_{\mathbf{c}}\delta\widehat{\mathbf{c}}_{\mathbf{R}_n} + \boldsymbol{\epsilon}_{\mathbf{E}_n} \tag{371}$$

Replace $\widehat{c}_{R_{m,n}}$ by $\widehat{c}_{\mathbf{G}_m}$ in equation (371) to obtain the error vector of the nth replication computed with the globally estimated value of parameter c_m, which is denoted by $\widehat{\mathbf{e}}_{G_{m,n}}$. From equations (368) to (371), the difference between error vectors $\widehat{\mathbf{e}}_{G_{m,n}}$ and $\widehat{\mathbf{e}}_{R_n}$ is given by

$$\widehat{\mathbf{e}}_{GR_{m,n}} = \mathbf{f}_{\mathbf{c}_m}\mathbf{p}_m^{\mathbf{T}}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}\left(\boldsymbol{\epsilon}_{\mathbf{E}_n} - \frac{1}{N}\mathbf{H}\boldsymbol{\epsilon}_{\mathbf{E}}\right) \tag{372}$$

where $\mathbf{f}_{\mathbf{c}_m}$ is the mth column of $\mathbf{F}_{\mathbf{c}}$.

Let $NK \times 1$ error vector $\widehat{\mathbf{e}}_{\mathbf{GR}_m} = \left[\widehat{\mathbf{e}}_{GR_{m,1}}^{\mathbf{T}} ... \widehat{\mathbf{e}}_{GR_{m,N}}^{\mathbf{T}}\right]^{\mathbf{T}}$, which can then be expressed in terms of $NK \times 1$ measurement error vector $\boldsymbol{\epsilon}_{\mathbf{E}}$ as

$$\widehat{\mathbf{e}}_{\mathbf{GR}_m} = \left(\mathbf{I}_{\mathbf{A}} - \frac{1}{N}\mathbf{H}^{\mathbf{T}}\mathbf{A}\mathbf{H}\right)\boldsymbol{\epsilon}_{\mathbf{E}} \tag{373}$$

where $K \times K$ matrix $\mathbf{A} = \mathbf{f}_{\mathbf{c}_m}\mathbf{p}_m^{\mathbf{T}}\mathbf{F}_{\mathbf{c}}^{\mathbf{T}}$ and $NK \times NK$ block diagonal matrix $\mathbf{I}_{\mathbf{A}}$ is defined as

$$\mathbf{I_A} = \begin{bmatrix} \mathbf{A} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{A} & \dots & \mathbf{0} \\ \vdots & \vdots & \dots & \vdots \\ \mathbf{0} & \mathbf{0} & \dots & \mathbf{A} \end{bmatrix} \tag{374}$$

It is seen that the inner product $\widehat{\mathbf{e}}^{\mathbf{T}}_{\mathbf{GR}_m}\widehat{\mathbf{e}}_{\mathbf{GR}_m}$ equals $(S_{SG_m} - S_{SR})$. Clearly $\mathbf{A}$ has rank 1. It follows from equation (280) that $\mathbf{p}^{\mathbf{T}}_m\mathbf{F}^{\mathbf{T}}_{\mathbf{c}}\mathbf{f}_{\mathbf{c}_m} = 1$. Hence,

$$\mathbf{AA} = \mathbf{f}_{\mathbf{c}_m}\mathbf{p}^{\mathbf{T}}_m\mathbf{F}^{\mathbf{T}}_{\mathbf{c}}\mathbf{f}_{\mathbf{c}_m}\mathbf{p}^{\mathbf{T}}_m\mathbf{F}^{\mathbf{T}}_{\mathbf{c}} = \mathbf{f}_{\mathbf{c}_m}\mathbf{p}^{\mathbf{T}}_m\mathbf{F}^{\mathbf{T}}_{\mathbf{c}} = \mathbf{A}$$

and $\mathbf{A}$ is idempotent. It can then be seen that $\mathbf{I_A}$ is idempotent with rank N, since $\mathbf{A}$ is idempotent with rank 1. Thus $\mathbf{I_A} - 1/\mathbf{NH^TAH}$ is idempotent with rank $(N-1)$, and therefore the inner product $\widehat{\mathbf{e}}^{\mathbf{T}}_{\mathbf{GR}_m}\widehat{\mathbf{e}}_{\mathbf{GR}_m}$ can be expressed as

$$S_{SG_m} - S_{SR} = \widehat{\mathbf{e}}^{\mathbf{T}}_{\mathbf{GR}_m}\widehat{\mathbf{e}}_{\mathbf{GR}_m} = \boldsymbol{\epsilon}^{\mathbf{T}}_{\mathbf{E}}\left(\mathbf{I_A} - \frac{1}{N}\mathbf{H^TAH}\right)\boldsymbol{\epsilon}_{\mathbf{E}} \tag{375}$$

It follows from Theorem 1 that $S_{SG_m} - S_{SR}$ is chi-square distributed with $N-1$ degrees of freedom.

The residual sum of squares of the nth replicated regression, $S_{SR_n} = \boldsymbol{\epsilon}^{\mathbf{T}}_{\mathbf{E}_n}\mathbf{W_K}\boldsymbol{\epsilon}_{\mathbf{E}_n}$, has been shown as chi-square distributed with $K - M_{\mathbf{z}}$ degrees of freedom. Because the error vectors $\boldsymbol{\epsilon}_{\mathbf{E}_n}$ are mutually independent, it follows from equation (366) and Theorem 2 that the total replicated sum of squares S_{SR} is chi-square distributed with $N(K - M_{\mathbf{z}})$ degrees of freedom. Therefore, if the following inequality is satisfied

$$T_{cm} = \frac{(S_{SG_m} - S_{SR})/(N-1)}{S_{SR}/[N(K - M_{\mathbf{z}})]} > F_{(N-1),\, N(K-M_{\mathbf{z}})}(\alpha) \tag{376}$$

then the null hypothesis that parameter c_m is stationary is rejected at confidence level α.

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13. ABSTRACT *(Maximum 200 words)*

Experimental aerodynamic researchers require estimated precision and bias uncertainties of measured physical quantities, typically at 95 percent confidence levels. Uncertainties of final computed aerodynamic parameters are obtained by propagation of individual measurement uncertainties through the defining functional expressions. In this paper, rigorous mathematical techniques are extended to determine precision and bias uncertainties of any instrument-sensor system. Through this analysis, instrument uncertainties determined through calibration are now expressed as functions of the corresponding measurement for linear and nonlinear univariate and multivariate processes. Treatment of correlated measurement precision error is developed. During laboratory calibration, calibration standard uncertainties are assumed to be an order of magnitude less than those of the instrument being calibrated. Often calibration standards do not satisfy this assumption. This paper applies rigorous statistical methods for inclusion of calibration standard uncertainty and covariance due to the order of their application. The effects of mathematical modeling error on calibration bias uncertainty are quantified. The effects of experimental design on uncertainty are analyzed. The importance of replication is emphasized; techniques for estimation of both bias and precision uncertainties using replication are developed. Statistical tests for stationarity of calibration parameters over time are obtained.

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