# IRREGULARITIES IN X(Y) FROM Y(X) IN LINEAR CALIBRATION

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Abstract. Let $X$ be an input measurement and $Y$ the output reading of a calibrated instrument, with $Y(X)$ as the calibration curve. Solving $X(Y)$ projects an instrumental reading back onto the scale of measurements as an object of pivotal interest. Arrays of instrumental readings are projected in this manner in practice, yielding arrays of calibrated measurements, typically subject to errors of calibration. Effects of calibration errors on properties of calibrated measurements are examined here under linear calibration. Irregularities arise as induced dependencies, inflated variances, nonstandard distributions, inconsistent sample means, the underestimation of measurement variance, and other unintended consequences. On the other hand, conventional properties are seen to remain largely in place in the use of selected regression diagnostics, and in one–way comparative experiments using calibrated data.

## 1. Introduction

Measurements enable the sciences and engineering, typically through calibrated instruments subject to errors of calibration. Statistical issues in calibration are considered in references [1]–[11], for example, all focused on the calibration of instruments *per se,* rather than their subsequent and repeated usage. All are linked to error–induced irregularities in arrays of calibrated measurements, but these largely have been overlooked in the archival literature. Our intent here is to bridge these gaps for the case of classically calibrated data, as are often encountered in practice.

To fix ideas, instrumental readings $\{U_1, \ldots, U_m\}$ during calibration are observed at measurements $\{X_1, \ldots, X_m\}$ without error, under the model $U(X)$, namely $\{U_i = \beta_0 + \beta_1 X_i + \epsilon_i; 1 \le i \le m\}$, giving the least–squares calibration line $\widehat{U} = \widehat{\beta}_0 + \widehat{\beta}_1 X$, together with the calibrated measurement $Y = \widehat{X}(U) = (U - \widehat{\beta}_0)/\widehat{\beta}_1$ from a subsequent instrumental reading $U$. For example, in calibrating a laboratory colorimeter for assessing phosphorus content, light transmittance $(U_i)$ from its photocell relates linearly (Beer's law) to input $(X_i)$ in known milligrams of phosphorus. Subsequent colorimetric readings $\{Z_1, \ldots, Z_n\}$, taken during the course of an experiment, then are projected back onto the scale of phosphorus measurements as $\{Y_i = (Z_i - \widehat{\beta}_0)/\widehat{\beta}_1; 1 \le i \le n\}$, to be analyzed as the calibrated entities of note. Periodic checks against a standard then determine when recalibration is required.

*Key words and phrases.* Linear calibration; Induced dependencies; Nonstandard distributions; Diagnostics; Case studies.

Often referred to as *classical calibration,* this is the model of choice here. In contrast, *inverse calibration*, as set forth in the cited references, is based on the *unconventional* model $\{X_i = \gamma_0 + \gamma_1 U_i + \epsilon_i;\, 1 \leq i \leq m\}$, unconventional in that $\{X_i; 1 \leq i \leq m\}$ continue to be taken as measured without error.

There is a long–standing but unresolved debate on the merits of classical versus inverse calibration; see the aforementioned references. Our choice here is guided by its tractability, resting on mathematical statistics *in lieu of* the simulation studies often employed in support of inverse regression. Moreover, parametric and nonparametric procedures often require that sample data $\{Y_1, \ldots, Y_n\}$ should be uncorrelated, or even independent. This clearly fails in calibrated data, regardless of the method of calibration, owing to the propagation of calibration errors across the calibrated measurements. Here we examine these and other irregularities attributable to errors of calibration.

To place the current work in perspective, the following antecedents are germane. As noted, references [1]–[11] focus exclusively on the calibration of instruments *per se,* rather than consequences of their subsequent usage, as found also in a burgeoning literature in the field of *chemometrics.* In contrast, subsequent effects of classical calibration errors are studied in [12], where actual levels for one–sample confidence intervals are found always less than nominal values, with further results regarding tolerance intervals. Moreover, findings in tandem with the present study are reported in [13], but for the case of *direct assays* taking $\{X_i = \gamma_0 + \gamma_1 U_i + \epsilon_i;\, 1 \leq i \leq m\}$ as a *conventional* model having chance variation in $X_i$ but with $\{U_i; 1 \leq i \leq m\}$ as regressors determined without error. The focus there is effects of calibration errors on subsequent statistical analyses, where mixing distributions are required to account properly for stochastic variation attributable to calibration errors. This feature carries over to the present study on subsequent effects of classical calibration errors, but with further technical complications surrounding the use of negative moments. An outline follows.

Section 2 develops notation and other technical support, to include the required mixing distributions of Equations (2.1) and (2.2). Section 3 reexamines the process of calibration, together with irregularities attributable to errors of calibration. Section 4 traces the imprint of these irregularities on various issues in statistical inference. These include inferences regarding the mean and variance in a single sample, with mixing distributions as given in Equations (4.1) and (4.2) of Theorem 3. Extensions include the near preservation of inferences for location and scale in comparative experiments, to include the analysis of one-way experiments as in Equations (4.6) and (4.7) of Theorem 4. The choice of truncation point for slope, as in Remark 1, is based on the correlation between $X$ and $U$. Section 5 examines the ability of model diagnostics to uncover violations incurred through classical calibration based on observations $Y = X(U)$. Section 6 enumerates a variety of illustrative case studies, and Section 7 ends on summary conclusions and a cautionary note. Some collateral details are referred to an Appendix, to include critical features of negative moments, their expansions and properties. A comprehensive list of references is cited encompassing supporting material.

## 2. Preliminaries

2.1. **Notation.** Designate $\mathbb{R}^n$ as Euclidean $n$–space, $\mathbb{R}^n_+$ as its positive orthant, $\mathbb{S}_n$ as the real symmetric $(n \times n)$ matrices, and $\mathbb{S}^+_n$ and $\mathbb{S}^0_n$ as their positive definite and positive semidefinite varieties. Arrays are set in bold type, to include the transpose $\boldsymbol{A}'$ and inverse $\boldsymbol{A}^{-1}$ of $\boldsymbol{A}$; the unit vector $\mathbf{1}_n = [1, \ldots, 1]' \in \mathbb{R}^n$; the identity matrix $\boldsymbol{I}_n$; a block–diagonal matrix $\mathrm{Diag}(\boldsymbol{A}_1, \ldots, \boldsymbol{A}_k)$; and $\boldsymbol{B}_n = (\boldsymbol{I}_n - n^{-1}\mathbf{1}_n\mathbf{1}'_n)$. The trace, determinant, and rank of $\boldsymbol{A}$ are $\mathrm{tr}(\boldsymbol{A})$, $|\,\boldsymbol{A}\,|$, and $\mathrm{r}(\boldsymbol{A})$. Eigenvalues of $\boldsymbol{A} \in \mathbb{S}_n$ are designated as $\{ch_i(\boldsymbol{A}); 1 \le i \le n\}$. Operators $E(\boldsymbol{Y})$ and $\mathrm{V}(\boldsymbol{Y})$ designate the expectation vector and dispersion matrix for $\boldsymbol{Y} \in \mathbb{R}^n$, with $E(Y)$ and $\mathrm{Var}(Y)$ as corresponding values on $\mathbb{R}^1$. Other moments, to include negative moments on $\mathbb{R}^1$, are $\{\mu_r(Z) = E(Z^r);\ r \in \{-2, -1, 1\}\}$ as moments about 0, and $\{\mu_r(Z) = E(Z - \mu_1)^r);\ r \in \{2, 3, 4\}\}$ as central moments. Specifically, let $\kappa_1 = \mu_{-1}(\widehat{\beta})$, $\kappa_2 = \mu_{-2}(\widehat{\beta})$, and $\kappa_{11} = \mathrm{Var}(\widehat{\beta}^{-1}) = \kappa_2 - \kappa_1^2$ in terms of an estimator $\widehat{\beta}$. Expansions and approximations to selected negative moments are undertaken in the Appendix.

2.2. **Special Distributions.** Probability density and cumulative distribution functions are identified as *pdf* and *cdf,* with $\mathcal{L}(\boldsymbol{Y})$ as the law of distribution of $\boldsymbol{Y} \in \mathbb{R}^n$. Distributions of note on $\mathbb{R}^1$ include $N_1(\mu, \sigma^2)$ as the Gaussian law with parameters $(\mu, \sigma^2)$; $N^b_a(\mu_T, \sigma^2_T)$ as $N_1(\mu, \sigma^2)$ restricted to $[a, b]$; and noncentral versions of Student's $t(\nu, \lambda)$, chi–squared $\chi^2(\nu, \lambda)$, and Snedecor–Fisher $F(\nu_1, \nu_2, \lambda)$ distributions, having $\{\nu, \nu_1, \nu_2\}$ as degrees of freedom and noncentrality $\lambda$. Specifically, $g_{t^2}(u; \nu, \lambda)$ and $g_F(u; \nu_1, \nu_2, \lambda)$ designate the densities corresponding to $t^2(\nu, \lambda)$ and $F(\nu_1, \nu_2, \lambda)$, respectively, and $\Gamma^d_c(\nu, \lambda)$ is the restriction of $\chi^2(\nu, \lambda)$ to the interval $[c, d]$ in $\mathbb{R}^1_+$.

Distributions on $\mathbb{R}^n$ include $N_n(\boldsymbol{\theta}, \boldsymbol{\Sigma})$ as the Gaussian law, and $g_n(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\Sigma})$ as its *pdf,* having location–scale parameters $(\boldsymbol{\theta}, \boldsymbol{\Sigma})$. Gaussian mixtures include

$$f_n(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\Sigma}, G_1) = \int_{-\infty}^{\infty} g_n(\boldsymbol{x}; t^{-1}\boldsymbol{\theta}, t^{-2}\boldsymbol{\Sigma})\, dG_1(t), \tag{2.1}$$

as translation–scale mixtures, with $G_1(\cdot)$ as a *cdf* on $\mathbb{R}^1$, giving purely scale mixtures on $\mathbb{R}^1_+$ when $\boldsymbol{\theta} = \mathbf{0}$. Distributions for quadratic forms emerge on letting $\mathcal{L}(U\,|\,w)$ be the scaled gamma density $g_0(u; \alpha, \beta/w) = (w/\beta)^\alpha u^{\alpha-1} e^{-wu/\beta}/\Gamma(\alpha)$, then compounding as

$$f(u; \alpha, \beta, G_2) = \frac{u^{\alpha-1}}{\beta^\alpha \Gamma(\alpha)} \int_0^\infty w^\alpha e^{-wx/\beta}\, dG_2(w) \tag{2.2}$$

with $G_2(w)$ as a *cdf* on $\mathbb{R}^1_+$.

2.3. **Structured Dispersion.** Errors having non–scalar dispersion matrices often are encountered in practice. Their relevance here is to examine the superposition of calibrative errors on such pre–existing structures. Accordingly, let $\Xi_0(n) = \{\boldsymbol{\Sigma}_0(\boldsymbol{\gamma}); \boldsymbol{\gamma} \in \Gamma_n\}$ comprise the matrices $\boldsymbol{\Sigma}_0(\boldsymbol{\gamma}) = (\boldsymbol{I}_n + \mathbf{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\mathbf{1}'_n - \bar{\gamma}\mathbf{1}_n\mathbf{1}'_n)$ in $\mathbb{S}^+_n$, such that $\boldsymbol{\gamma}' = [\gamma_1, \ldots, \gamma_n]$ and

$\bar{\gamma} = (\gamma_1 + \ldots + \gamma_n)/n$. Such matrices and their equivalents are considered in [14] in connection with the analysis of variance; they comprise the within-subject dispersion matrices preserving validity of $F$–tests in the analysis of repeated measurements [15,16]; and they determine equivalence classes of Pitman [17] estimators for a mean [18]. Related work [19]–[21] found Grubbs' [22] test for a single shifted outlier to be exact in level and power under normality for all dispersion matrices in $\Xi_0(n)$. The form $(\boldsymbol{D} + \mathbf{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\mathbf{1}_n')$ emerges in the study [23] of Euclidean distance matrices, having applications in linear inference [24].

Designate by $\Xi_1(n) = \{\boldsymbol{\Sigma}(\rho) = [(1-\rho)\boldsymbol{I}_n + \rho\mathbf{1}_n\mathbf{1}_n'];\ -(n-1)^{-1} < \rho < 1\}$ the equicorrelation matrices in $\mathbb{S}_n^+$, together with the ensemble $\Xi(n) = \{\boldsymbol{\Sigma}(\boldsymbol{\gamma}, \phi);\ (\boldsymbol{\gamma}, \phi) \in \Lambda_n\}$ in $\mathbb{S}_n^+$, such that $\boldsymbol{\Sigma}(\boldsymbol{\gamma}, \phi) = [\boldsymbol{I}_n + \mathbf{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\mathbf{1}_n' - \phi\mathbf{1}_n\mathbf{1}_n']$ is positive definite, where $\Xi_0(n) \subset \Xi(n)$ since $\boldsymbol{\Sigma}_0(\boldsymbol{\gamma}) = \boldsymbol{\Sigma}(\boldsymbol{\gamma}, \bar{\gamma})$. Eigenvalues and conditions for positive definiteness are found on writing $\boldsymbol{\Sigma}(\boldsymbol{\gamma}, \phi) = \boldsymbol{I}_n + \boldsymbol{A}_n(\boldsymbol{\gamma}, \phi)$ with $\boldsymbol{A}_n(\boldsymbol{\gamma}, \phi) = \mathbf{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\mathbf{1}_n' - \phi\mathbf{1}_n\mathbf{1}_n'$. To these ends let $\mathcal{A}_n = \{\boldsymbol{A}_n(\boldsymbol{\gamma}, \phi) = (\mathbf{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\mathbf{1}_n' - \phi\mathbf{1}_n\mathbf{1}_n'); (\boldsymbol{\gamma}, \phi) \in \Lambda_n\}$, and for each $\boldsymbol{A}_n(\boldsymbol{\gamma}, \phi)$, let $\tau_1 = \mathrm{tr}[\boldsymbol{A}_n(\boldsymbol{\gamma}, \phi)]$ $= 2(\gamma_1 + \ldots + \gamma_n) - n\phi = n(2\bar{\gamma} - \phi)$ and $\tau_2 = (\gamma_1 - \bar{\gamma})^2 + \ldots + (\gamma_n - \bar{\gamma})^2$. Essential properties follow.

**Lemma 1.** *Suppose that $\boldsymbol{\Sigma}(\boldsymbol{\gamma}, \phi) = \boldsymbol{I}_n + \boldsymbol{A}_n(\boldsymbol{\gamma}, \phi)$ with $\boldsymbol{A}_n(\boldsymbol{\gamma}, \phi) = \mathbf{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\mathbf{1}_n' - \phi\mathbf{1}_n\mathbf{1}_n'$, and let $\Xi(n)$ comprise all such matrices in $\mathbb{S}_n^+$.*

*(i) If $\boldsymbol{\gamma} \neq \mathbf{0}$, then $\boldsymbol{A}_n(\boldsymbol{\gamma}, \phi)$ has rank $r[\boldsymbol{A}_n(\boldsymbol{\gamma}, \phi)] = 2$; otherwise $r[\boldsymbol{A}_n(\mathbf{0}, \phi)] = 1$.*

*(ii) If $\boldsymbol{\gamma} \neq \mathbf{0}$, then $\boldsymbol{A}_n(\boldsymbol{\gamma}, \phi)$ is an indefinite matrix, its positive and negative eigenvalues given respectively by $\alpha_1 = [\tau_1 + (\tau_1^2 + 4n\tau_2)^{1/2}]/2$ and $\alpha_n = [\tau_1 - (\tau_1^2 + 4n\tau_2)^{1/2}]/2$.*

*(iii) The ordered eigenvalues $\{\xi_1 \geq \ldots \geq \xi_n\}$ of $\boldsymbol{\Sigma}(\boldsymbol{\gamma}, \phi)$ are given by $\{\xi_1 = 1 + \alpha_1,\ \xi_2 = \ldots = \xi_{n-1} = 1,\ \xi_n = 1 + \alpha_n\}$.*

*(iv) $\boldsymbol{\Sigma}(\boldsymbol{\gamma}, \phi) \in \Xi(n)$ if and only if $(\boldsymbol{\gamma}, \phi) \in \Lambda_n$, such that $\tau_1 > n\tau_2 - 1$, or equivalently, $2\bar{\gamma} - \phi > \tau_2 - 1/n$.*

**Proof.** (i) Write $\boldsymbol{A}_n(\boldsymbol{\gamma}, \phi) = \mathbf{1}_n(\boldsymbol{\gamma} - \eta\mathbf{1}_n)' + (\boldsymbol{\gamma} - \eta\mathbf{1}_n)\mathbf{1}_n' = \mathbf{1}_n\boldsymbol{\theta}' + \boldsymbol{\theta}\mathbf{1}_n$ with $\eta = \phi/2$ and $\boldsymbol{\theta} = (\boldsymbol{\gamma} - \eta\mathbf{1}_n)$. For $\boldsymbol{\gamma} \neq \mathbf{0}$ this clearly has rank 2; otherwise $\boldsymbol{A}_n(\mathbf{0}, \phi) = \phi\mathbf{1}_n\mathbf{1}_n'$ has unit rank. With $\boldsymbol{\gamma} \neq \mathbf{0}$, the leading terms of the characteristic polynomial $P_n(\cdot)$ for $\boldsymbol{A}_n(\boldsymbol{\gamma}, \phi)$ are $P_n(\boldsymbol{A}_n) = \alpha^n - c_1\alpha^{n-1} + c_2\alpha^{n-2}$, where $c_1 = \mathrm{tr}[\boldsymbol{A}_n(\boldsymbol{\gamma}, \phi)] = \tau_1$ and $c_2$ is the sum of all $(2 \times 2)$ principal minors. Further terms vanish since $\boldsymbol{A}_n(\boldsymbol{\gamma}, \phi)$ has rank 2. A typical principal $(2 \times 2)$ submatrix is $\boldsymbol{A}_n(i, j) = \begin{bmatrix} 2\gamma_i - c & \gamma_i + \gamma_j - c \\ \gamma_i + \gamma_j - c & 2\gamma_j - c \end{bmatrix}$ with $c = \phi$; and its minor is $\mid \boldsymbol{A}_n(i, j) \mid = -(\gamma_i - \gamma_j)^2$ independently of $c$, so that $c_2 = -\sum_{i<j}(\gamma_i - \gamma_j)^2 = -n\sum_{i=1}^{n}(\gamma_i - \bar{\gamma})^2 = -n\tau_2$ from a standard formula. It follows that $P_n(\boldsymbol{A}_n) = \alpha^{n-2}(\alpha^2 - \tau_1\alpha - n\tau_2)$, its roots as given in conclusion (ii). Conclusion (iii) follows directly since $\{ch_i(\boldsymbol{I}_n + \boldsymbol{A}_n(\boldsymbol{\gamma}, \phi)) = 1 + ch_i(\boldsymbol{A}_n(\boldsymbol{\gamma}, \phi)); 1 \leq i \leq n\}$, and conclusion (iv) from the requirement that $1 + \alpha_n = 1 + [\tau_1 - (\tau_1^2 + 4n\tau_2)^{1/2}]/2 > 0$ in order that $\boldsymbol{\Sigma}(\boldsymbol{\gamma}, \phi)$ should be positive definite. □

Conclusion (ii), and thus conclusion (iii), hold generally, whether $\boldsymbol{\gamma} = \mathbf{0}$ or not. For $\boldsymbol{\gamma} = \mathbf{0}$ implies $\tau_2 = 0$, so that $\alpha_1 = \tau_1 = n\phi$ and $\alpha_n = 0$, giving the well–known array $\{1 + n\phi, 1, \ldots, 1\}$ as eigenvalues of $\boldsymbol{\Sigma}(\mathbf{0}, \phi) = (\boldsymbol{I}_n + \phi\mathbf{1}_n\mathbf{1}_n')$.

Further reproductive, annihilative, and preservative properties are associated with $\mathcal{A}_n = \{\boldsymbol{A}_n(\boldsymbol{\gamma},\phi);(\boldsymbol{\gamma},\phi)\in\Lambda_n\}$. Let $\mathcal{G}_n = \{\boldsymbol{G}\in\mathbb{S}_n : \boldsymbol{G} = \xi_1\boldsymbol{e}\boldsymbol{e}' + \xi_2\boldsymbol{q}_2\boldsymbol{q}_2' + \cdots + \xi_n\boldsymbol{q}_n\boldsymbol{q}_n'\}$ comprise the matrices in $\mathbb{S}_n$ having orthonormal eigenvectors $\{\boldsymbol{e},\boldsymbol{q}_2,\ldots,\boldsymbol{q}_n\}$ such that $\boldsymbol{e} = n^{-1/2}\boldsymbol{1}_n$. For each $\boldsymbol{G}\in\mathcal{G}_n$ let $\boldsymbol{G}_1 = \xi_1\boldsymbol{e}\boldsymbol{e}'$ and $\boldsymbol{G}_2 = \boldsymbol{G}-\boldsymbol{G}_1$. Further partition $\boldsymbol{\gamma}' = [\boldsymbol{\gamma}_1',\ldots,\boldsymbol{\gamma}_k']$ with $\{\boldsymbol{\gamma}_i\in\mathbb{R}^{n_i};1\le i\le k\}$ and $n_1+\ldots+n_k = n$; let $\boldsymbol{L}_n' = \mathrm{Diag}(n_1^{-1}\boldsymbol{1}_{n_1}',\ldots,n_k^{-1}\boldsymbol{1}_{n_k}')$; and note that $\boldsymbol{L}_n'\boldsymbol{1}_n = \boldsymbol{1}_k$. Essential properties follow.

**Lemma 2.** *Let* $\mathcal{A}_n = \{\boldsymbol{A}_n(\boldsymbol{\gamma},\phi);(\boldsymbol{\gamma},\phi)\in\Lambda_n\}$; *consider* $\mathcal{G}_n = \{\boldsymbol{G}\in\mathbb{S}_n : \boldsymbol{G} = \xi_1\boldsymbol{e}\boldsymbol{e}' + \boldsymbol{G}_2\}$; *and let* $\boldsymbol{L}_n' = \mathrm{Diag}(n_1^{-1}\boldsymbol{1}_{n_1}',\ldots,n_k^{-1}\boldsymbol{1}_{n_k}')$.

*(i) For* $\boldsymbol{G} = (\boldsymbol{G}_1+\boldsymbol{G}_2)\in\mathcal{G}_n$, $\boldsymbol{G}_2$ *has the annihilative property that* $\boldsymbol{G}_2\boldsymbol{1}_n = \boldsymbol{0}$, *so that* $\boldsymbol{G}\boldsymbol{1}_n = (\boldsymbol{G}_1+\boldsymbol{G}_2)\boldsymbol{1}_n = \xi_1\boldsymbol{e}\boldsymbol{e}'\boldsymbol{1}_n = \xi_1\boldsymbol{1}_n$ *and* $\boldsymbol{G}_2\boldsymbol{A}_n(\boldsymbol{\gamma},\phi)\boldsymbol{G}_2 = \boldsymbol{0}$.

*(ii)* $\mathcal{A}_n$ *is closed under* $\boldsymbol{G}\in\mathcal{G}_n$ *acting by congruence, i.e.,* $\boldsymbol{G}\boldsymbol{A}_n(\boldsymbol{\gamma},\phi)\boldsymbol{G} = \boldsymbol{A}_n(\boldsymbol{\omega},\alpha)\in\mathcal{A}_n$ *with* $\boldsymbol{\omega} = \xi_1\boldsymbol{G}\boldsymbol{\gamma}$ *and* $\alpha = \phi\xi_1^2$ *for each* $\boldsymbol{G}\in\mathcal{G}_n$.

*(iii) The structure of* $\boldsymbol{A}_n(\boldsymbol{\gamma},\phi)\in\mathcal{A}_n$ *is preserved under* $\boldsymbol{A}_n(\boldsymbol{\gamma},\phi)\to\boldsymbol{L}_n'\boldsymbol{A}_n(\boldsymbol{\gamma},\phi)\boldsymbol{L}_n$ *in the sense that* $\boldsymbol{L}_n'\boldsymbol{A}_n(\boldsymbol{\gamma},\phi)\boldsymbol{L}_n = \boldsymbol{A}_k(\bar{\boldsymbol{\gamma}},\phi)\in\mathcal{A}_k$, *with* $\bar{\boldsymbol{\gamma}}' = [\bar{\gamma}_1,\ldots,\bar{\gamma}_k]$ *and* $\{\bar{\gamma}_i = (\gamma_{i1}+\ldots+\gamma_{in_i})/n_i;1\le i\le k\}$.

**Proof.** Conclusion (i) follows since $\boldsymbol{G}_2\boldsymbol{1}_n = (\xi_2\boldsymbol{q}_2\boldsymbol{q}_2' + \cdots + \xi_n\boldsymbol{q}_n\boldsymbol{q}_n')\boldsymbol{1}_n = \boldsymbol{0}$ from the orthonormality of $\{\boldsymbol{e},\boldsymbol{q}_2,\ldots,\boldsymbol{q}_n\}$, so that $(\boldsymbol{G}_1+\boldsymbol{G}_2)\boldsymbol{1}_n = \xi_1\boldsymbol{e}\boldsymbol{e}'\boldsymbol{1}_n = \xi_1\boldsymbol{1}_n$ and $\boldsymbol{G}_2\boldsymbol{A}_n(\boldsymbol{\gamma},\phi)\boldsymbol{G}_2 = \boldsymbol{0}$. To see conclusion (ii), write $\boldsymbol{G}\boldsymbol{A}_n(\boldsymbol{\gamma},\phi)\boldsymbol{G}$ as

$$\begin{aligned}\boldsymbol{G}(\boldsymbol{1}_n\boldsymbol{\gamma}'+\boldsymbol{\gamma}\boldsymbol{1}_n'-\phi\boldsymbol{1}_n\boldsymbol{1}_n')\boldsymbol{G} &= \boldsymbol{G}\boldsymbol{1}_n\boldsymbol{\gamma}'\boldsymbol{G}+\boldsymbol{G}\boldsymbol{\gamma}\boldsymbol{1}_n'\boldsymbol{G}-\phi\boldsymbol{G}\boldsymbol{1}_n\boldsymbol{1}_n'\boldsymbol{G}\\ &= \boldsymbol{G}_1\boldsymbol{1}_n\boldsymbol{\gamma}'\boldsymbol{G}+\boldsymbol{G}\boldsymbol{\gamma}\boldsymbol{1}_n'\boldsymbol{G}_1-\phi\boldsymbol{G}_1\boldsymbol{1}_n\boldsymbol{1}_n'\boldsymbol{G}_1\\ &= \xi_1\boldsymbol{1}_n\boldsymbol{\gamma}'\boldsymbol{G}+\boldsymbol{G}\boldsymbol{\gamma}\boldsymbol{1}_n'\xi_1-\phi\xi_1^2\boldsymbol{1}_n\boldsymbol{1}_n'\\ &= \boldsymbol{1}_n\boldsymbol{\omega}'+\boldsymbol{\omega}\boldsymbol{1}_n'-\alpha\boldsymbol{1}_n\boldsymbol{1}_n'\end{aligned}$$

from conclusion (i), with $\boldsymbol{\omega} = \xi_1\boldsymbol{G}\boldsymbol{\gamma}$ and $\alpha = \phi\xi_1^2$ as asserted. Conclusion (iii) follows directly on noting that $\boldsymbol{L}_n'\boldsymbol{1}_n = \boldsymbol{1}_k$ and $\boldsymbol{L}_n'\boldsymbol{\gamma} = \bar{\boldsymbol{\gamma}}\in\mathbb{R}^k$, to complete our proof. □

## 3. Calibration

We next seek properties of calibrated measurements $X(Y)$ under classical assays based on the calibration line $Y(X)$. A first look reexamines calibration itself.

3.1. **The Calibration Process.** Consider $\{U_i = \beta_0+\beta_1X_i+\epsilon_i;1\le i\le m\}$ under Gauss–Markov assumptions with $\{\mathrm{Var}(U_i) = \sigma_U^2;1\le i\le m\}$, giving $(\widehat{\beta}_0,\widehat{\beta}_1)$ as least–squares estimators, and collateral values $S_{uu} = \sum_{i=1}^m(U_i-\overline{U})^2$, $S_{xu} = \sum_{i=1}^m(X_i-\overline{X})(U_i-\overline{U})$, and $S_{xx} = \sum_{i=1}^m(X_i-\overline{X})^2$. Here $\mathrm{Var}(\widehat{\beta}_0) = \sigma_0^2$ and $\mathrm{Var}(\widehat{\beta}_1) = \sigma_1^2 = \sigma_U^2/S_{xx}$. *Gaussian calibration* refers to $\{\epsilon_1,\ldots,\epsilon_m\}$ as *iid* $N_1(0,\sigma_U^2)$ random variables. Subsequent readings $\{Z_1,\ldots,Z_n\}$, taken independently of $\{U_1,\ldots,U_m\}$, give the calibrated measurements $\{Y_i = (Z_i-\widehat{\beta}_0)/\widehat{\beta}_1;1\le i\le n\}$, or equivalently, $\boldsymbol{Y} = \widehat{\beta}_1^{-1}(\boldsymbol{Z}-\widehat{\beta}_0\boldsymbol{1}_n)$. If elements of $\boldsymbol{Z}' = [Z_1,\ldots,Z_n]$ have means $\boldsymbol{\mu}_Z' = [\mu_1,\ldots,\mu_n]$ and second moments $V(\boldsymbol{Z}) = \boldsymbol{\Sigma} = [\sigma_{ij}]$, independently of $(\widehat{\beta}_0,\widehat{\beta}_1)$, then conditional moments follow directly as

$$E(\boldsymbol{Y}\,|\,\widehat{\beta}_1) = \widehat{\beta}_1^{-1}[\boldsymbol{\mu}_Z - E(\widehat{\beta}_0\,|\,\widehat{\beta}_1)\boldsymbol{1}_n] \tag{3.1}$$

$$V(\boldsymbol{Y}\,|\,\widehat{\beta}_1) = \widehat{\beta}_1^{-2}[\boldsymbol{\Sigma} + \mathrm{Var}(\widehat{\beta}_0\,|\,\widehat{\beta}_1)\mathbf{1}_n\mathbf{1}_n']. \tag{3.2}$$

Expressions simplify if neither $E(\widehat{\beta}_0 \mid \widehat{\beta}_1)$ nor $\mathrm{Var}(\widehat{\beta}_0 \mid \widehat{\beta}_1)$ depends on $\widehat{\beta}_1$. This holds in Gaussian calibration where $\{X_1, \ldots, X_m\}$ have been centered to $\{(X_1 - \overline{X}), \ldots, (X_m - \overline{X})\}$, so that new outputs $\{Z_1, \ldots, Z_n\}$ first are projected onto the scale of measurements, then shifted by $\overline{X}$ units. For this case $\widehat{\beta}_0 = \overline{U}$; $\mathrm{Var}(\widehat{\beta}_0) = \sigma_0^2 = \sigma_U^2/m$; $\mathrm{Var}(\widehat{\beta}_1) = \sigma_1^2 = \sigma_U^2/S_{xx}$ as before; and $(\widehat{\beta}_0, \widehat{\beta}_1)$ are now uncorrelated and, under Gaussian calibration, are independent. We take the initial calibration to have been centered.

3.2. **Truncation.** Unconditional moments of $\{Y_1, \ldots, Y_n\}$, as crafted, are undefined, owing to outcomes of $\widehat{\beta}_1$ near zero. However, a routine exclusion rule accepts a provisional calibration if $\widehat{\beta}_1 \in [a, b]$ for fixed $a < b$ not spanning zero, and recalibrates otherwise. See [1,6,8], for example. This effectively truncates the distribution of $\widehat{\beta}_1$, guaranteeing in turn all moments of $\{Y_1, \ldots, Y_n\}$. Accordingly, let $I_{[a,\,b]}$ be the indicator of the set $[a,\, b] \in \mathbb{R}^1$ not spanning zero; designate $\widehat{\beta}_T = I_{[a,\,b]}\widehat{\beta}_1$ as the resulting restricted estimator; and let $\beta_T$ $= E(\widehat{\beta}_T)$ and $\sigma_T^2 = \mathrm{Var}(\widehat{\beta}_T)$. Clearly $\beta_T \in [a, b]$ and, under Gaussian calibration, $\mathrm{Var}(\widehat{\beta}_T)$ $= \sigma_T^2 < \sigma_1^2 = \mathrm{Var}(\widehat{\beta}_1)$, from a result of [25]. Moreover, the restriction $\mathcal{L}(\widehat{\beta}_T) = N_a^b(\beta_T, \sigma_T^2)$, together with $\mathcal{L}(\widehat{\beta}_1^2/\sigma_1^2) = \chi^2(1, \delta)$ with $\delta = \beta_1^2/\sigma_1^2$, is tantamount to restricting $(\widehat{\beta}_1^2/\sigma_1^2)$ to $[c, d]$, with $c = a^2/\sigma_1^2$ and $d = b^2/\sigma_1^2$, to be designated as $\mathcal{L}(\widehat{\beta}_1^2/\sigma_1^2 \in [c, d]) = \Gamma_c^d(1, \delta)$ in the parlance of Section 2.2. The following concept is germane.

**Definition 1.** Let $\mathcal{L}(W)$ be the distribution of $W \in \mathbb{R}^1$ having the density $f_W(\cdot)$; let $[a,\, b]$ be an interval of truncation; let $W_T = I_{[a,\,b]}W$; and let $\mathcal{L}(W\,|\,W \in [a,\, b]) = \mathcal{L}(W_T)$ designate the distribution of $W$ restricted to $[a,\, b]$. Then *coverage* is defined as $C_g = \int_a^b f_W(t)dt$, so that the density of $W_T$ is $f_{W_T}(\cdot) = C_g^{-1} f_W(\cdot)$ on $[a,\, b]$.

Guidelines are sought in choosing points of truncation. Without loss of generality we take $\widehat{\beta}_1 > 0$, correspondingly $S_{xu} > 0$; otherwise reflect $\{U_1, \ldots, U_m\}$ and $\{Z_1, \ldots, Z_n\}$ about zero; and take $[a,\, b] \in \mathbb{R}_+^1$ as points of truncation with $a > 0$. In practice it often suffices to restrict $\widehat{\beta}_1$ to $[c,\, \infty)$ with $c > 0$. Regarding the choice of $c$, we note that a typical calibration, if effective, will have squared correlation over 90%. Moreover, the squared correlation $R^2_{(X,U)}$ is functionally related to the *OLS* estimator $\widehat{\beta}_1$ by the standard relationship

$$R^2_{(X,U)} = \widehat{\beta}_1^2 \frac{S_{xx}}{S_{uu}}.$$

In order to assure finite negative moments $\{\mu_{-1}(\widehat{\beta}_T),\, \mu_{-2}(\widehat{\beta}_T)\}$, as required subsequently, we stipulate a working rule–of–thumb as follows, subject of course to user discretion.

**Remark 1. Rule–of–Thumb.** Take the squared correlation to satisfy $R^2_{(X,U)} > 5\%$. With $\{S_{xx},\, S_{uu}\}$ as given by the data, requiring that $5\% < R^2_{(X,U)}$ necessarily restricts $\widehat{\beta}_1$ to the interval $[\sqrt{0.05 S_{uu}/S_{xx}},\, \infty)$.

**Remark 2.** It is seen in Section 6 that this choice on occasion yields coverage near unity, so that $\mathcal{L}(\widehat{\beta}_T)$ and $\mathcal{L}(\widehat{\beta}_1)$ largely coincide.

3.3. **Error Analysis.** If instead $(\beta_0, \beta_1)$ were known, then $\{Y_i = (Z_i - \beta_0)/\beta_1; 1 \le i \le n\}$ would be recovered without errors of calibration, in which case $E(Y_i) = (\mu_i - \beta_0)/\beta_1 = \mu_Y(\beta_1)$, $\mathrm{Var}(Y_i) = \mathrm{Var}(Z_i)/\beta_1^2 = \sigma_Y^2(\beta_1)$, and $\rho(Y_i, Y_j) = \rho(Z_i, Z_j)$. This "ideal" case serves as reference against which recovery under calibrative errors may be gauged. From expression (3.2) the conditional correlation parameter becomes $\rho(Y_i, Y_j \mid \widehat{\beta}_1) = (\sigma_{ij} + \sigma_0^2)/[(\sigma_{ii} + \sigma_0^2)(\sigma_{jj} + \sigma_0^2)]^{1/2}$ independently of $\widehat{\beta}_1$. Even if $V(\boldsymbol{Z}) = \sigma_Z^2 \boldsymbol{I}_n$, where $\sigma_{ij} = 0$ for $i \ne j$, conditional correlations will have been induced through calibration. Unconditional properties of $\{Y_1, \ldots, Y_n\}$ follow through deconditioning, to include negative moments $\kappa_1 = \mu_{-1}(\widehat{\beta}_T)$, $\kappa_2 = \mu_{-2}(\widehat{\beta}_T)$, and $\kappa_{11} = \mathrm{Var}(\widehat{\beta}_T^{-1})$ of $\widehat{\beta}_T$, as follows.

**Theorem 1.** *Let $\{Y_i = (Z_i - \widehat{\beta}_0)/\widehat{\beta}_T; 1 \le i \le n\}$ be measurements inverse to outputs $\{Z_1, \ldots, Z_n\}$ from a calibrated instrument observed independently of $\{U_1, \ldots, U_m\}$, such that $E(\boldsymbol{Z}) = \boldsymbol{\mu}_Z$ and $V(\boldsymbol{Z}) = \boldsymbol{\Sigma}$; and let $\sigma_0^2 = \mathrm{Var}(\widehat{\beta}_0)$, $\sigma_T^2 = \mathrm{Var}(\widehat{\beta}_T)$, $\kappa_1 = \mu_{-1}(\widehat{\beta}_T)$, $\kappa_2 = \mu_{-2}(\widehat{\beta}_T)$, and $\kappa_{11} = \mathrm{Var}(\widehat{\beta}_T^{-1})$. Then unconditional moments, to be designated as $E(\boldsymbol{Y}) = \boldsymbol{\mu}_Y$ and $V(\boldsymbol{Y}) = \boldsymbol{\Xi}$, are given by*

*(i)* $\boldsymbol{\mu}_Y = \kappa_1(\boldsymbol{\mu}_Z - \beta_0 \mathbf{1}_n)$;

*(ii)* $\boldsymbol{\Xi} = \kappa_2(\boldsymbol{\Sigma} + \sigma_0^2 \mathbf{1}_n \mathbf{1}_n') + \kappa_{11}(\boldsymbol{\mu}_Z - \beta_0 \mathbf{1}_n)(\boldsymbol{\mu}_Z - \beta_0 \mathbf{1}_n)'$.

*(iii) Moreover, if $\mathcal{L}(\boldsymbol{Z}) = N_n(\boldsymbol{\mu}_Z, \boldsymbol{\Sigma})$ independently of Gaussian calibrative errors, with $\widehat{\beta}_T$ as $\widehat{\beta}_1$ restricted to $[a, b]$ in $\mathbb{R}_+^1$, then the unconditional joint density of the elements of $\boldsymbol{Y}$ is the translation–scale mixture*

$$f_n(\boldsymbol{y}; \boldsymbol{\mu}_Y, \boldsymbol{\Xi}, G_1) = C_g^{-1} \int_a^b g_n(\boldsymbol{y}; \boldsymbol{\mu}(t), \boldsymbol{\Xi}(t)) dG_1(t) \tag{3.3}$$

*as in (2.1), where $\boldsymbol{\mu}(t) = t^{-1}(\boldsymbol{\mu}_Z - \beta_0 \mathbf{1}_n)$, $\boldsymbol{\Xi}(t) = t^{-2}(\boldsymbol{\Sigma} + \sigma_0^2 \mathbf{1}_n \mathbf{1}_n')$, $C_g = \int_a^b dG_1(t)$, and with mixing distribution $G_1(\cdot) = N_1(\beta_1, \sigma_1^2)$.*

**Proof.** Conclusion (i) follows directly from (3.1), and conclusion (ii) from (3.2), on using $\mathrm{Cov}(Y_i, Y_j) = E_{\widehat{\beta}_T}[\mathrm{Cov}(Y_i, Y_j \mid \widehat{\beta}_T)] + \mathrm{Cov}_{\widehat{\beta}_T}[E(Y_i \mid \widehat{\beta}_T), E(Y_j \mid \widehat{\beta}_T)]$ for covariances, and similarly for variances. Noting for fixed $\widehat{\beta}_T$ that $\boldsymbol{Y}$ is a linear function of $(\boldsymbol{Z}, \widehat{\beta}_0)$, we see that $\mathcal{L}(\boldsymbol{Y} \mid \widehat{\beta}_T) = N_n(\boldsymbol{\mu}_Y(\widehat{\beta}_T), \boldsymbol{\Xi}(\widehat{\beta}_T))$ as in (3.1) and (3.2). Expression (3.3) now follows on mixing over the conditioning distribution. $\square$

Further irregularities, beyond induced correlations, are now apparent. Conclusion (ii) asserts that $\{\mathrm{Var}(Y_i) = \kappa_2(\sigma_{ii} + \sigma_0^2) + \kappa_{11}(\mu_i - \beta_0)^2; 1 \le i \le n\}$. Even if elements of $\{Z_1, \ldots, Z_n\}$ are homoscedastic, such that $V(\boldsymbol{Z}) = \sigma_Z^2 \boldsymbol{I}_n$, it follows that homogeneity of the unconditional variances of $\{Y_1, \ldots, Y_n\}$ is tantamount to homogeneity of their means. We next examine these and other issues incurred in the analysis and interpretation of measurements classically calibrated and subject to errors of calibration.

## 4. Topics in Inference

Model irregularities, to include induced correlations and possible heteroscedasticity, violate the tenets of conventional data analysis in estimation and hypothesis testing. We focus on normal–theory inferences, lacking the independence often required by nonparametrics. We next specialize earlier findings, as they apply in a single sample and in selected comparative experiments.

4.1. **Single Sample.** Elements of $\boldsymbol{Z} = [Z_1, \ldots, Z_n]'$ now are taken to be uncorrelated and homogeneous in mean and variance in keeping with conventional assumptions, *i.e.,* $E(\boldsymbol{Z}) = \mu_Z \mathbf{1}_n$ and $V(\boldsymbol{Z}) = \sigma_Z^2 \boldsymbol{I}_n$. At issue are properties of $\mathcal{L}(\boldsymbol{Y})$ and of $(\overline{Y}, S_Y^2, t_0^2, \boldsymbol{R})$ as the sample mean, the sample variance, Student's statistic $t_0^2 = n(\overline{Y} - \mu_Y^0)^2/S_Y^2$ with reference to two–sided alternatives, and $\boldsymbol{R} = [(Y_1 - \overline{Y}), \ldots, (Y_n - \overline{Y})]' = \boldsymbol{B}_n \boldsymbol{Y}$ as the ordinary residuals. Conditional and unconditional means are $E(\boldsymbol{Y} \mid \widehat{\beta}_T) = \widehat{\beta}_T^{-1}(\mu_Z - \beta_0)\mathbf{1}_n$ and $E(\boldsymbol{Y}) = \kappa_1(\mu_Z - \beta_0)\mathbf{1}_n$. Second moments exhibit common correlations, namely, $\mathrm{V}(\boldsymbol{Y} \mid \widehat{\beta}_T) = \boldsymbol{\Xi}(\widehat{\beta}_T) = \widehat{\beta}_T^{-2}(\sigma_Z^2 + \sigma_0^2)\boldsymbol{\Sigma}(\rho)$ with $\rho = \sigma_0^2/(\sigma_Z^2 + \sigma_0^2)$, and $\mathrm{V}(\boldsymbol{Y}) = \boldsymbol{\Xi} = \kappa_2(\sigma_Z^2 \boldsymbol{I}_n + \sigma_0^2 \mathbf{1}_n \mathbf{1}_n') + \kappa_{11}(\mu_Z - \beta_0)^2 \mathbf{1}_n \mathbf{1}_n'$, the latter with $\rho_0 = [\kappa_2 \sigma_0^2 + \kappa_{11}(\mu_Z - \beta_0)^2]/[\kappa_2(\sigma_Z^2 + \sigma_0^2) + \kappa_{11}(\mu_Z - \beta_0)^2]$. Recall here that $\kappa_1 = \mu_{-1}(\widehat{\beta}_1)$, $\kappa_2 = \mu_{-2}(\widehat{\beta}_1)$, and $\kappa_{11} = \mathrm{Var}(\widehat{\beta}_1^{-1}) = \kappa_2 - \kappa_1^2$. Means and variances of $\{Y_1, \ldots, Y_n\}$, both conditionally and unconditionally, are homogeneous; but correlations may become large. Essential moments and related properties are considered next; it is seen that $S_Y^2$ may grossly underestimate the actual measurement variance $\sigma_Y^2$, and that induced dependencies preempt conventional asymptotics for $\overline{Y}_n = (Y_1 + \ldots + Y_n)/n$.

**Theorem 2.** *Let* $\{Y_i = (Z_i - \widehat{\beta}_0)/\widehat{\beta}_T; 1 \leq i \leq n\}$ *be measurements inverse to outputs* $\{Z_1, \ldots, Z_n\}$ *from a calibrated instrument observed independently of* $\{U_1, \ldots, U_m\}$*, such that* $E(\boldsymbol{Z}) = \mu_Z \mathbf{1}_n$ *and* $V(\boldsymbol{Z}) = \sigma_Z^2 \boldsymbol{I}_n$*, and consider the sample quantities* $(\overline{Y}_n, S_Y^2, \boldsymbol{R})$*, with* $\boldsymbol{R}' = [(Y_1 - \overline{Y}), \ldots, (Y_n - \overline{Y})]$ *as the ordinary residuals. Then*

*(i)* $\overline{Y}_n$ *is unbiased but inconsistent for estimating* $E(Y_i) = \kappa_1(\mu_Z - \beta_0)$*;*

*(ii)* $E(S_Y^2) = \kappa_2 \sigma_Z^2 = \sigma_Y^2 - [\kappa_2 \sigma_0^2 + \kappa_{11}(\mu_Z - \beta_0)^2]$*, so that* $S_Y^2$ *underestimates* $\mathrm{Var}(Y_i) = \sigma_Y^2$.

*(iii)* $\{E(R_i) = 0; 1 \leq i \leq n\}$.

**Proof.** The unbiasedness of $\overline{Y}_n$ follows routinely, and its variance from

$$\begin{aligned}\mathrm{Var}(n^{-1}\mathbf{1}_n'\boldsymbol{Y}) &= n^{-2}\mathbf{1}_n'[\kappa_2(\sigma_Z^2 \boldsymbol{I}_n + \sigma_0^2 \mathbf{1}_n \mathbf{1}_n') + \kappa_{11}(\mu_Z - \beta_0)^2 \mathbf{1}_n \mathbf{1}_n']\mathbf{1}_n \\ &= n^{-1}\kappa_2 \sigma_Z^2 + \kappa_2 \sigma_0^2 + \kappa_{11}(\mu_Z - \beta_0)^2.\end{aligned}$$

Since $\lim_{n\to\infty} \mathrm{Var}(\overline{Y}_n) = [\kappa_2 \sigma_0^2 + \kappa_{11}(\mu_Z - \beta_0)^2] > 0$, its limit distribution is not degenerate at $\mu_Y$, so that consistency of $\overline{Y}_n$ holds neither in probability, nor in mean square, nor almost surely, in agreement with assertion (i). Conclusion (ii) follows on evaluating the expected value of the quadratic form $(n-1)S_Y^2 = \boldsymbol{Y}'\boldsymbol{B}_n\boldsymbol{Y}$ as $E[(n-1)S_Y^2] = \mathrm{tr}\, \boldsymbol{B}_n V(\boldsymbol{Y}) + \boldsymbol{\mu}_Y' \boldsymbol{B}_n \boldsymbol{\mu}_Y$. Details are

$$\begin{aligned}E[(n-1)S_Y^2] &= \mathrm{tr}\, \boldsymbol{B}_n[\kappa_2(\sigma_Z^2 \boldsymbol{I}_n + \sigma_0^2 \mathbf{1}_n \mathbf{1}_n') + \kappa_{11}(\mu_Z - \beta_0)^2 \mathbf{1}_n \mathbf{1}_n'] + \boldsymbol{\mu}_Y' \boldsymbol{B}_n \boldsymbol{\mu}_Y \\ &= (n-1)\kappa_2 \sigma_Z^2\end{aligned}$$

where $\boldsymbol{\mu}_Y'\boldsymbol{B}_n\boldsymbol{\mu}_Y = \kappa_1^2(\mu_Z-\beta_0)^2\mathbf{1}_n'\boldsymbol{B}_n\mathbf{1}_n = 0$, since $\boldsymbol{B}_n$ is idempotent of rank $(n-1)$ and $\boldsymbol{B}_n\mathbf{1}_n = \mathbf{0}$. Conclusion (iii) follows from $E(\boldsymbol{R}) = E(\boldsymbol{B}_n\boldsymbol{Y}) = \kappa_1(\mu_Z-\beta_0)\boldsymbol{B}_n\mathbf{1}_n = \mathbf{0}$, to complete our proof. □

The following consequences are noteworthy.

- Conclusion (i) preempts the usual expectation that lengths of $(1-\alpha)$ confidence intervals for $\mu_Y$ will decrease at the rate $O(n^{-1/2})$.
- Conclusion (ii) asserts that $S_Y^2$ underestimates $\mathrm{Var}(Y_i) = \sigma_Y^2$, with bias $B = [\kappa_2\sigma_0^2 + \kappa_{11}(\mu_Z-\beta_0)^2]$.

To continue, unconditional moments of calibrated measurements are seen to depend on those of the conditioning variable $\widehat{\beta}_T$. It remains to examine effects of calibration on unconditional distributions, to include those of the sample statistics $(\overline{Y}, S_Y^2, t_0^2, \boldsymbol{R})$. Under Gaussian calibration without exclusion, we have $\mathcal{L}(\widehat{\beta}_1) = N_1(\beta_1, \sigma_1^2)$ and $\mathcal{L}(\widehat{\beta}_1^2/\sigma_1^2) = \chi^2(1,\delta)$ with $\delta = \beta_1^2/\sigma_1^2$. With exclusion, the mixing distributions in expressions (2.1) and (2.2) now are $G_1(\widehat{\beta}_T) = N_a^b(\beta_T, \sigma_T^2)$, whereas $G_2(\widehat{\beta}_T^2;\delta)$ is a version of $\Gamma_c^d(1,\delta)$ found on restricting $\chi^2(1,\delta)$ to $[c,d]$ in $\mathbb{R}_+^1$. Details follow.

**Theorem 3.** *Let $\{Y_i = (Z_i - \widehat{\beta}_0)/\widehat{\beta}_T; 1 \le i \le n\}$ be calibrated measurements based on $\{Z_1,\dots,Z_n\}$ as iid $N_1(\mu_Z,\sigma_Z^2)$ random variables independent of $(\widehat{\beta}_0,\widehat{\beta}_T)$ under Gaussian calibration, with $\widehat{\beta}_T$ restricted to $[a,b]$ in $\mathbb{R}_+^1$, and let $\delta = \beta_1^2/\sigma_1^2$. Consider statistics $(\overline{Y}, S_Y^2, t_0^2, \boldsymbol{R})$, where $t_0^2 = n(\overline{Y}-\mu_Y^0)^2/S_Y^2$ and $\boldsymbol{R} = [(Y_1-\overline{Y}),\dots,(Y_n-\overline{Y})]'$ consists of ordinary residuals. Then the following properties hold.*

*(i) $\mathcal{L}(\overline{Y})$ has the density $f_1(u;\mu,\tau^2(n),G_1)$ as in (3.3) for distributions on $\mathbb{R}^1$, where $\mu = (\mu_Z-\beta_0)$ and $\tau^2(n) = n^{-1}(\sigma_Z^2 + n\sigma_0^2)$, with mixing distribution $G_1(t) = N_1(\beta_1,\sigma_1^2)$ on $\mathbb{R}^1$.*

*(ii) $\mathcal{L}(\boldsymbol{R})$ has the density*

$$f_n(\boldsymbol{r};\mathbf{0},\sigma_Z^2\boldsymbol{B}_n,G_1) = C_g^{-1}\int_a^b g_n(\boldsymbol{y};\mathbf{0},t^{-2}\sigma_Z^2\boldsymbol{B}_n)dG_1(t) \tag{4.1}$$

*as in (3.3), with mixing distribution $G_1(t) = N_1(\beta_1,\sigma_1^2)$ on $\mathbb{R}^1$.*

*(iii) $\mathcal{L}[(n-1)S_Y^2\sigma_1^2/\sigma_Z^2]$ has the density $f(u;\alpha,2,G_2) = \frac{u^{\alpha-1}}{\beta^\alpha\Gamma(\alpha)}\int_c^d w^\alpha e^{-wx/2}dG_2(w)$ as in (2.2) with $\alpha = \nu/2$ and $\nu = (n-1)$, and mixing distribution $G_2(\widehat{\beta}_1^2;\delta)$ as $\Gamma(1,\delta)$ on $\mathbb{R}_+^1$ such that $c = a^2/\sigma_1^2$ and $d = b^2/\sigma_1^2$.*

*(iv) The unconditional density of $t_0^2$ is the mixture*

$$g(u;\nu,\lambda,G_1) = C_g^{-1}\int_a^b kg_{t^2}(u;\nu,\lambda(t))dG_1(t) \tag{4.2}$$

*with $k = \sigma_Z^2/(\sigma_Z^2+n\sigma_0^2)$, $\nu = (n-1)$, noncentrality $\lambda(t) = n[(\mu_Z-\beta_0) - t\mu_Y^0]^2/(\sigma_Z^2+n\sigma_0^2)$, and mixing distribution $G_1(t) = N_1(\beta_1,\sigma_1^2)$ on $\mathbb{R}^1$*

**Proof.** Begin with $\mathcal{L}(\boldsymbol{Y}\,|\,\widehat{\beta}_T) = N_n[\widehat{\beta}_T^{-1}\mu\mathbf{1}_n, \widehat{\beta}_T^{-2}(\sigma_Z^2\boldsymbol{I}_n + \sigma_0^2\mathbf{1}_n\mathbf{1}_n')]$ to determine directly that $\mathcal{L}(\boldsymbol{R}\,|\,\widehat{\beta}_T) = N_n(\mathbf{0}, \widehat{\beta}_T^{-2}\sigma_Z^2\boldsymbol{B}_n)$, since $\boldsymbol{B}_n$ is idempotent and $\boldsymbol{B}_n\mathbf{1}_n = \mathbf{0}$; and that $\mathcal{L}(\overline{Y}\,|\,\widehat{\beta}_T) = N_1(\widehat{\beta}_T^{-1}\mu, \widehat{\beta}_T^{-2}\tau^2(n))$, where $\mu = (\mu_Z-\beta_0)$ and $\tau^2(n) = n^{-1}(\sigma_Z^2+n\sigma_0^2)$. The unconditional density of $\overline{Y}$ thus is $f_1(u;\mu,\tau^2(n),G_1)$ on specializing (3.3) from $\mathbb{R}^n$ to $\mathbb{R}^1$, to give conclusion (i) with mixing distribution as asserted. Conclusion (ii) follows similarly on mixing $\mathcal{L}(\boldsymbol{R}\,|\,\widehat{\beta}_T)$ over $G_1(t)$. Since $(n-1)S_Y^2 = \boldsymbol{R}'\boldsymbol{R}$, we infer that $\mathcal{L}(\boldsymbol{R}'\boldsymbol{R}\widehat{\beta}_1^2/\sigma_Z^2\,|\,\widehat{\beta}_1^2) = \chi^2(\nu,0)$ with $\nu = n-1$, so that $\mathcal{L}((n-1)S_Y^2/\sigma_Z^2\,|\,\widehat{\beta}_1^2)$ is a central chi–squared variate scaled by $\widehat{\beta}_1^2$. On identifying $(n-1)S_Y^2\sigma_1^2/\sigma_Z^2$ with $U$ and $(\widehat{\beta}_1^2/\sigma_1^2)$ with $w$ in developments leading to (2.2), we thus establish conclusion (iii) on specializing from gamma to chi–squared distributions under the restriction $\widehat{\beta}_T^2 \in [a^2,b^2]$ in $\mathbb{R}_+^1$, so that $(\widehat{\beta}_1^2/\sigma_1^2)$ is now restricted to $[a^2/\sigma_1^2, b^2/\sigma_1^2]$. To continue, observe that $\mathcal{L}[(\overline{Z}-\widehat{\beta}_0-\widehat{\beta}_T\mu_Y^0)\,|\,\widehat{\beta}_T] = N_1[(\mu_Z-\beta_0-\widehat{\beta}_T\mu_Y^0), n^{-1}(\sigma_Z^2+n\sigma_0^2)]$. Properly standardized, the quantity $t^2 = n[(\overline{Z}-\widehat{\beta}_0-\widehat{\beta}_T\mu_Y^0)^2/S_Z^2][\sigma_Z^2/(\sigma_Z^2+n\sigma_0^2)]$ conditionally has Student's distribution $\mathcal{L}(t^2\,|\,\widehat{\beta}_T) = t^2(\nu,\lambda(\widehat{\beta}_T))$ with $\nu=(n-1)$ and $\lambda(\widehat{\beta}_T) = n[(\mu_Z-\beta_0) - \widehat{\beta}_T\mu_Y^0]^2/(\sigma_Z^2+n\sigma_0^2)$, so that $t_0^2 = t^2/k$ with $k = \sigma_Z^2/(\sigma_Z^2+n\sigma_0^2)$. In particular, $\mathcal{L}(t_0^2\,|\,\widehat{\beta}_T) = \mathcal{L}(t^2/k\,|\,\widehat{\beta}_T)$. It follows on scaling and mixing that the unconditional density is (4.2), to complete our proof. $\square$

4.2. **Effective Calibration.** Enough evidence is now in hand to support a qualitative assessment of classical calibrations based on $X(Y)$ from the linear calibration $Y(X)$. Anomalies are seen to depend mainly on the parameters $\kappa_2 = \mu_{-2}(\widehat{\beta}_T)$, $\kappa_{11} = \mathrm{Var}(\widehat{\beta}_T^{-1})$, and $|\ \mu_Z-\beta_0\ |$ . Appendix Lemma 3 gives expansions approximating the negative moments $\{\kappa_1 = \mu_{-1}(\widehat{\beta}_T),\ \kappa_2 = \mu_{-2}(\widehat{\beta}_T),\ \kappa_{11} = \mathrm{Var}(\widehat{\beta}_T^{-1})\}$, together with orders $O(\cdot)$ of the approximations. The following consequences emerge from Section 4.1 and the aforementioned expansions.

- The parameter $\kappa_2 = \mu_{-2}(\widehat{\beta}_T) \approxeq \frac{1}{\beta_T^2} + \frac{3\sigma_T^2}{\beta_T^4}$ is increasing in $\sigma_T^2$ and decreasing in $|\,\beta_T\,|$, up to the order of approximation.
- The quantity $|\,\mu_Z-\beta_0\,|$ pertains to centering of the calibrating values $\{U_1,\ldots,U_m\}$ relative to subsequent readings $\{Z_1,\ldots,Z_n\}$. Here $|\,\mu_Z-\beta_0\,|$ becomes smaller, the more effectively are $\{U_1,\ldots,U_m\}$ centered near the mean $\mu_Z$ of $\{Z_1,\ldots,Z_n\}$.
- Effective centering in turn diminishes effects of extrapolating beyond the calibrating data.
- The bias $B = [\kappa_2\sigma_0^2 + \kappa_{11}(\mu_Z-\beta_0)^2]$ of $S_Y^2$ for estimating $\sigma_Y^2$, as in Theorem 2(ii), increases (i) with increasing uncertainty $(\sigma_0^2,\sigma_T^2)$ in estimating the line of calibration, (ii) with increasing $|\,\mu_Z-\beta_0\,|$, and (iii) with increasing $\{\kappa_2,\kappa_{11}\}$.
- On the other hand, the expectation $E(S_Y^2) = \kappa_2\sigma_Z^2$ may be compared with $\mathrm{Var}(Y_i) = \sigma_Z^2/\beta_1^2$, as the ideal variance to be attained under linear calibration with known $(\beta_0,\beta_1)$.
- The conditional correlation $\rho = \sigma_0^2/(\sigma_Z^2+\sigma_0^2)$ increases with decreasing $\sigma_Z^2/\sigma_0^2$.
- The unconditional correlation
$$\rho_0 = \frac{[\kappa_2\sigma_0^2 + \kappa_{11}(\mu_Z-\beta_0)^2]}{[\kappa_2(\sigma_Z^2+\sigma_0^2) + \kappa_{11}(\mu_Z-\beta_0)^2]}$$
increases (i) with increasing uncertainty in estimating $\beta_0$, (ii) with increasing $|\,\mu_Z - \beta_0\,|$, and (iii) with increasing $\{\kappa_2,\kappa_{11}\}$, with other parameters held fixed.

- The conditional noncentrality parameter $\lambda(\widehat{\beta}_T) = n\widehat{\beta}_T^2[\mu_Y(\widehat{\beta}_T) - \mu_Y^0]^2/(\sigma_Z^2 + n\sigma_0^2)$ is an increasing function of $|\,\widehat{\beta}_T\,|$ and the discrepancy $|\,\mu_Y(\widehat{\beta}_T) - \mu_Y^0\,|$, and it decreases with increasing $\sigma_Z^2$ and $\sigma_0^2$ with other parameters fixed, where $\mu_Y(\widehat{\beta}_T) = (\mu_Z–\beta_0)/\widehat{\beta}_T$.
- The expected value

$$E[\lambda(\widehat{\beta}_T)] = \frac{n\{\beta_T^2[\mu_Y(\beta_T) - \mu_Y^0]^2 + \sigma_T^2(\mu_Y^0)^2\}}{\sigma_Z^2 + n\sigma_0^2}$$

  is an increasing function of $|\,\beta_T\,|$, $|\,\mu_Y(\beta_T) - \mu_Y^0\,|$, and $\sigma_T^2$, and it decreases with increasing $\sigma_Z^2$ and $\sigma_0^2$ with other parameters fixed, where $\mu_Y(\beta_T) = (\mu_Z - \beta_0)/\beta_T$.

4.3. **One–Way Experiments.** We next model observations $\{Z_1, \ldots, Z_n\}$ as from a one–way experiment in $k$ samples of sizes $\{n_1, \ldots, n_k\}$, with $n_1 + \ldots + n_k = n$. Accordingly, partition $\boldsymbol{Z}' = [\boldsymbol{Z}_1', \ldots, \boldsymbol{Z}_k']$, such that $\{\boldsymbol{Z}_i' = [Z_{i1}, \ldots, Z_{in_i}]; 1 \leq i \leq k\}$; and similarly for $\boldsymbol{Y}'$ $= [\boldsymbol{Y}_1', \ldots, \boldsymbol{Y}_k']$, with $\{\boldsymbol{Y}_i' = [Y_{i1}, \ldots, Y_{in_i}]; 1 \leq i \leq k\}$. We suppose that $\{E(Z_{ij}) = \mu_i; 1 \leq j \leq n_i\}$, so that $\boldsymbol{\mu}_Z = [\mu_1\mathbf{1}_{n_1}', \ldots, \mu_k\mathbf{1}_{n_k}']'$. It is known that the normal–theory test for $H_0 : \mu_1 = \cdots = \mu_k$ is exact under $V(\boldsymbol{Z}) = \omega^2\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})$ as in Section 2.3. From its block–partitioned form we extract $\{\mathrm{V}(\boldsymbol{Z}_i) = \omega^2\boldsymbol{\Sigma}(\boldsymbol{\gamma}_i, \bar{\gamma}) = \omega^2(\boldsymbol{I}_{n_i} + \mathbf{1}_{n_i}\boldsymbol{\gamma}_i' + \boldsymbol{\gamma}_i\mathbf{1}_{n_i}' - \bar{\gamma}\mathbf{1}_{n_i}\mathbf{1}_{n_i}'); 1 \leq i \leq k\}$, where $\boldsymbol{\gamma}'$ $= [\boldsymbol{\gamma}_1', \ldots, \boldsymbol{\gamma}_k']$ has been partitioned conformably such that $\{\boldsymbol{\gamma}_i = [\gamma_{i1}, \ldots, \gamma_{in_i}]' \in \mathbb{R}^{n_i}; 1 \leq i \leq k\}$. Note that the test remains exact despite heterogeneity of the variances $\{\mathrm{Var}(Z_{ij}) = \omega^2(2\gamma_{ij} - \bar{\gamma}); 1 \leq j \leq n_i, 1 \leq i \leq k\}$ within and among samples, attributable to the structural parameters of $\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})$. We next proceed to examine consequences of superimposing calibrative errors onto those structures in the analysis of one–way experiments, to include conventional analysis of variance and comparisons among the sample means and variances.

Accordingly, take $V(\boldsymbol{Z}) = \omega^2\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})$ to model the ambient background experimental noise, subject to external scale changes for each of the $k$ designated samples. To model such changes, pre– and post–multiply $\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})$ by $\boldsymbol{D_{\omega I}} = \mathrm{Diag}(\omega_1\boldsymbol{I}_{n_1}, \ldots, \omega_k\boldsymbol{I}_{n_k})$ to get $\boldsymbol{\Xi}_n(\boldsymbol{\omega}, \boldsymbol{\gamma})$ $= \boldsymbol{D_{\omega I}}\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})\boldsymbol{D_{\omega I}}$, which in partitioned form is

$$\boldsymbol{\Xi}_n(\boldsymbol{\omega}, \boldsymbol{\gamma}) = \begin{bmatrix} \omega_1^2\boldsymbol{\Sigma}(\gamma_1, \bar{\gamma}) & \omega_1\omega_2\boldsymbol{A}_{12} & \ldots & \omega_1\omega_k\boldsymbol{A}_{1k} \\ \omega_2\omega_1\boldsymbol{A}_{21} & \omega_2^2\boldsymbol{\Sigma}(\boldsymbol{\gamma}_2, \bar{\gamma}) & \ldots & \omega_2\omega_k\boldsymbol{A}_{2k} \\ \cdots & \cdots & \cdots & \cdots \\ \omega_k\omega_1\boldsymbol{A}_{k1} & \omega_k\omega_2\boldsymbol{A}_{k2} & \ldots & \omega_k^2\boldsymbol{\Sigma}(\boldsymbol{\gamma}_k, \bar{\gamma}) \end{bmatrix} \tag{4.3}$$

with $\{\boldsymbol{\Sigma}(\boldsymbol{\gamma}_i, \bar{\gamma}); 1 \leq i \leq k\}$ as before, and with $\{\boldsymbol{A}_{ij} = \mathbf{1}_{n_i}\boldsymbol{\gamma}_j' + \boldsymbol{\gamma}_i\mathbf{1}_{n_j}' - \bar{\gamma}\mathbf{1}_{n_i}\mathbf{1}_{n_j}'\}$. Specializing from (3.1) and (3.2) gives the conditional moments

$$\begin{aligned} E(\boldsymbol{Y}\,|\,\widehat{\beta}_T) = \boldsymbol{\mu}_Y(\widehat{\beta}_T) &= \widehat{\beta}_T^{-1}(\boldsymbol{\mu}_Z - \beta_0\mathbf{1}_n) \\ &= \widehat{\beta}_T^{-1}[(\mu_1 - \beta_0)\mathbf{1}_{n_1}', \ldots, (\mu_k - \beta_0)\mathbf{1}_{n_k}']' \end{aligned} \tag{4.4}$$

$$\mathrm{V}(\boldsymbol{Y}\,|\,\widehat{\beta}_T) = \boldsymbol{\Sigma}(\widehat{\beta}_T) = \widehat{\beta}_T^{-2}[\boldsymbol{\Xi}_n(\boldsymbol{\omega}, \boldsymbol{\gamma}) + \sigma_0^2\mathbf{1}_n\mathbf{1}_n'], \tag{4.5}$$

together with $\mathcal{L}(\boldsymbol{Y}\,|\,\widehat{\beta}_T) = N_n(\boldsymbol{\mu}_Y(\widehat{\beta}_T), \boldsymbol{\Sigma}(\widehat{\beta}_T))$ under Gaussian errors. Unconditional moments are $E(\boldsymbol{Y}) = \kappa_1[(\mu_1 - \beta_0)\mathbf{1}_{n_1}', \ldots, (\mu_k - \beta_0)\mathbf{1}_{n_k}']'$ and $V(\boldsymbol{Y}) = \kappa_2[\boldsymbol{\Xi}_n(\boldsymbol{\omega}, \boldsymbol{\gamma}) + \sigma_0^2\mathbf{1}_n\mathbf{1}_n'] +$ $\kappa_{11}\boldsymbol{M}$, where $\boldsymbol{M} = [\boldsymbol{M}_{ij}] = (\boldsymbol{\mu}_Z - \beta_0\mathbf{1}_n)(\boldsymbol{\mu}_Z - \beta_0\mathbf{1}_n)'$ with $\boldsymbol{M}_{ij} = (\mu_i - \beta_0)(\mu_j - \beta_0)\mathbf{1}_{n_i}\mathbf{1}_{n_j}'$.

To examine effects of calibration on sample quantities of note, consider transformations such that $T_1(\boldsymbol{Y}) = \bar{\boldsymbol{Y}} = [\overline{Y}_1, \ldots, \overline{Y}_k]'$ comprise the $k$ sample means; $T_2(\boldsymbol{Y}) = \boldsymbol{R} = [\boldsymbol{R}_1', \ldots, \boldsymbol{R}_k']'$ consists of the ordinary within–sample residuals, with $\{\boldsymbol{R}_i = \boldsymbol{B}_{n_i}\boldsymbol{Y}_i; 1 \leq i \leq k\}$ and $\boldsymbol{B}_{n_i} = (\boldsymbol{I}_{n_i} - n_i^{-1}\mathbf{1}_{n_i}\mathbf{1}_{n_i}')$; and $T_3(\boldsymbol{Y}) = [\nu_1 S_1^2, \ldots, \nu_k S_k^2]'$ are the residual sums of squares $\{\nu_i S_i^2 = \boldsymbol{R}_i'\boldsymbol{R}_i = \boldsymbol{Y}_i'\boldsymbol{B}_{n_i}\boldsymbol{Y}_i; 1 \leq i \leq k\}$, with $\{\nu_i = n_i - 1; 1 \leq i \leq k\}$. We require $\boldsymbol{\theta} = [\bar{\gamma}_1, \ldots, \bar{\gamma}_k]'$ as means of the partitioned elements of $\boldsymbol{\gamma}' = [\boldsymbol{\gamma}_1', \ldots, \boldsymbol{\gamma}_k']$ as in Section 2.3. Essential properties follow.

**Theorem 4.** *Consider calibrated measurements* $\boldsymbol{Y}' = [\boldsymbol{Y}_1', \ldots, \boldsymbol{Y}_k']$ *from* $\boldsymbol{Z}' = [\boldsymbol{Z}_1', \ldots, \boldsymbol{Z}_k']$ *such that* $E(\boldsymbol{Z}) = \boldsymbol{\mu}_Z = [\mu_1\mathbf{1}_{n_1}', \ldots, \mu_k\mathbf{1}_{n_k}']'$ *and* $V(\boldsymbol{Z}) = \boldsymbol{\Xi}_n(\boldsymbol{\omega}, \boldsymbol{\gamma})$ *as in (4.3); let* $\boldsymbol{\mu} = [\mu_1, \ldots, \mu_k]'$; *and let* $T_1(\boldsymbol{Y}) = [\overline{Y}_1, \ldots, \overline{Y}_k]'$; $T_2(\boldsymbol{Y}) = \boldsymbol{R} = [\boldsymbol{R}_1', \ldots, \boldsymbol{R}_k']'$; *and* $T_3(\boldsymbol{Y}) = [\nu_1 S_1^2, \ldots, \nu_k S_k^2]'$, *with* $\{\nu_i = n_i - 1; 1 \leq i \leq k\}$. *Moreover, a Gaussian model asserts that* $\mathcal{L}(\boldsymbol{Z}) = N_n(\boldsymbol{\mu}_Z, \boldsymbol{\Xi}_n(\boldsymbol{\omega}, \boldsymbol{\gamma}))$ *independently of* $(\widehat{\beta}_0, \widehat{\beta}_T)$ *under Gaussian calibration.*

*(i) Conditional and unconditional means of* $T_1(\boldsymbol{Y}) = \bar{\boldsymbol{Y}}$ *are given by* $E(\bar{\boldsymbol{Y}} \mid \widehat{\beta}_T) = \boldsymbol{\tau}(\widehat{\beta}_T) = \widehat{\beta}_T^{-1}(\boldsymbol{\mu} - \beta_0\mathbf{1}_k)$ *and* $E(\bar{\boldsymbol{Y}}) = \boldsymbol{\tau} = \kappa_1(\boldsymbol{\mu} - \beta_0\mathbf{1}_k)$.

*(ii) Conditional dispersion parameters of* $\bar{\boldsymbol{Y}}$ *are* $V(\bar{\boldsymbol{Y}} \mid \widehat{\beta}_T) = \boldsymbol{\Xi}_1(\widehat{\beta}_T) = \widehat{\beta}_T^{-2}[\boldsymbol{\Xi}_k(\boldsymbol{\omega}, \boldsymbol{\theta}, \boldsymbol{n}) + \sigma_0^2\mathbf{1}_k\mathbf{1}_k']$, *where* $\boldsymbol{\Xi}_k(\boldsymbol{\omega}, \boldsymbol{\theta}, \boldsymbol{n}) = \boldsymbol{D}_{\boldsymbol{\omega}}[\boldsymbol{D}_{\boldsymbol{n}}^{-1} + \boldsymbol{A}_k(\boldsymbol{\theta}, \bar{\gamma})]\boldsymbol{D}_{\boldsymbol{\omega}}$, *with* $\boldsymbol{D}_{\boldsymbol{\omega}} = \mathrm{Diag}(\omega_1, \ldots, \omega_k)$, $\boldsymbol{D}_{\boldsymbol{n}} = \mathrm{Diag}(n_1, \ldots, n_k)$, *and* $\boldsymbol{A}_k(\boldsymbol{\theta}, \bar{\gamma}) = \mathbf{1}_k\boldsymbol{\theta}' + \boldsymbol{\theta}\mathbf{1}_k' - \bar{\gamma}\mathbf{1}_k\mathbf{1}_k'$, *where* $\boldsymbol{\theta} = [\bar{\gamma}_1, \ldots, \bar{\gamma}_k]'$ *are means of the partitioned elements of* $\boldsymbol{\gamma}' = [\boldsymbol{\gamma}_1', \ldots, \boldsymbol{\gamma}_k']$. *Unconditional dispersion parameters are* $V(\bar{\boldsymbol{Y}}) = \boldsymbol{\Xi}_1 = \kappa_2[\boldsymbol{\Xi}_k(\boldsymbol{\omega}, \boldsymbol{\theta}, \boldsymbol{n}) + \sigma_0^2\mathbf{1}_k\mathbf{1}_k'] + \kappa_{11}(\boldsymbol{\mu} - \beta_0\mathbf{1}_k)(\boldsymbol{\mu} - \beta_0\mathbf{1}_k)'$.

*(iii) Under Gaussian assumptions the unconditional density of* $\mathcal{L}(\bar{\boldsymbol{Y}})$ *is the translation–scale mixture*

$$f_k(\boldsymbol{u}; \boldsymbol{\tau}, \boldsymbol{\Xi}_1, G_1) = C_g^{-1}\int_a^b g_k(\boldsymbol{u}; \boldsymbol{\tau}(t), \boldsymbol{\Xi}_1(t))dG_1(t) \tag{4.6}$$

*with mixing distribution* $G_1(t) = N_1(\beta_1, \sigma_1^2)$ *on* $\mathbb{R}^1$ *as in (3.3), where* $\boldsymbol{\tau}(t) = t^{-1}(\boldsymbol{\mu} - \beta_0\mathbf{1}_k)$ *and* $\boldsymbol{\Xi}_1(t) = t^{-2}[\boldsymbol{\Xi}_k(\boldsymbol{\omega}, \boldsymbol{\theta}, \boldsymbol{n}) + \sigma_0^2\mathbf{1}_k\mathbf{1}_k']$ *as in conclusion (ii).*

*(iv) Conditional and unconditional means of the residuals are* $E(\boldsymbol{R} \mid \widehat{\beta}_T) = \mathbf{0} = E(\boldsymbol{R})$. *Dispersion parameters are* $V(\boldsymbol{R} \mid \widehat{\beta}_T) = \boldsymbol{\Xi}_2(\widehat{\beta}_T) = \widehat{\beta}_T^{-2}\mathrm{Diag}(\omega_1^2\boldsymbol{B}_{n_1}, \ldots, \omega_k^2\boldsymbol{B}_{n_k})$, *and* $V(\boldsymbol{R}) = \boldsymbol{\Xi}_2 = \kappa_2\mathrm{Diag}(\omega_1^2\boldsymbol{B}_{n_1}, \ldots, \omega_k^2\boldsymbol{B}_{n_k})$.

*(v) Under Gaussian errors the joint density of residuals* $\boldsymbol{R} = [\boldsymbol{R}_1', \ldots, \boldsymbol{R}_k']'$ *is given by* $f_n(\boldsymbol{r}; \mathbf{0}, \boldsymbol{\Xi}_2, G_1)$ *as in (3.3), with mixing distribution* $G_1(t) = N_1(\beta_1, \sigma_1^2)$ *on* $\mathbb{R}^1$, *where* $\boldsymbol{\Xi}_2(t) = t^{-2}\mathrm{Diag}(\omega_1^2\boldsymbol{B}_{n_1}, \ldots, \omega_k^2\boldsymbol{B}_{n_k})$.

*(vi) Under Gaussian errors the joint density of elements of* $[\nu_1 S_1^2\sigma_1^2/\omega_1^2, \ldots, \nu_k S_k^2\sigma_1^2/\omega_k^2]'$ *is given by*

$$f(\boldsymbol{u}; \nu_1, \ldots, \nu_k, G_2) = \int_c^d \prod_{i=1}^k g_0(u_i; \nu_i/2, 2/w)dG_2(w) \tag{4.7}$$

*with* $\{\nu_i = n_i - 1; 1 \leq i \leq k\}$ *and* $g_0(u_i; \alpha_i, \beta/w) = (w/\beta)^{\alpha_i}u_i^{\alpha_i - 1}e^{-wu_i/\beta}/\Gamma(\alpha_i)$, *having mixing distribution* $G_2(\widehat{\beta}_1^2; \delta)$ *as* $\Gamma(1, \delta)$ *on* $\mathbb{R}_+^1$ *such that* $[c, d] = [a^2/\sigma_1^2, b^2/\sigma_1^2]$, *with* $\delta = \beta_1^2/\sigma_1^2$.

**Proof.** Arguments follow step–by–step as in the proofs of Section 4.1. While details differ, proceed beginning with $E(\boldsymbol{Y} \mid \widehat{\beta}_T)$ from (4.4) and $\mathrm{V}(\boldsymbol{Y} \mid \widehat{\beta}_T)$ from (4.5). Observe that $\bar{\boldsymbol{Y}} = \boldsymbol{L}_n'\boldsymbol{Y}$ with $\boldsymbol{L}_n' = \text{Diag}(n_1^{-1}\mathbf{1}_{n_1}', \ldots, n_k^{-1}\mathbf{1}_{n_k}')$; and that $\boldsymbol{R} = \boldsymbol{B}\boldsymbol{Y}$ with $\boldsymbol{B} = \text{Diag}(\boldsymbol{B}_{n_1}, \ldots, \boldsymbol{B}_{n_k})$. Starting with $\boldsymbol{\Xi}_n(\boldsymbol{\omega}, \boldsymbol{\gamma}) = \boldsymbol{D}_{\boldsymbol{\omega}\boldsymbol{I}}\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})\boldsymbol{D}_{\boldsymbol{\omega}\boldsymbol{I}}$ from (4.3), where $\boldsymbol{\Sigma}_0(\boldsymbol{\gamma}) = \boldsymbol{I}_n + \boldsymbol{A}_n(\boldsymbol{\gamma}, \bar{\gamma}) = (\boldsymbol{I}_n + \mathbf{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\mathbf{1}_n' - \bar{\gamma}\mathbf{1}_n\mathbf{1}_n')$, we record the identities $\boldsymbol{L}_n'\boldsymbol{D}_{\boldsymbol{\omega}\boldsymbol{I}} = \boldsymbol{D}_{\boldsymbol{\omega}}\boldsymbol{L}_n'$, $\boldsymbol{L}_n'\boldsymbol{I}_n\boldsymbol{L}_n = \boldsymbol{D}_{\boldsymbol{n}}^{-1} = \text{Diag}(n_1^{-1}, \ldots, n_k^{-1})$, with $\boldsymbol{D}_{\boldsymbol{\omega}} = \text{Diag}(\omega_1, \ldots, \omega_k)$; and $\boldsymbol{L}_n'\boldsymbol{A}_n(\boldsymbol{\gamma}, \bar{\gamma})\boldsymbol{L}_n = \boldsymbol{A}_k(\boldsymbol{\theta}, \bar{\gamma})$ as in Lemma 2(iii), with $\boldsymbol{\theta} = [\bar{\gamma}_1, \ldots, \bar{\gamma}_k]'$ as means of the partitioned elements of $\boldsymbol{\gamma}' = [\boldsymbol{\gamma}_1', \ldots, \boldsymbol{\gamma}_k']$. It follows directly that $E(\bar{\boldsymbol{Y}} \mid \widehat{\beta}_T) = \widehat{\beta}_T^{-1}\boldsymbol{L}_n'[(\mu_1\mathbf{1}_{n_1}', \ldots, \mu_k\mathbf{1}_{n_k}')' + \beta_0\mathbf{1}_n] = \widehat{\beta}_T^{-1}(\boldsymbol{\mu} - \beta_0\mathbf{1}_k)$ with $\boldsymbol{\mu} = [\mu_1, \ldots, \mu_k]'$, and that $E(\bar{\boldsymbol{Y}}) = \kappa_1(\boldsymbol{\mu} - \beta_0\mathbf{1}_k)$ as stated in conclusion (i). Moreover, $\text{V}(\bar{\boldsymbol{Y}} \mid \widehat{\beta}_T) = \boldsymbol{\Xi}_1(\widehat{\beta}_T) = \widehat{\beta}_T^{-2}[\boldsymbol{\Xi}_k(\boldsymbol{\omega}, \boldsymbol{\theta}, \boldsymbol{n}) + \sigma_0^2\mathbf{1}_k\mathbf{1}_k']$, where $\boldsymbol{\Xi}_k(\boldsymbol{\omega}, \boldsymbol{\theta}, \boldsymbol{n}) = \boldsymbol{L}_n'\boldsymbol{\Xi}_n(\boldsymbol{\omega}, \boldsymbol{\gamma})\boldsymbol{L}_n = \boldsymbol{D}_{\boldsymbol{\omega}}[\boldsymbol{D}_{\boldsymbol{n}}^{-1} + \boldsymbol{A}_k(\boldsymbol{\theta}, \bar{\gamma})]\boldsymbol{D}_{\boldsymbol{\omega}}$, with $\boldsymbol{D}_{\boldsymbol{n}} = \text{Diag}(n_1, \ldots, n_k)$, and $\boldsymbol{A}_k(\boldsymbol{\theta}, \bar{\gamma}) = \mathbf{1}_k\boldsymbol{\theta}' + \boldsymbol{\theta}\mathbf{1}_k' - \bar{\gamma}\mathbf{1}_k\mathbf{1}_k'$. Unconditional dispersion parameters are $V(\bar{\boldsymbol{Y}}) = \boldsymbol{\Xi}_1 = \kappa_2[\boldsymbol{\Xi}_k(\boldsymbol{\omega}, \boldsymbol{\theta}, \boldsymbol{n}) + \sigma_0^2\mathbf{1}_k\mathbf{1}_k'] + \kappa_{11}(\boldsymbol{\mu} - \beta_0\mathbf{1}_k)(\boldsymbol{\mu} - \beta_0\mathbf{1}_k)'$, to give conclusion (ii). Conclusion (iii) follows directly as before, and conclusion (iv) on using $\text{V}(\boldsymbol{R} \mid \widehat{\beta}_T) = \widehat{\beta}_T^{-2}\boldsymbol{B}\text{V}(\boldsymbol{Y})\boldsymbol{B} = \widehat{\beta}_T^{-2}\text{Diag}(\omega_1^2\boldsymbol{I}_{n_1}, \ldots, \omega_k^2\boldsymbol{I}_{n_k})$ since $\boldsymbol{B}_{n_i}\boldsymbol{\Sigma}(\boldsymbol{\gamma}_i, \bar{\gamma})\boldsymbol{B}_{n_i} = \boldsymbol{B}_{n_i}$ and $\boldsymbol{B}_{n_i}\boldsymbol{A}_{ij}\boldsymbol{B}_{n_j} = \mathbf{0}$ from the idempotency of $\{\boldsymbol{B}_{n_1}, \ldots, \boldsymbol{B}_{n_k}\}$ and the annihilations $\{\boldsymbol{B}_{n_i}\mathbf{1}_{n_i} = \mathbf{0}; 1 \le i \le k\}$. Conclusion (v) follows directly from (iv). Conclusion (iv) asserts under Gaussian errors that $\{\boldsymbol{R}_1, \ldots, \boldsymbol{R}_k\}$, and thus $\{S_1^2, \ldots, S_k^2\}$, are conditionally independent given $\widehat{\beta}_T$. As in the proof for Theorem 3(iv), the marginal density of $\mathcal{L}(\nu_i S_i^2\sigma_1^2/\omega_i^2 \mid \widehat{\beta}_1)$ is the scaled chi–squared density $g_0(u_i; \nu_i/2, 2w)$ as defined preceding (2.2), with $w = (\widehat{\beta}_1^2/\sigma_1^2)$. Their unconditional joint density now follows on mixing as in Section 2.2, as asserted in conclusion (vi), to complete our proof. $\square$

We turn next to comparisons among $\{S_1^2, \ldots, S_k^2\}$. Recall from (4.5) that $\{\text{Var}(Y_{ij} \mid \widehat{\beta}_T) = \widehat{\beta}_T^{-2}\omega_i^2(2\gamma_{ij} - \bar{\gamma} + \sigma_0^2); 1 \le j \le n_i\}$ and $\{\text{Var}(Y_{ij}) = \kappa_2\omega_i^2(2\gamma_{ij} - \bar{\gamma} + \sigma_0^2) + \kappa_{11}(\mu_i - \beta_0)^2; 1 \le j \le n_i\}$, for each $\{i = 1, 2, \ldots, k\}$. These are heterogeneous within and among samples by virtue of the structural parameters $\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})$, even when the external scalings $\{\omega_1, \ldots, \omega_k\}$ are equal. However, Theorem 4(iv) establishes not only that $\mathcal{L}(S_1^2, \ldots, S_k^2)$ is independent of $\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})$, but that their scale parameters $\{\omega_1^2/\sigma_1^2, \ldots, \omega_k^2/\sigma_1^2\}$ are equal if and only if $\{\omega_1^2, \ldots, \omega_k^2\}$ are homogeneous. To continue, let $T_4(S_1^2, \ldots, S_k^2)$ be any scale–invariant statistic, *i.e.,* $T_4(cS_1^2, \ldots, cS_k^2) = T_4(S_1^2, \ldots, S_k^2)$ for $c \ne 0$. This is the substance of the following,

**Theorem 5.** *Let $\{S_1^2, \ldots, S_k^2\}$ be within–sample variances from the calibrated measurements $\{Y_{ij}; 1 \le j \le n_i, 1 \le i \le k\}$ in a one–way experiment; let $T_4(S_1^2, \ldots, S_k^2)$ be any scale–invariant statistic; and consider a Gaussian model with $\mathcal{L}(\boldsymbol{Z}) = N_n(\boldsymbol{\mu}_Z, \boldsymbol{\Xi}_n(\boldsymbol{\omega}, \boldsymbol{\gamma}))$ independently of $(\widehat{\beta}_0, \widehat{\beta}_1)$ under Gaussian calibration. Then the distribution of $T_4(S_1^2, \ldots, S_k^2)$ is identical to its conventional normal–theory form, as if $\{(Y_{ij} - \mu_i)/\sigma_i; 1 \le j \le n_i, 1 \le i \le k\}$ were iid $N_1(0, 1)$, independently of $(\widehat{\beta}_0, \widehat{\beta}_T)$ and $\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})$.*

**Proof.** Gaussian errors and Theorem 4(iv) assert that $\mathcal{L}(\widehat{\beta}_T\boldsymbol{R}_1/\omega_1, \ldots, \widehat{\beta}_T\boldsymbol{R}_k/\omega_k \mid \widehat{\beta}_T) = N_n(\mathbf{0}, \boldsymbol{B})$ with $\boldsymbol{B} = \text{Diag}(\boldsymbol{B}_{n_1}, \ldots, \boldsymbol{B}_{n_k})$, so that $\{(n_1 - 1)S_1^2\widehat{\beta}_T^2/\omega_1^2, \ldots, (n_k - 1)S_k^2\widehat{\beta}_T^2/\omega_k^2\}$ are conditionally independent chi–squared variables, given $\widehat{\beta}_T$. However, we have that

$$T_4(S_1^2\widehat{\beta}_T^2/\omega_1^2, \ldots, S_k^2\widehat{\beta}_T^2/\omega_k^2) = T_4(S_1^2/\omega_1^2, \ldots, S_k^2/\omega_k^2)$$

by its scale invariance, so that $\mathcal{L}[T_4(S_1^2,\ldots,S_k^2)\,|\,\widehat{\beta}_T] = \mathcal{L}[T_4(S_1^2,\ldots,S_k^2)]$ unconditionally, independently of $(\widehat{\beta}_0,\widehat{\beta}_T)$, and depending on $\boldsymbol{\Xi}_n(\boldsymbol{\omega},\boldsymbol{\gamma})$ only through $\boldsymbol{\omega} = [\omega_1,\ldots,\omega_k]'$, to complete our proof. □

Conventional comparisons among variances are necessarily scale–invariant. Moreover, it is seen that procedures based on $\{S_1^2,\ldots,S_k^2\}$ support tests for conditional hypotheses $H_0' : \widehat{\beta}_T^{-2}\omega_1^2 = \cdots = \widehat{\beta}_T^{-2}\omega_k^2$, or equivalently, $H_0 : \omega_1^2 = \omega_2^2 = \cdots = \omega_k^2$, against appropriate alternatives. Theorem 5 applies for both null and non–null distributions of invariant test statistics. Tests in common usage include

- Modifications of Bartlett's [26] likelihood ratio test;
- Cochran's [27] test based on $S_{max}^2/(S_1^2+\cdots+S_k^2)$;
- Hartley's [28] $F$–max test based on the maximal ratio $\max\{S_i^2/S_j^2\}$.
- Gnanadesikan's [29] simultaneous comparisons of treatment variances with a control.

In summary, in view of $\{\mathrm{Var}(Y_{ij}\mid\widehat{\beta}_T) = \widehat{\beta}_T^{-2}\omega_i^2(2\gamma_{ij}-\bar{\gamma}+\sigma_0^2); 1\le j\le n_i\}$, it is seen that conventional tests based on $\{S_1^2,\ldots,S_k^2\}$ cannot discern heterogeneity among variances owing to the structural parameters $\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})$, but only the external scalings $\{\omega_1,\ldots,\omega_k\}$ within the $k$ samples. Fortunately, it is seen next that the homogeneity of $\{\omega_1^2,\ldots,\omega_k^2\}$ is enough to validate the one–way analysis of variance, irrespective of the structural parameters $\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})$ and additional complications arising through classical calibration.

To examine effects of calibration on the one–way analysis of variance, we suppose that $\mathrm{V}(\boldsymbol{Z}) = \omega^2\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})$, so that $\mathrm{V}(\boldsymbol{Y}\,|\,\widehat{\beta}_T) = \widehat{\beta}_T^{-2}\omega^2[\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})+\sigma_0^2\mathbf{1}_n\mathbf{1}_n'] = \widehat{\beta}_T^{-2}\omega^2\boldsymbol{\Sigma}(\boldsymbol{\gamma},\phi)$ as in Section 2.3, with $\phi = \bar{\gamma}-\sigma_0^2/\omega^2$. Call this $\mathrm{V}(\boldsymbol{Y}\,|\,\widehat{\beta}_T) = \boldsymbol{\Xi}(\widehat{\beta}_T)$. We proceed to validate the analysis conditionally, given $\widehat{\beta}_T$, where $E(\boldsymbol{Y}\,|\,\widehat{\beta}_T) = \widehat{\beta}_T^{-1}(\boldsymbol{\mu}_Z-\beta_0\mathbf{1}_n)$ with $\boldsymbol{\mu}_Z = [\mu_1\mathbf{1}_{n_1}',\ldots,\mu_k\mathbf{1}_{n_k}']'$. Recall that $\boldsymbol{I}_n = \boldsymbol{A}_0+\boldsymbol{A}_1+\boldsymbol{A}_2$ partitions $\boldsymbol{Y}'\boldsymbol{I}_n\boldsymbol{Y} = \boldsymbol{Y}'\boldsymbol{A}_0\boldsymbol{Y}+\boldsymbol{Y}'\boldsymbol{A}_1\boldsymbol{Y}+\boldsymbol{Y}'\boldsymbol{A}_2\boldsymbol{Y}$ such that $\boldsymbol{Y}'\boldsymbol{A}_0\boldsymbol{Y} = n\overline{Y}^2$, with $\overline{Y}$ as the grand mean and $\boldsymbol{A}_0 = n^{-1}\mathbf{1}_n\mathbf{1}_n'$; $\boldsymbol{Y}'\boldsymbol{A}_1\boldsymbol{Y} = \sum_{i=1}^k n_i(\overline{Y}_i-\overline{Y})^2$; and $\boldsymbol{Y}'\boldsymbol{A}_2\boldsymbol{Y} = \sum_{i=1}^k\sum_{j=1}^{n_i}(Y_{ij}-\overline{Y}_i)^2$. Here $\{\boldsymbol{A}_0,\boldsymbol{A}_1,\boldsymbol{A}_2\}$ are idempotent matrices of ranks $\{1,k-1,n-k\}$ such that $\{\boldsymbol{A}_i\boldsymbol{A}_j = \mathbf{0}; i\ne j\}$ and thus $\{\boldsymbol{A}_i\mathbf{1}_n = \mathbf{0}; i=1,2\}$ since $\boldsymbol{A}_0 = n^{-1}\mathbf{1}_n\mathbf{1}_n'$. In particular, we partition $\boldsymbol{Y}'(\boldsymbol{I}_n-\boldsymbol{A}_0)\boldsymbol{Y}$ as $\boldsymbol{Y}'\boldsymbol{B}_n\boldsymbol{Y} = \boldsymbol{Y}'\boldsymbol{A}_1\boldsymbol{Y}+\boldsymbol{Y}'\boldsymbol{A}_2\boldsymbol{Y}$. To validate the Fisher–Cochran theorem conditionally requires that $\{\boldsymbol{A}_i\boldsymbol{\Xi}(\widehat{\beta}_T)\boldsymbol{A}_j = \mathbf{0}; i\ne j\}$ with $\{i,j\in\{1,2\}\}$. Moreover, scale parameters to be associated with the quadratic forms are found as $\{\xi_i^2\boldsymbol{G} = \boldsymbol{G}\boldsymbol{\Xi}(\widehat{\beta}_T)\boldsymbol{G}; \boldsymbol{G}\in\{\boldsymbol{A}_1,\boldsymbol{A}_2,\boldsymbol{B}_n\}\}$; their degrees of freedom are determined by ranks; and noncentrality parameters derive from expected mean squares. This program of study is carried out next in support of the following.

**Theorem 6.** *Let $\{Y_{ij} = \widehat{\beta}_T^{-1}(Z_{ij}-\widehat{\beta}_0); 1\le j\le n_i, 1\le i\le k\}$ be calibrated measurements in a one–way experiment such that $\mathcal{L}(\boldsymbol{Z}) = N_n(\boldsymbol{\mu}_Z,\omega^2\boldsymbol{\Sigma}_0(\boldsymbol{\gamma}))$ independently of Gaussian errors of calibration, where $\boldsymbol{\mu}_Z = [\mu_1\mathbf{1}_{n_1}',\ldots,\mu_k\mathbf{1}_{n_k}']'$, so that $\boldsymbol{\mu}_Y(\widehat{\beta}_T) = E(\boldsymbol{Y}\mid\widehat{\beta}_T) = \widehat{\beta}_T^{-1}(\boldsymbol{\mu}_Z-\beta_0\mathbf{1}_n)$ and $\mathrm{V}(\boldsymbol{Y}\,|\,\widehat{\beta}_T) = \boldsymbol{\Xi}(\widehat{\beta}_T) = \widehat{\beta}_T^{-2}\omega^2\boldsymbol{\Sigma}(\boldsymbol{\gamma},\phi)$ with $\phi = \bar{\gamma}-\sigma_0^2/\omega^2$.*

*(i) To test equality of elements $\kappa_1[\mu_1,\ldots,\mu_k]'$ of $\boldsymbol{\mu}_Y = \kappa_1[\mu_1\mathbf{1}_{n_1}',\ldots,\mu_k\mathbf{1}_{n_k}']'$, pertaining to the group means of calibrated measurements, the analysis of variance test is identical in level and power to its conventional normal–theory form where $\mathcal{L}(\boldsymbol{Y}) = N_n(\boldsymbol{\mu}_Y,\sigma_Y^2\boldsymbol{I}_n)$.*

*(ii) Supporting tests, based on linear contrasts among the group means, are identical in level and power to their normal–theory forms, as if* $\mathcal{L}(\boldsymbol{Y}) = N_n(\boldsymbol{\mu}_Y, \sigma_Y^2 \boldsymbol{I}_n)$.

**Proof.** Given the partition $\boldsymbol{Y}'\boldsymbol{B}_n\boldsymbol{Y} = \boldsymbol{Y}'\boldsymbol{A}_1\boldsymbol{Y} + \boldsymbol{Y}'\boldsymbol{A}_2\boldsymbol{Y}$, we proceed conditionally, given $\widehat{\beta}_T$, to examine (i) consistency of their scale parameters, (ii) the conditional independence of $\boldsymbol{Y}'\boldsymbol{A}_1\boldsymbol{Y}$ and $\boldsymbol{Y}'\boldsymbol{A}_2\boldsymbol{Y}$, and (iii) conditional expectations of $\{\boldsymbol{Y}'\boldsymbol{A}_1\boldsymbol{Y}, \boldsymbol{Y}'\boldsymbol{A}_2\boldsymbol{Y}, \boldsymbol{Y}'\boldsymbol{B}_n\boldsymbol{Y}\}$. Accordingly, scale parameters are found as $\{\xi_i^2\boldsymbol{G} = \boldsymbol{G}\boldsymbol{\Xi}(\widehat{\beta}_T)\boldsymbol{G}; \boldsymbol{G} \in \{\boldsymbol{A}_1, \boldsymbol{A}_2, \boldsymbol{B}_n\}\}$, where $\boldsymbol{G}\boldsymbol{\Xi}(\widehat{\beta}_T)\boldsymbol{G} = \widehat{\beta}_T^{-2}\omega^2\boldsymbol{G}(\boldsymbol{I}_n + \boldsymbol{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\boldsymbol{1}_n' - \phi\boldsymbol{1}_n\boldsymbol{1}_n')\boldsymbol{G} = \widehat{\beta}_T^{-2}\omega^2\boldsymbol{G}$ since $\boldsymbol{G}$ is idempotent and $\boldsymbol{G}\boldsymbol{1}_n = \boldsymbol{0}$ for $\boldsymbol{G} \in \{\boldsymbol{A}_1, \boldsymbol{A}_2, \boldsymbol{B}_n\}$, thus confirming that their scale parameters are equal, namely, $\widehat{\beta}_T^{-2}\omega^2$. The conditional independence of $\{\boldsymbol{Y}'\boldsymbol{A}_1\boldsymbol{Y}, \boldsymbol{Y}'\boldsymbol{A}_2\boldsymbol{Y}\}$ follows since $\boldsymbol{A}_1\boldsymbol{\Xi}(\widehat{\beta}_T)\boldsymbol{A}_2 = \widehat{\beta}_T^{-2}\omega^2\boldsymbol{A}_1(\boldsymbol{I}_n + \boldsymbol{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\boldsymbol{1}_n' - \phi\boldsymbol{1}_n\boldsymbol{1}_n')\boldsymbol{A}_2 = \widehat{\beta}_T^{-2}\omega^2\boldsymbol{A}_1\boldsymbol{A}_2 = \boldsymbol{0}$ and $\boldsymbol{A}_1\boldsymbol{1}_n = \boldsymbol{0}$ $= \boldsymbol{A}_2\boldsymbol{1}_n$. Conditional expectations of $\{\boldsymbol{Y}'\boldsymbol{A}_1\boldsymbol{Y}, \boldsymbol{Y}'\boldsymbol{A}_2\boldsymbol{Y}, \boldsymbol{Y}'\boldsymbol{B}_n\boldsymbol{Y}\}$ are found as

$$\{E(\boldsymbol{Y}'\boldsymbol{G}\boldsymbol{Y} \,|\, \widehat{\beta}_T) = \mathrm{tr}\boldsymbol{G}\boldsymbol{\Xi}(\widehat{\beta}_T) + [\boldsymbol{\mu}_Y(\widehat{\beta}_T)]'\boldsymbol{G}[\boldsymbol{\mu}_Y(\widehat{\beta}_T)]; \boldsymbol{G} \in \{\boldsymbol{A}_1, \boldsymbol{A}_2, \boldsymbol{B}_n\}\},$$

where $\mathrm{tr}\boldsymbol{G}\boldsymbol{\Xi}(\widehat{\beta}_T)\boldsymbol{G} + [\boldsymbol{\mu}_Y(\widehat{\beta}_T)]'\boldsymbol{G}[\boldsymbol{\mu}_Y(\widehat{\beta}_T)] = \widehat{\beta}_T^{-2}\omega^2\mathrm{tr}\boldsymbol{G}(\boldsymbol{I}_n + \boldsymbol{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\boldsymbol{1}_n' - \phi\boldsymbol{1}_n\boldsymbol{1}_n') + \widehat{\beta}_T^{-2}(\boldsymbol{\mu}_Z - \beta_0\boldsymbol{1}_n)'\boldsymbol{G}(\boldsymbol{\mu}_Z - \beta_0\boldsymbol{1}_n) = \widehat{\beta}_T^{-2}\omega^2\mathrm{tr}\boldsymbol{G} + \widehat{\beta}_T^{-2}\boldsymbol{\mu}_Z'\boldsymbol{G}\boldsymbol{\mu}_Z$ since $\boldsymbol{G}\boldsymbol{1}_n = \boldsymbol{0}$ and $\mathrm{tr}\boldsymbol{G}\boldsymbol{\gamma}\boldsymbol{1}_n' = \boldsymbol{1}_n'\boldsymbol{G}\boldsymbol{\gamma}' = \boldsymbol{0}$ for $\boldsymbol{G} \in \{\boldsymbol{A}_1, \boldsymbol{A}_2, \boldsymbol{B}_n\}$. Moreover, the quadratic forms are those for the one–way analysis of $\{Z_{ij}; 1 \le j \le n_i, 1 \le i \le k\}$, namely, $\boldsymbol{\mu}_Z'\boldsymbol{A}_1\boldsymbol{\mu}_Z = \sum_{i=1}^k n_i(\mu_i - \bar{\mu})^2$, with $\bar{\mu} = n^{-1}\sum_{i=1}^k n_i\mu_i$; $\boldsymbol{\mu}_Z'\boldsymbol{A}_2\boldsymbol{\mu}_Z = 0$; and $\boldsymbol{\mu}_Z'\boldsymbol{B}_n\boldsymbol{\mu}_Z = \sum_{i=1}^k n_i(\mu_i - \bar{\mu})^2$. Now combine these facts into the conditional test statistic

$$F(\widehat{\beta}_T) = \frac{\boldsymbol{Y}'\boldsymbol{A}_1\boldsymbol{Y}\widehat{\beta}_T/(k-1)\omega^2}{\boldsymbol{Y}'\boldsymbol{A}_2\boldsymbol{Y}\widehat{\beta}_T/(n-k)\omega^2}$$

such that $\mathcal{L}[F(\widehat{\beta}_T) \,|\, \widehat{\beta}_T] = F(k-1, n-k, \lambda(\widehat{\beta}_T))$, with $\lambda(\widehat{\beta}_T) = \widehat{\beta}_T^{-2}\sum_{i=1}^k n_i(\mu_i - \bar{\mu})^2/\widehat{\beta}_T^{-2}\omega^2 = \sum_{i=1}^k n_i(\mu_i - \bar{\mu})^2/\omega^2$. It follows that $\mathcal{L}[F(\widehat{\beta}_T) \,|\, \widehat{\beta}_T] = F(k-1, n-k, \lambda)$ unconditionally, with $\lambda = \sum_{i=1}^k n_i(\mu_i - \bar{\mu})^2/\omega^2$, to establish conclusion (i). To continue, let $\boldsymbol{C}'\bar{\boldsymbol{Y}}$ be a collection of linear contrasts among the within–sample calibrated means, and let $S_Y^2 = \boldsymbol{Y}'\boldsymbol{A}_2\boldsymbol{Y}/(n-k)$ be the pooled within–sample variance. The test for conditional independence of $(\boldsymbol{C}'\bar{\boldsymbol{Y}}, S_Y^2)$ is that $\boldsymbol{C}'\boldsymbol{L}_n'\boldsymbol{\Xi}(\widehat{\beta}_T)\boldsymbol{A}_2 = \boldsymbol{0}$, with $\boldsymbol{L}_n' = \mathrm{Diag}(n_1^{-1}\boldsymbol{1}_{n_1}', \ldots, n_k^{-1}\boldsymbol{1}_{n_k}')$. We directly evaluate $\boldsymbol{C}'\boldsymbol{L}_n'(\boldsymbol{I}_n + \boldsymbol{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\boldsymbol{1}_n' - \phi\boldsymbol{1}_n\boldsymbol{1}_n')\boldsymbol{A}_2 = \boldsymbol{C}'\boldsymbol{L}_n'\boldsymbol{A}_2 + \boldsymbol{C}'\boldsymbol{1}_k\boldsymbol{\gamma}'\boldsymbol{A}_2 = \boldsymbol{0}$ since $\boldsymbol{L}_n'\boldsymbol{A}_2 = \boldsymbol{0}$, $\boldsymbol{1}_n'\boldsymbol{A}_2 = \boldsymbol{0}$, $\boldsymbol{L}_n'\boldsymbol{1}_n = \boldsymbol{1}_k$, and $\boldsymbol{C}'\boldsymbol{1}_k = \boldsymbol{0}$ as linear contrasts, so that $(\boldsymbol{C}'\bar{\boldsymbol{Y}}, S_Y^2)$ are conditionally independent given $\widehat{\beta}_T$. It follows that the standardized variables $\boldsymbol{C}'\bar{\boldsymbol{Y}}/S_Y$ satisfy $\widehat{\beta}_T^{-1}\boldsymbol{C}'(\bar{\boldsymbol{Z}} - \widehat{\beta}_0\boldsymbol{1}_k)/\widehat{\beta}_T^{-1}S_Z = \boldsymbol{C}'\bar{\boldsymbol{Z}}/S_Z$, their conditional and unconditional distributions being identical to their normal–theory forms when $\mathcal{L}(\boldsymbol{Y}) = N_n(\boldsymbol{\mu}_Y, \sigma_Y^2\boldsymbol{I}_n)$, to establish conclusion (ii) and thus complete our proof. □

## 5. Diagnostics

At issue is the capacity of available diagnostics to uncover the types of model violations induced through calibration based on $X(Y)$. If effective, then the routine use of these diagnostics in the past would have alerted users to such anomalies. We now face these concerns with regard to induced correlations and nonnormality of calibrated data. This assessment is carried out in the context of a single sample as in Section 4.1, where correlations may be attributed exclusively to calibration.

5.1. **Detecting Correlation.** Correlations induced through calibration clearly may be excessive. Conventional tests for correlation invoke matrices $V(\boldsymbol{Y}) = \tau^2\boldsymbol{\Xi}(\omega) = \tau^2(\boldsymbol{I}_n + \omega\boldsymbol{A})$, with $\boldsymbol{A}$ fixed and $\omega$ such that $\boldsymbol{\Xi}(\omega) \in \mathbb{S}_n^+$. Specializing gives $\tau^2\boldsymbol{\Xi}(\omega)$ as $\boldsymbol{\Sigma}(\rho)$ under equicorrelation. Tests due to [30]–[34], and others, utilize versions of von Neumann's [35] ratio $U = \boldsymbol{R}'\boldsymbol{B}\boldsymbol{R}/\boldsymbol{R}'\boldsymbol{R}$, with $\boldsymbol{R}$ as the observed residuals and with $\boldsymbol{B}(n \times n)$ fixed. See [36] for example. Here the unconditional distributions $\mathcal{L}(U)$ are all identical to their normal–theory forms, as if $\boldsymbol{R} = \boldsymbol{B}_n\boldsymbol{Z}$ with $\mathcal{L}(\boldsymbol{Z}) = N_n(\mu_Z\boldsymbol{1}_n, \sigma_Z^2\boldsymbol{I}_n)$, so that $\mathcal{L}(\boldsymbol{R}) = N_n(\boldsymbol{0}, \sigma_Z^2\boldsymbol{B}_n)$. This is seen from the proof for Theorem 3, where $\mathcal{L}(\boldsymbol{R}\,|\,\widehat{\beta}_T) = N_n(\boldsymbol{0}, \widehat{\beta}_T^{-2}\sigma_Z^2\boldsymbol{B}_n)$, together with the scale–invariance of $U = \boldsymbol{R}'\boldsymbol{B}\boldsymbol{R}/\boldsymbol{R}'\boldsymbol{R}$, assuring that $\mathcal{L}(\boldsymbol{R}'\boldsymbol{B}\boldsymbol{R}/\boldsymbol{R}'\boldsymbol{R}\,|\,\widehat{\beta}_T) = \mathcal{L}(\boldsymbol{R}'\boldsymbol{B}\boldsymbol{R}/\boldsymbol{R}'\boldsymbol{R})$ unconditionally. Accordingly, all such diagnostics for correlative dependencies are blind to the induced correlation structures of Section 4.1. In short, correlative dependencies induced through classical calibration, however excessive, cannot be discerned through the use of conventional diagnostics.

5.2. **Detecting Nonnormality.** Conventional diagnostics for normality include graphics and hypothesis tests. Graphics utilize plots of ordered residuals against their normal–theory expectations, to include the scaled residuals $\{R_i/S_Y; 1\leq i\leq n\}$, or the Studentized residuals $\{W_iR_i/S_Y; i = 1, 2, \ldots, n\}$, standardized so that $\mathrm{Var}(W_iR_i) = \sigma_Y^2$. See Sections 2.12 and 5.7 of [37], for example. However, in calibrated data these residual plots are indistinguishable from those for the conventional Gaussian model $N_n(\mu\boldsymbol{1}_n, \sigma^2\boldsymbol{I}_n)$, whatever be the joint mixture density of type (2.1) for the calibrated measurements $\{Y_i = (Z_i - \widehat{\beta}_0)/\widehat{\beta}_T; 1\leq i\leq n\}$. This follows from the fact that $\mathcal{L}(\boldsymbol{R}/(\boldsymbol{R}'\boldsymbol{R})^{1/2}\,|\,\widehat{\beta}_T) = \mathcal{L}(\boldsymbol{R}/(\boldsymbol{R}'\boldsymbol{R})^{1/2})$ from scale invariance, having a scaled multivariate Student's $t$–distribution with $\nu = n - 1$ degrees of freedom, depending on neither $\widehat{\beta}_T$ nor $\sigma_Y^2$.

The regression tests of [38] utilize the statistic $W = (\sum_{i=1}^n w_iY_{[i]})^2/(n-1)S_Y^2$, where $\{Y_{[1]} \leq Y_{[2]} \leq \ldots \leq Y_{[n]}\}$ are the ordered values of $\{Y_1, \ldots, Y_n\}$, and $\{w_1, \ldots, w_n\}$ are fixed weights. These tests are powerful against a wide range of alternatives, especially against skewed distributions or those having short or very long tails, even in small samples. See [39], for example. Accordingly, these would appear to be promising for detecting nonstandard mixture distributions of type (2.1) for classically calibrated measurements. For the latter we have

$$W = \frac{(\sum_{i=1}^n w_iY_{[i]})^2}{(n-1)S_Y^2} = \frac{[(\sum_{i=1}^n w_iZ_{[i]} - \widehat{\beta}_0\sum_{i=1}^n w_i)]^2}{(n-1)S_Y^2\widehat{\beta}_T^2}. \tag{5.1}$$

However, since $\sum_{i=1}^n w_i = 0$ for the regression tests of [38], and since $S_Y^2\widehat{\beta}_T^2 = S_Z^2$, we infer that $W = [(\sum_{i=1}^n w_iZ_{[i]}]^2/(n-1)S_Z^2$, so that $\mathcal{L}(W \mid \widehat{\beta}_T) = \mathcal{L}(W)$ holds unconditionally from cancellation. Accordingly, these regression tests fail to distinguish between Gaussian distributions, and Gaussian mixtures of type (2.1) from classically calibrated data. On the other hand, these tests do offer a clear check on normality of $\mathcal{L}(Z_1, \ldots, Z_n)$, on which the mixtures (2.1) are predicated. Variations on these regression tests are surveyed in [40], none able to distinguish between Gaussian data and the mixtures (2.1) induced through calibration.

Hypothesis tests based on the central moment ratios $\{b_1 = m_3^2/m_2^3,\, b_2 = m_4/m_2^2\}$, where $m_r = \sum_{i=1}^{n}(Y_i - \overline{Y})^r$, are especially useful for distinguishing between Gaussian and skewed distributions, or against distributions having excessive or short tails; see [40]. These ratios, when based on classically calibrated measurements $\{Y_1, \ldots, Y_n\}$, are precisely those obtainable from $\{Z_1, \ldots, Z_n\}$, so that their null distributions are identical to those under conventional assumptions where $\mathcal{L}(\boldsymbol{Y}) = N_n(\mu\mathbf{1}_n, \sigma^2\boldsymbol{I}_n)$, whatever be the actual joint mixture distribution of type (2.1) stemming from calibration.

In short, conventional diagnostics for normality, as listed, cannot distinguish between Gaussian errors, and Gaussian mixtures of type (2.1). Thus radical departures from conventional Gaussian models, as induced through the use of calibrated instruments, cannot be discerned through routine screening using any of the listed diagnostic tools.

In Section 5 we have reexamined the capacity for conventional diagnostics to detect the correlations and nonnormality induced through calibration. Even radical departures from conventional assumptions cannot be discerned through routine screening using any of the listed diagnostic tools.

## 6. NUMERICAL STUDIES

We next examine effects of calibration in two case studies. Case 1 couples octane number $(U)$ with percent purity $(X)$ in gasoline. Since octane numbers are evaluated routinely in production, it is expedient to use these quantities as surrogates to access percent purity through calibration. Case 2 typifies the universal calibration of laboratory and field instruments, specifically, the calibration of a colorimeter in the determination of phosphorus. Here the milligrams $(X)$ of phosphorus were measured directly on an analytical balance; an added reagent then developed a yellow solution; and the transmittance $(U)$ from the photocell of the colorimeter was observed for each specimen. Linearity of the calibration is known from Beer's Law, stating that intensity of transmitted light relates inversely to phosphorus concentration.

For a calibration $\{U_i = \beta_0 + \beta_1 X_i + \epsilon_i; 1 \le i \le m\}$, we denote as before the *OLS* estimators $\{\widehat{\beta}_0, \widehat{\beta}_1\}$, and their values $\{b_0, b_1\}$ as computed from the data. Collateral values from Section 3.1 include $S_{uu} = \sum_{i=1}^{m}(U_i - \overline{U})^2$, $S_{xu} = \sum_{i=1}^{m} X_i(U_i - \overline{U})$, and $S_{xx} = \sum_{i=1}^{m}(X_i - \overline{X})^2$, with $\overline{X} = 0$ as in Section 3.1. Moreover, $S_U^2$ is the residual mean square and $R^2_{(X,U)}$ the squared correlation between $X$ and $U$. The data are reported in Table 1, and the summary statistics $\{m,\, b_0,\, b_1,\, S_U^2, S_{xx}, S_{uu}, S_U/\sqrt{S_{xx}},\, R^2_{(X,U)}\}$ are listed in Table 2 from the linear calibration.

Much less scatter appears in the phosphorus data of Case 2 than the octane data of Case 1, as is borne out in scatter plots not shown, and by the squared correlations given in the last column of Table 2. By comparison, the estimated slope is considerably greater in the gasoline data of Case 1, with estimated standard error of the slope as given by $S_{\widehat{\beta}_1} = S_U/\sqrt{S_{xx}} = 0.1848$; in contrast, $S_{\widehat{\beta}_1} = 0.003335$ for Case 2. Both features influence

TABLE 1. Case 1: Percent purity ($X$) and octane number ($U$) of gasoline. Case 2: Milligrams phosphorus ($X$) and transmittance ($U$) in calibrating a laboratory colorimeter.

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Case | $X$ | 99.8 | 99.7 | 99.6 | 99.5 | 99.4 | 99.3 | 99.2 | 99.1 | 99.0 | 98.9 | 98.8 |
| 1 | $U$ | 87.6 | 87.4 | 87.2 | 87.4 | 87.2 | 86.8 | 86.5 | 86.3 | 86.4 | 86.6 | 86.1 |
| Case | $X$ | 0.00 | 2.28 | 4.56 | 6.84 | 9.12 | 11.40 | 13.68 | 15.96 | 18.24 | 22.80 | 27.36 |
| 2 | $U$ | 0.00 | 0.56 | 1.02 | 1.74 | 2.01 | 2.68 | 3.28 | 3.87 | 4.32 | 5.23 | 6.38 |

TABLE 2. Summary statistics for Case 1 and Case 2.

| Case | $m$ | $b_0$ | $b_1$ | $S_U^2$ | $S_{xx}$ | $S_{uu}$ | $S_U/\sqrt{S_{xx}}$ | $R^2_{(X,U)}$ |
|---|---|---|---|---|---|---|---|---|
| 1 | 11 | 86.8636 | 1.4545 | 0.037580 | 1.10 | 2.6655 | 0.184800 | 87.3% |
| 2 | 11 | 2.8264 | 0.2330 | 0.008219 | 739.12 | 40.1875 | 0.003335 | 99.8% |

the magnitudes of irregularities in calibrated data, which we next examine numerically for the two case studies.

To continue, consider cut–off values $[c, \infty)$. Invoking the Rule–of–Thumb of Remark 1 with $\{S_{xx}, S_{uu}, \widehat{\beta}_1\}$ as given, for Case 1 the rule $5\% \leq R^2_{(X,U)}$ restricts $\widehat{\beta}_1 \in [0.3481, \infty)$. For Case 2, the restriction is $\widehat{\beta}_1 \in [0.01166, \infty)$. These correspond to the interval $[a, b]$ in Section 3.1 that defines the exclusion rule for $\mathcal{L}(\widehat{\beta}_T) = \mathcal{L}(\widehat{\beta}_1 \mid \widehat{\beta}_1 \in [a, b])$ for the restricted estimator $\widehat{\beta}_T$.

Estimates for the inverse moments $\{\mu_{-1}(\widehat{\beta}_T),\, \mu_{-2}(\widehat{\beta}_T)\}, \mathrm{Var}(\widehat{\beta}_T^{-1})\}$ for the two case studies are reported in Table 3. These are approximated using inverse moment estimators in expressions from Lemma 3, Appendix A, assuming Gaussian errors during calibration with $\mu_3(\widehat{\beta}_1) = 0$ and $\mu_4(\widehat{\beta}_1) = 3[\mu_2(\widehat{\beta}_1)]^2$, equivalently, with skewness $\gamma_1(\widehat{\beta}_1) = 0$ and kurtosis $\gamma_2(\widehat{\beta}_1) = 3$. These assumptions are shown to be justified for $\widehat{\beta}_T$ by computing the skewness and kurtosis for the truncated distribution of $\widehat{\beta}_T$. Table 3 reports these values, which were computed with Maple, to be $\{0,\, 3.0000\}$ for both Cases 1 and 2.

**Remark 3.** This in part exemplifies Remark 2. For both Cases 1 and 2 the coverage exceeds 0.9999. Using extended precision in Maple, the estimates $\widehat{\beta}_1$ and $\widehat{\beta}_T$ differ in the ninth decimal place for Case 1, as do their estimated standard deviations.

TABLE 3. Estimates for inverse moments of $\widehat{\beta}_T$ from Lemma 3 when $\mu_3(\widehat{\beta}_T) = 0$ and $\mu_4(\widehat{\beta}_T) = 3[\mu_2(\widehat{\beta}_T)]^2$, and values for $\{\gamma_1(\widehat{\beta}_T), \gamma_2(\widehat{\beta}_T)\}$.

| Case | $\mu_{-1}(\widehat{\beta}_T)$ | $\mu_{-2}(\widehat{\beta}_T)$ | $\mathrm{Var}(\widehat{\beta}_T^{-1})$ | $\gamma_1(\widehat{\beta}_T)$ | $\gamma_2(\widehat{\beta}_T)$ |
|---|---|---|---|---|---|
| 1 | 0.6992 | 0.4974 | 0.008606 | 0 | 3.0000 |
| 2 | 4.2935 | 18.4376 | 0.003782 | 0 | 3.0000 |

Estimates for $\mu_{-1}(\widehat{\beta}_T)$ and $\mu_{-2}(\widehat{\beta}_T)$ are considerably greater for the phosphorus data than for the octane data, reflecting the smaller slope of the former. Conversely, $\mathrm{Var}(\widehat{\beta}_T^{-1})$ is smaller in the phosphorus data, no doubt reflecting the substantially smaller value for $S_U/\sqrt{S_{xx}}$.

Further computations take $\sigma_Z^2 = \sigma_U^2$, as estimated by $S_U^2$ during calibration. Note, however, that this equality might be contraindicated in the calibration of some biomedical instruments, where $\{\sigma_U^2 << \sigma_Z^2\}$ often obtains [7]. The initial calibration is assumed to have been centered with $\overline{X} = 0$, so that $\widehat{\beta}_0 = \overline{U}$ and $\mathrm{Var}(\widehat{\beta}_0) = \sigma_0^2 = \sigma_U^2/m$, as estimated by $S_U^2/m$. The variance of $\{Y_i;\ 1 \le i \le n\}$, under $\sigma_Z^2 = \sigma_U^2$ and the additional assumption that $\{U_1, \ldots, U_m\}$ and $\{Z_1, \ldots, Z_n\}$ have been centered such that $E(U_i) = E(Z_i)$, is estimated by $\kappa_2 S_U^2(1 + 1/m)$ from Theorem 1, and is listed under $\sigma_Y^2(\theta_0)$ in Table 5.

To demonstrate the accuracy of estimates for the inverse moments of $\widehat{\beta}_T$ from Lemma 3, we used Maple software to compute the inverse moments $\{\kappa_1, \kappa_2, \mathrm{Var}(\widehat{\beta}_T^{-1})\}$ of $\widehat{\beta}_T$, having restricted $\widehat{\beta}_T$ to $[c, \infty) = [0.3481, \infty)$ for Case 1 and to $[0.01166, \infty)$ for Case 2, as noted. These ranges have coverage over 0.9999; that is, for Case 2 $\Pr[\widehat{\beta}_1 \in [c, \infty)] > 0.9999$, with $(\widehat{\beta}_1 - b_1)/(S_U/\sqrt{S_{xx}}) = (\widehat{\beta}_1 - 0.2330)/(0.003335)$ as an approximate standard normal distribution. Table 4 reports the inverse moments for $\widehat{\beta}_T \in [c, \infty)$, as computed from $\mathcal{L}(\widehat{\beta}_T)$ $= N_c^{\infty}(\mu_T, \sigma_T^2)$, as $N_1(\mu, \sigma^2)$ restricted to $[c, \infty]$. The inverse moment estimators in Table 3 all agree (to the accuracy of the data) with the inverse moments, using Maple, for the truncated distribution $\mathcal{L}(\widehat{\beta}_T)$, as shown in Table 4.

TABLE 4. Inverse moments of $\widehat{\beta}_T$ for the distribution $\mathcal{L}(\widehat{\beta}_T) = N_c^{\infty}(\beta_T, \sigma_T^2)$ restricted to $\widehat{\beta}_1 \in [c, \infty)$.

| Case | $\mu_{-1}(\widehat{\beta}_T)$ | $\mu_{-2}(\widehat{\beta}_T)$ | $\mathrm{Var}(\widehat{\beta}_T^{-1})$ |
|---|---|---|---|
| 1 | 0.6992 | 0.4976 | 0.008606 |
| 2 | 4.2935 | 18.4376 | 0.003782 |

To study unconditional moments for $\{Y_i = (Z_i - \widehat{\beta}_0)/\widehat{\beta}_T;\ 1 \le i \le n\}$ as in Theorem 1, it is germane to examine parameters common to $\{Y_1, \ldots, Y_n\}$ as the bias $\theta = |\mu_Z - \beta_0|$ is allowed to vary. We treat four cases, namely, $\theta \in [\theta_0, \theta_1, \theta_2, \theta_3] = [0,\ \sigma_Z^2/2,\ \sigma_Z^2,\ 3\sigma_Z^2/2]$ so as to adjust for scale, with corresponding estimates as fractions of $S_U^2$. Estimates for the unconditional means $\mu_Y(\theta) = \kappa_1\theta$ and unconditional variances $\sigma_Y^2(\theta) = \kappa_2(\sigma_Z^2 + \sigma_0^2) + \kappa_{11}\theta^2$ common to $\{Y_1, \ldots, Y_n\}$, derived using the inverse moment estimates $\{\kappa_1, \kappa_2, \kappa_{11}\}$ of $\widehat{\beta}_T$ from Table 3, are reported in Table 5 for each of the two case studies.

The unconditional mixture distribution for $\{Y_i = (Z_i - \widehat{\beta}_0)/\widehat{\beta}_T;\ 1 \le i \le n\}$ from Equation (3.3) can be computed using Maple. The unconditional mixture distribution for $Y$ uses as parameters $\{\mu_Z \doteqdot \widehat{\beta}_0,\ \sigma_Z^2 = \sigma_U^2 \doteqdot S_U^2,\ \sigma_0^2 \doteqdot S_U^2/m,\ \sigma_1^2 \doteqdot S_U^2/S_{xx}\}$.] From the unconditional mixture distribution, estimates for the mean and variance of $\mathcal{L}(Y|\theta)$, with bias $\theta = |\mu_Z - \beta_0|$, are denoted as $\{E(Y|\theta),\ V_Y(\theta) = \mathrm{Var}(Y|\theta)\}$, and are shown in Tables 5 and 6 for $\theta \in [\theta_0, \theta_1, \theta_2, \theta_3] = [0, \sigma_Z^2/2, \sigma_Z^2, 3\sigma_Z^2/2]$.

The estimates $\{\mu_Y(\theta_i);\ i=0,...,3\}$ using the inverse moments estimates from Table 3 agree (to the accuracy of the data) with the corresponding estimators $\{E(Y|\theta_i);\ i=0,...,3\}$, computed using Maple and the unconditional mixture distribution for $Y$ from Equation (3.3), while the corresponding variance estimator $\sigma_Y^2(\theta)$, using the inverse moment estimators from Table 3, show an overestimation compared to $\mathrm{Var}(Y|\theta)$ from the unconditional mixture distribution. The skewness $\{\gamma_1(Y\,|\,\theta_i)\}$ and kurtosis $\gamma_2(Y\,|\,\theta_i)$ for the unconditional mixture distribution $\mathcal{L}(Y\,|\,\theta_i)$ for Case 1 and Case 2 were computed using Maple for values $\theta \in [\theta_0,\theta_1,\theta_2,\theta_3] = [0,\sigma_Z^2/2,\sigma_Z^2,3\sigma_Z^2/2]$, and are given in Table 7. These show an increase in both skewness and kurtosis as the bias is increased.

Table 5. Estimates $\{\mu_Y(\theta_i\}$ for the unconditional moments of $\mathcal{L}(Y)$ using the inverse moments from Table 3 and estimates $\{E(Y|\theta_i)\}$ from Theorem 1, where $\theta = |\mu_Z - \beta_0|$ takes values $\theta \in [\theta_0,\theta_1,\theta_2,\theta_3] = [0,\sigma_Z^2/2,\sigma_Z^2,3\sigma_Z^2/2]$ and $S_U$ is used for $\sigma_Z$.

| Case | $\mu_Y(\theta_0)$ | $E(Y\|\theta_0)$ | $\mu_Y(\theta_1)$ | $E(Y\|\theta_1)$ | $\mu_Y(\theta_2)$ | $E(Y\|\theta_2)$ | $\mu_Y(\theta_3)$ | $E(Y\|\theta_3)$ |
|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 0.06776 | 0.06777 | 0.13550 | 0.13550 | 0.20330 | 0.20330 |
| 2 | 0 | 0 | 0.19460 | 0.19460 | 0.38920 | 0.38920 | 0.58390 | 0.58390 |

Table 6. Estimates $\{\sigma_Y^2(\theta_i)\}$ for the unconditional moments of $\mathcal{L}(Y)$ using the inverse moments from Table 3, and estimates $\{V_Y(\theta_i) = \mathrm{Var}(Y|\theta_i\}$ from Theorem 1, where $\theta = |\mu_Z - \beta_0|$ takes values in $[\theta_0,\theta_1,\theta_2,\theta_3] = [0,\sigma^2/2,\sigma_Z^2,3\sigma_Z^2/2]$ and $S_U$ replaces $\sigma_Z$.

| Case | $\sigma_Y^2(\theta_0)$ | $V_Y(\theta_0)$ | $\sigma_Y^2(\theta_1)$ | $V_Y(\theta_1)$ | $\sigma_Y^2(\theta_2)$ | $V_Y(\theta_2)$ | $\sigma_Y^2(\theta_3)$ | $V_Y(\theta_3)$ |
|---|---|---|---|---|---|---|---|---|
| 1 | 0.02039 | 0.02040 | 0.02254 | 0.02048 | 0.02900 | 0.02073 | 0.03975 | 0.02033 |
| 2 | 0.16530 | 0.16530 | 0.16630 | 0.16530 | 0.16910 | 0.16540 | 0.17380 | 0.16540 |

Table 7 reports the skewness $\gamma_1(Y|\theta_i)$ and kurtosis $\gamma_2(Y|\theta_i)$ for the unconditional mixture distribution $\mathcal{L}(Y\,|\,\theta_i)$ from Theorem 1 using Maple, with bias $\theta = |\mu_Z - \beta_0|$ taking values in $[\theta_0,\theta_1,\theta_2,\theta_3] = [0,\sigma_Z^2/2,\sigma_Z^2,3\sigma_Z^2/2]$.

Table 7. Estimates for the skewness $\{\gamma_1(\theta_i) \equiv \gamma_1(Y|\theta_i)\}$ and kurtosis $\{\gamma_2(\theta_i) \equiv \gamma_2(Y|\theta_i)\}$ parameters for the unconditional mixture distribution $\mathcal{L}(Y\,|\,\theta_i)$ using Maple where $\theta = |\mu_Z - \beta_0|$ takes values $\theta \in [\theta_0,\theta_1,\theta_2,\theta_3] = [0,\sigma_Z^2/2,\sigma_Z^2,3\sigma_Z^2/2]$

| Case | $\gamma_1(\theta_0)$ | $\gamma_2(\theta_0)$ | $\gamma_1(\theta_1))$ | $\gamma_2(\theta_1)$ | $\gamma_1(\theta_2)$ | $\gamma_2(\theta_2)$ | $\gamma_1(\theta_3))$ | $\gamma_2(\theta_3)$ |
|---|---|---|---|---|---|---|---|---|
| 1 | 0.0000 | 3.2360 | 0.05311 | 3.2413 | 0.1056 | 3.2568 | 0.1571 | 3.2821 |
| 2 | 0.0000 | 3.0025 | 0.0006 | 3.0025 | 0.0012 | 3.0025 | 0.0018 | 3.0025 |

We next examine the underestimation of $\mathrm{Var}(Y_i)$ by $S_Y^2$ as shown in Theorem 2. To these ends we estimate $E(S_Y^2) = \sigma_Z^2\mu_{-2}(\widehat{\beta}_T)$ using $S_U^2$ in lieu of $\sigma_Z^2$, and $\mu_{-2}(\widehat{\beta}_T)$ as estimated in Table 3. These values are listed in the second column of Table 8. Observe from Theorem 2 that the bias may be written as $B(\theta) = \sigma_0^2\mu_{-2}(\widehat{\beta}_T)+\theta^2\mathrm{Var}(\widehat{\beta}_T)$, with $\theta = |\mu_Z - \beta_0|$ as before. Values for the bias for $\theta \in [\theta_0, \theta_1, \theta_2, \theta_3] = [0, \sigma^2/2, \sigma_Z^2, 3\sigma_Z^2/2]$ are estimated as fractions of $S_U^2$, as reported in succeeding columns of Table 8. In parentheses are the fractional errors $B(\theta)/\sigma_Y^2(\theta)$, with denominators taken from Table 5. The values in brackets in Table 8 are the fractional errors $B(\theta)/\mathrm{Var}(Y|\theta)$ using the estimates for the denominator from Table 5 for the unconditional mixture distribution $\mathcal{L}(Y|\theta)$ from Theorem 1 computed with Maple. When the bias $\theta$ is zero, the fractional error is

$$\frac{B(0)}{\sigma_Y^2(0)} = \frac{\kappa_2\sigma_0^2}{\kappa_2(\sigma^2+\sigma_0^2)} = \frac{\sigma^2/m}{\sigma^2+\sigma^2/m} = \frac{1}{m+1} = 0.08333.$$

and similarly $B(0)/\mathrm{Var}(\widehat{\beta}_T|\theta = 0) = 1/(m+1)$. Column 3 of Table 8 reports these values for the fractional errors. This concludes our numerical studies.

TABLE 8. Estimates for $E(S_Y^2)$ and its bias $B(\theta)$ for estimating $\mathrm{Var}(Y|\theta)$ with $\theta = |\mu_Z - \beta_0|$ taking values in $[\theta_0, \theta_1, \theta_2, \theta_3] = [0, \sigma^2/2, \sigma_Z^2, 3\sigma_Z^2/2]$ as estimated using $S_U^2$ for $\sigma_Z^2$. The fractional errors in parentheses are $B(\theta)/\sigma_Y^2(\theta)$ and in brackets are $B(\theta)/\mathrm{Var}(Y|\theta)$ from Table 5.

| Study | $\sigma_Z^2\mu_{-2}(\widehat{\beta}_T)$ | $B(\theta_0)$ | $B(\theta_1)$ | $B(\theta_2)$ | $B(\theta_3)$ |
|---|---|---|---|---|---|
| Case 1 | 0.01870 | 0.001699 | 0.002020 | 0.002983 | 0.004588 |
| | | (0.08333) | (0.08962) | (0.10290) | (0.11540) |
| | | [0.08333] | [0.09867] | [0.14390] | [0.21700] |
| Case 2 | 0.15150 | 0.01378 | 0.01378 | 0.01378 | 0.01378 |
| | | (0.08333) | (0.08286) | (0.08147) | (0.07926) |
| | | [0.08333] | [0.08333] | [0.08332] | [0.08330] |

## 7. CONCLUSIONS

Our findings bear variously on contemporary statistical practice. In statistical process control, for example, evidence for a tightened process resides in the sample variance $S_Y^2$, often monitored using an $S^2$–chart. For calibrated data, underestimation of the actual variance by $S_Y^2$ would tend to present an overly optimistic view that the target variance had been achieved when, in fact, it had not. In consequence, the average run lengths of such charts typically would be longer than intended, even when the process is in control.

To continue, the means of measured product characteristics are routinely monitored using $\overline{X}$–charts, which are tantamount to monitoring a succession of Student–t statistics. But our studies in Theorem 3 show that these statistics are inflated in magnitude, so that the lower and upper control limits for such charts will be exceeded more frequently than intended.

In consequence, the average run lengths would be smaller, perhaps much smaller, than intended even when the process is in control. This fact alone could wreak havoc in the use of three–sigma or six–sigma control limits.

In summary, the widespread and necessary use of calibration may have devastating effects, even on elementary data–analytic procedures pertaining to location and scale parameters. It is unfortunate that these difficulties cannot be flagged by the ever expanding use of available diagnostic tools. It thus is incumbent on knowledgeable users of statistical methodology, and the statistical consultants advising them, to assess the extent of these difficulties as they might impact the analysis and interpretation of a particular set of calibrated data.

## Appendix A

We require various moments $\mu_r(\cdot)$, to include negative moments. In particular, $\{\mu_r(Z) = E(Z^r);\ r \in [-2,-1,1]\}$ designate moments about 0, whereas $\{\mu_r(Z) = E(Z-\mu_1)^r;\ r \in [2,3,4]\}$ identify central moments. Approximations to selected negative moments are undertaken in the following. We apply the Delta Method for the fourth order ($q = 4$) Taylor series approximation on the transformation $g(t) = 1/t$.

**Lemma 3.** *For a random sample of size $n$, let $Z_n \in \mathbb{R}^1$ be a statistic with range $[c,\infty) \subset (0,\infty)$ for some $c > 0$, and with finite moments up to order $2(q+1) = 10$ such that $E(|Z_n - \mu_1|^{10}) = O(n^{-5})$. Then fourth order ($q = 4$) approximations to $\mu_{-1}(Z_n)$, $\mu_{-2}(Z_n)$, and $Var(Z_n^{-1})$ are given by*

$$\begin{aligned}
\mu_{-1}(Z_n) &= \frac{1}{\mu_1} + \frac{\mu_2}{\mu_1^3} - \frac{\mu_3}{\mu_1^4} + \frac{\mu_4}{\mu_1^5} + O(n^{-5/2}) \\
\mu_{-2}(Z_n) &= \frac{1}{\mu_1^2} + \frac{3\mu_2}{\mu_1^4} - \frac{4\mu_3}{\mu_1^5} + \frac{5\mu_4}{\mu_1^6} + O(n^{-5/2}) \\
Var(Z_n^{-1}) &= \frac{\mu_2}{\mu_1^4} - \frac{2\mu_3}{\mu_1^5} + \frac{3\mu_4 - \mu_2^2}{\mu_1^6} + \frac{2\mu_2\mu_3}{\mu_1^7} - \frac{2\mu_2\mu_4 + \mu_3^2}{\mu_1^8} + \frac{2\mu_3\mu_4}{\mu_1^9} - \frac{\mu_4^2}{\mu_1^{10}} + O(n^{-3}).
\end{aligned}$$

**Proof**. As the distribution $Z_n$ has range $[c,\infty) \subset (0,\infty)$, the delta method for bounded functions with bounded derivatives can be applied with the transformation $g(t) = 1/t$; for example see [41] and [42]. We compute the fourth degree ($q = 4$) Taylor series expansion for $\{Z_n^{-1}, Z_n^{-2}\}$ with error bound, as shown in Equation (1) of [41] and in Equation (3) of [42], to be

$$\begin{aligned}
E(Z_n^{-1}) &= \frac{1}{\mu_1} + \frac{\mu_2}{\mu_1^3} - \frac{\mu_3}{\mu_1^4} + \frac{\mu_4}{\mu_1^5} + O(n^{-(4+1)/2}) \\
E(Z_n^{-2}) &= \frac{1}{\mu_1^2} + \frac{3\mu_2}{\mu_1^4} - \frac{4\mu_3}{\mu_1^5} + \frac{5\mu_4}{\mu_1^6} + O(n^{-(4+1)/2}).
\end{aligned}$$

Expanding $\mathrm{Var}(Z_n^{-1}) = \mu_{-2}(Z_n) - [\mu_{-1}(Z_n)]^2$ yields the Taylor series estimate for $\mathrm{Var}(Z_n^{-1})$,

$$\mathrm{Var}(Z_n^{-1}) = \frac{\mu_2}{\mu_1^4} - \frac{2\mu_3}{\mu_1^5} + \frac{3\mu_4 - \mu_2^2}{\mu_1^6} + \frac{2\mu_2\mu_3}{\mu_1^7} - \frac{2\mu_2\mu_4 + \mu_3^2}{\mu_1^8} + \frac{2\mu_3\mu_4}{\mu_1^9} - \frac{\mu_4^2}{\mu_1^{10}} + O(n^{-(4+2)/2}),$$

where the bound $O(n^{-(4+2)/2})$ is given in Equation (2) of [41]. $\square$

**Remark 4.** For developments leading to the Case Studies of Section 6, identify $n$ of Lemma 3 with the sample size $m$ in determining the calibration line, and let $\widehat{\beta}_1(m) \equiv \widehat{\beta}_{1,n}$ be its slope and $\sigma_{1,n}$ its standard deviation, with $\sigma_{1,n}^2 = \sigma^2/S_{xx}(n)$ depending on $n$. Then the truncated distribution is that of $Z_n = \widehat{\beta}_{T,n}$ with $\mathcal{L}(\widehat{\beta}_{T,n}) = \mathcal{L}(\widehat{\beta}_{1,n}|\widehat{\beta}_{1,n} \in [c,\infty))$, and with the untruncated distribution $\mathcal{L}(\widehat{\beta}_{1,n}) = N_1(\beta_1, \sigma_{1,n}^2)$ having finite moments for $p \geq 1$ as given by

$$E(|\widehat{\beta}_{1,n} - \beta_1|^p) = \sigma_{1,n}^p \frac{2^{\frac{p}{2}}\Gamma(\frac{p+1}{2})}{\sqrt{\pi}} = O((\sigma_{1,n}^2)^{\frac{p}{2}}).$$

To apply Lemma 3 for $Z_n = \widehat{\beta}_{T,n}$, the requirement that $E(|Z_n - \mu_1|^{10}) = O(n^{-5})$ is verified as follows.

**Lemma 4.** *Let $Z_n = \widehat{\beta}_{T,n}$ such that $\mathcal{L}(\widehat{\beta}_{T,n}) = \mathcal{L}(\widehat{\beta}_{1,n}|\widehat{\beta}_{1,n} \in [c,\infty))$, with $\mathcal{L}(\widehat{\beta}_{1,n}) = N_1(\beta_1, \sigma_{1,n}^2)$. Then $E(|\widehat{\beta}_{T,n} - E(\widehat{\beta}_{T,n})|^{10}) = O(n^{-5})$.*

**Proof**. To continue, we assume that the data $\{X_1, \ldots, X_n\}$ have comparable variation such that $S_{xx}(n)/n \xrightarrow{n} Q_{xx}$ with $\{A_1, A_2\}$ such that for all $n$, $0 < A_1 \leq \frac{S_{xx}(n)}{n} \leq A_2$, equivalently, that $0 < \sigma^2/(nA_2) \leq \sigma^2_{\widehat{\beta}_{1,n}} = \frac{\sigma^2}{S_{xx}(n)} \leq \sigma^2/(nA_1)$; and in particular,

$$E(|\widehat{\beta}_{1,n} - \beta_1|^p) = O(n^{-\frac{p}{2}}).$$

The *OLS* estimator for the slope is a consistent estimator with $\sqrt{n}(\widehat{\beta}_{1,n} - \beta_1) \xrightarrow{d} N(0, \sigma^2/Q_{xx})$. We have assumed that $c < \beta_1$, so the coverages $\Pr[c < \widehat{\beta}_{1,n}] = \Pr[\sqrt{n}(c-\beta_1)/\sqrt{\sigma^2/Q_{xx}} < \sqrt{n}(\widehat{\beta}_{1,n} - \beta_1)/\sqrt{\sigma^2/Q_{xx}}] \xrightarrow{n} 1$. In particular, the coverages $\{C_g(n)\}$ are bounded away from zero with $0 < B < \Pr[\widehat{\beta}_{1,n} \in [c,\infty)]$. For the truncated distribution we have

$$\begin{aligned} E(|\widehat{\beta}_{T,n} - \beta_1|^p) &= \frac{1}{C_g(n)} \int_c^\infty |t - \beta_1|^p f_{\widehat{\beta}_{1,n}}(t)dt \\ &\leq \frac{1}{B} \int_{-\infty}^\infty |t - \beta_1|^p f_{\widehat{\beta}_{1,n}}(t)dt \\ &= \frac{1}{B} E(|\widehat{\beta}_{1,n} - \beta_1|^p) = O(n^{-\frac{p}{2}}). \end{aligned}$$

By Hölder's inequality

$$|E(\widehat{\beta}_{T,n}) - \beta_1| = |E(\widehat{\beta}_{T,n} - \beta_1)| \leq \Big(E(|\widehat{\beta}_{T,n} - \beta_1|^p)\Big)^{\frac{1}{p}}$$

so

$$|E(\widehat{\beta}_{T,n}) - \beta_1|^p \leq E(|\widehat{\beta}_{T,n} - \beta_1|^p) = O(n^{-\frac{p}{2}}).$$

To apply Lemma 3 to the truncated statistic $\widehat{\beta}_{T,n}$, the requirement that $E(|Z_n - \mu_1|^{10}) = O(n^{-5})$ is verified through the binomial expansion by

$$\begin{aligned} E(|\widehat{\beta}_{T,n} - E(\widehat{\beta}_{T,n})|^p) &= E(|\widehat{\beta}_{T,n} - \beta_1 + \beta_1 - E(\widehat{\beta}_{T,n})|^p) \\ &\leq \sum_{r=0}^{p} \binom{p}{r} \Big(E(|\widehat{\beta}_{T,n} - \beta_1|^r)\Big) \Big(|E(\widehat{\beta}_{T,n}) - \beta_1|^{p-r}\Big) \\ &= \sum_{r=0}^{p} O(n^{-\frac{r}{2}}) O(n^{-\frac{p}{2}+\frac{r}{2}}) = O(n^{-\frac{p}{2}}), \end{aligned}$$

to complete our proof. □

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