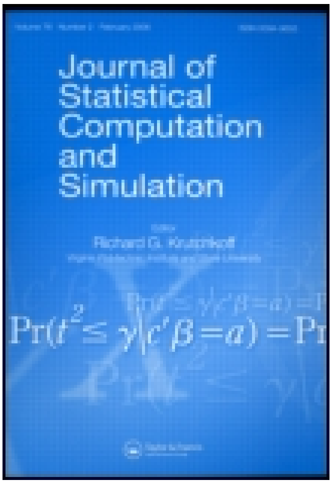

Journal of Statistical Computation and Simulation
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gscs20

Irregularities in X(Y) from Y(X) in linear calibration

D. R. Jensen [a] & D. E. Ramirez [a]

[a] Department of Mathematics, University of Virginia, PO Box 400137, Charlottesville, VA, 22904-4137, USA

Published online: 26 Mar 2012.

To cite this article: D. R. Jensen & D. E. Ramirez (2013) Irregularities in X(Y) from Y(X) in linear calibration, Journal of Statistical Computation and Simulation, 83:10, 1807-1828, DOI: 10.1080/00949655.2012.671324

To link to this article: http://dx.doi.org/10.1080/00949655.2012.671324

Journal of Statistical Computation and Simulation, 2013
Vol. 83, No. 10, 1807–1828, http://dx.doi.org/10.1080/00949655.2012.671324

Irregularities in $X(Y)$ from $Y(X)$ in linear calibration

D.R. Jensen and D.E. Ramirez*

Department of Mathematics, University of Virginia, PO Box 400137, Charlottesville, VA 22904-4137, USA

(*Received 5 October 2011; final version received 26 February 2012*)

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. The arrays of instrumental readings are projected in this manner in practice, yielding arrays of calibrated measurements, typically subject to errors of calibration. The effects of calibration errors on the properties of calibrated measurements are examined here under linear calibration. Irregularities arise as induced dependencies, inflated variances, non-standard 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.

Keywords: linear calibration; induced dependencies; non-standard distributions; diagnostics; case studies

1. Introduction

Measurements enable the sciences and engineering, typically through calibrated instruments subject to errors of calibration. Statistical issues in calibration were considered in [1–11]; for example, all focused on the calibration of instruments *per se* rather than on their subsequent and repeated usage. All are linked to error-induced irregularities in arrays of calibrated measurements, but these have been largely 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 $\{U_1, \dots, U_m\}$ during calibration are observed at measurements $\{X_1, \dots, X_m\}$ without error, under the model $U(X)$, namely $\{U_i = \beta_0 + \beta_1 X_i + \epsilon_i; 1 \leq i \leq m\}$, giving the least-squares calibration line $\hat{U} = \hat{\beta}_0 + \hat{\beta}_1 X$, together with the calibrated measurement $Y = \hat{X}(U) = (U - \hat{\beta}_0)/\hat{\beta}_1$ 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 $\{Z_1, \dots, Z_n\}$, taken during the course of an experiment, then are projected back onto the scale of phosphorus measurements as $\{Y_i = (Z_i - \hat{\beta}_0)/\hat{\beta}_1; 1 \leq i \leq n\}$, to be analysed as the calibrated entities of note. Periodic checks against a standard then determine when recalibration is required. Often referred to as *classical calibration,* this is the model of choice here. In contrast, *inverse calibration*, as set forth in the above-cited references, is based on the

*Corresponding author. Email: der@virginia.edu *unconventional* model $\{X_i = \gamma_0 + \gamma_1 U_i + \epsilon_i; 1 \le i \le m\}$, unconventional in that $\{X_i; 1 \le i \le m\}$ 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 non-parametric procedures often require that sample data $\{Y_1, \ldots, Y_n\}$ 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 previously, [1–11] focused exclusively on the calibration of instruments *per se* rather than on the consequences of their subsequent usage, as also found in a burgeoning literature in the field of *chemometrics.* In contrast, subsequent effects of classical calibration errors were studied in [12], where actual levels for one-sample confidence intervals were found to be 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 $\{X_i = \gamma_0 + \gamma_1 U_i + \epsilon_i; 1 \le i \le m\}$ as a *conventional* model having chance variation in X_i but with $\{U_i; 1 \le i \le m\}$ as regressors determined without error. The focus there was on the effects of calibration errors on subsequent statistical analyses, where mixing distributions are required to properly account 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 (1) and (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 (6) and (7) 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 (11) and (12) 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 the 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 $\mathbb{S}_n^0$ 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 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 tr $(\boldsymbol{A})$, $|\ \boldsymbol{A}\ |$, and $r(\boldsymbol{A})$, respectively. The 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 $V(\boldsymbol{Y})$ designate the expectation vector and dispersion matrix for $\boldsymbol{Y} \in \mathbb{R}^n$, with $E(Y)$ and Var (Y) as the 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 zero and $\{\mu_r(Z) = E(Z - \mu_1)^r); r \in \{2, 3, 4\}\}$ as central moments. Specifically, let $\kappa_1 = \mu_{-1}(\hat{\beta})$, $\kappa_2 = \mu_{-2}(\hat{\beta})$, and $\kappa_{11} = \mathrm{Var}\,(\hat{\beta}^{-1}) = \kappa_2 - \kappa_1^2$ in terms of an estimator $\hat{\beta}$. Expansions and approximations to selected negative moments are given in Appendix 1.

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 (μ, σ^2); $N_a^b(\mu_T, \sigma_T^2)$ as $N_1(\mu, \sigma^2)$ restricted to $[a, b]$; and non-central 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 non-centrality λ. 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 $\Gamma_c^d(\nu, \lambda)$ 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

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

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

$$f(u; \alpha, \beta, G_2) = \frac{u^{\alpha-1}}{\beta^\alpha \Gamma(\alpha)} \int_0^\infty w^\alpha \mathrm{e}^{-wx/\beta}\, \mathrm{d}G_2(w) \tag{2}$$

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 $\boldsymbol{\Sigma}_0(\boldsymbol{\gamma}) = (\boldsymbol{I}_n + \boldsymbol{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\boldsymbol{1}_n' - \bar{\gamma}\boldsymbol{1}_n\boldsymbol{1}_n')$ in $\mathbb{S}_n^+$, such that $\boldsymbol{\gamma}' = [\gamma_1, \ldots, \gamma_n]$ and $\bar{\gamma} = (\gamma_1 + \cdots + \gamma_n)/n$. Such matrices and their equivalents were 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 $(\boldsymbol{D} + \boldsymbol{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\boldsymbol{1}_n')$ emerges in the study [23] of Euclidean distance matrices, having applications in linear inference [24].

Designate by $\Xi_1(n) = \{\boldsymbol{\Sigma}(\rho) = [(1-\rho)\boldsymbol{I}_n + \rho\boldsymbol{1}_n\boldsymbol{1}_n']; -(n-1)^{-1} < \rho < 1\}$ 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 $\boldsymbol{\Sigma}(\boldsymbol{\gamma}, \phi) = [\boldsymbol{I}_n + \boldsymbol{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\boldsymbol{1}_n' - \phi\boldsymbol{1}_n\boldsymbol{1}_n']$ 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 $\boldsymbol{A}_n(\boldsymbol{\gamma}, \phi) = \boldsymbol{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\boldsymbol{1}_n' - \phi\boldsymbol{1}_n\boldsymbol{1}_n'$. To these ends, let $\mathcal{A}_n = \{\boldsymbol{A}_n(\boldsymbol{\gamma}, \phi) = (\boldsymbol{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\boldsymbol{1}_n' - \phi\boldsymbol{1}_n\boldsymbol{1}_n'); (\boldsymbol{\gamma}, \phi) \in \Lambda_n\}$, and for each $\boldsymbol{A}_n(\boldsymbol{\gamma}, \phi)$, let $\tau_1 = \mathrm{tr}\,[\boldsymbol{A}_n(\boldsymbol{\gamma}, \phi)] = 2(\gamma_1 + \cdots + \gamma_n) - n\phi = n(2\bar{\gamma} - \phi)$ and $\tau_2 = (\gamma_1 - \bar{\gamma})^2 + \cdots + (\gamma_n - \bar{\gamma})^2$. 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, with 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* $\{\xi_1 \geq \cdots \geq \xi_n\}$ *of* $\boldsymbol{\Sigma}(\boldsymbol{\gamma},\phi)$ *are given by* $\{\xi_1 = 1+\alpha_1, \xi_2 = \cdots = \xi_{n-1} = 1, \xi_n = 1+\alpha_n\}$.
(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 $c_1 = \text{tr}\,[\boldsymbol{A}_n(\boldsymbol{\gamma},\phi)] = \tau_1$ and c_2 is the sum of all (2×2) principal minors. Further terms vanish since $\boldsymbol{A}_n(\boldsymbol{\gamma},\phi)$ has rank 2. A typical principal (2×2) 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 $|\boldsymbol{A}_n(i,j)| = -(\gamma_i - \gamma_j)^2$ 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 $P_n(\boldsymbol{A}_n) = \alpha^{n-2}(\alpha^2 - \tau_1\alpha - n\tau_2)$, with 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) follows from the requirement that $1 + \alpha_n = 1 + [\tau_1 - (\tau_1^2 + 4n\tau_2)^{1/2}]/2 > 0$ in order that $\boldsymbol{\Sigma}(\boldsymbol{\gamma},\phi)$ be positive definite. ■

Conclusion (ii) and thus conclusion (iii) hold generally, whether $\boldsymbol{\gamma} = \mathbf{0}$ or not. Here, $\boldsymbol{\gamma} = \mathbf{0}$ 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 $\boldsymbol{e} = n^{-1/2}\mathbf{1}_n$. 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 $\{\boldsymbol{\gamma}_i \in \mathbb{R}^{n_i}; 1 \leq i \leq k\}$ and $n_1 + \cdots + n_k = n$; let $\boldsymbol{L}_n' = \text{Diag}\,(n_1^{-1}\mathbf{1}_{n_1}', \ldots, n_k^{-1}\mathbf{1}_{n_k}')$; and note that $\boldsymbol{L}_n'\mathbf{1}_n = \mathbf{1}_k$. 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* $\boldsymbol{L}_n' = \text{Diag}\,(n_1^{-1}\mathbf{1}_{n_1}', \ldots, n_k^{-1}\mathbf{1}_{n_k}')$.

(i) *For* $\boldsymbol{G} = (\boldsymbol{G}_1 + \boldsymbol{G}_2) \in \mathcal{G}_n$, $\boldsymbol{G}_2$ *has the annihilative property that* $\boldsymbol{G}_2\mathbf{1}_n = \mathbf{0}$, *so that* $\boldsymbol{G}\mathbf{1}_n = (\boldsymbol{G}_1 + \boldsymbol{G}_2)\mathbf{1}_n = \xi_1\boldsymbol{e}\boldsymbol{e}'\mathbf{1}_n = \xi_1\mathbf{1}_n$ *and* $\boldsymbol{G}_2\boldsymbol{A}_n(\boldsymbol{\gamma},\phi)\boldsymbol{G}_2 = \mathbf{0}$.
(ii) $\mathcal{A}_n$ *is closed under* $\boldsymbol{G} \in \mathcal{G}_n$ *acting by congruence, that is,* $\boldsymbol{G}\boldsymbol{A}_n(\boldsymbol{\gamma},\phi)\boldsymbol{G} = \boldsymbol{A}_n(\boldsymbol{\omega},\alpha) \in \mathcal{A}_n$ *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* $\{\bar{\gamma}_i = (\gamma_{i1} + \cdots + \gamma_{in_i})/n_i; 1 \leq i \leq k\}$.

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

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

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 $\boldsymbol{L}_n'\mathbf{1}_n = \mathbf{1}_k$ and $\boldsymbol{L}_n'\boldsymbol{\gamma} = \bar{\boldsymbol{\gamma}} \in \mathbb{R}^k$, to complete our proof. ■

3. Calibration

Here, we seek the 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 $\{U_i = \beta_0 + \beta_1 X_i + \epsilon_i; 1 \le i \le m\}$ under Gauss–Markov assumptions with $\{\mathrm{Var}\,(U_i) = \sigma_U^2; 1 \le i \le m\}$, giving $(\hat\beta_0, \hat\beta_1)$ as least-squares estimators, and collateral values $S_{uu} = \sum_{i=1}^m (U_i - \bar U)^2$, $S_{xu} = \sum_{i=1}^m (X_i - \bar X)(U_i - \bar U)$, and $S_{xx} = \sum_{i=1}^m (X_i - \bar X)^2$. Here, $\mathrm{Var}\,(\hat\beta_0) = \sigma_0^2$ and $\mathrm{Var}\,(\hat\beta_1) = \sigma_1^2 = \sigma_U^2/S_{xx}$. *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 $\{Y_i = (Z_i - \hat\beta_0)/\hat\beta_1; 1 \le i \le n\}$, or equivalently $\boldsymbol{Y} = \hat\beta_1^{-1}(\mathbf{Z} - \hat\beta_0\mathbf{1}_n)$. If elements of $\boldsymbol{Z}' = [Z_1,\ldots,Z_n]$ have means $\boldsymbol{\mu}_Z' = [\mu_1,\ldots,\mu_n]$ and second moments $V(\mathbf{Z}) = \mathbf{\Sigma} = [\sigma_{ij}]$, independently of $(\hat\beta_0, \hat\beta_1)$, then conditional moments follow directly as

$$E(\boldsymbol{Y} \mid \hat\beta_1) = \hat\beta_1^{-1}[\boldsymbol{\mu}_Z - E(\hat\beta_0 \mid \hat\beta_1)\mathbf{1}_n], \tag{3}$$

$$V(\boldsymbol{Y} \mid \hat\beta_1) = \hat\beta_1^{-2}[\mathbf{\Sigma} + \mathrm{Var}\,(\hat\beta_0 \mid \hat\beta_1)\mathbf{1}_n\mathbf{1}_n']. \tag{4}$$

Expressions simplify if neither $E(\hat\beta_0 \mid \hat\beta_1)$ nor $\mathrm{Var}\,(\hat\beta_0 \mid \hat\beta_1)$ depends on $\hat\beta_1$. This holds in Gaussian calibration where $\{X_1,\ldots,X_m\}$ have been centred to $\{(X_1 - \bar X),\ldots,(X_m - \bar X)\}$, so that new outputs $\{Z_1,\ldots,Z_n\}$ first are projected onto the scale of measurements and then shifted by $\bar X$ units. For this case, $\hat\beta_0 = \bar U$; $\mathrm{Var}\,(\hat\beta_0) = \sigma_0^2 = \sigma_U^2/m$; $\mathrm{Var}\,(\hat\beta_1) = \sigma_1^2 = \sigma_U^2/S_{xx}$ as before; and $(\hat\beta_0, \hat\beta_1)$ are now uncorrelated and, under Gaussian calibration, are independent. We take the initial calibration to have been centred.

3.2. *Truncation*

Unconditional moments of $\{Y_1,\ldots,Y_n\}$, as crafted, are undefined, owing to outcomes of $\hat\beta_1$ near zero. However, a routine exclusion rule accepts a provisional calibration if $\hat\beta_1 \in [a,b]$ for fixed $a < b$ not spanning zero and recalibrates otherwise; see [1,6,8], for example. This effectively truncates the distribution of $\hat\beta_1$, 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 $\hat\beta_T = I_{[a,b]}\hat\beta_1$ as the resulting restricted estimator; and let $\beta_T = E(\hat\beta_T)$ and $\sigma_T^2 = \mathrm{Var}\,(\hat\beta_T)$. Clearly, $\beta_T \in [a,b]$ and, under Gaussian calibration, $\mathrm{Var}\,(\hat\beta_T) = \sigma_T^2 < \sigma_1^2 = \mathrm{Var}\,(\hat\beta_1)$, from a result reported in [25]. Moreover, the restriction $\mathcal{L}(\hat\beta_T) = N_a^b(\beta_T, \sigma_T^2)$, together with $\mathcal{L}(\hat\beta_1^2/\sigma_1^2) = \chi^2(1,\delta)$ with $\delta = \beta_1^2/\sigma_1^2$, is tantamount to restricting $(\hat{\beta}_1^2/\sigma_1^2)$ to $[c, d]$, with $c = a^2/\sigma_1^2$ and $d = b^2/\sigma_1^2$, to be designated as $\mathcal{L}(\hat{\beta}_1^2/\sigma_1^2 \in [c, d]) = \Gamma_c^d(1, \delta)$ 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 $\mathcal{L}(W \mid W \in [a, b]) = \mathcal{L}(W_T)$ designate the distribution of W restricted to $[a, b]$. Then,* coverage *is defined as $C_g = \int_a^b f_W(t)\,\mathrm{d}t$, 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 $\hat{\beta}_1 > 0$, 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 $\hat{\beta}_1$ 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 $\hat{\beta}_1$ by the standard relationship

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

In order to assure finite negative moments $\{\mu_{-1}(\hat{\beta}_T), \mu_{-2}(\hat{\beta}_T)\}$, 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 $\hat{\beta}_1$ to the interval $[\sqrt{0.05 S_{uu}/S_{xx}}, \infty)$.

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

3.3. *Error analysis*

If instead (β_0, β_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 $E(Y_i) = (\mu_i - \beta_0)/\beta_1 = \mu_Y(\beta_1)$, $\text{Var}\,(Y_i) = \text{Var}\,(Z_i)/\beta_1^2 = \sigma_Y^2(\beta_1)$, and $\rho(Y_i, Y_j) = \rho(Z_i, Z_j)$. This 'ideal' case serves as a reference against which recovery under calibrative errors may be gauged. From expression (4), the conditional correlation parameter becomes $\rho(Y_i, Y_j \mid \hat{\beta}_1) = (\sigma_{ij} + \sigma_0^2)/[(\sigma_{ii} + \sigma_0^2)(\sigma_{jj} + \sigma_0^2)]^{1/2}$ independently of $\hat{\beta}_1$. Even if $V(\mathbf{Z}) = \sigma_Z^2 \mathbf{I}_n$, where $\sigma_{ij} = 0$ for $i \neq j$, conditional correlations will have been induced through calibration. Unconditional properties of $\{Y_1, \ldots, Y_n\}$ follow through deconditioning, to include negative moments $\kappa_1 = \mu_{-1}(\hat{\beta}_T)$, $\kappa_2 = \mu_{-2}(\hat{\beta}_T)$, and $\kappa_{11} = \text{Var}\,(\hat{\beta}_T^{-1})$ of $\hat{\beta}_T$, as follows.

THEOREM 1 *Let $\{Y_i = (Z_i - \hat{\beta}_0)/\hat{\beta}_T; 1 \le i \le n\}$ be the measurements inverse to outputs $\{Z_1, \ldots, Z_n\}$ from a calibrated instrument observed independently of $\{U_1, \ldots, U_m\}$, such that $E(\mathbf{Z}) = \boldsymbol{\mu}_Z$ and $V(\mathbf{Z}) = \boldsymbol{\Sigma}$; and let $\sigma_0^2 = \text{Var}\,(\hat{\beta}_0)$, $\sigma_T^2 = \text{Var}\,(\hat{\beta}_T)$, $\kappa_1 = \mu_{-1}(\hat{\beta}_T)$, $\kappa_2 = \mu_{-2}(\hat{\beta}_T)$, and $\kappa_{11} = \text{Var}\,(\hat{\beta}_T^{-1})$. Then, unconditional moments, to be designated as $E(\mathbf{Y}) = \boldsymbol{\mu}_Y$ and $V(\mathbf{Y}) = \boldsymbol{\Xi}$, 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* $\hat{\beta}_T$ *as* $\hat{\beta}_1$ *restricted to* $[a,b]$ *in* $\mathbb{R}^1_+$, *then the unconditional joint density of the elements of* $\boldsymbol{Y}$ *is the translation–scale mixture*

$$f_n(\boldsymbol{y}; \boldsymbol{\mu}_Y, \boldsymbol{\Xi}, G_1) = C_g^{-1} \int_a^b g_n(\boldsymbol{y}; \boldsymbol{\mu}(t), \boldsymbol{\Xi}(t))\, \mathrm{d}G_1(t) \tag{5}$$

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

Proof Conclusion (i) follows directly from Equation (3), and conclusion (ii) from Equation (4), on using $\mathrm{Cov}\,(Y_i, Y_j) = E_{\hat{\beta}_T}[\mathrm{Cov}\,(Y_i, Y_j \mid \hat{\beta}_T)] + \mathrm{Cov}_{\hat{\beta}_T}[E(Y_i \mid \hat{\beta}_T), E(Y_j \mid \hat{\beta}_T)]$ for covariances and similarly for variances. Noting for fixed $\hat{\beta}_T$ that $\boldsymbol{Y}$ is a linear function of $(\boldsymbol{Z}, \hat{\beta}_0)$, we see that $\mathcal{L}(\boldsymbol{Y} \mid \hat{\beta}_T) = N_n(\boldsymbol{\mu}_Y(\hat{\beta}_T), \boldsymbol{\Xi}(\hat{\beta}_T))$ as in Equations (3) and (4). Expression (5) now follows on mixing over the conditioning distribution. ■

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 the elements of $\{Z_1, \ldots, Z_n\}$ are homoscedastic, such that $V(\boldsymbol{Z}) = \sigma_Z^2 \boldsymbol{I}_n$, it follows that the homogeneity of the unconditional variances of $\{Y_1, \ldots, Y_n\}$ is tantamount to the 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 non-parametrics. We next specialize earlier findings, as they apply in a single sample and in selected comparative experiments.

4.1. *Single sample*

The 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, that is, $E(\boldsymbol{Z}) = \mu_Z \mathbf{1}_n$ and $V(\boldsymbol{Z}) = \sigma_Z^2 \boldsymbol{I}_n$. At issue are the properties of $\mathcal{L}(\boldsymbol{Y})$ and of $(\bar{Y}, S_Y^2, t_0^2, \boldsymbol{R})$ as the sample mean, the sample variance, Student's statistic $t_0^2 = n(\bar{Y} - \mu_Y^0)^2 / S_Y^2$ with reference to two-sided alternatives, and $\boldsymbol{R} = [(Y_1 - \bar{Y}), \ldots, (Y_n - \bar{Y})]' = \boldsymbol{B}_n \boldsymbol{Y}$ as the ordinary residuals. Conditional and unconditional means are $E(\boldsymbol{Y} \mid \hat{\beta}_T) = \hat{\beta}_T^{-1}(\mu_Z - \beta_0)\mathbf{1}_n$ and $E(\boldsymbol{Y}) = \kappa_1(\mu_Z - \beta_0)\mathbf{1}_n$. Second moments exhibit common correlations, namely $V(\boldsymbol{Y} \mid \hat{\beta}_T) = \boldsymbol{\Xi}(\hat{\beta}_T) = \hat{\beta}_T^{-2}(\sigma_Z^2 + \sigma_0^2)\boldsymbol{\Sigma}(\rho)$ with $\rho = \sigma_0^2/(\sigma_Z^2 + \sigma_0^2)$ and $V(\boldsymbol{Y}) = \boldsymbol{\Xi} = \kappa_2(\sigma_Z^2 \boldsymbol{I}_n + \sigma_0^2 \mathbf{1}_n \mathbf{1}_n') + \kappa_{11}(\mu_Z - \beta_0)^2 \mathbf{1}_n \mathbf{1}_n'$, 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 $\kappa_1 = \mu_{-1}(\hat{\beta}_1)$, $\kappa_2 = \mu_{-2}(\hat{\beta}_1)$, and $\kappa_{11} = \mathrm{Var}\,(\hat{\beta}_1^{-1}) = \kappa_2 - \kappa_1^2$. The 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 σ_Y^2 and that induced dependencies preempt conventional asymptotics for $\bar{Y}_n = (Y_1 + \cdots + Y_n)/n$.

Theorem 2 *Let* $\{Y_i = (Z_i - \hat{\beta}_0)/\hat{\beta}_T; 1 \le i \le n\}$ *be the 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 $(\bar{Y}_n, S_Y^2, \boldsymbol{R})$, with $\boldsymbol{R}' = [(Y_1 - \bar{Y}), \ldots, (Y_n - \bar{Y})]$ as the ordinary residuals. Then,

(i) *$\bar{Y}_n$ 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* Var $(Y_i) = \sigma_Y^2$.
(iii) $\{E(R_i) = 0; 1 \leq i \leq n\}$.

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

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

Since $\lim_{n\to\infty}$ Var $(\bar{Y}_n) = [\kappa_2\sigma_0^2 + \kappa_{11}(\mu_Z - \beta_0)^2] > 0$, its limit distribution is not degenerate at μ_Y, so that the consistency of $\bar{Y}_n$ does not hold in probability or in mean square or, 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 $E[(n-1)S_Y^2] = \text{tr}\,\boldsymbol{B}_n V(\boldsymbol{Y}) + \boldsymbol{\mu}_Y'\boldsymbol{B}_n\boldsymbol{\mu}_Y$. The details are

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

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 μ_Y will decrease at the rate $O(n^{-1/2})$.
- Conclusion (ii) asserts that S_Y^2 underestimates 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 $\hat{\beta}_T$. It remains to examine the effects of calibration on unconditional distributions, to include those of the sample statistics $(\bar{Y}, S_Y^2, t_0^2, \boldsymbol{R})$. Under Gaussian calibration without exclusion, we have $\mathcal{L}(\hat{\beta}_1) = N_1(\beta_1, \sigma_1^2)$ and $\mathcal{L}(\hat{\beta}_1^2/\sigma_1^2) = \chi^2(1,\delta)$ with $\delta = \beta_1^2/\sigma_1^2$. With exclusion, the mixing distributions in expressions (1) and (2) now are $G_1(\hat{\beta}_T) = N_a^b(\beta_T, \sigma_T^2)$, whereas $G_2(\hat{\beta}_T^2;\delta)$ 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 $\{Y_i = (Z_i - \hat{\beta}_0)/\hat{\beta}_T; 1 \leq i \leq n\}$ be the calibrated measurements based on $\{Z_1, \ldots, Z_n\}$ as iid $N_1(\mu_Z, \sigma_Z^2)$ random variables independent of $(\hat{\beta}_0, \hat{\beta}_T)$ under Gaussian calibration, with $\hat{\beta}_T$ restricted to $[a,b]$ in $\mathbb{R}_+^1$, and let $\delta = \beta_1^2/\sigma_1^2$. Consider statistics $(\bar{Y}, S_Y^2, t_0^2, \boldsymbol{R})$, where $t_0^2 = n(\bar{Y} - \mu_Y^0)^2/S_Y^2$ and $\boldsymbol{R} = [(Y_1 - \bar{Y}), \ldots, (Y_n - \bar{Y})]'$ consists of ordinary residuals. Then, the following properties hold.*

(i) *$\mathcal{L}(\bar{Y})$ has the density $f_1(u;\mu,\tau^2(n),G_1)$ as in Equation (5) 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*

$$f_n(\boldsymbol{r};\boldsymbol{0},\sigma_Z^2\boldsymbol{B}_n,G_1) = C_g^{-1}\int_a^b g_n(\boldsymbol{y};\boldsymbol{0},t^{-2}\sigma_Z^2\boldsymbol{B}_n)\,\mathrm{d}G_1(t) \quad (6)$$

as in Equation (5), *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* $f(u;\alpha,2,G_2) = (u^{\alpha-1}/\beta^\alpha\Gamma(\alpha))\int_c^d w^\alpha \mathrm{e}^{-wx/2}\,\mathrm{d}G_2(w)$ *as in Equation* (2) *with* $\alpha = \nu/2$ *and* $\nu = (n-1)$ *and mixing distribution* $G_2(\hat{\beta}_1^2;\delta)$ *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*

$$g(u;\nu,\lambda,G_1) = C_g^{-1}\int_a^b k g_{t^2}(u;\nu,\lambda(t))\,\mathrm{d}G_1(t) \quad (7)$$

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

Proof Begin with $\mathcal{L}(\boldsymbol{Y} \mid \hat{\beta}_T) = N_n[\hat{\beta}_T^{-1}\mu\boldsymbol{1}_n, \hat{\beta}_T^{-2}(\sigma_Z^2\boldsymbol{I}_n + \sigma_0^2\boldsymbol{1}_n\boldsymbol{1}_n')]$ to determine directly that $\mathcal{L}(\boldsymbol{R} \mid \hat{\beta}_T) = N_n(\boldsymbol{0}, \hat{\beta}_T^{-2}\sigma_Z^2\boldsymbol{B}_n)$, since $\boldsymbol{B}_n$ is idempotent and $\boldsymbol{B}_n\boldsymbol{1}_n = \boldsymbol{0}$ and that $\mathcal{L}(\bar{Y} \mid \hat{\beta}_T) = N_1(\hat{\beta}_T^{-1}\mu, \hat{\beta}_T^{-2}\tau^2(n))$, where $\mu = (\mu_Z - \beta_0)$ and $\tau^2(n) = n^{-1}(\sigma_Z^2 + n\sigma_0^2)$. The unconditional density of $\bar{Y}$ thus is $f_1(u;\mu,\tau^2(n),G_1)$ on specializing Equation (5) from $\mathbb{R}^n$ to $\mathbb{R}^1$, to give conclusion (i) with mixing distribution as asserted. Conclusion (ii) follows similarly on mixing $\mathcal{L}(\boldsymbol{R} \mid \hat{\beta}_T)$ over $G_1(t)$. Since $(n-1)S_Y^2 = \boldsymbol{R}'\boldsymbol{R}$, we infer that $\mathcal{L}(\boldsymbol{R}'\boldsymbol{R}\hat{\beta}_1^2/\sigma_Z^2 \mid \hat{\beta}_1^2) = \chi^2(\nu,0)$ with $\nu = n-1$, so that $\mathcal{L}((n-1)S_Y^2/\sigma_Z^2 \mid \hat{\beta}_1^2)$ is a central chi-squared variate scaled by $\hat{\beta}_1^2$. On identifying $(n-1)S_Y^2\sigma_1^2/\sigma_Z^2$ with U and $(\hat{\beta}_1^2/\sigma_1^2)$ with w in developments leading to Equation (2), we thus establish conclusion (iii) on specializing from gamma to chi-squared distributions under the restriction $\hat{\beta}_T^2 \in [a^2,b^2]$ in $\mathbb{R}_+^1$, so that $(\hat{\beta}_1^2/\sigma_1^2)$ is now restricted to $[a^2/\sigma_1^2, b^2/\sigma_1^2]$. To continue, observe that $\mathcal{L}[(\bar{Z} - \hat{\beta}_0 - \hat{\beta}_T\mu_Y^0) \mid \hat{\beta}_T] = N_1[(\mu_Z - \beta_0 - \hat{\beta}_T\mu_Y^0), n^{-1}(\sigma_Z^2 + n\sigma_0^2)]$. Properly standardized, the quantity $t^2 = n[(\bar{Z} - \hat{\beta}_0 - \hat{\beta}_T\mu_Y^0)^2/S_Z^2][\sigma_Z^2/(\sigma_Z^2 + n\sigma_0^2)]$ conditionally has Student's distribution $\mathcal{L}(t^2 \mid \hat{\beta}_T) = t^2(\nu,\lambda(\hat{\beta}_T))$ with $\nu = (n-1)$ and $\lambda(\hat{\beta}_T) = n[(\mu_Z - \beta_0) - \hat{\beta}_T\mu_Y^0]^2/(\sigma_Z^2 + n\sigma_0^2)$, so that $t_0^2 = t^2/k$ with $k = \sigma_Z^2/(\sigma_Z^2 + n\sigma_0^2)$. In particular, $\mathcal{L}(t_0^2 \mid \hat{\beta}_T) = \mathcal{L}(t^2/k \mid \hat{\beta}_T)$. It follows on scaling and mixing that the unconditional density is Equation (7), to complete our proof. ■

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 $\kappa_2 = \mu_{-2}(\hat{\beta}_T)$, $\kappa_{11} = \mathrm{Var}\,(\hat{\beta}_T^{-1})$, and $|\mu_Z - \beta_0|$. Lemma A.1 gives expansions approximating the negative moments $\{\kappa_1 = \mu_{-1}(\hat{\beta}_T), \kappa_2 = \mu_{-2}(\hat{\beta}_T), \kappa_{11} = \mathrm{Var}\,(\hat{\beta}_T^{-1})\}$, together with orders $O(\cdot)$ of the approximations. The following consequences emerge from Section 4.1 and the aforementioned expansions.

- The parameter $\kappa_2 = \mu_{-2}(\hat{\beta}_T) \approxeq 1/\beta_T^2 + 3\sigma_T^2/\beta_T^4$ is increasing in σ_T^2 and decreasing in $|\beta_T|$, up to the order of approximation.
- The quantity $|\mu_Z - \beta_0|$ pertains to centring 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 $\{U_1,\ldots,U_m\}$ centred near the mean μ_Z of $\{Z_1,\ldots,Z_n\}$.
- Effective centring in turn diminishes the 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 σ_Y^2, as in Theorem 2(ii), increases (i) with increasing uncertainty (σ_0^2, σ_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 Var $(Y_i) = \sigma_Z^2/\beta_1^2$, as the ideal variance to be attained under linear calibration with known (β_0, β_1).
- The conditional correlation $\rho = \sigma_0^2/(\sigma_Z^2 + \sigma_0^2)$ increases with decreasing σ_Z^2/σ_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 β_0, (ii) with increasing $|\mu_Z - \beta_0|$, and (iii) with increasing $\{\kappa_2, \kappa_{11}\}$, with other parameters held fixed.
- The conditional non-centrality parameter $\lambda(\hat{\beta}_T) = n\hat{\beta}_T^2[\mu_Y(\hat{\beta}_T) - \mu_Y^0]^2/(\sigma_Z^2 + n\sigma_0^2)$ is an increasing function of $|\ \hat{\beta}_T\ |$ and the discrepancy $|\mu_Y(\hat{\beta}_T) - \mu_Y^0|$, and it decreases with increasing σ_Z^2 and σ_0^2 with other parameters fixed, where $\mu_Y(\hat{\beta}_T) = (\mu_Z - \beta_0)/\hat{\beta}_T$.
- The expected value

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

is an increasing function of $|\ \beta_T\ |$, $|\mu_Y(\beta_T) - \mu_Y^0|$, and σ_T^2, and it decreases with increasing σ_Z^2 and σ_0^2 with other parameters fixed, where $\mu_Y(\beta_T) = (\mu_Z - \beta_0)/\beta_T$.

4.3. *One-way experiments*

Here, we model observations $\{Z_1, \ldots, Z_n\}$ as from a one-way experiment in k samples of sizes $\{n_1, \ldots, n_k\}$, with $n_1 + \cdots + n_k = n$. Accordingly, partition $\boldsymbol{Z}' = [\boldsymbol{Z}_1', \ldots, \boldsymbol{Z}_k']$, such that $\{\boldsymbol{Z}_i' = [Z_{i1}, \ldots, Z_{in_i}]; 1 \le i \le k\}$, and similarly $\boldsymbol{Y}' = [\boldsymbol{Y}_1', \ldots, \boldsymbol{Y}_k']$, with $\{\boldsymbol{Y}_i' = [Y_{i1}, \ldots, Y_{in_i}]; 1 \le i \le k\}$. We suppose that $\{E(Z_{ij}) = \mu_i; 1 \le j \le n_i\}$, 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 $\{V(\boldsymbol{Z}_i) = \omega^2\boldsymbol{\Sigma}(\boldsymbol{\gamma}_i, \bar{\gamma}) = \omega^2(\boldsymbol{I}_{n_i} + \mathbf{1}_{n_i}\boldsymbol{\gamma}_i' + \boldsymbol{\gamma}_i\mathbf{1}_{n_i}' - \bar{\gamma}\mathbf{1}_{n_i}\mathbf{1}_{n_i}'); 1 \le i \le k\}$, where $\boldsymbol{\gamma}' = [\boldsymbol{\gamma}_1', \ldots, \boldsymbol{\gamma}_k']$ has been partitioned conformably such that $\{\boldsymbol{\gamma}_i = [\gamma_{i1}, \ldots, \gamma_{in_i}]' \in \mathbb{R}^{n_i}; 1 \le i \le k\}$. Note that the test remains exact despite heterogeneity of the variances $\{\text{Var}\ (Z_{ij}) = \omega^2(2\gamma_{ij} - \bar{\gamma}); 1 \le j \le n_i, 1 \le i \le k\}$ within and among samples, attributable to the structural parameters of $\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})$. We next proceed to examine the 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 $\boldsymbol{D}_{\boldsymbol{\omega I}} = \text{Diag}\ (\omega_1\boldsymbol{I}_{n_1}, \ldots, \omega_k\boldsymbol{I}_{n_k})$ to get $\boldsymbol{\Xi}_n(\boldsymbol{\omega}, \boldsymbol{\gamma}) = \boldsymbol{D}_{\boldsymbol{\omega I}}\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})\boldsymbol{D}_{\boldsymbol{\omega I}}$, which in partitioned form is

$$\boldsymbol{\Xi}_n(\boldsymbol{\omega}, \boldsymbol{\gamma}) = \begin{bmatrix} \omega_1^2\boldsymbol{\Sigma}(\gamma_1, \bar{\gamma}) & \omega_1\omega_2\boldsymbol{A}_{12} & \ldots & \omega_1\omega_k\boldsymbol{A}_{1k} \\ \omega_2\omega_1\boldsymbol{A}_{21} & \omega_2^2\boldsymbol{\Sigma}(\boldsymbol{\gamma}_2, \bar{\gamma}) & \ldots & \omega_2\omega_k\boldsymbol{A}_{2k} \\ \ldots & \ldots & \ldots & \ldots \\ \omega_k\omega_1\boldsymbol{A}_{k1} & \omega_k\omega_2\boldsymbol{A}_{k2} & \ldots & \omega_1^k\boldsymbol{\Sigma}(\boldsymbol{\gamma}_k, \bar{\gamma}) \end{bmatrix} \quad (8)$$

with $\{\boldsymbol{\Sigma}(\boldsymbol{\gamma}_i,\bar{\gamma});1\le i\le k\}$ 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 Equations (3) and (4) gives the conditional moments

$$E(\boldsymbol{Y}\mid\hat{\beta}_T)=\boldsymbol{\mu}_Y(\hat{\beta}_T)=\hat{\beta}_T^{-1}(\boldsymbol{\mu}_Z-\beta_0\mathbf{1}_n)$$
$$=\hat{\beta}_T^{-1}[(\mu_1-\beta_0)\mathbf{1}_{n_1}',\ldots,(\mu_k-\beta_0)\mathbf{1}_{n_k}']', \tag{9}$$
$$V(\boldsymbol{Y}\mid\hat{\beta}_T)=\boldsymbol{\Sigma}(\hat{\beta}_T)=\hat{\beta}_T^{-2}[\boldsymbol{\Xi}_n(\boldsymbol{\omega},\boldsymbol{\gamma})+\sigma_0^2\mathbf{1}_n\mathbf{1}_n'], \tag{10}$$

together with $\mathcal{L}(\boldsymbol{Y}\mid\hat{\beta}_T)=N_n(\boldsymbol{\mu}_Y(\hat{\beta}_T),\boldsymbol{\Sigma}(\hat{\beta}_T))$ 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 the effects of calibration on sample quantities of note, consider transformations such that $T_1(\boldsymbol{Y})=\bar{\boldsymbol{Y}}=[\bar{Y}_1,\ldots,\bar{Y}_k]'$ 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 $\{\boldsymbol{R}_i=\boldsymbol{B}_{n_i}\boldsymbol{Y}_i;1\le i\le k\}$ and $\boldsymbol{B}_{n_i}=(\boldsymbol{I}_{n_i}-n_i^{-1}\mathbf{1}_{n_i}\mathbf{1}_{n_i}')$; and $T_3(\boldsymbol{Y})=[\nu_1S_1^2,\ldots,\nu_kS_k^2]'$ are the residual sums of squares $\{\nu_iS_i^2=\boldsymbol{R}_i'\boldsymbol{R}_i=\boldsymbol{Y}_i'\boldsymbol{B}_{n_i}\boldsymbol{Y}_i;1\le i\le k\}$, with $\{\nu_i=n_i-1;1\le i\le k\}$. We require $\boldsymbol{\theta}=[\bar{\gamma}_1,\ldots,\bar{\gamma}_k]'$ as the 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 Equation* (8); *let* $\boldsymbol{\mu}=[\mu_1,\ldots,\mu_k]'$; *and let* $T_1(\boldsymbol{Y})=[\bar{Y}_1,\ldots,\bar{Y}_k]'$, $T_2(\boldsymbol{Y})=\boldsymbol{R}=[\boldsymbol{R}_1',\ldots,\boldsymbol{R}_k']'$, *and* $T_3(\boldsymbol{Y})=[\nu_1S_1^2,\ldots,\nu_kS_k^2]'$, *with* $\{\nu_i=n_i-1;1\le i\le k\}$. *Moreover, a Gaussian model asserts that* $\mathcal{L}(\boldsymbol{Z})=N_n(\boldsymbol{\mu}_Z,\boldsymbol{\Xi}_n(\boldsymbol{\omega},\boldsymbol{\gamma}))$ *independently of* $(\hat{\beta}_0,\hat{\beta}_T)$ *under Gaussian calibration.*

(i) *Conditional and unconditional means of* $T_1(\boldsymbol{Y})=\bar{\boldsymbol{Y}}$ *are given by* $E(\bar{\boldsymbol{Y}}\mid\hat{\beta}_T)=\boldsymbol{\tau}(\hat{\beta}_T)=\hat{\beta}_T^{-1}(\boldsymbol{\mu}-\beta_0\mathbf{1}_k)$ *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* $V(\bar{\boldsymbol{Y}}\mid\hat{\beta}_T)=\boldsymbol{\Xi}_1(\hat{\beta}_T)=\hat{\beta}_T^{-2}[\boldsymbol{\Xi}_k(\boldsymbol{\omega},\boldsymbol{\theta},\boldsymbol{n})+\sigma_0^2\mathbf{1}_k\mathbf{1}_k']$, *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 the 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*

$$f_k(\boldsymbol{u};\boldsymbol{\tau},\boldsymbol{\Xi}_1,G_1)=C_g^{-1}\int_a^b g_k(\boldsymbol{u};\boldsymbol{\tau}(t),\boldsymbol{\Xi}_1(t))\,\mathrm{d}G_1(t) \tag{11}$$

with mixing distribution $G_1(t)=N_1(\beta_1,\sigma_1^2)$ *on* $\mathbb{R}^1$ *as in Equation* (5), *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* $E(\boldsymbol{R}\mid\hat{\beta}_T)=\mathbf{0}=E(\boldsymbol{R})$. *Dispersion parameters are* $V(\boldsymbol{R}\mid\hat{\beta}_T)=\boldsymbol{\Xi}_2(\hat{\beta}_T)=\hat{\beta}_T^{-2}\mathrm{Diag}\,(\omega_1^2\boldsymbol{B}_{n_1},\ldots,\omega_1^k\boldsymbol{B}_{n_k})$, *and* $V(\boldsymbol{R})=\boldsymbol{\Xi}_2=\kappa_2\mathrm{Diag}\,(\omega_1^2\boldsymbol{B}_{n_1},\ldots,\omega_1^k\boldsymbol{B}_{n_k})$.

(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 Equation* (5), *with mixing distribution* $G_1(t)=N_1(\beta_1,\sigma_1^2)$ *on* $\mathbb{R}^1$, *where* $\boldsymbol{\Xi}_2(t)=t^{-2}\mathrm{Diag}\,(\omega_1^2\boldsymbol{B}_{n_1},\ldots,\omega_1^k\boldsymbol{B}_{n_k})$.

(vi) *Under Gaussian errors, the joint density of elements of* $[\nu_1S_1^2\sigma_1^2/\omega_1^2,\ldots,\nu_kS_k^2\sigma_1^2/\omega_1^k]'$ *is given by*

$$f(\boldsymbol{u};\nu_1,\ldots,\nu_k,G_2)=\int_c^d\prod_{i=1}^k g_0\left(u_i;\frac{\nu_i}{2},\frac{2}{w}\right)\mathrm{d}G_2(w) \tag{12}$$

with $\{\nu_i = n_i - 1; 1 \le i \le k\}$ *and* $g_0(u_i; \alpha_i, \beta/w) = (w/\beta)^{\alpha_i} u_i^{\alpha_i - 1} \mathrm{e}^{-wu_i/\beta} / \Gamma(\alpha_i)$, *having mixing distribution* $G_2(\hat{\beta}_1^2; \delta)$ *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 given in Section 4.1. While details differ, proceed beginning with $E(\boldsymbol{Y} \mid \hat{\beta}_T)$ from Equation (9) and $V(\boldsymbol{Y} \mid \hat{\beta}_T)$ from Equation (10). Observe that $\bar{\boldsymbol{Y}} = \boldsymbol{L}_n'\boldsymbol{Y}$ with $\boldsymbol{L}_n' = \mathrm{Diag}\,(n_1^{-1}\mathbf{1}_{n_1}', \ldots, n_k^{-1}\mathbf{1}_{n_k}')$ and that $\boldsymbol{R} = \boldsymbol{B}\boldsymbol{Y}$ with $\boldsymbol{B} = \mathrm{Diag}\,(\boldsymbol{B}_{n_1}, \ldots, \boldsymbol{B}_{n_k})$. Starting with $\boldsymbol{\Xi}_n(\boldsymbol{\omega}, \boldsymbol{\gamma}) = \boldsymbol{D}_{\boldsymbol{\omega I}}\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})\boldsymbol{D}_{\boldsymbol{\omega I}}$ from Equation (8), 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 $\boldsymbol{L}_n'\boldsymbol{D}_{\boldsymbol{\omega I}} = \boldsymbol{D}_{\boldsymbol{\omega}}\boldsymbol{L}_n'$, $\boldsymbol{L}_n'\boldsymbol{I}_n\boldsymbol{L}_n = \boldsymbol{D}_{\boldsymbol{n}}^{-1} = \mathrm{Diag}\,(n_1^{-1}, \ldots, n_k^{-1})$, with $\boldsymbol{D}_{\boldsymbol{\omega}} = \mathrm{Diag}\,(\omega_1, \ldots, \omega_k)$, 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 the means of the partitioned elements of $\boldsymbol{\gamma}' = [\boldsymbol{\gamma}_1', \ldots, \boldsymbol{\gamma}_k']$. It follows directly that $E(\bar{\boldsymbol{Y}} \mid \hat{\beta}_T) = \hat{\beta}_T^{-1}\boldsymbol{L}_n'[(\mu_1\mathbf{1}_{n_1}', \ldots, \mu_k\mathbf{1}_{n_k}')' + \beta_0\mathbf{1}_n] = \hat{\beta}_T^{-1}(\boldsymbol{\mu} - \beta_0\mathbf{1}_k)$ 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, $V(\bar{\boldsymbol{Y}} \mid \hat{\beta}_T) = \boldsymbol{\Xi}_1(\hat{\beta}_T) = \hat{\beta}_T^{-2}[\boldsymbol{\Xi}_k(\boldsymbol{\omega}, \boldsymbol{\theta}, \boldsymbol{n}) + \sigma_0^2\mathbf{1}_k\mathbf{1}_k']$, 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 $\boldsymbol{D}_{\boldsymbol{n}} = \mathrm{Diag}\,(n_1, \ldots, n_k)$, and $\boldsymbol{A}_k(\boldsymbol{\theta}, \bar{\gamma}) = \mathbf{1}_k\boldsymbol{\theta}' + \boldsymbol{\theta}\mathbf{1}_k' - \bar{\gamma}\mathbf{1}_k\mathbf{1}_k'$. 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 $V(\boldsymbol{R} \mid \hat{\beta}_T) = \hat{\beta}_T^{-2}\boldsymbol{B}V(\boldsymbol{Y})\boldsymbol{B} = \hat{\beta}_T^{-2}\mathrm{Diag}\,(\omega_1^2\boldsymbol{I}_{n_1}, \ldots, \omega_1^k\boldsymbol{I}_{n_k})$ 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 conclusion (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 $\hat{\beta}_T$. As in the proof for Theorem 3(iv), the marginal density of $\mathcal{L}(\nu_i S_i^2\sigma_1^2/\omega_i^2 \mid \hat{\beta}_1)$ is the scaled chi-squared density $g_0(u_i; \nu_i/2, 2w)$ as defined in (2), with $w = (\hat{\beta}_1^2/\sigma_1^2)$. Their unconditional joint density now follows on mixing as in Section 2.2, as asserted in conclusion (vi), to complete our proof. ■

We turn next to comparisons among $\{S_1^2, \ldots, S_k^2\}$. Recall from Equation (10) that $\{\mathrm{Var}\,(Y_{ij} \mid \hat{\beta}_T) = \hat{\beta}_T^{-2}\omega_i^2(2\gamma_{ij} - \bar{\gamma} + \sigma_0^2); 1 \le j \le n_i\}$ and $\{\mathrm{Var}\,(Y_{ij}) = \kappa_2\omega_i^2(2\gamma_{ij} - \bar{\gamma} + \sigma_0^2) + \kappa_{11}(\mu_i - \beta_0)^2; 1 \le j \le n_i\}$, 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 $\{\omega_1^2/\sigma_1^2, \ldots, \omega_1^k/\sigma_1^2\}$ are equal if and only if $\{\omega_1^2, \ldots, \omega_1^k\}$ are homogeneous. To continue, let $T_4(S_1^2, \ldots, S_k^2)$ be any scale-invariant statistic, that is, $T_4(cS_1^2, \ldots, cS_k^2) = T_4(S_1^2, \ldots, S_k^2)$ for $c \neq 0$. This is the substance of the following.

Theorem 5 *Let* $\{S_1^2, \ldots, S_k^2\}$ *be the 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* $(\hat{\beta}_0, \hat{\beta}_1)$ *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* $(\hat{\beta}_0, \hat{\beta}_T)$ *and* $\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})$.

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

$$T_4\left(\frac{S_1^2\hat{\beta}_T^2}{\omega_1^2}, \ldots, \frac{S_k^2\hat{\beta}_T^2}{\omega_1^k}\right) = T_4\left(\frac{S_1^2}{\omega_1^2}, \ldots, \frac{S_k^2}{\omega_1^k}\right)$$

by its scale invariance, so that $\mathcal{L}[T_4(S_1^2,\ldots,S_k^2)\mid\hat\beta_T]=\mathcal{L}[T_4(S_1^2,\ldots,S_k^2)]$ unconditionally, independently of $(\hat\beta_0,\hat\beta_T)$, 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' : $\hat\beta_T^{-2}\omega_1^2=\cdots=\hat\beta_T^{-2}\omega_1^k$ or, equivalently, $H_0:\omega_1^2=\omega_2^2=\cdots=\omega_1^k$ against appropriate alternatives. Theorem 5 applies for both null and non-null distributions of invariant test statistics. Tests in common usage include the following:

- 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 $\{\mathrm{Var}\,(Y_{ij}\mid\hat\beta_T)=\hat\beta_T^{-2}\omega_i^2(2\gamma_{ij}-\bar\gamma+\sigma_0^2);1\le j\le n_i\}$, 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 $\{\omega_1^2,\ldots,\omega_1^k\}$ 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 the effects of calibration on the one-way analysis of variance, we suppose that $V(\boldsymbol{Z})=\omega^2\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})$, so that $V(\boldsymbol{Y}\mid\hat\beta_T)=\hat\beta_T^{-2}\omega^2[\boldsymbol{\Sigma}_0(\boldsymbol{\gamma})+\sigma_0^2\mathbf{1}_n\mathbf{1}_n']=\hat\beta_T^{-2}\omega^2\boldsymbol{\Sigma}(\boldsymbol{\gamma},\phi)$ as in Section 2.3, with $\phi=\bar\gamma-\sigma_0^2/\omega^2$. Call this $V(\boldsymbol{Y}\mid\hat\beta_T)=\boldsymbol{\Xi}(\hat\beta_T)$. We proceed to validate the analysis conditionally, given $\hat\beta_T$, where $E(\boldsymbol{Y}\mid\hat\beta_T)=\hat\beta_T^{-1}(\boldsymbol{\mu}_Z-\beta_0\mathbf{1}_n)$ 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 $\boldsymbol{Y}'\boldsymbol{A}_0\boldsymbol{Y}=n\bar Y^2$, with $\bar Y$ as the grand mean and $\boldsymbol{A}_0=n^{-1}\mathbf{1}_n\mathbf{1}_n'$; $\boldsymbol{Y}'\boldsymbol{A}_1\boldsymbol{Y}=\sum_{i=1}^k n_i(\bar Y_i-\bar Y)^2$; and $\boldsymbol{Y}'\boldsymbol{A}_2\boldsymbol{Y}=\sum_{i=1}^k\sum_{j=1}^{n_i}(Y_{ij}-\bar Y_i)^2$. 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 $\boldsymbol{Y}'\boldsymbol{B}_n\boldsymbol{Y}=\boldsymbol{Y}'\boldsymbol{A}_1\boldsymbol{Y}+\boldsymbol{Y}'\boldsymbol{A}_2\boldsymbol{Y}$. The validation of the Fisher–Cochran theorem conditionally requires that $\{\boldsymbol{A}_i\boldsymbol{\Xi}(\hat\beta_T)\boldsymbol{A}_j=\mathbf{0};i\ne j\}$ with $\{i,j\in\{1,2\}\}$. Moreover, scale parameters to be associated with the quadratic forms are found as $\{\xi_i^2\boldsymbol{G}=\boldsymbol{G}\boldsymbol{\Xi}(\hat\beta_T)\boldsymbol{G};\boldsymbol{G}\in\{\boldsymbol{A}_1,\boldsymbol{A}_2,\boldsymbol{B}_n\}\}$; their degrees of freedom are determined by ranks; and non-centrality parameters derive from the expected mean squares. This programme of study is carried out next in support of the following.

THEOREM 6 *Let* $\{Y_{ij}=\hat\beta_T^{-1}(Z_{ij}-\hat\beta_0);1\le j\le n_i,1\le i\le k\}$ *be the 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* $\boldsymbol{\mu}_Y(\hat\beta_T)=E(\boldsymbol{Y}\mid\hat\beta_T)=\hat\beta_T^{-1}(\boldsymbol{\mu}_Z-\beta_0\mathbf{1}_n)$ *and* $V(\boldsymbol{Y}\mid\hat\beta_T)=\boldsymbol{\Xi}(\hat\beta_T)=\hat\beta_T^{-2}\omega^2\boldsymbol{\Sigma}(\boldsymbol{\gamma},\phi)$ *with* $\phi=\bar\gamma-\sigma_0^2/\omega^2$.

(i) *To test the 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 $\hat\beta_T$, 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 $\{\xi_i^2\boldsymbol{G}=\boldsymbol{G}\boldsymbol{\Xi}(\hat\beta_T)\boldsymbol{G};\boldsymbol{G}\in\{\boldsymbol{A}_1,\boldsymbol{A}_2,\boldsymbol{B}_n\}\}$, where $\boldsymbol{G}\boldsymbol{\Xi}(\hat\beta_T)\boldsymbol{G}=\hat\beta_T^{-2}\omega^2\boldsymbol{G}(\boldsymbol{I}_n+$

$\mathbf{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\mathbf{1}_n' - \phi\mathbf{1}_n\mathbf{1}_n')\boldsymbol{G} = \hat{\beta}_T^{-2}\omega^2\boldsymbol{G}$ since $\boldsymbol{G}$ is idempotent and $\boldsymbol{G}\mathbf{1}_n = \mathbf{0}$ for $\boldsymbol{G} \in \{\boldsymbol{A}_1, \boldsymbol{A}_2, \boldsymbol{B}_n\}$, thus confirming that their scale parameters are equal, namely $\hat{\beta}_T^{-2}\omega^2$. The conditional independence of $\{\boldsymbol{Y}'\boldsymbol{A}_1\boldsymbol{Y}, \boldsymbol{Y}'\boldsymbol{A}_2\boldsymbol{Y}\}$ follows since $\boldsymbol{A}_1\,\Xi\,(\hat{\beta}_T)\boldsymbol{A}_2 = \hat{\beta}_T^{-2}\omega^2\boldsymbol{A}_1(\boldsymbol{I}_n + \mathbf{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\mathbf{1}_n' - \phi\mathbf{1}_n\mathbf{1}_n')\boldsymbol{A}_2 = \hat{\beta}_T^{-2}\omega^2\boldsymbol{A}_1\boldsymbol{A}_2 = \mathbf{0}$ and $\boldsymbol{A}_1\mathbf{1}_n = \mathbf{0} = \boldsymbol{A}_2\mathbf{1}_n$. 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

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

where $\operatorname{tr}\boldsymbol{G}\,\Xi\,(\hat{\beta}_T)\boldsymbol{G} + [\boldsymbol{\mu}_Y(\hat{\beta}_T)]'\boldsymbol{G}[\boldsymbol{\mu}_Y(\hat{\beta}_T)] = \hat{\beta}_T^{-2}\omega^2\operatorname{tr}\boldsymbol{G}(\boldsymbol{I}_n + \mathbf{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\mathbf{1}_n' - \phi\mathbf{1}_n\mathbf{1}_n') + \hat{\beta}_T^{-2}(\boldsymbol{\mu}_Z - \beta_0\mathbf{1}_n)'\boldsymbol{G}(\boldsymbol{\mu}_Z - \beta_0\mathbf{1}_n) = \hat{\beta}_T^{-2}\omega^2\operatorname{tr}\boldsymbol{G} + \hat{\beta}_T^{-2}\boldsymbol{\mu}_Z'\boldsymbol{G}\boldsymbol{\mu}_Z$ since $\boldsymbol{G}\mathbf{1}_n = \mathbf{0}$ and $\operatorname{tr}\boldsymbol{G}\boldsymbol{\gamma}\mathbf{1}_n' = \mathbf{1}_n'\boldsymbol{G}\boldsymbol{\gamma}' = \mathbf{0}$ 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

$$F(\hat{\beta}_T) = \frac{\boldsymbol{Y}'\boldsymbol{A}_1\boldsymbol{Y}\hat{\beta}_T/(k-1)\omega^2}{\boldsymbol{Y}'\boldsymbol{A}_2\boldsymbol{Y}\hat{\beta}_T/(n-k)\omega^2} \tag{13}$$

such that $\mathcal{L}[F(\hat{\beta}_T) \mid \hat{\beta}_T] = F(k-1, n-k, \lambda(\hat{\beta}_T)$, with $\lambda(\hat{\beta}_T) = \hat{\beta}_T^{-2}\sum_{i=1}^k n_i(\mu_i - \bar{\mu})^2/\hat{\beta}_T^{-2}\omega^2 = \sum_{i=1}^k n_i(\mu_i - \bar{\mu})^2/\omega^2$. It follows that $\mathcal{L}[F(\hat{\beta}_T) \mid \hat{\beta}_T] = F(k-1, n-k, \lambda(\hat{\beta}_T))$ 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 variances. The test for conditional independence of $(\boldsymbol{C}'\bar{\boldsymbol{Y}}, S_Y^2)$ is that $\boldsymbol{C}'\boldsymbol{L}_n'\,\Xi\,(\hat{\beta}_T)\boldsymbol{A}_2 = \mathbf{0}$, with $\boldsymbol{L}_n' = \operatorname{Diag}(n_1^{-1}\mathbf{1}_{n_1}, \ldots, n_k^{-1}\mathbf{1}_{n_k}')$. We directly evaluate $\boldsymbol{C}'\boldsymbol{L}_n'(\boldsymbol{I}_n + \mathbf{1}_n\boldsymbol{\gamma}' + \boldsymbol{\gamma}\mathbf{1}_n' - \phi\mathbf{1}_n\mathbf{1}_n')\boldsymbol{A}_2 = \boldsymbol{C}'\boldsymbol{L}_n'\boldsymbol{A}_2 + \boldsymbol{C}'\mathbf{1}_k\boldsymbol{\gamma}'\boldsymbol{A}_2 = \mathbf{0}$ since $\boldsymbol{L}_n'\boldsymbol{A}_2 = \mathbf{0}$, $\mathbf{1}_n'\boldsymbol{A}_2 = \mathbf{0}$, $\boldsymbol{L}_n'\mathbf{1}_n = \mathbf{1}_k$, and $\boldsymbol{C}'\mathbf{1}_k = \mathbf{0}$ as linear contrasts, so that $(\boldsymbol{C}'\bar{\boldsymbol{Y}}, S_Y^2)$ are conditionally independent given $\hat{\beta}_T$. It follows that the standardized variables $\boldsymbol{C}'\bar{\boldsymbol{Y}}/S_Y$ satisfy $\hat{\beta}_T^{-1}\boldsymbol{C}'(\bar{\boldsymbol{Z}} - \hat{\beta}_0\mathbf{1}_k)/\hat{\beta}_T^{-1}S_Z = \boldsymbol{C}'\bar{\boldsymbol{Z}}/S_Z$, with 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 non-normality 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 $V(\boldsymbol{Y}) = \tau^2\,\Xi\,(\omega) = \tau^2(\boldsymbol{I}_n + \omega\boldsymbol{A})$, with $\boldsymbol{A}$ fixed and ω such that $\Xi\,(\omega) \in \mathbb{S}_n^+$. Specializing gives $\tau^2\,\Xi\,(\omega)$ as $\boldsymbol{\Sigma}(\rho)$ under equicorrelation. Tests due to Durbin and Watson [30–32], Anderson and Anderson [33], Theil [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 $\mathcal{L}(\boldsymbol{Z}) = N_n(\mu_Z\mathbf{1}_n, \sigma_Z^2\boldsymbol{I}_n)$, so that $\mathcal{L}(\boldsymbol{R}) = N_n(\mathbf{0}, \sigma_Z^2\boldsymbol{B}_n)$. This is seen from the proof for Theorem 3, where $\mathcal{L}(\boldsymbol{R} \mid \hat{\beta}_T) = N_n(\mathbf{0}, \hat{\beta}_T^{-2}\sigma_Z^2\boldsymbol{B}_n)$, together with the scale invariance of $U = \boldsymbol{R}'\boldsymbol{B}\boldsymbol{R}/\boldsymbol{R}'\boldsymbol{R}$, assuring that $\mathcal{L}(\boldsymbol{R}'\boldsymbol{B}\boldsymbol{R}/\boldsymbol{R}'\boldsymbol{R} \mid \hat{\beta}_T) = \mathcal{L}(\boldsymbol{R}'\boldsymbol{B}\boldsymbol{R}/\boldsymbol{R}'\boldsymbol{R})$ unconditionally. Accordingly, all such diagnostics for correlative dependencies are blind to the induced correlation structures given in 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 non-normality*

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 $\{R_i/S_Y; 1 \le i \le n\}$, 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 in [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 (1) for the calibrated measurements $\{Y_i = (Z_i - \hat{\beta}_0)/\hat{\beta}_T; 1 \le i \le n\}$. This follows from the fact that $\mathcal{L}(\boldsymbol{R}/(\boldsymbol{R}'\boldsymbol{R})^{1/2} \mid \hat{\beta}_T) = \mathcal{L}(\boldsymbol{R}/(\boldsymbol{R}'\boldsymbol{R})^{1/2})$ from scale invariance, having a scaled multivariate Student's t-distribution with $\nu = n - 1$ degrees of freedom, depending on neither $\hat{\beta}_T$ nor σ_Y^2.

The regression tests of Shapiro and Wilk [38] utilize the statistic $W = (\sum_{i=1}^n w_iY_{[i]})^2/(n-1)S_Y^2$, where $\{Y_{[1]} \le Y_{[2]} \le \cdots \le Y_{[n]}\}$ are the ordered values of $\{Y_1, \ldots, Y_n\}$ and $\{w_1, \ldots, w_n\}$ are the 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 non-standard mixture distributions of type (2.1) for classically calibrated measurements. For the latter, we have

$$W = \frac{(\sum_{i=1}^n w_iY_{[i]})^2}{(n-1)S_Y^2} = \frac{[(\sum_{i=1}^n w_iZ_{[i]} - \hat{\beta}_0\sum_{i=1}^n w_i)]^2}{(n-1)S_Y^2\hat{\beta}_T^2}. \tag{14}$$

However, since $\sum_{i=1}^n w_i = 0$ for the regression tests of [38], and since $S_Y^2\hat{\beta}_T^2 = S_Z^2$, we infer that $W = [(\sum_{i=1}^n w_iZ_{[i]}]^2/(n-1)S_Z^2$, so that $\mathcal{L}(W \mid \hat{\beta}_T) = \mathcal{L}(W)$ holds unconditionally from cancellation. Accordingly, these regression tests fail to distinguish between Gaussian distributions and Gaussian mixtures of type (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 (1) are predicated. Variations on these regression tests were surveyed in [40], with none being able to distinguish between Gaussian data and the mixtures (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 $m_r = \sum_{i=1}^n (Y_i - \bar{Y})^r$, are especially useful for distinguishing between Gaussian and skewed distributions or against distributions having excessive or short tails [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 $\mathcal{L}(\boldsymbol{Y}) = N_n(\mu\boldsymbol{1}_n, \sigma^2\boldsymbol{I}_n)$, whatever be the actual joint mixture distribution of type (1) stemming from calibration.

In short, conventional diagnostics for normality, as listed, cannot distinguish between Gaussian errors and Gaussian mixtures of type (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 non-normality 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

Here, we examine the 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 the intensity of the transmitted light relates inversely to phosphorus concentration.

For a calibration $\{U_i = \beta_0 + \beta_1 X_i + \epsilon_i; 1 \leq i \leq m\}$, we denote as before the OLS estimators $\{\hat{\beta}_0, \hat{\beta}_1\}$ and their values $\{b_0, b_1\}$ as computed from the data. Collateral values given in Section 3.1 include $S_{uu} = \sum_{i=1}^{m}(U_i - \bar{U})^2$, $S_{xu} = \sum_{i=1}^{m} X_i(U_i - \bar{U})$, and $S_{xx} = \sum_{i=1}^{m}(X_i - \bar{X})^2$, with $\bar{X} = 0$ 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 out in Table 2 from the linear calibration.

Much less scatter appears in the phosphorus data of Case 2 than in the octane data of Case 1, as is borne out in the 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 $S_{\hat{\beta}_1} = S_U/\sqrt{S_{xx}} = 0.1848$; in contrast, $S_{\hat{\beta}_1} = 0.003335$ for Case 2. Both features influence 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 $\{S_{xx}, S_{uu}, \hat{\beta}_1\}$ as given, for Case 1, the rule $5\% \leq R^2_{(X,U)}$ restricts $\hat{\beta}_1 \in [0.3481, \infty)$. For Case 2, the restriction is $\hat{\beta}_1 \in [0.01166, \infty)$. These correspond to the interval $[a, b]$ given in Section 3.1 that defines the exclusion rule for $\mathcal{L}(\hat{\beta}_T) = \mathcal{L}(\hat{\beta}_1 \mid \hat{\beta}_1 \in [a, b])$ for the restricted estimator $\hat{\beta}_T$.

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

Table 1. Percent purity (X) and octane number (U) of gasoline for Case 1 and milligrams phosphorus (X) and transmittance (U) in calibrating a laboratory colorimeter for Case 2.

Case 1	X	99.8	99.7	99.6	99.5	99.4	99.3	99.2	99.1	99.0	98.9	98.8
	U	87.6	87.4	87.2	87.4	87.2	86.8	86.5	86.3	86.4	86.6	86.1
Case 2	X	0.00	2.28	4.56	6.84	9.12	11.40	13.68	15.96	18.24	22.80	27.36
	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

Table 3. Estimates for inverse moments of $\hat{\beta}_T$ from Lemma A.1 when $\mu_3(\hat{\beta}_T) = 0$ and $\mu_4(\hat{\beta}_T) = 3[\mu_2(\hat{\beta}_T)]^2$ and values for $\{\gamma_1(\hat{\beta}_T), \gamma_2(\hat{\beta}_T)\}$.

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

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

The estimates for $\mu_{-1}(\hat{\beta}_T)$ and $\mu_{-2}(\hat{\beta}_T)$ are considerably greater for the phosphorus data than for the octane data, reflecting the smaller slope of the former. Conversely, Var $(\hat{\beta}_T^{-1})$ 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 $\{\sigma_U^2 \ll \sigma_Z^2\}$ is often obtained [7]. The initial calibration is assumed to have been centred with $\bar{X} = 0$, so that $\hat{\beta}_0 = \bar{U}$ and Var $(\hat{\beta}_0) = \sigma_0^2 = \sigma_U^2/m$, 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 centred such that $E(U_i) = E(Z_i)$, is estimated by $\kappa_2 S_U^2(1 + 1/m)$ from Theorem 1 and is given under $\sigma_Y^2(\theta_0)$ in Table 5.

To demonstrate the accuracy of the estimates for the inverse moments of $\hat{\beta}_T$ from Lemma A.1, we used Maple software to compute the inverse moments $\{\kappa_1, \kappa_2, \text{Var}(\hat{\beta}_T^{-1})\}$ of $\hat{\beta}_T$, having restricted $\hat{\beta}_T$ 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, $\Pr[\hat{\beta}_1 \in [c, \infty)] > 0.9999$, with $(\hat{\beta}_1 - b_1)/(S_U/\sqrt{S_{xx}}) = (\hat{\beta}_1 - 0.2330)/(0.003335)$ as an approximate standard normal distribution. Table 4 reports the inverse moments for $\hat{\beta}_T \in [c, \infty)$, as computed from $\mathcal{L}(\hat{\beta}_T) = N_c^{\infty}(\mu_T, \sigma_T^2)$, as $N_1(\mu, \sigma^2)$ restricted to $[c, \infty]$. The inverse moment estimators given in Table 3 are in agreement (to the accuracy of the data) with the inverse moments, using Maple, for the truncated distribution $\mathcal{L}(\hat{\beta}_T)$, as shown in Table 4.

To study the unconditional moments for $\{Y_i = (Z_i - \hat{\beta}_0)/\hat{\beta}_T; 1 \le i \le n\}$ as in Theorem 1, it is germane to examine the 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. The 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 $\hat{\beta}_T$ given in Table 3, are reported in Table 5 for each of the two case studies.

The unconditional mixture distribution for $\{Y_i = (Z_i - \hat{\beta}_0)/\hat{\beta}_T; 1 \le i \le n\}$ from Equation (5) can be computed using Maple. The unconditional mixture distribution for Y uses as parameters $\{\mu_Z \doteqdot \hat{\beta}_0, \sigma_Z^2 = \sigma_U^2 \doteqdot S_U^2, \sigma_0^2 \doteqdot S_U^2/m, \sigma_1^2 \doteqdot S_U^2/S_{xx}\}$.] From the unconditional mixture distribution, the estimates for the mean and variance of $\mathcal{L}(Y|\theta)$, with bias $\theta = |\mu_Z - \beta_0|$, are

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

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

Table 5. Estimates $\{\mu_Y(\theta_i\}$ for the unconditional moments of $\mathcal{L}(Y)$ using the inverse moments taken 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 σ_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 taken from Table 3 and estimates $\{V_Y(\theta_i) = \text{Var}\,(Y|\theta_i\}$ 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 σ_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. 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 $\mathcal{L}(Y \mid \theta_i)$ 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	0.0531	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

denoted as $\{E(Y|\theta), V_Y(\theta) = \text{Var}\,(Y|\theta)\}$ and are given 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 $\{\mu_Y(\theta_i); i = 0, \ldots, 3\}$ using the inverse moment estimates given in Table 3 are in agreement (to the accuracy of the data) with the corresponding estimators $\{E(Y|\theta_i); i = 0, \ldots, 3\}$, computed using Maple and the unconditional mixture distribution for Y from Equation (5), while the corresponding variance estimator $\sigma_Y^2(\theta)$, using the inverse moment estimators given in Table 3, show an overestimation compared with Var $(Y|\theta)$ from the unconditional mixture distribution. The skewness $\{\gamma_1(Y \mid \theta_i)\}$ and kurtosis $\gamma_2(Y \mid \theta_i)$ for the unconditional mixture distribution $\mathcal{L}(Y \mid \theta_i)$ 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 7 reports the skewness $\gamma_1(Y|\theta_i)$ and kurtosis $\gamma_2(Y|\theta_i)$ for the unconditional mixture distribution $\mathcal{L}(Y \mid \theta_i)$ from Theorem 1 using Maple, with bias $\theta = |\mu_Z - \beta_0|$ taking values in $[\theta_0, \theta_1, \theta_2, \theta_3] = [0, \sigma_Z^2/2, \sigma_Z^2, 3\sigma_Z^2/2]$.

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

Table 8. Estimates for $E(S_Y^2)$ and its bias $B(\theta)$ for estimating 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 σ_Z^2.

Study	$\sigma_Z^2 \mu_{-2}(\hat{\beta}_T)$	$B(\theta_0)$	$B(\theta_1)$	$B(\theta_2)$	$B(\theta_3)$
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]

Note: The fractional errors within the parentheses are $B(\theta)/\sigma_Y^2(\theta)$ and those in the brackets are $B(\theta)/\mathrm{Var}\,(Y|\theta)$ taken from Table 5.

bias θ 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 $B(0)/\mathrm{Var}\,(\hat{\beta}_T|\theta = 0) = 1/(m+1)$. The third column of Table 8 reports these values for the fractional errors. This concludes our numerical studies.

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 the measured product characteristics are routinely monitored using $\bar{X}$-charts, which are tantamount to monitoring a succession of Student's t-statistics. But our studies on 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-analytical 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 is thus 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.

References

[1] R.G. Krutchkoff, *Classical and inverse regression methods of calibration*, Technometrics 9 (1967), pp. 425–439.
[2] R.G. Krutchkoff, *A note on the calibration problem*, Technometrics 10 (1968), pp. 430–431.
[3] R.G. Krutchkoff, *Classical and inverse regression methods of calibration in extrapolation*, Technometrics 11 (1969), pp. 605–608.
[4] R.G. Krutchkoff, *Letter to the editor*, Technometrics 12 (1970), pp. 433–434.

[5] R.G. Krutchkoff, *The calibration problem and closeness*, J. Stat. Comput. Simul. 1 (1971), pp. 87–95.
[6] L.M. Ott and R.H. Myers, *Optimal experimental designs for estimating the independent variable in regression*, Technometrics 10 (1968), pp. 811–823.
[7] J. Berkson, *Estimation of a liner function for a calibration line: Consideration of a recent proposal*, Technometrics 11 (1969), pp. 649–660.
[8] E.J. Williams, *A note on regression methods in calibration*, Technometrics 11 (1969), pp. 189–192.
[9] M. Halperin, *On inverse estimation in linear regression*, Technometrics 12 (1970), pp. 727–736.
[10] S.-C. Chow and J. Shao, *On the difference between the classical and inverse methods of calibration*, Appl. Stat. 11 (1990), pp. 649–660.
[11] V. Centner, D.L. Massart, and S. deJong, *Inverse calibration predicts better than classical calibration*, Fresenius' J. Anal. Chem. 361 (1998), pp. 2–9.
[12] J.M. Mulrow, D.F. Vecchia, J.P. Buonaccorsi, and H.K. Iyer, *Problems with interval estimation when data are adjusted via calibration*, J. Qual. Technol. 20 (1988), pp. 233–247.
[13] D.R. Jensen and D.E. Ramirez, *Anomalies in the analysis of calibrated data*, J. Stat. Comput. Simul. 79 (2009), pp. 299–314.
[14] B. Baldessari, *Analysis of variance of dependent data*, Statistica (Bologna) 26 (1966), pp. 895–903.
[15] H. Huynh and L.S. Feldt, *Conditions under which mean square ratios in repeated measurements designs have exact F-distributions*, J. Amer. Statist. Assoc. 65 (1970), pp. 1582–1589.
[16] H. Rouanet and D. Lépine, *Comparison between treatments in a repeated-measurement disign: ANOVA and multivariate methods*, British J. Math. Statist. Psych. 23 (1970), pp. 147–163.
[17] E.J.G. Pitman, *The estimation of location- and scale-parameters of a continuous population of any given form*, Biometrika 30 (1938), pp. 390–421.
[18] D.R. Jensen and S.S. Srinivasan, *Matrix equivalence classes with applications*, Linear Algebra Appl. 388 (2004), pp. 249–260.
[19] M.S. Srivastava, *Effect of equicorrelation in detecting a spurious observation*, Canad. J. Statist. 8 (1980), pp. 249–251.
[20] D.M. Young, R. Pavur, and V.R. Marco, *On the effect of correlation and unequal variances in detecting a spurious observation*, Canadian J. Statist. 17 (1989), pp. 103–105.
[21] J.K. Baksalary and S. Puntanen, *A complete solution to the problem of robustness of Grubbs's test*, Canad. J. Statist. 18 (1990), pp. 285–287.
[22] F.E. Grubbs, *Criteria for testing outlying observations*, Ann. Math. Statist. 21 (1950), pp. 27–58.
[23] J.C. Gower, *Euclidean distance geometry*, Math. Sci. 7 (1982), pp. 1–14.
[24] R.W. Farebrother, *Linear unbiased approximators of the disturbances in the standard linear model*, Linear Algebra Appl. 67 (1985), pp. 259–274.
[25] M. Kanter and H. Proppe, *Reduction of variance for Gaussian densities via restriction to convex sets*, J. Multivariate Anal. 7 (1977), pp. 74–87.
[26] M.S. Bartlett, *Properties of sufficiency and statistical tests*, Proc. R. Soc. A 160 (1937), pp. 268–282.
[27] W.G. Cochran, *The distribution of the largest of a set of estimated variances as a fraction of their total*, Ann. Eugenics 11 (1941), pp. 47–52.
[28] H.O. Hartley, *The maximum F-ratio as short-cut test for heterogeneity of variances*, Biometrika 37 (1950), pp. 308–312.
[29] R. Gnanadesikan, *Equality of more than two variances and more than two dispersion matrices against certain alternatives*, Ann. Math. Statist. 30 (1959), pp. 177–184.
[30] J. Durbin and G.S. Watson, *Testing for serial correlation in least squares regression. I*, Biometrika 37 (1950), pp. 409–428.
[31] J. Durbin and G.S. Watson, *Testing for serial correlation in least squares regression. II*, Biometrika 38 (1951), pp. 159–178.
[32] J. Durbin and G.S. Watson, *Testing for serial correlation in least squares regression. III*, Biometrika 58 (1971), pp. 1–19.
[33] R.L. Anderson and T.W. Anderson, *Distribution of the circular serial correlation for residuals from a fitted fourier series*, Ann. Math. Statist. 21 (1950), pp. 59–81.
[34] H. Theil, *The analysis of disturbances in regression analysis*, J. Amer. Statist. Assoc. 60 (1965), pp. 1067–1079.
[35] J. von Neumann, *Distribution of mean square successive difference to the variance*, Ann. Math. Statist. 12 (1941), pp. 367–395.
[36] T. Kariya, *A robustness property of the tests for serial correlation*, Ann. Statist. 5 (1977), pp. 1212–1220.
[37] R.H. Myers, *Classical and Modern Regression with Applications*, 2nd ed., PWS-Kent, Boston, MA, 1990.
[38] S.S. Shapiro and M.B. Wilk, *An analysis of variance test for normality (complete samples)*, Biometrika 52 (1965), pp. 591–611.
[39] J.P. Royston, *Shapiro–Wilk W statistics*, in *Encyclopedia of Statistical Sciences*, Vol. 8, S. Kotz, N.L. Johnson, and C.B. Read, eds., Wiley, New York, 1988, pp. 430–431.
[40] R.B. D'Agostino, *Tests for Departures from Normality*, in *Encyclopedia of Statistical Sciences*, Vol. 2, S. Kotz, N.L. Johnson, and C.B. Read, eds., Wiley, New York, 1982, pp. 315–324.
[41] J. Hurt, *Asymptotic expansions of functions of statistics*, Appl. Math. 21 (1976), pp. 444–456.
[42] G.W. Oehlert, *A note on the delta method*, Amer. Statist. 46 (1992), pp. 27–29.

Appendix 1

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 zero, 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 A.1 *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, the fourth-order ($q = 4$) approximations to $\mu_{-1}(Z_n)$, $\mu_{-2}(Z_n)$, and* Var (Z_n^{-1}) *are given by*

$$\mu_{-1}(Z_n) = \frac{1}{\mu_1} + \frac{\mu_2}{\mu_1^3} - \frac{\mu_3}{\mu_1^4} + \frac{\mu_4}{\mu_1^5} + O(n^{-5/2}),$$

$$\mu_{-2}(Z_n) = \frac{1}{\mu_1^2} + \frac{3\mu_2}{\mu_1^4} - \frac{4\mu_3}{\mu_1^5} + \frac{5\mu_4}{\mu_1^6} + O(n^{-5/2}),$$

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

Proof As the distribution Z_n has a 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 [41,42]. 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) in [41] and in Equation (3) in [42], to be

$$E(Z_n^{-1}) = \frac{1}{\mu_1} + \frac{\mu_2}{\mu_1^3} - \frac{\mu_3}{\mu_1^4} + \frac{\mu_4}{\mu_1^5} + O(n^{-(4+1)/2}),$$

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

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

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

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

Remark A.1 For developments leading to the case studies described in Section 6, identify n of Lemma A.1 with the sample size m in determining the calibration line, and let $\hat{\beta}_1(m) \equiv \hat{\beta}_{1,n}$ 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 $Z_n = \hat{\beta}_{T,n}$ with $\mathcal{L}(\hat{\beta}_{T,n}) = \mathcal{L}(\hat{\beta}_{1,n}|\hat{\beta}_{1,n} \in [c, \infty))$ and with the untruncated distribution $\mathcal{L}(\hat{\beta}_{1,n}) = N_1(\beta_1, \sigma_{1,n}^2)$ having finite moments for $p \geq 1$ as given by

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

To apply Lemma A.1 for $Z_n = \hat{\beta}_{T,n}$, the requirement that $E(|Z_n - \mu_1|^{10}) = O(n^{-5})$ is verified as follows.

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

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, $0 < A_1 \leq S_{xx}(n)/n \leq A_2$, equivalently, that $0 < \sigma^2/(nA_2) \leq \sigma_{\hat{\beta}_{1,n}}^2 = \sigma^2/S_{xx}(n) \leq \sigma^2/(nA_1)$, and in particular,

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

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

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

By Hölder's inequality

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

so

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

To apply Lemma A.1 to the truncated statistic $\hat{\beta}_{T,n}$, the requirement that $E(|Z_n - \mu_1|^{10}) = O(n^{-5})$ is verified through the binomial expansion by

$$\begin{aligned} E(|\hat{\beta}_{T,n} - E(\hat{\beta}_{T,n})|^p) &= E(|\hat{\beta}_{T,n} - \beta_1 + \beta_1 - E(\hat{\beta}_{T,n})|^p) \\ &\leq \sum_{r=0}^{p} \binom{p}{r} (E(|\hat{\beta}_{T,n} - \beta_1|^r))(|E(\hat{\beta}_{T,n}) - \beta_1|^{p-r}) \\ &= \sum_{r=0}^{p} O(n^{-r/2}) O(n^{-p/2+r2}) = O(n^{-p/2}), \end{aligned}$$

to complete our proof. ■