Peelle's Pertinent Puzzle in Nuclear Safeguards Measurements

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Abstract:

In nuclear safeguards, two measurement methods are sometimes used to infer nuclear material mass. Suppose that the method 1 and 2 estimates are 1.0 kg and 1.5 kg, respectively. Using generalized least squares (GLS) to combine two estimates has a long history dating to its development by Gauss in 1795. In some settings, GLS exhibits curious behaviour, as described in Peelle's Pertinent Puzzle (PPP) where the GLS estimate to combine the 1.0 and 1.5 estimates is 0.88. PPP was introduced in 1987 in the context of combining two or more estimates of fundamental parameters that arise in nuclear interaction experiments. When PPP occurs, the GLS estimate is outside the range of the data, which has led to concerns that GLS estimation is flawed. This paper describes GLS estimation and PPP and points out that PPP can only occur if the two estimates are highly correlated and have different variances. Next, this paper shows that PPP can arise in an example from safeguards, in which the goal is to estimate the average nuclear material mass in N items. A sample of n_1 items from the population of N items is measured by a lower-quality assay method; a subsample n_2 of the n_1 sampled items is also measured by a higher-quality assay method. This paper shows that PPP can arise in applying GLS to combine the estimates from the lower-quality and higher-quality assay methods, for any of three different measurement error models. Model A is the same as that used by a conventional safeguards model. Model B is a modification of model A. Model C arises when both assay methods are calibrated using reverse regression, which in recent uncertainty quantification studies has been shown to outperform classical regression followed by inversion.

Keywords: combining two measurements, generalized least squares, Peelle's pertinent puzzle

1. Introduction

Nuclear safeguards aim to verify that nuclear materials are used exclusively for peaceful purposes. To ensure that States are honouring their safeguards obligations, measurements of nuclear material inventories and flows are needed. Statistical analyses used to support conclusions require uncertainty quantification (UQ), usually by estimating the relative standard deviation (RSD) in random and systematic errors associated with each measurement method [1-10].

This paper uses a safeguards quantitative verification measurement example to show the importance of accurate UQ of measurement errors and to show that although PPP can arise, GLS is still an effective option to combine two or more measurements of the same unknown true quantify.

The safeguards example modified slightly from [1] is as follows. The average nuclear material mass in *N* items is to be estimated by selecting n_1 items at random and measuring these items with measurement method #1, a non-destructive assay (NDA) device, such as a neutron multiplicity counter. The NDA device is then re-calibrated by randomly selecting a subset n_2 of the n_1 items and measuring them by measurement method #2, a destructive assay (DA) method, a balance and mass spectrometer. The problem is to estimate the population mean using the (n_1 + n_2) measurement results and to determine the variance of the estimate. As a specific example, the population may be *N* containers of U. The quality characteristic is the average mass of U-235.

Suppose in this example that the method 1 estimate is 1.0 kg and the method 2 estimate is 1.5 kg. For a particular covariance matrix [2] that contains the variances of the two estimates on the diagonal (0.1134 and 0.0505) and the covariance between the two estimates on the off-diagonal (0.06), the GLS estimate that combines the 1.0 and 1.5 estimates is 0.88. Under what conditions is it reasonable for the GLS estimate to be less than the smaller of the two measurements of nuclear material (NM), or greater than the larger of the two measurements? As [3] explains, the 0.88 estimate is reasonable if the two methods have large positive correlation and method 1 has smaller variance. Note that if the GLS estimate fell between 1.0 and 1.5, it would appear that the two methods have negative correlation. Because 0.88 is smaller than both 1.0 and 1.5, it appears that the two methods have a strong positive correlation, which is indeed the case. The unequal variances of method 1 and 2 provide information regarding whether the population NM mass is more likely to be less than the minimum or greater than the maximum of the two estimates.

Bonner, E., Burr, T., & Norman, C. (2018). Peelle's Pertinent Puzzle in Nuclear Safeguards Measurements. *ESARDA Bulletin - The International Journal of Nuclear Safeguards and Non-proliferation*, 57, 60-65. https://doi.org/10.3011/ ESARDA.IJNSNP.2018.11

In this case, the 0.88 estimate is closer to the method 1 estimate, which has smaller variance than the method 2 estimate.

This paper is organized as follows. Section two reviews GLS and PPP. Section three describes the safeguards example from [1], and modifies the measurement error assumptions from the example. Section four presents simulation results and shows that PPP can arise in the safeguards example. Section five summarizes and emphasizes the importance of accurate UQ.

2. Generalized Least Squares (GLS) and Peelle's Pertinent Puzzle (PPP)

2.1 GLS

GLS for parameter estimation has a long history dating to its development by Gauss and Legendre in the early 1800s [11]. PPP was introduced in the context of estimating fundamental parameters that arise in nuclear interaction experiments [2]. In PPP, the GLS estimate is outside the range of the data, eliciting concerns that GLS is flawed [4,5]. Reference [3] defended GLS in the PPP context and provided an example when PPP can occur. Although PPP examples remain relatively rare, the present paper illustrates that PPP can occur in the example from [1], and also defends GLS as an effective option to combine two (or more) estimates of the same quantity, regardless of whether PPP occurs.

To illustrate GLS, denote the results of two assay methods on the same item as X_1 and X_2. GLS applied to X_1 and X_2 provides the best linear unbiased estimate (BLUE) $\hat{\mu}$ of μ, regardless of whether PPP occurs [6]. Here, "best" means minimum variance and unbiased means that the average of $\hat{\mu}$ across many realizations of the same procedure is the true value μ. Note that one can write $\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \begin{pmatrix} \mu \\ \mu \end{pmatrix} + \begin{pmatrix} e_1 \\ e_2 \end{pmatrix}$ where $\begin{pmatrix} e_1 \\ e_2 \end{pmatrix} = \begin{pmatrix} R_1 \\ R_2 \end{pmatrix}$, or if there are also systematic errors, $\begin{pmatrix} e_1 \\ e_2 \end{pmatrix} = \begin{pmatrix} S_1 \\ S_2 \end{pmatrix} + \begin{pmatrix} R_1 \\ R_2 \end{pmatrix}$, where S_1 is the systematic error of method 1, R_1 is the random error of method 1, and similarly for method 2 [7-10]. This paper uses either μ or T, depending on the context, to denote the true NM mass in an item. Denote the 2-by-2 covariance of $\begin{pmatrix} X_1 \\ X_2 \end{pmatrix}$ as Σ with the method variances $\sigma_{1,1}^2$ and $\sigma_{2,2}^2$ as the diagonal entries and the method covariance $\sigma_{1,2}^2 = \sigma_{2,1}^2$ as the off-diagonal entries. The well-known GLS estimate is $\hat{\mu} = cG^T\Sigma^{-1}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$, where $G^T = (1,1)$ $c = (G^T\Sigma^{-1}G)^{-1}$, and the variance of $\hat{\mu}$ is $\sigma^2 = (G^T\Sigma^{-1}G)^{-1}$.

In the example, μ is the unknown and writing $\hat{\mu} = a_1X_1 + (1-a_1)X_2$, note that $\sigma_{\hat{\mu}}^2 = a_1^2\sigma_{X_1}^2 + (1-a_1)^2\sigma_{X_2}^2 + 2a_1(1-a_1)\sigma_{X_1,X_2}^2$. Then the GLS solution $\hat{\mu} = cG^T\Sigma^{-1}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ arises from standard calculus (by setting the derivative of $\sigma_{\hat{\mu}}^2$ with respect to a_1 to zero and solving for a_1) or from projection matrix results in linear algebra. The result is $a_1 = c_1$, where $c = (c_1, c_2) = (c_1, 1-c_1) = (G^T\Sigma^{-1}G)^{-1}G^T\Sigma^{-1}$.The estimate $\hat{\mu}$ is a weighted average of the two estimates, with weights summing to 1. In the case of uncorrelated measurements, with zeros on the off-diagonals of Σ, the weights are proportional to the inverse of the respective variances, so $a_1 = c_1 = \sigma_2^2 / (\sigma_1^2 + \sigma_2^2)$. If the measurements are uncorrelated, then the GLS estimate is guaranteed to be between the two estimates.

2.2 PPP

PPP is defined as either $\hat{\mu} > max(x_1, x_2)$ or $\hat{\mu} < \min(x_1, x_2)$. Sivia [12] gave a condition on Σ for which PPP cannot occur, expressed as: if $\rho \le min(\frac{\sigma_1}{\sigma_2}, \frac{\sigma_2}{\sigma_1})$ then PPP cannot occur. In practice, entries in Σ are estimated, and so [3] shows that there are situations where it appears that PPP occurs when it does not, and vice versa. A theorem in [3] shows that if a_1 and $a_2 = 1 - a_1$ have opposite signs, then PPP occurs:

Theorem 1. Suppose a_1 and $a_2 = 1 - a_1$have opposite signs. Then either $\hat{\mu} > max(x_1, x_2)$ or $\hat{\mu} < \min(x_1, x_2)$. That is, $\hat{\mu}$will always fall outside the range of (x_1, x_2). The simple proof from [3] of Theorem 1 is given here.

Proof. First assume $a_1 > 1$ and $a_2 < 0$. If $x_1 < x_2$ then $\hat{\mu} = a_1x_1 + a_2x_2 < a_1x_1 + a_2x_1 = x_1$ because $a_2 < 0$. Similarly, if $x_1 > x_2$ then $\hat{\mu} = a_1x_1 + a_2x_2 > a_1x_1 + a_2x_1 = x_1$ because $a_2 < 0$. The proof is completed by next assuming $a_1 < 0$ and $a_2 > 1$, and following similar steps.

3. The Safeguards Example

Jaech [1] used the following model, Eq. (1) for the better (DA) measurement and Eq. (2) for the worse (NDA) measurement:

$$X_{1i} = T_i + S_1 + R_{1i} \quad (1),$$

$$X_{2i} = \beta T_i + R_{2i} \quad (2),$$

where T_i is the true value (in kg) of item i, S_1 is the systematic error of method 1, R_{1i} is the random error of method 1, β is a constant that is estimated from calibration data. Estimation error in $\hat{\beta}$ leads to systematic error in method 2. In this context, $\hat{\beta}$ is estimated using $\hat{\beta} = \sum_{i=1}^{n_2} X_{2,i} \Big/ \sum_{i=1}^{n_2} X_{1,i}$, which is a ratio of random variables. In many applications, including this one, the variance of a ratio of random variables must be estimated by simulation because the estimate of variance based on the linear first-term Taylor series approximation is not accurate [8-10]. Then, the method 1 estimate of the population mean is $\hat{\mu}_1 = \sum_{i=1}^{n_2} X_{1,i} / n_2$ and the method 2 estimate is $\hat{\mu}_2 = \frac{1}{\hat{\beta}} \sum_{i=1}^{n_1} X_{2,i} / n_1$. This example involves measurement error in both X_1 and X_2, so the literature on "errors-in-predictors" is relevant [13,14] , and the variance in $\frac{1}{\hat{\beta}}$ is estimated by simulation in Section 4.

Rather than the way that GLS was presented in Section 2.1, GLS is often presented in the context of estimating β in a linear regression relating response Y to, for example, predictors X_1 and X_2, denoted $Y = \beta X + e$ [6], where X is a matrix with n rows containing X_1 values in column 1 and X_2 values in column 2. Perhaps this is why [1] did not recognize this safeguards example as one for which known GLS results apply (as shown in Section 2.1). So, instead of applying known GLS results, [1] re-derived the GLS solution, by setting the derivative of an approximate expression for $\sigma^2_{\hat{\mu}}$ with respect to a_1 equal to zero to solve for the value a_1 that minimizes the approximate expression for $\sigma^2_{\hat{\mu}}$. The approximation result from [1], which is evaluated in Section 4, is $\sigma^2_{\hat{\mu}} \approx \{\frac{na^2 + n_1 - 2an_1}{n_1(n-n_1)} - 1/N\}\sigma^2_{\mu} + \sigma^2_{S1} + \frac{\sigma^2_{R1}}{n_1} + \frac{n(1-a)^2\sigma^2_{R2}}{n_1(n-n_1)\beta^2}$ (3), where $\sigma^2_{\mu} = \sum_{i=1}^{N} (T_i - \bar{T})^2 / (N-1)$ (4).

To arrive at Eq. (3), reference [1] ignored estimate error in $\hat{\beta}$, assumed $\hat{\beta} = \beta$, and applied standard error variance propagation to a linear Taylor-series approximation of $\hat{\mu}$. Simulations in Section 4 show that estimation errors in the covariance matrix Σ can lead to the belief that PPP occurs when it does not, and vice versa.

This paper uses three distinct error models for example 1. Jaech's [1] Equations (1) and (2) will be referred to as model A. As model B, instead of Equations (1) and (2), one could use the more common error models [7]:

$$X_{1i} = T_i + S_1 + R_{1i} \quad (5),$$
$$X_{2i} = T_i + S_2 + R_{2i} \quad (6),$$

where Eq. (5) is the same as Eq. (2), and Eq. (6) explicitly provides the systematic error for method 2. Again, T_i is the true value of item i, $S_{X_1} \sim N(0,\sigma_{S_1})$,is the short-term systematic error of method 1, $R_{X_{1i}} \sim N(0,\sigma_{R_1})$ is the random error of method 1, and similarly for method 2 in Eq. (6). Note that model B is not the same as model A unless $S_2 = T(\beta - 1)$, which is a relative error model for S_2

As for model C, the data that were used to calibrate methods 1 and 2 prior to measuring the sampled items could be used. Recent numerical evaluations of four calibration options have led a recommendation to use reverse calibration [8-10], using n (X_{1i},T_i) pairs to fit $T_i = \beta_{1,0} + \beta_1 X_{1i} + R_{1_i}$ and n (X_{2i},T_i) pairs to fit $T_i = \beta_{2,0} + \beta_{2,1} X_{2i} + R_{2_i}$ for method two. The calibration options evaluated in [8] are to apply classical regression, fitting $X_{1i} = \alpha_0 + \alpha_1 T + R_{1_i}$, and then inverting to solve $\hat{T} = (X_{1i} - \hat{\alpha}_0)/\hat{\alpha}_1$ (and similarly for method two), or to apply reverse calibration, directly fitting $T_i = \beta_0 + \beta_1 X_{1i} + R_{1_i}$. Both options can adjust for errors in predictors or not, so there is a total of four calibration options. The reverse calibration option without adjusting for errors in predictors (but using simulation with errors in predictors to accurately evaluate the behaviour of the estimate) has been found to have the same or smaller estimation error, so it is the only option evaluated in Section 4. Figure 1 plots the observed bias in 1 (of 10^5) simulation with 3 standards, and as shown in [8], model C can be expressed as:

$$X_{1i} = T_i + S_{1,1} + S_{1,2}(T_i - \bar{T}) + R_{1i} \quad (7),$$
$$X_{2i} = T_i + S_{2,1} + S_{2,2}(T_i - \bar{T}) + R_{2i} \quad (8),$$

with both additive and multiplicative systematic errors. The additive systematic error arises from estimation error in the intercept. The multiplicative systematic error arises from estimation error in the slope, increasing from 0 at the middle of the calibration data to large positive or negative values near the ends of the calibration data. Some of the well-known results for least squares regression are relevant for evaluating calibration data; however, reverse calibration is not a straight-forward application of regression because of the errors in predictors, and [8-10] recommend simulation for accurate model fitting and uncertainty quantification arising from calibration data.

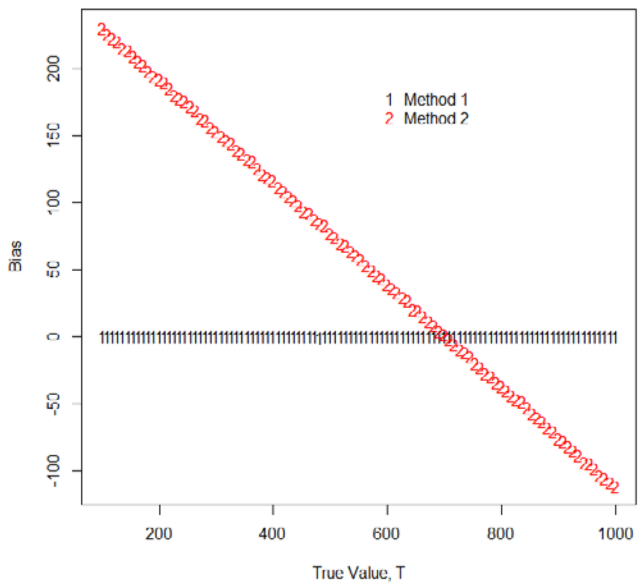

Figure 1: Bias versus true value for method 1 and method 2 in one calibration.

4. Simulation Results for the Safeguards Example

Recall that PPP was introduced in [2] for $\Sigma = \begin{pmatrix} 0.1134 & 0.06 \\ 0.06 & 0.0506 \end{pmatrix}$ for which the values $a_1 = 1.22, a_2 = -0.22$, minimize $\sigma^2_{\hat{\mu}}$ and $\hat{\mu} = 1.22 \times 1 - 0.22 \times 1.5 = 0.88$. Estimation errors in the sample covariance matrix $\hat{\Sigma}$ to estimate Σ can make it appear that PPP does not occur. For example, in 10^5 simulations in R with n = 10, 100, and 1000 (X_1, X_2) pairs, the relative frequency that $\hat{\Sigma}$ leads to the wrong conclusion that PPP does not occur is 72%, 40%, and 0%, respectively. Estimation errors in the sample covariance matrix $\hat{\Sigma}$ to estimate Σ can also make it appear that PPP does occur when it does not. For example, with $\Sigma = \begin{pmatrix} 0.1134 & 0.0506 \\ 0.0506 & 0.06 \end{pmatrix}$, $a_1 = 0.13, a_2 = 0.87$, so PPP does not occur, but in 10^5 simulations in R [15] with n = 10, 100, and 1000 (X_1, X_2) pairs, the relative frequency that $\hat{\Sigma}$ leads to the wrong conclusion that PPP does occur is 32%, 14%, and 0%, respectively.

It was found using 10^6 simulations in R [14] that PPP can occur for models A, B, and C. It was also found that Eq. (3) is not sufficiently accurate for $\sigma^2_{\hat{\mu}}$ (see results in Sections 4.1-4.3). The values in the covariance matrices given below are repeatable to the number of digits shown across sets of 10^6 simulations. In all the results below, $N = 100, \overline{T} = 100, \sigma_T = 50$.

4.1 Model A

The example from [1] was evaluated by simulation in R [15] using $n_1 = 30, n_2 = 5, \sigma_{S1} = 1, \sigma_{R1} = 0.1, \beta = 1.1, \sigma_{R2} = 0.1$. The estimated covariance matrix is $\hat{\Sigma} = \begin{pmatrix} 384 & 399 \\ 399 & 838 \end{pmatrix}$, which implies that the correlation between Method 1 and 2 is 0.70, and that $a_1 = 1.04, a_2 = -0.04$, so by Theorem 1, PPP occurs. Figure 2 plots the root mean squared estimation error in $\hat{\mu}$ versus a_1.

Figure 3 plots the observed and predicted $\sigma_{\hat{\mu}}$ using Eq. (3) from [1] versus a_1. Note that Eq. (3) from [1] is not an accurate approximation. It is noted here that reference [1] did not use $\hat{\mu}_2 = \frac{1}{\hat{\beta}} \sum_{i=1}^{n_1} X_{2,i} / n_1$, but instead used $\hat{\mu}_2 = \frac{1}{\hat{\beta}} \sum_{i=1}^{n_1 - n_2} X_{2,i} / (n_2 - n_1)$, which uses only those NDA measurements that were not used to estimate β.
All simulations evaluated both options. It was found that both options can lead to PPP, but the first option has smaller estimation error, so the reported results all used $\hat{\mu}_2 = \frac{1}{\hat{\beta}} \sum_{i=1}^{n_1} X_{2,i} / n_1$. However, Figure 3 used $\hat{\mu}_2 = \frac{1}{\hat{\beta}} \sum_{i=1}^{n_1 - n_2} X_{2,i} / (n_2 - n_1)$ because Eq. (3) from [1] was for $\hat{\mu}_2 = \frac{1}{\hat{\beta}} \sum_{i=1}^{n_1 - n_2} X_{2,i} / (n_2 - n_1)$.

4.2 Model B

The modified example from [1] was evaluated by simulation in R [15] using n_1=20, n_2=5, $\sigma_{S1} = 1, \sigma_{R1} = 1, \sigma_{S1} = 2, \sigma_{R2} = 2$. The estimated covariance matrix is $\hat{\Sigma} = \begin{pmatrix} 333 & 343 \\ 343 & 784 \end{pmatrix}$, which implies that the correlation between Method 1 and 2 is 0.67, and that $a_1 = 1.02, a_2 = -0.02$. so by Theorem 1, PPP occurs.

4.3 Model C

The modified example from [1] was evaluated by simulation in R [15] using N = 100, n_1=20, n_2=10, $\overline{T} = 100$, $\sigma_T = 50$, $\beta_0 = 1, \beta_1 = 100$, $\sigma_{T1} = 0.003, \sigma_{R1} = 0.003, \sigma_{T2} = 0.04$, $\sigma_{R2} = 0.04$. There were 3 calibration items, with true values of 100, 550, and 1000 grams. The estimated covariance matrix is $\hat{\Sigma} = \begin{pmatrix} 835 & 850 \\ 850 & 1357 \end{pmatrix}$ which implies that the correlation between Method 1 and 2 is 0.80, and that $a_1 = 1.03, a_2 = -0.03$, so by Theorem 1, PPP occurs.

Models A, B, and C can all exhibit PPP and for the numerical examples chosen, models A, B, and C have $a_1 = 1.04, a_2 = -0.04$, $a_1 = 1.02, a_2 = -0.02$, and $a_1 = 1.03, a_2 = -0.03$, respectively.

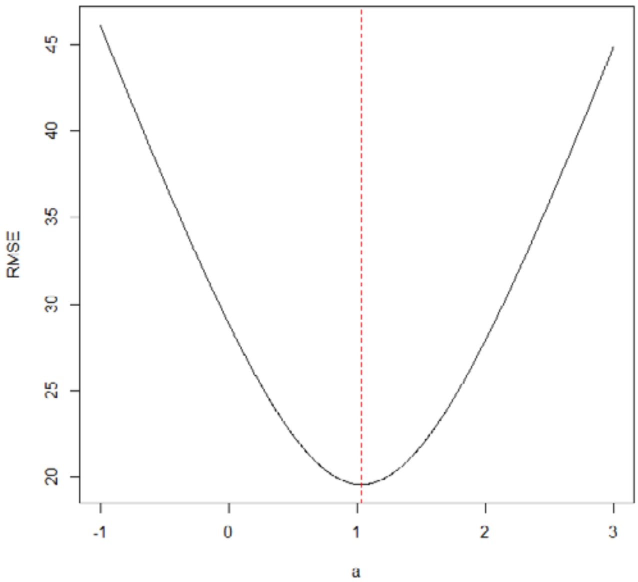

Figure 2: The RMSE versus a_1 for model A. The minimum RMSE occurs at $a_1 = 1.03, a_2 = -0.03$.

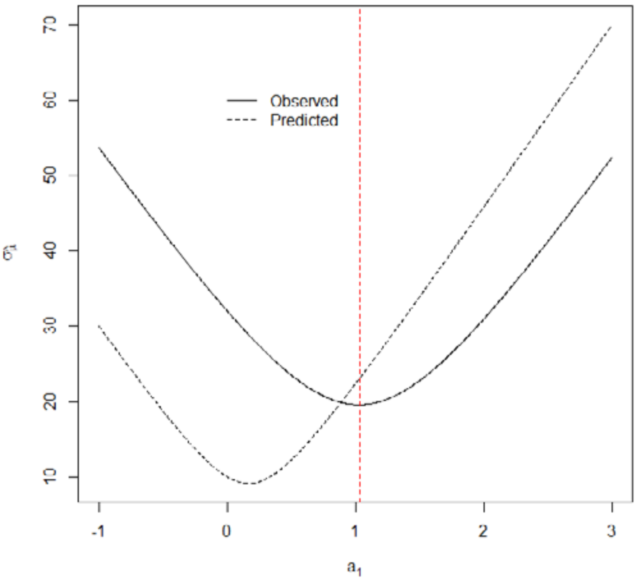

Figure 3: Observed and predicted value for Model A (from Eq. (3) from reference [1]) of $\sigma_{\hat{\mu}}$ versus a_1.

5. Summary

Recent work on uncertainty quantification [8-10] for NDA has found that simulation is needed for high-quality uncertainty quantification. This paper provides another example where simulation is needed for high-quality estimation of the 2-by-2 covariance matrix Σ of two assay methods. The example was a safeguards measurement example from [1] in which a sample of items was assayed using both a lower uncertainty (DA) method and a higher uncertainty (NDA) method was re-evaluated. First, it was shown that generalized least squares can be applied to optimally combine the resulting two estimates, $\hat{\mu}_1$ and $\hat{\mu}_2$ of the population mean. μ. Second, it was shown using simulation for any of three measurement error models, that there is large positive covariance between the two estimates, $\hat{\mu}_1$ and $\hat{\mu}_2$, and one estimate has much larger variance than the other. Third, it was shown that PPP can occur for all three models. Because PPP is a somewhat rare phenomenon, this finding is of interest. However, safeguards analysts need not be concerned if PPP occurs in such an example; because it is an understandable behaviour of GLS [2-4,16] in examples with large positive covariance matrices. Analysts are advised to use simulation to ensure high-quality estimates of Σ so that analysts know when PPP does occur. Reference [16] considers alternatives to PPP when there is non-negligible estimation error in $\hat{\Sigma}$.

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