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Statistical Analysis in Nuclear Accountability: A Simulation Approach

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ABSTRACT

This paper describes a computer simulation approach to modeling material balances and to deriving the limits of error attributable to measurement procedures. A new probability distribution is presented which is useful in the computer simulations. This distribution permits the investigator to assess the sensitivity of initial distributional assumptions on the computed limits of error. The simulation approach is illustrated with a case study example.

1. INTRODUCTION

In this paper we discuss the statistical treatment of the numbers arising from the process of nuclear accountability. Our goal is to decide whether a given amount of material unaccounted for (MUF) is actually missing from the facility or is apparently missing because of combined measurement errors.

If the MUF falls within certain computed limits, we conclude that it is within measurement error. If outside these limits, we conclude that some material is missing. Our approach in calculating these limits on measurement error is first to model the given process. This involves analyzing the flow of material in the process and the associated measurement instruments and practices (including calibration techniques). We model each measurement in the process with a random variable whose expected value is the true value to be measured and whose probability distribution reflects the likely variability in the observed value. We then employ a computer

program to simulate the process and to generate many realizations of the MUF. Given the simulated MUFs from a model which assumes no missing material, we readily can see the variability which can be expected in the normal course of events. Intervals containing the middle 95% and 99% of the generated MUF values yield reasonable estimates of the "warning" and "out of control" limits, respectively.

A much simpler approach to estimating these limits is to assign a standard deviation (or precision) to each measurement in the process and then to assimilate this information in an overall standard deviation by propagation of error. While this gives an estimate of the variance, it is not known how to use such an estimate to form a confidence interval for the mean. The usual practice of taking 2 or 3 estimated standard deviations on either side of the mean as "warning" or "out of control" limits depends heavily on the assumption of normality. Although this approach is easy to carry out, the resulting limits may be poor estimates of the overall measurement error. Frequently, measurements are the product of two values (for example, weight and concentration) which can lead to non-normal probability distributions. Another major difficulty with this approach is its inability to handle calibration errors. Since calibration curves are estimated from the measurement of standards (material with a "known" value), the mere assignment of standard deviations to individual measurements does not accurately incorporate calibration errors.

The simulation approach requires considerable expertise in modeling a given process, but leads to reasonable estimates of the overall measurement error. A desirable feature of this approach is that we can test the effect of our distributional assumptions on our estimates of measurement error. In particular, we can investigate the effects of departures from the normal distribution assumption. This test is performed by exercising our computer model for a variety of assumed probability distributions. For each computer run, the estimated measurement error is obtained. The complete set of these estimates indicates the effect of the distributional assumptions. In the desirable situation, the set of estimates do not vary dramatically so that we can conclude that the results are not sensitive to the initial assumptions. Sensitivity analysis is an essential tool in evaluating the simulation model and assessing the appropriateness of the estimates of measurement error.

In section 2 we describe a new family of symmetric univariate probability distributions which can enhance sensitivity analysis studies, as described above. This family is particularly useful in analyzing quantitatively the effect of departures from normality on the estimates of measurement error. The proposed family includes as special cases the uniform and normal probability distributions, which are commonly used in nuclear accountability. The kurtosis of the family (i.e., the fourth standardized moment) which is an indicator of tail weight, varies from 1.8 (the uniform) to 3.0 (the normal) to 5.4 (a heavy-tailed distribution). Hence, the family includes a broad spectrum of probability distributions.

Random variates from the proposed family are easy to generate, and thus, they can be used in the computer simulation model.

The simulation approach together with the new family of distributions leads to robust estimates of the overall measurement error. In section 3 we describe in detail a case study in which measurement errors for a particular process were estimated by simulation. We conclude that our approach leads to reasonable estimates of overall measurement error.

2. PROPERTIES OF THE NEW DISTRIBUTION

The proposed distribution has probability density function

$$f(x) = \frac{\sqrt{\alpha}\,\Gamma(\alpha-1/2)}{2\sigma\,\Gamma(\alpha)\sqrt{3}}\left[1 - H\left(\frac{2\alpha(x-\mu)^2}{3\sigma^2}\right)\right],$$

for $\alpha > 1/2$, $-\infty < x < \infty$. H is the distribution function of a gamma random variable with shape parameter $\alpha - 1/2$ and scale parameter 2. Numerous properties of this distribution are derived in [1, 2]. Properties of importance to nuclear materials simulation applications are enumerated below.

1. A random variable X with the density f is symmetric and all moments exist. In particular, the mean of X is μ, the variance is σ^2, the skewness is 0, and the kurtosis is $1.8(\alpha + 1)/\alpha$.

2. The kurtosis can assume any value in the interval [1.8, 5.4). For a specified kurtosis, say β_2, set $\alpha = 1.8/(\beta_2 - 1.8)$.

3. A range of distributional properties is obtained by appropriate choice of parameters. For $\alpha = 1.5$, a normal distribution is obtained. As α tends to infinity, f approaches a uniform distribution. More generally, the probability in the tails can be regulated by the choice of α: large α gives light tails, α near 1.5 gives medium tails, and heavy tails are obtained for α near 0.5.

4. The proposed distribution can be easily generated on a digital computer. One algorithm is as follows: Generate a gamma variate x_1 with shape parameter α and scale parameter 2. Then, generate conditionally a uniform variate x_2 on the interval $(-\sqrt{x_1}, \sqrt{x_1})$. A random variate with density f is $\sqrt{(1.5\alpha)}\sigma x_2 + \mu$. Recommendations for the appropriate gamma generation algorithm are given in [3].

5. By using a computer simulation program for a range of α values, one can assess the effects of almost any type of symmetric non-normality on the simulated results.

3. CASE STUDY

In this section we describe the methodology for computing limits of error (LE) in a process for recovering uranium from metal scrap. We first describe the physical material. We then discuss the material balance areas and the measurement devices and practices. Finally, we present results from a computer simulation model which is used to estimate LE.

3.1. Physical Material

A part of the uranium reprocessing operations at the Los Alamos Scientific Laboratory consists of recovering uranium from turnings created in machining uranium metal. After burning to eliminate oily residues, this material is stored in cans in a vault for possibly several months. Periodically, several cans are removed and their contents dissolved. Ultimately, fairly pure uranium oxide is precipitated.

3.2. Material Balances and Measurements

We concentrate on two material balances in the recovery process. Before a can is placed in the vault, its contents are burned to an oxide and a non-destructive assay is performed using a random driver device. This device is calibrated with standards of 250g, 500g, 1000g, 1500g and 2000g uranium per can. There are five replications per can during the calibration run. Each can in the vault usually contains 1500g to 2000g uranium. One material balance area is defined by considering a processing batch of 4 or 5 cans. The corresponding MUF is the difference between the total uranium assays at the times of putting the cans in the vault and taking them out of the vault.

The batch can usually be completely dissolved in a nitric acid solution. The volume of the solution is typically 30 to 40 liters and is obtained from reading graduated cylinders (especially designed for radioactive solutions). The concentration is determined from a non-destructive uranium solution assay device (USAD) using a 20 ml sample. The calibration standards used for this device are 150, 250, 300 and 350 grams uranium per liter solutions with five replications each. The product of the volume and the concentration yield an estimate of the uranium in solution. The second material balance area is defined by the material as it leaves the vault and the uranium in the solution.

3.3. Computer Simulation Model

The problem is to derive LE for each of the material balance areas defined in section 3.2. Under the assumption of no hold up or diversion, the corresponding MUFs can be modeled, as follows:

$$MUF1 = \sum_{i=1}^{n} \left(\frac{x_i - a_1}{b_1}\right) - \sum_{i=1}^{n} \left(\frac{y_i - a_2}{b_2}\right)$$

$$MUF2 = \sum_{i=1}^{n} \left(\frac{y_i - a_2}{b_2}\right) - V \cdot \left(\frac{C - a_3}{b_3}\right),$$

where

x_i = random driver measurement for i^{th} can as it enters the vault

y_i = random driver measurement for i^{th} can as it leaves the vault

n = number of cans

a_i, b_i = estimated calibration constants assuming a linear relationship $y_i = b_i x_i + a_i$

V = volume measurement

C = concentration measurement.

We can treat each of the measurements and estimates as random variables, with a variance derived from historical or designed experimentation. For investigating particular MUFs, we use the observed measurements as the means of the random variables. For the estimated calibration "constants," we simulate readings for the standards and fit a line to them. The slope of the fitted line is b_i; the intercept is a_i. Since the sets of random driver measurements are taken months apart, different calibration constants are simulated for the repeated measurements on a batch of cans.

The next step in the methodology is to simulate in a computer program the models for MUF1 and MUF2. Naturally, we use the proposed distribution of section 2 to model the individual random variables. From the previous paragraph, the values of μ and σ^2 are determined, and the parameter α gives us a degree of freedom in a sensitivity analysis. In particular, we can select, say, five kurtosis values 1.8, 2.5, 3., 4. and 5.3 with corresponding α values ∞, 2.57, 1.5, 0.818 and 0.514. Eventually, we compare five sets of estimates of LE. The details are apparent from the subsequent example.

Consider, for illustration, four cans with initial random driver measurements 1688g, 1676g, 1723g and 1705g and with later random driver measurements 1735g, 1719g, 1719g, and 1682g, respectively. The MUF for this material balance area is 63g gain. The solution assay is 6504g with a volume measurement of 26.2ℓ. Thus, the second material balance area has a MUF of 271g loss. Are these MUFs within their limits of error?

Our approach to the question is to simulate five replications of 1000 samples of MUF1 and MUF2. Each set of 1000 values is sorted, and the 5th, 25th, 975th and 995th observations provide estimates of the 0.5, 2.5, 97.5 and 99.5 percentiles. Denote the four estimates as p_i, q_i, r_i and s_i, respectively, where i is the replication. Since the limits are symmetric, we can justify estimates of the 95% warnings limits as $\pm$ [median $|q_i|$ + median r_i]/2 and the 99% out of control limits as $\pm$ [median $|p_i|$ + median s_i]/2. Certainly, other estimates could be proposed, but our experience indicates these

to be robust.

The resulting estimates [illegible] he simulation run are given in Tables I and II.

From these simulation results, we can observe that the 63q MUF gain and the 271q MUF loss are within their respective LE for all distributions sampled. We conclude the MUFs represent material apparently missing because of combined measurement errors. We also notice that the LE estimates are reasonably stable over the range of distributions sampled.

4. CONCLUSIONS

In this paper we have presented a computer simulation methodology for determining limits of error for material unaccounted for. This approach is straightforward, leads to reasonable LE estimates, and can incorporate measurement errors induced by calibration. The new probability distribution can be used effectively to assess the impact of non-normal distributional assumptions. This facilitates the analysis of computed warning and out of control limits. An example has been given which illustrates the methodology.

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TABLE I. MUF1 RESULTS.

β_2	Est. 95% Limits	Est. 99% Limits
1.8	±319g	±419g
2.5	±331g	±435g
3.0	±328g	±436g
4.0	±341g	±452g
5.3	±313g	±443g

TABLE II. MUF2 RESULTS.

β_2	Est. 95% Limits	Est. 99% Limits
1.8	±273g	±355g
2.5	±272g	±360g
3.0	±274g	±356g
4.0	±279g	±370g
5.3	±280g	±378g