Proceedings of the INMM & ESARDA Joint Virtual Annual Meeting August 23-26 & August 30-September 1, 2021

Statistical Analysis Of Convergence And Error Propagation In Stochastic Model For Safeguards Inspection

L. Annadevula[1], S. K. Aghara[1], K. Jarman[2], and L. Joyce[1]

[1]University of Massachusetts Lowell, Lowell, MA, USA

[2]Pacific Northwest National Laboratory, Richland, WA, USA

ABSTRACT

IAEA safeguards experts use detection probability (DP) as the primary effectiveness metric for nuclear material inventory and flow verification activities. The DP is calculated over a spectrum of diversion scenarios (from a few items with gross defects to a large number of items with bias defects), and the worst-case (lowest) DP is reported. Deterministic models using statistical distributions are generally used to compute achieved DP for individual nuclear material strata to assess the effectiveness of the IAEA verification inspections. The models get involved as the total number of defect types in the multi-defect sample space increases. The model must first calculate the item selection probability as well as the identification probability at each step in each stratum. Once done, the model then aggregates the DP from each stratum to calculate an aggregate detection probability (ADP) for the entire facility. The model must consider the broad range of ways in which material could be diverted within the facility to add up to that total and determine the minimum ADP over all possible diversion strategies. The stochastic approach to simulating inspection of items in a nuclear facility involves random selection of items containing nuclear material and predicting the results of measurements for these samples. Stochastic methods offer greater flexibility to model scenario development to simulate different diversion strategies and measurement characteristics. Stochastic methods rely on multiple simulations for each scenario to generate a distribution of DP values to compute the average and the uncertainty. A critical attribute of stochastic methods for such an application is a rigorous analysis of convergence (in terms of number of stochastic "trials") and error, or precision in the estimated DP. This paper describes the method and its application to international safeguards inspection performance evaluation.

INTRODUCTION

In IAEA nuclear safeguards and inspections, a state is a collection of facilities, a facility is a collection of strata and a stratum is a collection of items and batches. Diversion strategies at stratum level involve different ways of acquiring the goal material from the items or batches and detection strategies involve different selection and identification procedures the inspectors perform to identify the defected items. The Defect detection probability (DP) is considered as a metric in quantifying the effectiveness of various detection strategies on the stratum which was put through specific limiting case diversion strategies [1 - 3]. At facility or state level, the diversion strategies involve different ways of splitting the total goal diversion amount into total number of strata and acquiring the stratum specific goal amounts using the stratum specific diversion strategies which when inspected will result in stratum specific DPs for each stratum which will be aggregated to yield a facility level detection probability metric using event independence principle. Among all possible ways or combinations of splitting the total goal amount among existing strata there exists one combination which poses maximum proliferation risk yielding minimum aggregate detection probability (Min ADP). Thus, Min ADP is used as limiting case metric to evaluate the combined and overall effectiveness of stratum specific detection strategies at facility or state levels.

Deterministic models [1,2] use statistical distributions, like multi-variate hypergeometric distributions for computing selection probabilities and normal, step distributions for computing identification probabilities, in the quest to compute DP for individual nuclear material stratum to assess the effectiveness of the IAEA verifications employed on the stratum which was subjected to diversion strategy. Developing computational algorithms for multi stratum facilities, such as enrichment and reprocessing, with multi-defect sample space of items/batches to compute the DPs in individual stratum become exceedingly complex when approached deterministically. The solution gets more involved as the total number of defect types in the multi-defect sample space increases. The model must identify all possible relevant defect outcomes and calculate the item selection probability as well as the identification probability at each outcome to get the overall DP. So far there is no single overarching model that can compute DPs when a stratum is subjected to wide range of diversion and detection strategies, not to mention the task of identifying all possible outcomes to compute selection probabilities is by itself computationally expensive. As such the inspection verification problem which has randomness involved in the item selection process is ideally suited for a stochastic approach. This involves repeating a series of random selections of items from the set of all items in the stratum, followed by measurements of the selected items. For each simulation or trial, a DP value (the outcome) is calculated. Through large number of trials, a distribution of DP values (the stochastic solutions) are obtained when averaged shall yield required Detection probability (DP) for the specified inspection campaign data. Since stochastic process is random there is an error and uncertainty associated with the result and is depended on the total number of trials. A set of statistical checks must be performed to evaluate convergence, accuracy and precision of the computed results. Similarly, all the stratum level DP curves thus produced by stochastic model with their associated errors when in turn aggregated to facility level causes the errors to propagate to yield final Aggregate Detection Probability value (ADP) with its own error accumulated from all individual stratum level errors. This paper will describe the statistical DP Error Convergence and the ADP Error Propagation tools developed for the stochastic model. Inspection examples will be described along with necessary results and plots to describe the significance of the tools.

STOCHASTIC MODEL - WITH “TRIALS” ANALOGY

The Stochastic approach to inspection [3] involves simulating the inspection process i.e., randomly choosing a fixed number of items from sample space and performing measurements for these samples. For each random outcome, a DP value is calculated. Multiple such Simulations/Trials are performed on the same sample space to get multiple DP values. The final Detection Probability is given by the Average or First Moment of all the individual DP values and the standard error of all individual DP values gives the error in the final DP estimate.

For i^{th} simulation or trial, the obtained DP estimate is taken as X_i and ‘N’ such simulations are performed such that ‘i’ takes the values of 1 to ‘n’. Mean of all X_i values equation (1) gives the final DP estimate and the standard error of all X_i values equation (2) gives the required error in the estimated DP value.

$$\hat{\mu} = \bar{X} = \frac{1}{N}\sum_{i} X_i \qquad (1)$$

$$s^2 = \frac{1}{N-1}\sum_{i}(X_i - \bar{X})^2$$

$$se(\hat{\mu}) = \frac{s}{\sqrt{N}} \qquad (2)$$

NEED FOR ERROR CONVERGENCE IMPLEMENTATION

From equation (2) it is clear that increasing the number of trials ‘N’ will lower the standard error in the final result and figure (1) demonstrates the convergence of error with increase in number of trials. Through the error converges by increasing the trials, in order to conserve the computational resources, it is necessary for the model to be able to run precisely required number of trials not more nor less in order to achieve certain set error in DP estimate. Unfortunately, the required number of trials needed to achieve certain error in DP estimates vary with type of inspection problem which can be observed in figure (1). Different falsified pin examples converge to different errors when model runs same number of trials. To achieve the set error in DP the viability of the following two options has been explored:

1. Pre-compute minimum trials or
2. Perform running standard error estimations.

Building a package that pre-computes minimum trials require the evaluation of dependances of final detection probability on different input variables. This is a difficult task as the number of variables involved keep varying from problem to problem. Mainly number of item types in the sample space and number of instruments used in the inspection process keep changing with different diversion and detection strategies applied to the stratum. Thus, building a package that can predict minimum trials, required to reach certain error, for any inspection scenario is not a viable option. The more efficient and practical option is to remodel the existing stochastic model from “Trials” analogy to “Trials-Batches” analogy and estimate running standard error allowing the code to decide when to stop running additional batches once the set error in DP estimate has been achieved.

STOCHASTIC MODEL - WITH “TRIALS & BATCHES” ANALOGY

Statistical DP Error Convergence package has been developed, allows the model to converge to the required accuracy without the need to quantify the minimum trials. The tool makes use of Batches-Trials analogy with each batch containing fixed number of trials/simulations performed yielding a DP estimate and an error estimate at the end of each batch. The code, runs one batch at a time and a running estimate of DP and its standard error are computed using individual estimates from each batch, continues to run more batches until the error converges to set value. This Batch-Trial analogy allows the code to be efficient with computational resources and at the same time reach the set accuracy of final result without the need to compute minimum number of trials. This running estimate of DP and its standard error is computed using the one-way balanced ANOVA derivation[4].

Estimating running DP and standard error using ANOVA

Let X_{ij} represent DP for the i^{th} Trial of j^{th} Batch. The values for i range from 1 to N trials and j takes values from 1 to M batches. Assume that the X_{ij} are independent and identically distributed random variables with mean μ and variance σ^2. The complete set of DP values can be represented in terms of the following matrix:

$$\begin{pmatrix} X_{11} & X_{12} & \cdots & X_{1M} \\ X_{21} & X_{22} & \cdots & X_{2M} \\ \vdots & \vdots & \ddots & \vdots \\ X_{N1} & X_{N2} & \cdots & X_{NM} \end{pmatrix}$$

Each Batch consists of 'N' DP values. For the jth batch, the mean, standard deviation and standard error in the mean are as follows:

$$\hat{\mu}_j = \bar{X}_{.j} = \frac{1}{N}\sum_i X_{ij}$$

$$s_j^2 = \frac{1}{N-1}\sum_i \left(X_{ij} - \bar{X}_{.j}\right)^2$$

$$se\left(\hat{\mu}_j\right) = \frac{s_j}{\sqrt{N}}$$

Aggregate mean, standard deviation, and standard error across the batches may be computed as follows:

$$\hat{\mu}_{avg} = \bar{X}_{..} = \frac{1}{M}\sum_j \bar{X}_{.j} = \hat{\mu} \tag{3}$$

$$s_{avg}^2 = \frac{1}{M-1}\sum_j \left(X_{.j} - \bar{X}_{..}\right)^2$$

$$se\left(\hat{\mu}_{avg}\right) = \frac{s_{avg}}{\sqrt{M}}.$$

The breakdown of the complete set of simulations into multiple subsets of batches is similar to the "within-group" and "across-group" calculations used in analysis of variance (ANOVA). We apply the same calculations used in ANOVA to compute overall statistics. First, the overall mean is simply the average of batch means as noted by $\hat{\mu}_{avg}$. The overall standard error is computed as follows:

$$se(\hat{\mu}) = \sqrt{\frac{(N-1)\,\overline{se\left(\hat{\mu}_j\right)^2}}{MN-1} + \frac{(M-1)\,se\left(\hat{\mu}_{avg}\right)^2}{MN-1}} \tag{4}$$

where,

$$\overline{se\left(\hat{\mu}_j\right)^2} = \frac{1}{M}\sum_j se\left(\hat{\mu}_j\right)^2$$

When number of batches M = 1, the second term in equation (4) disappears and the equation (4) reduces to equation (2) i.e., the standard error is simply the error of all simulations in batch-01. When number of trials per batch N =1, the first term in equation (4) disappears and the standard error is simply the standard error of individual values taken across all batches.

ADP ERROR PROPAGATION

The problem of ADP error propagation using stochastic DP results is addressed using both deterministic and stochastic methods. **Deterministically**, the propagation of error for ADP where component variables are in simple product with each other,

$$(1 - ADP) = \prod_{i=1}^{n}(1 - DP_i)$$

For functions $f = \prod_{i=1}^{n} X_i$ with independent variables, relative error in f is given by [5,6].

$$\left(\frac{SE_f}{f}\right)^2 = \sum_{i=1}^{n}\left(\frac{SE_i}{X_i}\right)^2$$

By rearranging and simplifying above expression with ADP & DP terms the final Standard error in ADP is given by the formula below,

$$\boldsymbol{SE_{ADP} = (1 - ADP)\sqrt{\sum_{i=1}^{n}\left(\frac{SE_i}{1 - DP_i}\right)^2}} \tag{5}$$

Stochastically, for all strata, normal distributions with DP_i as mean and SE_i as standard deviations are built. At each stochastic trial/simulation a single DP value is sampled randomly from each of the distributions and with the obtained set of DPs a single ADP value is computed. By using sufficiently large number of trials/simulations enough number of ADP values are generated in similar manner which in turn resemble a new normal distribution whose mean and standard deviation gives the final ADP and its standard error, respectively.

RESULTS

The convergence of standard error is demonstrated using the 'varying falsified pins' example inspection case described in paper Krieger et al. [1]. The spent fuel pond contains $N = 2500$ spent fuel assemblies (SFAs) with each assembly containing $L = 96$ fuel pins and in terms of material each assembly contains 2 kg or 0.25 SQ ($\bar{x}$) of Pu. A total goal amount (G) of 1 SQ or 8 Kg of Pu is chosen to be diverted by removing r_{pins} pins from each assembly. To acquire 1 SQ would require r_{SFA} assemblies from which r_{pins} pins are removed while the remaining $N - r_{\text{SFA}}$ assemblies remain untouched. Multiple example diversion strategies are considered where the falsified pins per assembly r_{pins} are chosen to be 2, 3, 5, 28 and 96 pins, which makes the total number of falsified assemblies r_{SFA} required to divert 1 SQ to be 192, 128, 77, 14 and 4 SFAs respectively computed based on the equation below.

$$\boldsymbol{r_{SFA}(r_{pins}) = ceil\left(\frac{G * L}{\bar{x} * r_{pins}}\right)}$$

Out of 2500 SFAs, the inspector verifies 10 SFAs with the ICVD, 65 SFAs with the DCVD, and 25 SFAs with the PGET, with their respective Identification probabilities discussed in the same paper, where per verified SFA only one measurement instrument is applied.

Error Convergence using Trials Analogy.

The initial stochastic model allows the user to set the number of trials used for computing DP results. The model simulates the above examples by varying the trials in logarithmic fashion from 10 to 100000 trials. The DP and standard error are computed using equations (1) & (2) respectively. Convergence in standard error to lower values can be seen in figure 1, the figure also demonstrates the fact that using same number of trials different examples converge to different standard error values which means using Trials only analogy the user must have an idea of number of trials he or she need to specify in order to get to required standard error for all examples. The goal of being able to compute DP values with required standard error is being achieved using Trials-Batches Analogy has been incorporated into the model. The added capability initiates new batch of trials and estimates running standard error using equations (3) & (4) until the error reaches set value making the model more practical to use for any user.

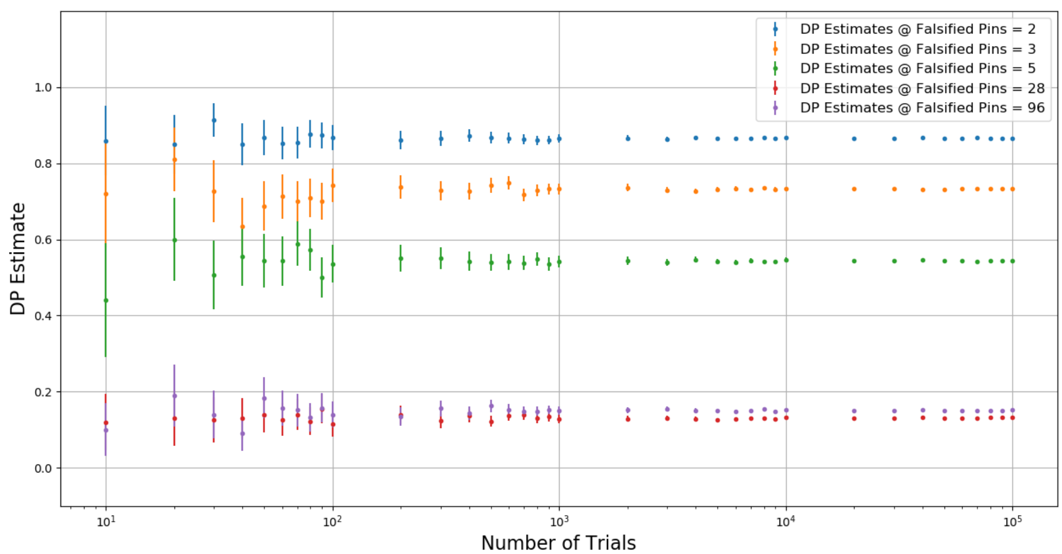

Figure 1. DP error convergence plot showing reduction of standard error with increase in number of Trials.

Error Convergence using Trials-Batches Analogy

The stochastic model updated with error convergence package simulates the above examples using 2000 trials per batch with a target standard error set to 0.002. The running DP & standard error is computed using equations (3) & (4) respectively. The code automatically generates and runs new batches until the standard error is equal to or less than the set value. Convergence in standard error to the set value can be seen in Figure 2, demonstrating the significance of the error convergence tool in conserving resources and bypassing extra steps required in computation of number of trials.

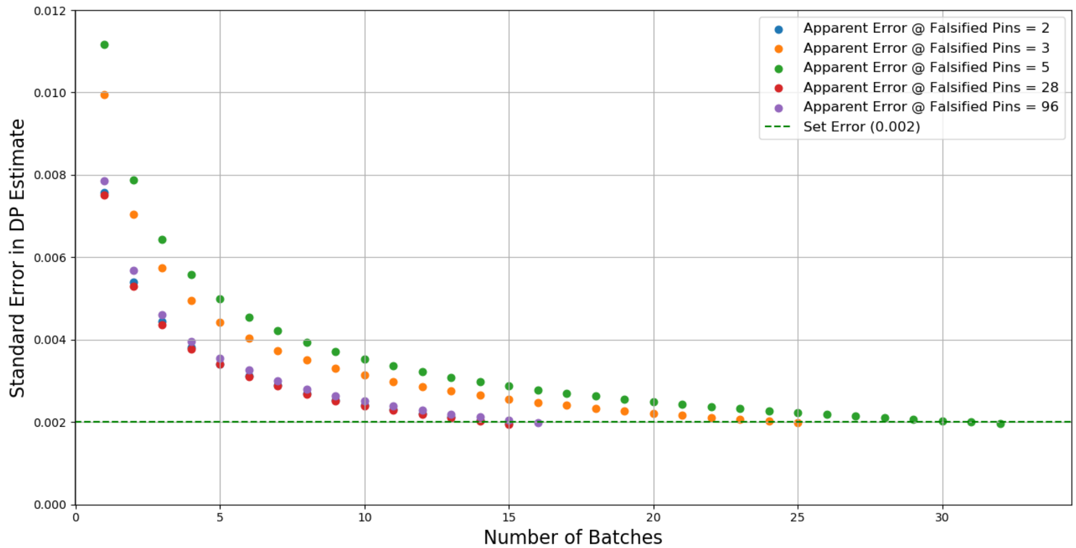

Figure 2. DP error convergence plot for various examples with code initiating new batches and terminating once the apparent error reaches set value (0.002)

<u>ADP Error Propagation Results</u>

A 10 Strata example with following set of DPs & Errors is considered and final ADP & its error is estimated using both deterministic formula & stochastic propagation tool discussed earlier. The results are compared below and found to agree with each other.

Combination DPs: [0, 0.5, 0, 0.6, 0, 0, 0, 0, 0, 0];

Combination Errors: [0, 0.002, 0, 0.0025, 0, 0, 0, 0, 0, 0].

Using Stochastic error propagation with 100,000 Trials, the final ADP is computed to be 0.80000032 $\pm$ 0.0014843. Whereas the Deterministically using equation (5), computed ADP value is 0.8 $\pm$ 0.00148408 are in agreement with each other. The deterministic error computation is much faster than stochastic error propagation and is chosen for practical applications.

CONCLUSIONS

Statistical balanced ANOVA derivation allows the estimation of running error in Trials-Batches Analogy, allows the user to skip the steps required to compute number of trials needed to reach certain error in DP estimates. Aggregating stochastic DP results requires the propagation of error, which is achieved deterministically and stochastically. Addition of the error convergence & error propagation packages standardizes the stochastic model built for IAEA Inspection Problems.

RECOMMENDATIONS AND FUTURE WORK

Currently, the model is built such that required error is set by user and the model stops running additional batches once the running error is less than or equal to set value. The future work involves development of similar framework which allows the user to set time and the code stops running when the execution time approaches the set time.

REFERENCES

1. T. Krieger, K. Aymanns, Rezniczek, and I. Niemeyer; “Optimal Sampling Plans for Inventory Verification of Spent Fuel Ponds”: Article 01; ESARDA Vol 58; June 2019; ISSN:1977-5296.
2. T. Krieger, T. L. Burr, "Comparison of an Exact to an Approximate Sample Size Calculation for Attribute Testing," Journal of Nuclear Materials Management, vol. 3, no. XLIV, 2016.
3. C. Gazze et al., "Stochastic Approaches for Calculating and Aggregating Detection Probabilities for Nuclear Material Diversion," BNL-211980-2019-INRE, 2019.
4. C. M. Douglas, G. C. Runger, "The Analysis of Variance," in Applied Statistics and Probability for Engineers, 7th ed.: Wiley, 2018, ch. 13th, pp. 472-475.
5. Anon,2020. “Propagation of Error,” Available at: https://chem.libretexts.org/@go/page/353 [Accessed August 4, 2021].
6. “Error Propagation tutorial" (PDF). Foothill College. October 9, 2009. Retrieved 2012-03-01.