A Neural Network Approach to the Detection of Nuclear Material Losses

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A series of repeated nuclear material balances forms a time series of often autocorrelated observations. Outliers, deviations from an in-control production process or time series pattern, indicate an out-of-control situation relative to the process norm. In this paper various methods, especially neural networks, will be examined with respect to their use to detect nuclear material diversions or losses more rapidly and accurately than currently used methods. The neural network technique will be enhanced with the use of a simulation computer program for creating the training data set. This simulation approach provides the opportunity of including outliers of various types in a data set for training the neural network because an actual process data set used for training possibly may not have outliers. In this paper, the methods will be compared on their ability to identify outliers and reduce false alarms. These methods were tested on data sets of nuclear material balances with known removals, and the results are tabulated and described. Based on these results, we believe the algorithms used will assist the nuclear industry in process control, provide a new approach to nuclear material safeguards, and also provide a new approach to training neural networks for process control applications.

A. INTRODUCTION

In Nuclear Materials Accounting the objective is to accurately determine if there have been material diversions or losses (e.g., leakage or theft) as soon as possible to minimize the threat to the environment and the public. Even though some progress has been made in this area, the control measures against leakage, theft, or other loss of radioactive material has continued to be of concern. The international crisis concerning the monitoring and safeguarding of nuclear material in the former Soviet Union has been highlighted by several instances of nuclear material from the former Soviet Union being found in Germany.[19,25,43,44] Furthermore, the National Academy of Sciences (NAS) has warned that a "clear and present danger to national and international security is posed".[25] In addition, the leakage of radioactive material into the environment has the potential to adversely affect the well-being of the world's population. Therefore, any method that could detect losses or diversions quickly and accurately would indeed provide a significant contribution to nuclear safeguards as well as public safety.

This paper demonstrates that nuclear material loss or diversion can be detected through the detection of statistical outliers.[3,23,41] Outliers may be thought of as observations in a set of data which appear to be inconsistent with the remainder of the data set. Traditional statistical process control (SPC) charts which attempt to detect outliers as do other current methods are generally based on two assumptions. First, that the system's observations in a time series are independent[2] and identically distributed (IID) about the process mean at any time, *t*. Second, that the underlying distribution is normal when the process is in statistical control.[39]

In the language of Control Charts, points that are outside three standard deviations of the process mean are usually considered to be process disturbances (outliers). When this situation exists, the process is said to be "out-of-control" and thus, there is a significant adverse process change due to usually an assignable cause. Otherwise, we say the process is in control, i.e., operating within its control limits.

In reality, the IID assumption of conventional control chart methods does not always hold. Therefore, traditional SPC procedures may be ineffective and inappropriate for monitoring and/or controlling the production process in these situations.[39] A process operator often uses sensitizing rules to interpret these charts. The sensitizing rules are as follows: (1) One point plots outside the 3-sigma control limits. (2) Two out of three consecutive points plot beyond the 2-sigma warning limits. (3) Four out of five consecutive points plot a distance of 1-sigma or beyond the center line. (4) Eight consecutive points plot on one side of the center line.[24] Based on such methods, the operator will decide from the analysis of the control charts whether a process correction is necessary. However, the operator can get a misleading indication of the process condition from his/her analysis if the IID, normal assumptions are violated.

B. NUCLEAR MATERIAL SAFEGUARDS AND RELATED RESEARCH METHODS

In 1982, Goldman et al.[15] reviewed the origins and development of nuclear material safeguards including the role of statistics. Nuclear material safeguards are tools used by nuclear material accounting managers to detect and prevent losses or diversions. In 1983, Marshall[22] faulted the International Atomic Energy Agency (IAEA) for what he regarded as its inadequate safeguards in dealing with the theft or loss of Special Nuclear Material (SNM). Despite such criticism of the safeguards in place, preventative control of diversion or loss continues to be a problem.

Customary statistical problems in material balance accounting are discussed by Goldman et al. In addition, Speed and Culpin[36] noted that the differentiation between a

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systematic error over several periods and an outright diversion or loss is difficult to identify. Bowen and Bennett[8] concurred with these findings. All authors agreed that improvement in statistical methods was necessary. Today, particular statistical methods [the Shewhart Control Chart, the cumulative summation (CUSUM) chart, the sequential probability ratio test, the power-one test, page test, robust test, etc.] are used for detecting significant shifts in the process mean or protracted losses. Nevertheless, Goldman et al. as well as Speed and Culpin concluded that there were problems with all of these methods.

Speed and Culpin also observed that none of the methods mentioned above considered prior probabilities of a diversion, nor took into account the cost of a false alarm concerning a diversion. These two are crucial in order to set the control limits for the process and thus establish the sensitivity of the methods. Picard[27] also determined that the CUSUM method was insensitive to protracted losses of material from large inventories.

In nuclear material accounting, the material balance equations[10,34] are used to monitor and control nuclear material within a facility. The nuclear industry does often use other equations instead of the material balance equations which are called the material unaccounted for (MUF) equations. The MUF equations are equal to the material balance equations multiplied by a negative one. The positive MUF equation equates to a loss or removal of material. Thus, the results based on these equations could be a negative material balance, a positive material balance, or zero (which indicates no material loss). A negative material balance can occur because of leakage, theft, accounting errors, operator errors, etc. A positive material balance results from a hidden gain because of a systematic measurement error or an unaccounted for measurement for an abnormal amount of material in the process that later reversed itself (e.g., caking). Sebastian et al.[34] provides an in-depth discussion of this topic.

In order for a material balance to be documented, hundreds of measurements and estimates are often necessary. This large amount of data and related sources of error create difficulty in measuring the dependency among observations. Outliers can distort these parameters and affect the standard error value and thus, inaccurate conclusions may result. The advantage of the methods demonstrated in this paper is that they detect the effect of these outlying ("out-of-control") observations.

Booth[5,6] details the relationship between time series outlier types and nuclear material accounting. An additive outlier (AO) affects a single observation. It is an abrupt removal or one time loss or theft. An innovative outlier (IO) affects sequential observations. This type can indicate leakage or systematic theft over a period of time. Thus, the early identification of an outlier and its type will minimize any loss or theft because the organization using this process would have the necessary information to deal with the problem effectively and quickly.

Prasad et al.[30] tested the joint estimation procedure[9] on nuclear material inventory data sets and achieved satisfactory results. This procedure was used because of its ability to handle deviations from any type of time series model of a process. Also, it is a robust and discriminating process which identifies outlier types, using standard hypothesis testing—not only additive (an abrupt removal or one time loss) and innovative (a continuing loss of short duration) but also temporary change (TC) (a continuing loss of longer duration) and level shift (LS) (a long term protracted removal or continuing loss throughout the remaining series) outlier types can be observed.

Sebastian et al.[34] recently tested polynomial smoothing algorithms and data bounding algorithms for nuclear material inventory data sets again with satisfactory results. A polynomial smoothing algorithm combines a commonly used smoother with an "outlier detection procedure for process control". A data bounding algorithm is essentially a means of adjusting data points that lie beyond certain limits, thus smoothing significant peaks and troughs. These methods have been adapted to outlier detection in safeguards development. Thus with the proper fine-tuning of the sensitivity constants for these algorithms, the process engineer can choose the algorithm which is best suited for the application.

The problem of Nuclear Materials Accounting procedures and the estimation of associated parameter values constitutes an unique application of outlier detection to a crucial societal problem. Previously, the joint estimation procedure, data bounding, polynomial smoothing, and neural networks have been successfully tested on conventional industrial process control data sets with known process disturbances (outliers).[17,29,31,32,33] In this paper, we discuss an enhancement to the neural network approach for use in nuclear material accounting and, in fact, any process control problem. This enhancement is based on a new simulation algorithm. This simulation algorithm creates a training data set from an actual data set of any size. The importance of this algorithm is that outliers can be incorporated into a training data set for a neural network, while an actual process data set used for training may not include outliers. Thus, the simulation algorithm provides a crucial enhancement to the neural network method in early and more accurate detection of outliers (i.e., process disturbances) while reducing the possibility of false alarms. This procedure in conjunction with the neural network approach has also been successfully tested on production process data sets of various sizes with known process disturbances.[16] Based on our results, we show that these methods, especially the neural network with the simulation enhancement feature, can be applied to nuclear material processes.

C. NEURAL NETWORK ALGORITHM FOR THE DETECTION OF PROCESS DISTURBANCE POINTS (OUTLIERS)

Today, neural network technology has become one of the most widely investigated topics in process control. The fascination with this field is based on the neural network's ability to learn from being exposed to information or data and then to utilize the information or data to make decisions in a manner that is similar to that performed by a human brain. R. Hecht-Nielsen[18] provided a definition that supports this idea: "A neural network is a computing system made up of a number of simple, highly interconnected processing elements, which processes information by its dynamic state response to external inputs".

This unique capability of a neural network for processing information provides specific advantages. These advantages include adaptive learning, self-organization, fault tolerance via redundant coding, real-time operating ability, and ease of insertion into existing technologies.[21] Beside these

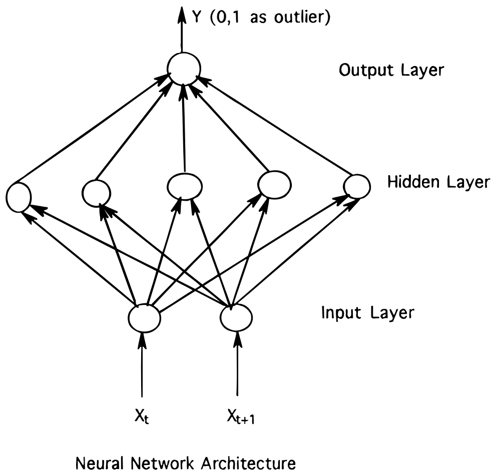

Figure 1.

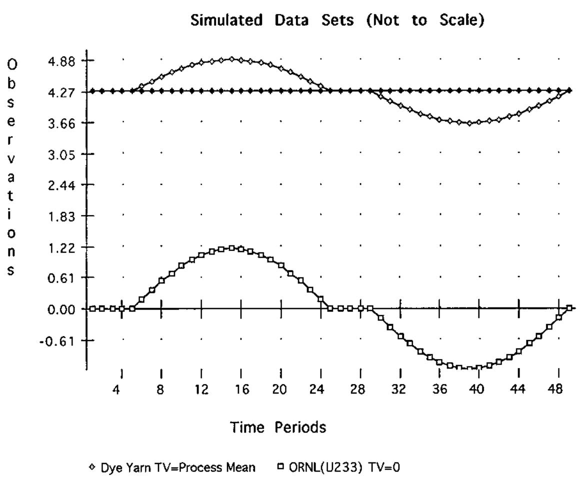

Figure 2.

advantages, there are other major reasons for using neural networks in process control. For example, a process expert is not necessary. The algorithm learns a process on its own. The approach works with any product. It anticipates process disturbances. Finally, it solves difficult problems in less time. Thus, the neural network's ability to respond to process changes satisfies the goal of obtaining faster and more complete solutions to process problems.

The neural network algorithm used in this study was developed by J. Denton.[12] The program formulates a set of network weights using standard back propagation training or nonlinear optimization algorithms and line searches in conjunction with backward error propagation. The algorithm requires various parameters to be established like the number of input nodes, output nodes, hidden nodes, and training and testing tolerances, etc.

For this paper, a particular neural network architecture was selected to satisfy the two criteria of time period shifts and proper number of hidden nodes. Thus, the network architecture used consisted of two input nodes, one output node, and five hidden nodes. The two nodes in the input layer were chosen because the vast majority of known data sets for this problem are AR(1), thus making the use of x_t and x_{t+1} for the two input nodes reasonable. The five hidden nodes were chosen based on the "$2n+1$ rule".[27] With this type of a network architecture (see Figure 1) a thorough analysis could be accomplished and firm conclusions drawn.

In performing the training phase, the neural network is presented a data set with various process disturbance points to achieve a particular outcome. This training is important because it sets up the neural network to look at streams of data coming from an actual process and identifying process disturbances early enough to prevent a problem from occurring and in turn reducing false alarms. The data set presented to the neural network is defined as the training data set and is composed of column vectors with the first two columns being the input data and the third column being the output data (see Appendix for details). Each output data point is a zero if that data point is within the control limits and a one if that data point is outside the control limits. However, a problem could arise with using actual data sets in two ways. First, the actual data set may not have enough data points for both the training and the testing of a neural network. Second, the actual data set may possibly not have any process disturbance points (i.e., outliers) for the proper training of the neural network. Therefore, a method that would provide a training data set based on actual data from a production process and one that is sure to contain all needed examples of process problems would be of great benefit to the statistical process control industry for use in applying neural networks. In response to this idea, we have developed such an approach based on simulation, which is described in the appendix. The basic idea behind the simulation is that control process data sets do not always contain outliers (i.e., out-of-control points). However, the purpose of the training phase is to train the neural network to detect outliers. Thus we use a simulation based on real control process data to generate an appropriate training data set containing outliers.

The neural network computer program provides various outputs such as the final weights of the training phase and the results of the training and testing phases. The results of the neural network computer program applied to the data sets in this study can be seen in the various Tables. Again, it must be stressed that due to the importance of not overlooking an outlier, as in the case of production processes, management must be willing to tolerate a certain frequency of false alarms. Thus a questionable outlier can serve as an early warning signal that the production process might be deteriorating. Management is then able to be more aware of a potential abnormal situation, and the operator can examine the critical points in the process, look for leaks, and monitor the process more closely.

D. COMPARING THE VARIOUS METHODS FOR OUTLIER DETECTION BASED ON DATA SETS WITH KNOWN DIVERSIONS

To accomplish a more decisive comparison, nuclear material balance data sets with known outliers (i.e., removals) were used. These data sets were taken from actual nuclear inventories known to have protracted removals of nuclear material. To illustrate the capabilities of the neural network approach, two particular cases of nuclear material removal have been selected. Each case will be discussed briefly. A discussion of the testing of various methods on the data set from each case will be presented in the next section.

In 1980, at the AGNS Barnwell Nuclear Fuels Plant[11] a series of experiments were performed in order to improve the detection of nuclear material losses or diversions in the

Table 1. Location and Timing of the Removals

experiment	location	start time/date	end time/day	total removal vol. (L)	total removal U. (kg)	OBS.
minirun 3C		0815/07/18	1204/07/21			
	pulse col. (2AP)	1645/07/18	0845/07/19	96	4.224	8−24
	pulse col. (3AP)	1645/07/18	1645/07/19	96	4.253	8−32
	surge tk. (1BP)	1615/07/18	0850/07/21	96	5.722	56−72
	"U" settled on bottom of acid concentrators = 120 kg					
minirun 5B		1600/11/18	1630/11/21			
	surge tk. (1BP)	0000/11/19	1200/11/19	174	10.2	9−20
	surge tk. (1BP)	1445/11/19	0115/11/20	177.2	11.1	23−34

different unit process accounting areas (UPAA). The material balance data were recorded periodically on a near-real-time basis with the aid of a computerized nuclear materials control and accounting system.

The experiments involved the physical removal of nuclear material in different forms from a Plutonium Purification Process (PPP). Also, location of removals, time, quantity, concentration, and type of diversion were noted. These experiments dealt with the second and the third plutonium cycles that use natural uranium solutions. The original researchers called these experiments "miniruns".

In 1977, the Energy Research and Development Administration issued a report titled "Report on Strategic Special Nuclear Material Inventory Differences".[10] In this report, data were presented on inventory differences for plutonium, enriched uranium, U-233, and Pu-238 from 1949 to 1976 from various sites. These sites included Los Alamos Scientific Laboratory (LASL), Oak Ridge National Laboratory (ORNL), Richland Hanford, and Savannah River. The Nuclear Regulatory Commission (NRC) has the responsibility for checking on nuclear material stored at their facilities. Thus, when the nuclear material inventory at a facility has a change, the NRC must investigate to determine the type of change. A negative change corresponds to possible losses or thefts, while a positive change corresponds to a gain. This pattern is the reverse of the MUF direction. This data was initially used by Chernick et al.[10] in their study of nuclear material safeguards.

We first consider miniruns 3C and 5B of the AGNS study. Table 1 presents the location and timing of removals for the two minirun data sets. The total protracted removal across the extended time period by volume of solution and the corresponding uranium content is recorded in column 5.

We also considered four of the seven nuclear material inventory differences (data sets) from Chernick et al.[10] These data sets were chosen at random and include U-233 from LASL, U-233 from Richland, U-233 from ORNL, and Pu-238 from the Savannah River. Even though the data of the material balances presented are on an annual basis, it is still useful for testing the neural network algorithm and comparing it to other algorithms. However, due to the time period, a host of assignable causes are possible and consequently timely corrective actions are precluded except for after the most recent observation. In the article, Chernick et al.[10] used the Influence Function Matrix approach to detect outliers in the nuclear material balance.

We will compare various methods on the tabulated results of these data sets for their ability to detect outliers but also to reduce false alarms. We are primarily comparing the neural network approach with the simulation enhancement against other approaches developed by our research group. Previous publications show that these methods are as good or better than those currently in use.[29−35] The analysis will be based on the following notation:

TOI = total outliers identified

T+OI = total positive outliers identified

NA+I = number of actual positive outliers identified

NFA = number of false alarms

N+OM = number of positive outliers missed

The most crucial analysis will be based on the detection of outliers as early as possible within the protracted period of removals. Due to the fact that the data is in MUF form, positive outliers will be of particular interest because they indicate a removal or loss.

E. TESTING THE VARIOUS METHODS FOR OUTLIER DETECTION BASED ON DATA SETS WITH KNOWN DIVERSIONS

Minirun 3C. Tables 1 and 2 show that there are three protracted removals from three locations in this experiment, two of which are in part simultaneous: 0.4186 Kg/h during observations 8−24; 0.1701 Kg/h during observations 25−32; and 0.3366 Kg/h during observations 56−72. The 120 Kg that settled out in the concentrators averages to 1.58 Kg/h. Over the entire period, the separated solids (120 Kg) and the amount removed (14.199 Kg) or 134.2 Kg should be an average for the material unaccounted for (MUF) of 1.77 Kg/h over the 76 observations.

Neural network (1.1 SD, see Appendix for definitions), data bounding and polynomial smoothing detected the very first observation (no. 8) in the initial protracted removal period. The joint estimation procedure and neural network (2.5 SD) missed the first observation but did detect no. 10, the negative observation. The joint estimation procedure detected the first positive protracted removal at no. 14, while the neural network (2.5 SD) detected it at no. 61. The neural network (1.1 SD) not only had the highest percentage of actual positive outliers identified but also had the highest percentage of false alarms. CUSUM missed the initial protracted removal period completely but did very well on the final protracted removal period.

Ideally, any comparison of results among different methods should be established upon equal attributes. However, the proposed methods do not have easily comparable attributes. Each method requires a different number of sensitivity constants. Even though the different methods are not exactly comparable, the comparisons done give a reasonable idea of their relative performances.

Minirun 5B. This run has two protracted removal periods with only a two hour interruption separating them, as can

Table 2. Minirun 3C-UPAA PPP(2AP, 3AP, 1BP) Detection of Outliers among Uranium Inventory Differences (MUF) − AGNS Barnwell Nuclear Fuels Plant[a−c]

time period	MUF	DB 1.1SD ref 35	poly smooth 1.1SD ref 35	joint estim ref 35	CUSUM ref 35	NN 2.5SD	NN 1.1SD	assigned cause
4	−6.5	*	*				*	none/unknown
8	5.5	*	*				*	protracted
10	−8.0	*	*	*		*	*	removal
13	1.8							0.4186 Kg/h
14	4.7			*			*	OBS. 8−24
								17 periods
15	4.4							17 periods
16	6.2							17 periods
17	2.8							17 periods
18	5.2						*	17 periods
19	6.7	*	*				*	17 periods
20	3.1							17 periods
22	1.1							17 periods
23	3.1							17 periods
24	1.3							17 periods
25	5.3	*	*				*	protracted
26	0.3							removal
29	−7.8	*	*	*			*	0.1701 Kg/h
30	0.3							OBS. 25−32
31	1.9							8 periods
37	5.4	*	*				*	none/unknown
39	7.2	*	*	*			*	none/unknown
42	6.6	*	*				*	none/unknown
45	7.0			*			*	none/unknown
56	0.45							protracted
58	−5.0	*					*	removal
59	3.0							0.3366Kg/h
								OBS. 56−72
60	1.8							17 periods
61	15.1	*+	*+	*	*	*	*	17 periods
62	−5.2	*	*				*	17 periods
63	3.6				*			17 periods
64	2.4				*			17 periods
65	3.6				*			17 periods
66	−1.0				*			17 periods
67	1.4				*			17 periods
68	1.6				*			17 periods
69	−2.3				*			17 periods
70	0.0				*			17 periods
71	0.7				*			17 periods
72	−40.0	*+	*+	*	*	*	*	17 periods
74	−5.2			*			*	none/unknown
total (TOI)		13	12	8	11	3	17	
total (T+OI)		7	7	4	7	1	10	
actual (NA+I)		4(15.4%)	4(15.4%)	2(7.7%)	7(26.9%)	1(3.8%)	6(23.1%)	
false (N+FA)		3(14.3%)	3(14.3%)	2(9.5%)	0	0	4(19%)	
missed (N+OM)		22	22	24	19	25	20	

[a] * = detection of outlier; *+ = detection of outlier beyond TV ± 3(MSD) for data bounding or polynomial smoothing; total number of data points = 76; min. value = −40 Kg, max. value = 15.1 Kg, target value(TV) = 0; total no. of observations during removal periods = 42; total no. of observations during nonremoval periods = 34; no. of + observations during removal periods = 26(61.9%); no. of + observations during nonremoval periods = 21(61.8%); amount of uranium that settled out = 120 Kg or 1.6 Kg/h. [b] Data bounding and polynomial smoothing: modified process average = 1.145; modified standard deviation = ±3.571 with %drop = 5%(4); median = 1.65. [c] Neural networks: weighted process mean = 1.616; SD = ±3.855.

be seen in Tables 1 and 3. Both protracted removals are from the surge tank (1BP): 10.2 Kg (0.850 Kg/h) during observations 9−20, and 11.1 Kg (0.925 Kg/h) during observations 23−34. The protracted removal periods had proportionally less positive MUF's then the nonremoval periods, making it very difficult to detect true losses while minimizing false alarms.

The neural network algorithms (2.5 SD) and (0.9 SD) (for definitions see the Appendix) immediately detected a negative outlier at point no. 1 while data bounding and polynomial smoothing detected a negative outlier at point no. 9. None of these methods detected a positive outlier until observations no. 17 and no. 18. The joint estimation procedure only detected negative outliers at observations no. 19 and no. 20.[30] This result could have occurred because the sensitivity constants may not be comparable to the other methods. All five methods failed to detect any loss in the second removal period (nos. 23−34) until observation no. 33. Again, CUSUM was not useful since it detected 56 consecutive outliers from observations nos. 3-58, well before and past the removal periods.

Chernick et al. Data Sets. In examining the comparison results presented in Tables 4−7, it can be seen that the neural network approach did detect the same outliers as the influence function matrix approach. However, the neural network approach in Tables 4−6 also detected additional

Table 3. Minirun 5B-UPAA PPP(1BP) Detection of Outliers among Uranium Inventory Differences (MUF) − AGNS Barnwell Nuclear Fuels Plant[a−c]

time period	MUF	DB 0.9SD ref 35	poly smooth 0.9SD ref 35	joint estim ref 35	CUSUM ref 35	NN 2.5SD	NN 0.9SD	assigned cause
1	−1.5					*	*	none/unknown
2	−1.7					*	*	none/unkonwn
3	−2.8	*+	*+		*	*	*	none/unknown
4	−1.8	*			*	*	*	none/unknown
9	−1.1	*	*		*	*	*	protracted
13	0.05				*			removal
14	0.18				*			0.850 Kg/h
15	0.1				*			OBS. 9−20
16	0.3				*			OBS. 9−20
17	0.75	*			*		*	OBS. 9−20
18	0.95	*	*		*		*	OBS. 9−20
19	−0.35			*	*			OBS. 9−20
20	−1.3	*	*	*	*	*	*	OBS. 9−20
30	0.15				*			protracted
31	0.2				*			removal
33	0.8	*	*	*	*		*	0.925 Kg/h
								OBS. 23−34
43	1.0	*			*		*	none/unknown
48	0.85	*			*		*	none/unknown
49	1.3	*			*	*	*	none/unknown
58	0.5						*	none/unknown
total (TOI)		10	5	3	56	7	13	
total (T+OI)		6	2	1	28	1	7	
actual (NA+I)		3(33.3%)	2(22.2%)	1(11%)	9(100%)	0	3(33.3%)	
false (N+FA)		3(11.5%)	0	0	19(73.1%)	1(3.8%)	4(15.4%)	
missed (N+OM)		6	7	8	0	9	6	

[a] * = detection of outlier; *+ = detection of outlier beyond TV ± 3(MSD) for data bounding or polynomial smoothing; total number of data points = 68; min. value = −2.8 Kg, max. value = 1.3 Kg, target value(TV) = 0; total no. of observations during removal periods = 24; total no. of observations during nonremoval periods = 44; no. of + observations during removal periods = 9(37.5%); no. of + observations during nonremoval periods = 26(59.1%). [b] Data bounding and polynomial smoothing: modified process average = 0.04; modified standard deviation = ± 0.613 with %drop = 2%(2); median = 0.075. [c] Neural networks: weighted process mean = 0.036; SD = ±0.482.

Table 4. Detection of Outliers in LASL U-233 Material Balances[a]

period	MB	influence function matrix ref 10	neural network 1.5 SD
1952	0.0		
1953	−5.7		
1954	−8.1	*	*
1955	−0.4		
1956	0.9		
1957	−3.6		
1958	−9.3	*	*
1959	−2.1		
1960	−4.9		
1961	−3.1		
1962	−6.8		*
1963	−1.5		
1967	−1.0		
1968	3.2		*
1969	0.2		
1970	1.9		
1971	−0.1		
1972	6.1	*	*
1973	−1.3		
total(TOI)		3	5

[a] * = detection of outlier; total number of data points = 29; min. value = −9.3, max. value = 6.1, target value = process mean; weighted process mean = −2.008; standard deviation = 2.817.

Table 5. Detection of Outliers in Richland U-233 Material Balances[a]

period	MB	influence function matrix ref 10	neural network 1.5 SD
1958	−86.4		
1959	−90.1		
1960	−143.7	*	*
1961	−169.2	*	*
1962	−106.8		*
1963	−66.9		
1964	−94.9	*	
1965	−118.8	*	*
1966	17.2		
1967	−1.5		
1968	−32.0		
1969	62.9		*
1970	−9.0		
total(TOI)		4	5

[a] * = detection of outliers; total number of data points = 29; min. value = −169.2, max. value = 62.9, target value = process mean; weighted process mean = −35.495; standard deviation = 36.620.

outliers, and this difference in number could be related to different sensitivity constants and quantifiable attributes used by each method. Even with this possible difference between methods, there are certain observations that can be made. In Table 4, the two additional points detected by the neural network approach could be indicating additional outlying points that are an indication of a problem in the material balance at LASL. In Table 5, the influence function matrix approach indicates period 1964 (−94.9) as an outlier and 1962 (−106.8) as a point within the control limits. However, the neural network approach detected the points in just the opposite way. The most significant observation to be made concerns Table 6. Here the authors state, “Year 77 is worth noting because it illustrates the outlier being detected at the time of occurrence”. Therefore, with the neural network approach’s ability to detect the last observation (1977) as an outlier, it demonstrated its capabilities for use in real-time on-line process control.

Table 6. Detection of Outliers in ORNL U-233 Material Balances[a]

period	MB	influence function matrix ref 10	neural network 1.5 SD
1957	0.1		
1958	−0.8		*
1959	−1.4	*	*
1960	−0.05		
1963	−0.1		
1964	−0.9		*
1965	−0.6		*
1966	0.3		
1976	−0.05		
1977	−3.3	*	*
total(TOI)		2	5

[a] * = detection of outlier; total number of data points = 26; min. value = −3.3, max. value = 0.3, target value = 0; weighted process mean = −0.221; standard deviation = 0.297.

Table 7. Detection of Outliers in Savannah PU-238 Material Balances[a]

period	MB	influence function matrix ref 10	neural network 1.5 SD
1969	−1.7		
1970	−19.6	*	*
1971	−2.9		
total(TOI)	−2.9		

[a] * = detection of outlier; total number of data points = 19; min. value = −19.6, max. value = 2.1, target value = 0; weighted process mean = −0.576; standard deviation = 2.076.

Table 8.

column 1	column 2	column 3
X_t	X_{t+1}	
X_{t+1}	X_{t+2}	
X_{t+2}	X_{t+3}	
X_{t+3}	X_{t+4}	
etc.	etc.	

Analysis. The outliers in the minirun data sets were difficult to identify because each removal per period was minute and generally did not exceed the normal in-control fluctuations. In fact, the removals were within the (0.2 SD) of the target value. The percentages of positive material unaccounted for (MUF) observations during the removal and nonremoval periods are similar, making it difficult to detect losses. In minirun 3C (Table 2), for example, little difference can be seen between removal and nonremoval periods. Then too, in minirun 5B, there is a greater frequency of positive MUF's during the removal periods.

Even though the five methods adapt to process change as though it were a new process, the joint estimation procedure does this to a greater extent. Thus, the joint estimation procedure will detect only the first outlier during a protracted removal period. Then, when the process reverts back to its normal state, it may also detect that change as an outlier. Finally, the joint estimation procedure did have a lower incidence of false alarms.

Precipitated Solids. In minirun 3C, outlier detection was further hampered by 120 Kg of uranium solids settling to the bottom of the concentrators. If this process was in a steady state condition or at equilibrium, the precipitation of solids would have been no problem. However, new material was constantly entering the process. Since these solids apparently were not considered in the nuclear inventories, both positive and negative MUF's would be recorded. However, it is assumed that the original researchers conducted the experiments properly and removed the solids from the concentrators before the beginning of each run. Nevertheless, there is no way of knowing at what rate the particles settled out. If the rate was constant, then the uranium precipitated out of solution at a rate of 1.58 Kg/h for one period in minirun 3C. This precipitation exceeded the rate of the protracted removals which ranged from 0.170 Kg/h to 0.735 Kg/h which certainly complicates outlier detection.

Doubt continues to exist as to whether an identified outlier represents a loss (removal) or simply solids that have precipitated out of the solution. Thus, a number of the false alarms could be expected. However, the methods should be able to adapt to the settled precipitation of solids if the rate of precipitation is a relatively constant part of the process.

Again, all of the methods had difficulties in detecting all of the known outliers. However, in comparison to other methods, neural networks did quite well, though care must be exercised because of the different sensitivity constants that each method uses. Finally, the joint estimation procedure is more adaptable to detecting the first outlier of an adverse process change because it is adapting to what is essentially a new process.

F. DISCUSSION

A drawback of some methods is in the fact that neither neural network, data bounding, nor polynomial smoothing as discussed in this paper can identify the outlier type directly. On the other hand, the joint estimation procedure, utilizing complex statistical mathematics and mathematically modeling the process, can identify the type of outlier. However, we believe that the neural network method could be trained to identify the type of outlier by the use of a simulated training data set incorporating the mathematical formula for each type of outlier. We are currently developing such an approach.

In process control, especially in dealing with nuclear material, we believe that both primary and secondary control procedures should be in place. The primary control procedure could be either a neural network, joint estimation, or polynomial smoothing which would have the main responsibility of controlling the process. The secondary control procedure could be one of the procedures just mentioned, CUSUM, traditional Control Charts, or other nuclear material accounting procedures. The secondary control method would function either as a backup in case of a failure of the primary control procedure or a verification of the primary control procedure. The various methods should be examined for use in a particular process prior to complete implementation.

The neural network approach, as the primary control method, can be trained, possibly with the use of simulation, to adjust to an out-of-control situation, especially in the case of consecutive outliers, as though they represent a new process or process adjustment. However, when the primary method is the joint estimation approach, it will usually only detect the beginning of a protracted removal or leakage situation. When the leakage stops and the process is brought back into control there is another process change back to the original condition. Therefore, the next point may appear as an outlier to the primary control method. Since the outliers during the adverse process change period may have gone undetected if the Joint Estimation is monitoring the new out-of-control process, the secondary control method is indispensable to keep beta (probability of a type II error) low.

Real-Time On-Line Process Control Capability. The results from the methods presented in this paper may lead the reader to conclude that the methods may only apply to retrospective control. However, these algorithms are capable of handling end points. Further, they can also apply to real-time on-line process control. Tables 2, 3, and 6 demonstrate that any outlier identified would have been detected by the neural network method if it were a final point. All identified outliers with assigned causes, except for possibly two exceptions, could be considered final points and thus a test could be conducted.

If an outlier is found by both the primary and secondary control methods, the practitioner can feel more assured that the process disturbance point is indeed an outlier and not a false alarm. Thus using the simulated data set for training a neural network to accurately pinpoint the outlier would eliminate some of the false alarms.

Any of the previous methods may confirm the indications of the neural network or vice versa to minimize alpha (the probability of a type I error) when a false alarm could have a major economical impact. Similarly, a second method, whether it be a neural network or not, could be used as a means of outlier detection to minimize beta (probability of type II error) if the economical impact of overlooking an outlier is crucial. By using a secondary confirmation method to detect outliers, the process control operator has at hand a large amount of information on a pending process disturbance. Therefore, future research will be required to verify the aforementioned statements.

Summary. The methods presented in this paper are effective across diverse applications. The neural network approach is particularly useful in the case of autocorrelated data. It can handle severely abnormal distribution situations which are due to the presence of many outliers. Further, the neural network approach is enhanced by the simulation computer program in the detection of outliers and the reduction of false alarms.

Neural networks have certain advantages that the other techniques do not. First, a process expert is not necessary for the neural network to function. However, someone knowledgeable about the process should of course check the neural network's results. Second, the network learns about the current process on its own; as well as making adjustments in its learning to account for process changes. Third, an overall knowledge of mathematical or scientific theory is not important for daily application of the neural network. Fourth, the type of product has no impact on the neural network performance because the network is directly controlling the process, and thereby indirectly maintaining the product quality. Fifth, the network lessens the possibility of human error because there is no necessary intervention or interaction by a person if a feedback loop is constructed. Sixth, it anticipates the abnormalities in order to correct for them within the process because it has the ability to learn and adjust to process changes without outside interference. Seventh, it removes the need for trial and error in establishing the optimum control for the process because it learns the information from the process itself.[4] In general, neural networks have been seen to be able to solve the more difficult problems in less time than other conventional methods.[14]

The simulation computer program provides important features in developing a training data set for a neural network. First, the amount of actual data required for both training and testing is not important because the simulated data set can be used strictly for testing. Second, the target value selection of the robust process mean or zero is easily entered. Third, the control limits for in-control versus out-of-control data points are calculated by the program. Fourth, the functional curve can be changed depending on the researcher's requirements. Fifth, the program has the potential of incorporating formulas for detecting particular outlier types. This is currently under test. Sixth, the program does calculate its own robust process mean and robust standard deviation for the actual data set. Overall, the simulation computer program provides a researcher with flexibility in developing a training data set for a neural network based on the researcher's needs.

It cannot be overly stressed that the most important feature of these methods which have been presented is the ability to identify outliers well within the usual three standard deviations from a target value. They are a favorable addition to those methods already available to the process control industry involved in nuclear material safeguards.

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APPENDIX: THE SIMULATION APPROACH TO TRAINING THE NEURAL NETWORK

The simulation computer program begins by reading two files. One file contains the total number of data points, the multiplying factor of the robust standard deviation based on the desired control limits for the process and the selected control method's sensitivity (e.g., 2.5 (robust standard deviation)), and the indication of the target value (zero or the robust process mean). The robust process mean and robust standard deviation are described below. The target value or center line represents the average level or value for the production process from which the control limits are calculated (e.g., target value ± 2.5 (robust standard deviation)). The second file is the complete data set. After reading these two files, the computer program then splits the data set into two (2) groups, A and B. A contains the first 80% of the observations and B contains the remaining 20%. Other splits are of course possible. A robust process mean and robust standard deviation were computed from the A set as described in ref 7. These two values are used as the basis for developing our simulated training data set.

After calculating the robust process mean and the robust standard deviation, the simulated data set can be developed by the computer program. The simulated data set is created by using the sine function (i.e., to generate both $+$ and $-$ outliers). The sine function provides a means to provide outlying data points and balance them above and below the target value as depicted in Figure 2. First, the maximum plus and minus variation about the robust process mean or target value is established. These values are calculated by multiplying the robust standard deviation by four. This multiplying factor of four was selected because a data point located within three standard deviations is considered an in-control point. Thus, by using a value of four we insure that there will be simulated outliers to train on in our new simulated data set. Now, the simulation program can start to create the simulated training data set. The simulated data set is divided into 60 individual time periods. The simulated data set could be divided into any number of individual time periods depending on the application. We felt that 60 individual periods were reasonable for a sine function with our data sets. For the first nine time periods, the data points for the simulated data set are equal to the robust process mean. Next, for the periods 10−30, the data points for the simulated data set are calculated using the upper half of the sine function from zero to π. The result from calculating the sine function for each period of time is multiplied by the maximum plus limit of four times the robust standard deviation. The resultant value is added to the robust process mean to generate + outliers. For the periods 31−39, the data points for the simulated data set are again equal to the robust process mean. Finally, for the periods 40−60, the lower half of the sine function from $\pi-2\pi$ is used to calculate a value for each period of time. This resultant value is multiplied by the minimum negative limit of four times the robust standard deviation and then added to the robust process mean to get the final data points (the lower outliers) for the simulated data set.

With the simulated data set complete and if the target value is selected at zero, the robust process mean will be subtracted from each simulated data point forming a new simulated data set. However, if the target value is to be the robust process mean, the formulated simulated data set will not be altered (see Figure 2). The sine function was selected in order to assure that outliers would be in the training data set. We are currently developing methods to completely simulate different outlier types using this approach. Hopefully then the simulation computer program will have the potential of incorporating the equations for the outlier types as described by Thome[37] and Chen et al.[42] and, in turn, training the neural network to identify any particular type of outlier. This will allow the analyst to be sure that he/she can detect any expected process problem type. Finally, the training data set for our program is organized from the simulated data set by three column vectors. The first two columns are the input data for training and the third column vector is the output data for training. The first column contains the simulated data set. The second column is the simulated data set points but shifted forward one observation to account for a time period change. Thus, if we call the simulated data X, we have the situation as shown in Table 8. In Table 8, column three is the output data for training which contains a zero for a point inside the established control limits and a one for a point outside the established control limits (an outlier). Thus, the training data set will contain outliers. The test data column vectors are formed in the same way using the test data sets (A Union B) except that column three initially contains all zeros. As the algorithm discovers outliers those observations are changed to ones and thus the outliers are identified. The reason that the form of the first two vectors in Table 8 was used is that the vast majority of real data we have worked with are AR(1) and therefore a one period lag is appropriate. We started the subscripts at t rather than zero to indicate that we can start this procedure anywhere in the series.

Now, at this point we have three data sets per application, simulated, A, and B. We train on the simulated data set and test on the union of A and B. Notice that we are not using the A set as the training data set (we only use its robust process mean and robust standard deviation to develop the simulated training data set). Thus, we are not training and testing on the same data set.

In order to actually run the neural network algorithm, we do the following. First, the neural network computer program requires that a definition file be created. This file specifies training parameters, instructions for node connections, and/or output control information. It further contains the specified neural network architecture, (In this case it is two input nodes, one output node, and five hidden nodes.) the tolerance for training and testing phases, and the number of test sets. The computer program does contain default values from unspecified parameters. When the computer program is initiated, the program reads the definition file, makes sure there is a training set and the correct number of test sets. Further it establishes the initial neural network weights using a default seed parameter provided by the computer clock to start randomly generating these weights via a uniform distribution centered at zero. The seed parameter is a unique value for each run unless fixed in the definition file because the seed parameter selection is important in the successful training of a neural network and its repeatability.

Using this approach, we are able to develop a complete training set of data containing outliers, even if all the process data available is in control.

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