INEEL/CON-98-00692
CONF-980733--

EXPERT SYSTEM TECHNOLOGY FOR NONDESTRUCTIVE WASTE ASSAY

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ABSTRACT
Nondestructive assay waste characterization data generated for use in the National TRU Program must be of known and demonstrable quality. Each measurement is required to receive an independent technical review by a qualified expert. An expert system prototype has been developed to automate waste NDA data review of a passive/active neutron drum counter system. The expert system is designed to yield a confidence rating regarding measurement validity. Expert system rules are derived from data in a process involving data clustering, fuzzy logic, and genetic algorithms. Expert system performance is assessed against confidence assignments elicited from waste NDA domain experts. Performance levels varied for the active, passive shielded, and passive system assay modes of the drum counter system, ranging from 78% to 94% correct classifications.

INTRODUCTION
Management of U. S. Department of Energy (DOE) defense generated containerized transuranic (TRU) waste requires determination of the entrained TRU mass and associated parameters. Nondestructive assay (NDA) techniques are the most common and efficient means to determine the TRU material quantity. Quality assurance objectives (QAOs) for NDA techniques used to characterize TRU waste destined for the Waste Isolation Pilot Plant are delineated in the National TRU Program Transuranic Waste Characterization Quality Assurance Program Plan (QAPP) [1].

Technically justifying compliance with applicable requirements and QAOs for TRU waste forms in the DOE inventory can be a complex process. Some waste form configurations manifest NDA system response complexities that diminish the ability to clearly establish compliance. Such complexities lead to the requirement that technical reviews be performed at the data generation level for each assay to ensure operational boundaries are maintained relative to QAPP requirements.

Technical review of waste NDA measurement data, though warranted with respect to present day waste NDA system capabilities, is labor intensive. Hence it is desirable to have an automated system to perform the technical review. The automated system must be capable of providing a comprehensive waste assay data assessment, and must be reproducible, auditable and compatible with the overall throughput requirements of the waste characterization process. Therefore, an evaluation of expert system technology was undertaken.

EXPERT SYSTEM
The expert system design is predicated on the SWEPP Assay System (SAS) passive/active neutron counter operating principles. The means by which the SAS detects the presence of TRU materials, processes detected signals and reduces the information to a mass estimate defines the attainable performance and associated data validity. Hence, the SAS data input to the expert system must embed base SAS response to allow for proper data evaluation. The expert system described is an evaluation of the technology, and is not intended for deployment at this stage.

Knowledge represented in the expert system was derived using methods of automatic fuzzy rule generation from data[2, 3]. The automatic rule generation process is an instance of supervised learning; therefore, correctly classified input data elicited from NDA experts was required. The expert system input data is a set of figures of merit that a domain expert has deemed significant. This section first discusses selection of the expert system input variables. Classification of the training and testing data is then discussed. Finally, the expert system training algorithm is presented. The training algorithm is discussed in detail in [4]; modifications to the initial procedure are discussed in this paper.

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EXPERT SYSTEM INPUT VARIABLES

A number of signals from the SAS signal processing modules provide output carrying the response of the passive and active detection assemblies. These signals are combined into figures of merit that contain system response information. These figures of merit are the expert system input variables. A fuzzy rule set is then defined in terms of these input variables. A set of expert system input variables has been determined for each of the three SAS measurement modes: passive system, passive shielded and active, as listed in Table 1. Ranges that define regions of acceptable operation based on the physical design of the SAS neutron detection system can be specified for each input variable. These regions can be defined either by the functional limits of the detection system components or response perturbations from waste form parameters such as matrix density. The selected variables are not intended to be all inclusive, but a reasonable set containing sufficient SAS neutron response information to develop and analyze expert system utility for assay data assessments. In particular, gamma spectroscopy data was unavailable during initial testing.

Table 1
Expert System Input Variables

Input Variable	Derivation
Passive System Mode	
Passive System Total Rate	System Total Count/(10 kHz clock ticks/10000)
System Total/Gated Event Ratio	System Total/Long Gate System Events
Early Barrel/Cavity Count Ratio	Barrel Flux Monitor/Flux Monitor
Passive Shielded Mode	
Passive Shielded Total Rate	Shielded Total Count/(10 kHz clock ticks/10000)
Shielded Total/Gated Event Ratio	Shielded Total/Short Gate Shielded Events
Early Barrel/Cavity Count Ratio	Barrel Flux Monitor/Flux Monitor
Active Mode	
Early/Late Count Ratio	Shielded Counts/Shielded Bkg
Early Barrel/Cavity Count Ratio	Barrel Flux Monitor/Flux Monitor

The variables chosen to represent passive system neutron function are system total rate, system total/gated event ratio and active early barrel/cavity count ratio. The passive shielded input variables are analogous to the passive system variables except that shielded detector data are used. The system total rate is used to assess SAS function using the known count rate limitations of the detection and data acquisition system. Count rate limits may be defined that identify rates that are too low to provide statistically meaningful mass estimations and too high such that saturation of the coincidence circuitry occurs and dead-time corrections begin to have large uncertainties or are inapplicable.

The system total/gated event ratio is a convenient ratio for assessing the quality of the coincidence count measure. In general, above a certain value, this variable indicates that an (α,n) component of the emitted neutron spectrum is degrading the coincidence measure. Low values of this variable indicate high count rates beyond the capabilities of the coincidence counting circuitry and associated dead-time correction. Mid-range values of this variable generally indicate proper system function and provide substantive evidence of data integrity.

The third passive system variable is the active early gate barrel/cavity count ratio. This ratio carries information on the macroscopic neutron transport characteristics of the waste matrix. Low values of this ratio indicate either strong neutron absorption or high moderator matrix properties, or both. Medium values indicate somewhat better neutron transport in the matrix, and high values represent minimum neutron loss in the matrix. Hence, this ratio provides information on the ability of emitted neutrons to leak from the matrix and be detected.

The active mode input variables consist of the early/late count ratio and the early barrel/cavity count ratio. The early/late count ratio, for certain waste configurations, is a reasonable representation of neutron lifetime in the matrix. For all but matrices with high concentrations of moderating materials, a longer neutron lifetime generally indicates good active neutron interrogation. A high value of this ratio indicates a matrix composition that quickly absorbs the interrogating flux, and to a certain extent, lack of a strong (α,n) neutron component. Finally, the early barrel/cavity count ratio provides information regarding the neutronic characteristics of the matrix (i.e., scatterer or absorber). The higher the ratio, the greater the transport mean free path of the matrix, which in general means better interrogation of the matrix.

Each of the input variables described above carries some information regarding system response. No single variable is sufficient to characterize the performance of the system for a given waste container assay. The variables each contribute information on system function and must therefore be processed as a cohesive set. The selected input variables are a reasonable attempt to extract pertinent response information from the system to support an assessment of data validity. As the SAS does not provide unique response data that can be used to account for all possible interferences, the input variable set does not support a rigorous performance assessment over all possible waste configurations. If existing analytical methods were capable of this, it is expected that they would be incorporated into the algorithms of present day waste NDA systems.

TRAINING AND TEST SET CLASSIFICATION

A panel of three waste NDA experts was assembled and given a set of SAS generated waste assays to assign validity confidence ratings, on a scale from zero to ten. They rated their confidence in each of the three measurement modes of the system, for each assay. The set contained 99 assays evenly selected from the graphite, combustibles, and glass waste types. Disagreement existed between the experts as to the proper classification of each assay, due partly to differing internal scales of judgment used by each expert, and partly to uncertainty associated with the interpretation of NDA results. A normalization procedure was adopted to reduce the scaling bias of each expert. Assays with normalized scores that did not agree were removed from the test set.

The score sets for each confidence value were normalized as follows. The mean and standard deviation for each expert's score set, and for the total population were calculated. Each expert's score set was adjusted by scaling factors to have the mean and standard deviation of the total population. Where there was good agreement for each confidence value between all three experts the normalized confidence scores were considered reliable. Assays for which disagreement occurred were removed, yielding a total of 67 scored assays. Sixteen assays were used for training, and 51 for testing. The training sets were selected to represent the spectrum of confidence values.

AUTOMATIC RULE GENERATION ALGORITHM

Classified training data are viewed as input/output vectors in a hyperspace, the dimension of which is the sum of the number of input and output elements. A cluster of data points represents an approximate relationship from input to output, a relationship that can be represented as a rule. A parameter called the cluster radius, discussed below, determines how many clusters will be found. A fuzzy clustering algorithm is used in the current application, producing a set of fuzzy rules.

Fuzzy sets are used extensively in control, decision-support, and pattern recognition. Fuzzy sets represent classes of items that are separated by imprecise boundaries, such as "the set of tall men". Fuzzy sets are used in data clustering applications where the data do not necessarily form distinct clusters. Likewise, fuzzy rules are used in expert systems when distinct decision boundaries are not present. There are no hard or precise boundaries separating regions of acceptable and unacceptable performance of the SAS, therefore the use of fuzzy methods is justified. See Zadeh's seminal paper for information regarding fuzzy sets [6].

A genetic algorithm is used to determine the cluster radius. Genetic algorithms are a class of optimization techniques that are broadly applicable to many types of problems. Their usefulness derives from the fact that they do not rely on gradient information, but instead attempt to imitate the forces of natural selection in seeking out superior solutions to problems. When using genetic algorithms, a data structure ("chromosome") to represent the problem and an objective function that measures the performance level ("fitness") of a solution to the problem must be specified. The genetic algorithm generates and evaluates a large number of these data structures ("population") and employs the objective function to select superior solutions. The population of solutions is evolved by recombination of superior solutions in a manner that simulates the genetic processes of crossover and mutation. Detailed discussion of genetic algorithms is beyond the scope of this paper. Interested readers are referred to the classic text by Goldberg [7].

For n input elements in each datum, the generated fuzzy rules take the following form:

if (x_1 matches A_1) and ... (x_n matches A_n) then (y is B), where
- $x_1 \ldots x_n$ are normalized rule input values,
- $A_1 \ldots A_n$ are exponential membership functions,
- y is the rule output, and
- B is a symmetric membership function.

Using a standard method of defuzzification (the center of gravity algorithm), y is found from:

$y = \Sigma_{i=1}(\mu_i y_i^*)/\Sigma_{i=1}\mu_i$, i=1...l, where
y_i^* is a vector of output membership function centroids, and
$\mu(x_j) = \exp(-.5\ \Sigma\ ((x_j - x_j^*)/\ \sigma_j)^2)$, j=1...n.

The parameters x_j^*, y_i^* and σ_j are initialized using subtractive clustering[3], a fuzzy data clustering routine, and optimized in a procedure involving backpropagation [5] and genetic algorithms. See [4] for a more thorough discussion of the rule-generation procedure.

The cluster radius, and the learning rate and the convergence criteria from the backpropagation routine must be chosen. These parameters uniquely determine a solution, and are represented in the genetic algorithm as a real-valued array. Determination of the cluster radius sets the number of data clusters. Many cluster validity indices have been proposed to deal with this issue [8]. The Xie-Beni index [9], S_{XB}, has been proposed for evaluating the validity of fuzzy clusters. This index is the ratio of the compactness of the clusters (a measure of the variance of the data points from the centers of the data clusters) to the square of the minimum distance between the cluster centers. In general, small values of S_{XB} indicate well-formed data clusters, provided the number of clusters does not approach the number of data points in the training data. Therefore, S_{XB} may be used as a principle component of the objective function.

An objective function employing the information embodied in S_{XB} was sought. S_{XB} is small for low compactness and large minimum inter-cluster distance. Figure 1 defines S_{XB} and illustrates the remainder of the discussion in this paragraph. The compactness generally decreases with increased cluster number, whereas the minimum inter-cluster distance generally increases with decreased cluster number. Because S_{XB} measures two opposing trends, Pareto optimization [7] was employed on these two trends simultaneously. Pareto optimization ranks data into subsets of approximately equal worth with respect to multiple criteria. The criteria used were the reciprocal of the numerator of S_{XB}, and the denominator of S_{XB}. Maximizing these quantities tends to reduce S_{XB}. Pareto rankings were combined with S_{XB} in the objective function. The objective function is shown in Figure 1, and was designed such that maximizing the function resulted in small S_{XB}. As shown in the following section, this composite objective function resulted in calculations in which S_{XB} averaged over an entire generation of solutions converged on a low value. The solution from the convergence generation with the minimum S_{XB} was chosen as the solution to the problem.

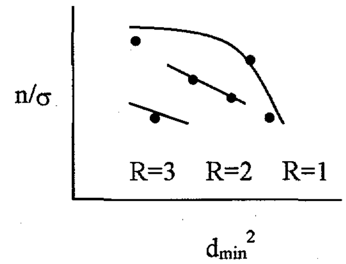
SYSTEM PERFORMANCE

Expert system performance for each measurement mode indicates the level of agreement between the manually classified test set and the classifications produced by the expert system. A simple function has been used to roll system performance into a single number:

performance = 4*number of data points in test set agreeing within 10% +
2* number of remaining data points agreeing within 25% +
1* number of remaining data points.

compactness
= variance/number of data points, σ/n

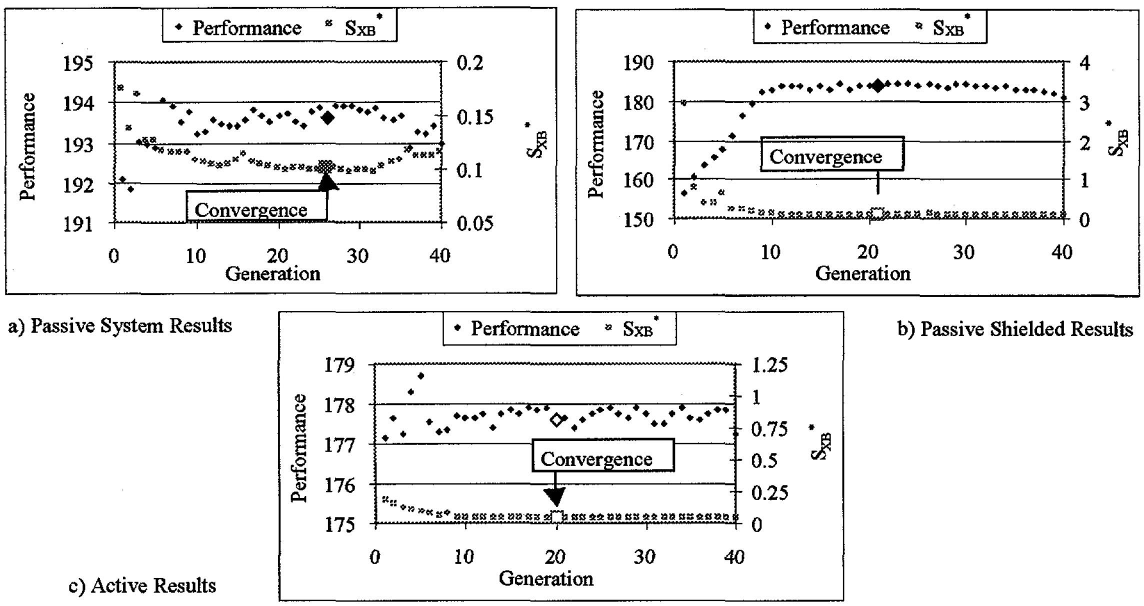
$S_{XB} = (\sigma/n)/d_{min}^2$, where
d_{min} = minimum inter-cluster distance



objective
= f(Pareto rank, S_{XB})
= f(R, S_{XB})
= Rmax – R + c ($1/S_{XB}$), where
c is a scaling constant.

Fig. 1 Definition of the Genetic Algorithm Objective Function

In words, points with a lesser degree of agreement receive less weight in the performance total. The performance of every solution produced during operation of the genetic algorithm was calculated and has been used to evaluate the quality of the final solution arrived at by the method described in the preceding section. Pareto optimization resulted in generations with steadily decreasing average S_{XB}, S_{XB}^*, as shown in Figure 2. It is also observed in the figure that the performance averaged over all solutions in a given generation tended to increase through the generations. The genetic algorithm is considered to have converged when the ratio of the current S_{XB}^*, to the ten-generation average of S_{XB}^* is less than 0.01. The point of convergence is indicated on each plot.



a) Passive System Results

b) Passive Shielded Results

c) Active Results

Fig. 2 Observed Trends in the Generation Average Performance and S_{XB}

Table 2 lists the average, maximum, and selected solution performance from the generation at which convergence occurred, for each measurement mode. It is observed that the selected solution (minimum S_{XB}) is the solution with maximum performance in two out of three cases, and a high performer in the remaining case. The Xie-Beni index and Pareto optimization combined produce a good objective function for guiding genetic algorithms to find well-formed clusters in subtractive data clustering. The expert system resulting from rules formed from this clustering procedure can achieve a high, if not optimal, level of performance.

CONCLUSIONS

An expert system was developed to operate on data acquired from a waste NDA system. The system performed well, especially considering that only partial waste NDA data was available for expert system processing (i.e. neutron data only). System performance was benchmarked against domain expert assessments of the quality of the test and training data.

Initial requirements on the function of the expert system have for the most part been demonstrated. These requirements include representation of domain expert NDA knowledge, and reasoning with supplied data and represented knowledge. At the present time there is ample indication that the expert system technique can be refined to accommodate the balance of available NDA data (e.g., gamma measurements), needed to make a comprehensive assessment of waste NDA data quality in accordance with the National TRU Program requirements.

The Xie-Beni index has been shown to be useful in determining the cluster radius used in subtractive clustering. The components of the index, the compactness of a set of fuzzy clusters and the square of the minimum distance between the centers of the fuzzy clusters, were used to perform Pareto optimization on the training data. The Pareto rankings determined in the optimization were then combined with the Xie-Beni index to obtain an objective function. This objective function was used by a genetic algorithm to determine the rule generation parameters of the subtractive clustering method. Three independent test sets were shown to be classified with 78% to 94% accuracy.

Table 2
Unique Values of S_{XB} and Performance at Convergence

	Passive System			Passive Shielded			Active		
Performance	**Perf.**	**S**	**% Correct**	**Perf.**	**S**	**% Correct**	**Perf.**	**S**	**% Correct**
Selected	194	0.095	94	184	0.101	80	178	0.046	78
Maximum	194	0.095	94	186	0.108	82	178	0.046	78
Average	193.6	0.101	--	184.0	0.116	--	177.6	0.047	--

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