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14. ABSTRACT
This was a short-term proof-of-concept project with the goal of demonstrating the feasibility of, and lay the theoretical foundations for, integration of predictive neural networks into Bayesian networks as a means of generating probability distribution functions and likelihood tables. The challenges were two-fold: first, developing a way to convert XY data output from an instrument to a probability density function using a neural network and secondly, fusing this and other types of sensor output into a single probabilistic evaluation of multiple sensor

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Final Report

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Report Title

Final Report: Technical Topic 3.2.2.d Bayesian and Non-parametric Statistics: Integration of Neural Networks with Bayesian Networks for Data Fusion and Predictive Modeling

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This was a short-term proof-of-concept project with the goal of demonstrating the feasibility of, and lay the theoretical foundations for, integration of predictive neural networks into Bayesian networks as a means of generating probability distribution functions and likelihood tables. The challenges were two-fold: first, developing a way to convert XY data output from an instrument to a probability density function using a neural network and secondly, fusing this and other types of sensor output into a single probabilistic evaluation of multiple sensor outputs. Ultimately, this would be useful in application such as networked sensor arrays such as might be deployed to detect chemical agents in a subway system for example. Figures 1-4 lay out the approach proposed.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received   Paper

TOTAL:

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received   Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received   Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received   Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received   Paper

TOTAL:

Number of Manuscripts:

Books

Received   Book

TOTAL:

<u>Received</u>　　　<u>Book Chapter</u>

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
New Entry	0.00	
Andrew Jefferson	0.13	
FTE Equivalent:	**0.13**	
Total Number:	**2**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics
This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME   PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

See attached.

Technology Transfer

N/A

Final Report:
STIR: Integration of Neural Networks with Bayesian Networks for Data Fusion and Predictive Modeling
Dr. Suzanne Bell, West Virginia University

1. Basis of the Project

        This was a short-term proof-of-concept project with the goal of demonstrating the feasibility of, and lay the theoretical foundations for, integration of predictive neural networks into Bayesian networks as a means of generating probability distribution functions and likelihood tables. The challenges were two-fold: first, developing a way to convert XY data output from an instrument to a probability density function using a neural network and secondly, fusing this and other types of sensor output into a single probabilistic evaluation of multiple sensor outputs. Ultimately, this would be useful in application such as networked sensor arrays such as might be deployed to detect chemical agents in a subway system for example. Figures 1-4 lay out the approach proposed.

Figure 1: Conversion of sensor outputs to probability density functions

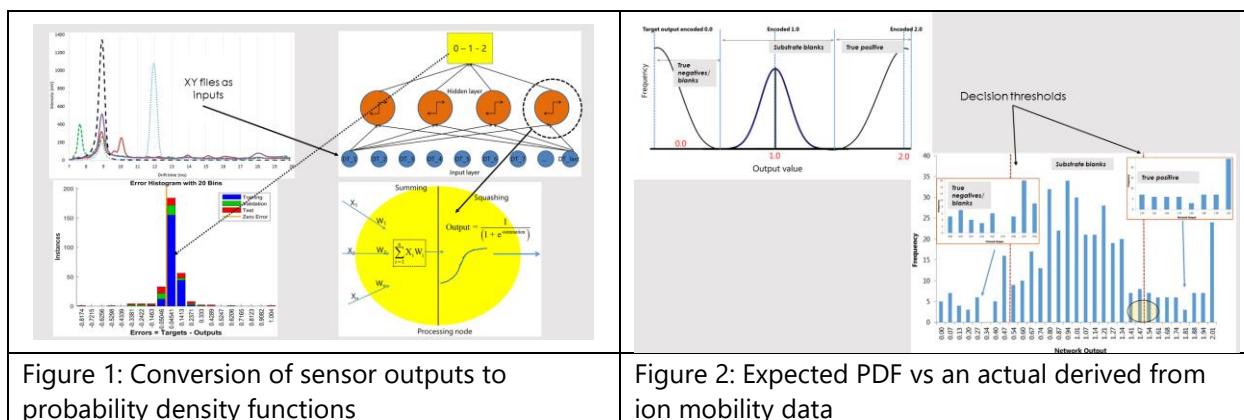Figure 2: Expected PDF vs an actual derived from ion mobility data

        Figure 1 illustrates how a neural network model is exploited to convert a database of spectra (as XY files) into a probability density function. Spectra are obtained across a variety of conditions, concentrations, and substrates to capture the variation expected in a realistic deployment; not all spectra associated with a given target compound will be identical. However, since all are obtained under controlled conditions, all can be assigned to a desired output. For example, the analyte TNT would be associated with dozens of spectra obtained from TNT placed on different substrates at different concentrations and at different times. Thus, the model, which is based on supervised learning, would be trained to produce the same output for all of these samples. For example, if all TNT spectra are assigned a desired output value of 1.0, it is expected that when the model is applied to these spectra, there will be a central tendency for output values around 1.0. If the training set is properly designed and the data space is sampled adequately, it is reasonable to convert a histogram of outputs into a PDF. Figure 2 shows

an example of a case in which a network has been trained to differentiate three types of spectral data: those associated with laboratory blanks (output of 0.0), matrix blanks (on substrates, 1.0), and true positives. The upper left is the hypothesized distribution and the lower right is the actual. The goal of the project was to generate data sets such as this for a set of 10 explosive compounds using the substrates described above using the three instruments.

This project was halted about half-way through (2014). The doctoral student who was working on the project and trained on the instruments left the university abruptly and unexpectedly. An undergraduate was able to complete one aspect of the data collection (IR spectra) but that was all we were able to do. The results of these experiments and data collection are described below.

Experimental Results and Discussion

The analyte class selected for testing was explosives as this is a common target analyte set amenable to multiple sensors. The instrument sensors identified for study were:

1. Infrared (IR) spectrometer

2. Differential ion mobility spectrometer (DMS)

3. Raman spectrometer

An in-house Perkin Elmer IR spectrometer was used along with a loaned DMS instrument (Chemring®) and a loaned Raman spectrometer from BWTEK. The first stage of the project involved preparing samples to be characterized with the instruments.

Dilute solutions of explosives and propellants were obtained from Accustandard® and included explosives such as TATP, HMTD, RDX, RDX, ammonium nitrate, potassium perchlorate, potassium nitrate, sugar, and TNT. The approach taken was to characterize the neat standard first as a positive control. For purposes of statistical analysis, the analytes were spiked onto substances that were meant to mimic what would be expected in a normal background environment. For the IR, potassium bromide (KBr) was selected as a blank substrate as it produces no peaks under IR analytical conditions. The other substrates were dust (standard reference material from the National Institute of Standards and Technology (NIST SRM), soil (NIST SRM), and laboratory grade sand. Mixtures of these were also prepared as substrates to include binary combinations of each in ranges of 10-90% by weight. A total of 112 samples consisting of substrate and explosives at various levels were prepared. For example, ~ 2g of 30% soil, 30% sand, and 40% potassium nitrate by weight would be one sample.

The standard reference materials were used to insure that the background was consistent, homogenous, and well-characterized. To construct a neural network model, a large number of samples

are needed that represent the range of expected instrumental responses under a given set of environmental conditions. The algorithm used (backpropagation neural networks) is a supervised learning algorithm in which examples are provided to the network along with the target output. Training involves iterative adjustment of weights to obtain the desired numerical output. For the model to be of practical use, it must be provided with the widest anticipated range of responses that could be associated with a positive or negative result. The network solution can only generalize to the extent that the training set captures anticipated ranges of positive responses. That is why each explosive was analyzed using many different substrates and concentrations and over different days.

For the sample analysis on each instrument, the first step was analysis of controls (blanks, substrate blanks, and explosives alone). Once performance was verified, the samples were analyzed using the standard operating procedure established. All data was obtained for all samples using the IR spectrometer, resulting in collection of several hundred spectra. However, distinct spectral features were observed for only the pure samples and in some cases, those in which the target analyte was in excess of 60% by weight. There were not enough viable spectra to pursue a neural network model using this sensor.

The next instrument selected was the Raman spectrometer. The first set of blanks and pure samples were analyzed with mixed success; only a few pure samples yielded viable spectra. That was as far as the project progressed before the manpower issue forced a halt to work.

2. Army/DoD Collaborations

We did not develop any DOD collaborations.

3. Transitions:

None of this technology was transferred.

4. Awards/honors: None

5. Metrics related to your grant

    a. Number peer-reviewed papers (related to this grant: 0

    b. Number of manuscripts (related to this grant): 0

    c. Number of presentations (related to this grant): 0

    d. Patents submitted (funded by this grant): 0

    e. Number grad students/yr (funded by this grant): 1 student for about 4 months

f. Number postdocs/yr (funded by this grant): 0

g. Number PhD degrees awarded (funded by this grant): 0

h. Number MS degrees awarded (funded by this grant): 0

6. Other notes?

One undergraduate worked on this project for two semesters as part of undergraduate research in the chemistry department. She picked up the grad student's work and finished what she could.