Radio Nuclide Identification for Mindless Automatons

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Goals

- Present the challenges in automated nuclide identification
- Define common terms required to discuss identification algorithms
- Demonstrate the need for Metrics and Test Benches
Problem Statement

What challenges we face.
What is the value of nuclide identification?

- The goal of any protection system is to recommend a course of action to maximize the probability that a threat will be caught.
  - Minimize unnecessary searches of non-threatening material
  - Raising response appropriately on potentially threatening sources

- The limiting resource is the number of secondary inspections

- The brightest sources are either RDD potentials or medical sources

- Nuclide Identification is simply a means to achieve our ends
Errors

- **False Negative**
  - Incorrectly omitting a nuclide that is present
  - Allows a threat to pass

- **False Positive**
  - Incorrectly reporting a nuclide that is not present
  - Results in an unnecessary search

- **Errors**
  - Result from overlap in statistical distributions
  - Can be minimized but never eliminated
Ambiguity

- Ambiguity – an observation can be reasonably interpreted in more than one way.
  - As the source counts are reduced distributions grow wider
  - Nuclides become more difficult to separate
  - Numbers of errors increase
Domain
Source Sample Space

Medical sources

Count rate

Radiography Sources & RDD

Pu Threats

Insufficient cnts For ID

U

K40

Th

Typical Detection Threshold

Energy
## Risk Categories

<table>
<thead>
<tr>
<th><strong>HIGH</strong></th>
<th><strong>MEDIUM</strong></th>
<th><strong>LOW</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Must do secondary inspection</td>
<td></td>
<td>May avoid secondary inspection</td>
</tr>
<tr>
<td>• High confidence threatening ID</td>
<td>• Ambiguous ID with more counts than expected from background</td>
<td>• Apparent Background</td>
</tr>
<tr>
<td>• Highly shielded ID (RDD)</td>
<td></td>
<td>• High confidence non-threatening sources</td>
</tr>
<tr>
<td>• High count rate, no ID</td>
<td></td>
<td></td>
</tr>
<tr>
<td>• Suspect Mixture</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Improvements in spectral id => Fewer errors + Minimize ambiguous cases
=> Reduced number of unnecessary secondary inspections
Identification Components

What makes mindless automatons tick?
Template Algorithm Types

**CLASSIFIERS**
- Asks
  - *What template best fits the observation?*
- Properties
  - Produces a list of templates ranked by fitness to the observation
  - Template library must fully span input domain, including naturally occurring mixtures

**ESTIMATORS**
- Asks
  - *What weighted sum of templates best represents the observation?*
- Properties
  - Produces a weighting vector
  - Mixture can span into novel and unanticipated situations
  - Best solution may not represent the true solution (No ranking)

**CLASSIFIER**
- Has Ranking
- Limited Solutions

**ESTIMATOR**
- Lacks Ranking
- Unlimited Solutions
Identification Methods

- Feature Extractors
  - Channel Decimation
  - PCA
  - Peak Extractor

- Feature enhancers
  - Deconvolution

- Other
  - Multi-detector Spectral Comparison
  - Asymmetric Detector Nuclide Identification/ Deconvolution

Identification Algorithms

- Classifiers
  - Neural Networks
  - Bayes Classifier
  - Nearest Neighbor

- Estimators
  - Multiple linear regression (Fittodb)
  - Gauss-Newton
  - Expectation Maximization

- Heuristics
  - Energy Banding
  - Peak identification

- Other
  - Shielding Estimators (MBS)
Domain of Nuclide Identifiers

- As number of counts increase, un-modeled effects become visible
  - Ground Bounce, Scattering in Environment, Age, Trace isotopes
- Template algorithms fail due to inadequate modeling

![Diagram showing the domain of nuclide identifiers with categories: Spectral Comparison, Classifier, Estimator, Deconvolution, and Peak Identifier. The x-axis represents counts ranging from 10 to 100k.](image-url)
Performance Testing

How well do automatons work under pressure?
## Characteristics of methods

<table>
<thead>
<tr>
<th></th>
<th>GADRAS</th>
<th>PCA Classifier</th>
<th>MLG</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Type</strong></td>
<td>Estimator</td>
<td>Classifier</td>
<td>Hybrid</td>
</tr>
<tr>
<td><strong>Algorithm</strong></td>
<td>MLR</td>
<td>PCA/MSE (dot prod)</td>
<td>Gauss-Newton ML/LBF</td>
</tr>
<tr>
<td><strong>Metric</strong></td>
<td>Chi Squared</td>
<td>Poisson Likelihood</td>
<td>AIC</td>
</tr>
<tr>
<td><strong>Groups/Trials</strong></td>
<td>5</td>
<td>528</td>
<td>25</td>
</tr>
<tr>
<td><strong>Nuclide Output</strong></td>
<td>Composition</td>
<td>1 Library Element</td>
<td>1 Nuclide Group</td>
</tr>
<tr>
<td><strong>Reports “No Detection”</strong></td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td><strong>Reports “Unknown”</strong></td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td><strong>Additional Output</strong></td>
<td>SNM catagory</td>
<td>Sorted Library List</td>
<td>Fitness of each Isotope Group</td>
</tr>
<tr>
<td><strong>Run Speed</strong></td>
<td>1 – 3 seconds</td>
<td>0.5 seconds</td>
<td>0.25 seconds</td>
</tr>
</tbody>
</table>
Evaluation methodology

- Evaluated on two sets
  - Verification – library elements as inputs to algorithm
  - Test – set of similar inputs representing real world inputs
- Ran 100 trials for each using Poisson random draws
- Varied the expected input signal from 50 to 1000 counts for test set
- Background added to sample was Poisson random draw with expected 400 counts
- Reference background was Poisson random draw with expected 120000 counts
- Produced
  - Score based on exact matches or inclusion
  - Cross Correlation Matrix of outputs produced by sample
  - Threat class based assignment
Verification results

- When given library elements and asked figure out which one, we expect nearly perfect performance.
- We didn’t get it.

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>False Negative</th>
<th>False Positive</th>
</tr>
</thead>
<tbody>
<tr>
<td>GADRAS</td>
<td>29%</td>
<td>34%</td>
</tr>
<tr>
<td>PCA</td>
<td>10%</td>
<td>10%</td>
</tr>
<tr>
<td>MLG</td>
<td>7%</td>
<td>6%</td>
</tr>
</tbody>
</table>

(at 300 cps)
Verification results

- PCA and MLG both performed significantly better than GADRAS (1/3 total number of errors)
- Some items failed to identify or were labeled as mixtures by all methods.

\[
\begin{align*}
232\text{Th} & \leftrightarrow 228\text{Th} \\
201\text{TI} & \leftrightarrow 139\text{Ce} \\
226\text{Ra} & \leftrightarrow 252\text{Cf} \\
192\text{Ir} & \leftrightarrow 237\text{Np} \\
67\text{Ga} & \leftrightarrow 237\text{Np} \\
133\text{Ba} & \leftrightarrow 131\text{I}
\end{align*}
\]

Implies library contains indistinguishable nuclides that cannot be resolved with NaI resolution.
Choice of test cases

Sources
- Most commonly detected medical isotopes
  - $^{99m}$Tc
  - $^{131}$I
  - $^{201}$Tl
  - $^{67}$Ga
- Common industrial and potential RDD, $^{137}$Cs
- Natural nuisance sources
  - Bananas
  - Wood
  - Fertilizer w/ potash
- Weapon surrogates with and without lead shielding
  - HEU
  - Virgin HEU
  - Weapons grade Pu
  - Reactor grade Pu
Correlation Result for Tests

Outputs are 90% identification point with noted errors. Best is overall performance at all count levels.

<table>
<thead>
<tr>
<th>Isotope</th>
<th>GADRAS</th>
<th>PCA</th>
<th>MLG</th>
<th>Best</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{99m}$Tc</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>PCA</td>
</tr>
<tr>
<td>$^{131}$I</td>
<td>1000</td>
<td>$^{133}$Ba</td>
<td>1000 $^{133}$Ba</td>
<td>PCA</td>
</tr>
<tr>
<td>$^{201}$Tl</td>
<td>$^{139}$Ce</td>
<td>300</td>
<td>200</td>
<td>MLG</td>
</tr>
<tr>
<td>$^{67}$Ga</td>
<td>300</td>
<td>$^{237}$Np 32%</td>
<td>300</td>
<td>MLG</td>
</tr>
<tr>
<td>$^{137}$Cs</td>
<td>200</td>
<td>100</td>
<td>100</td>
<td>MLG</td>
</tr>
<tr>
<td>Bananas</td>
<td>300</td>
<td>500</td>
<td>300</td>
<td>GAD</td>
</tr>
<tr>
<td>Wood</td>
<td>300</td>
<td>500</td>
<td>500</td>
<td>GAD</td>
</tr>
<tr>
<td>Potash</td>
<td>500</td>
<td>$^{152}$Eu 70%</td>
<td>$^{152}$Eu 30%</td>
<td>GAD</td>
</tr>
<tr>
<td>HEU</td>
<td>300</td>
<td>200</td>
<td>200</td>
<td>GAD</td>
</tr>
<tr>
<td>Virgin HEU</td>
<td>300</td>
<td>200</td>
<td>300</td>
<td>GAD</td>
</tr>
<tr>
<td>RG Pu</td>
<td>1000</td>
<td>$^{40}$K 30%</td>
<td>$^{137}$Cs 12%</td>
<td>MLG</td>
</tr>
<tr>
<td>WG Pu</td>
<td>500</td>
<td>300</td>
<td>500</td>
<td>PCA</td>
</tr>
<tr>
<td>HEU 1” Pb</td>
<td>$^{232}$U 84%</td>
<td>$^{232}$U 55%</td>
<td>$^{232}$U 55%</td>
<td>none</td>
</tr>
<tr>
<td>Virgin HEU 1” Pb</td>
<td>$^{238}$U 100%</td>
<td>$^{238}$U 100%</td>
<td>$^{238}$U 100%</td>
<td>none</td>
</tr>
<tr>
<td>RG Pu 1” Pb</td>
<td>$^{232}$Th 79%</td>
<td>$^{232}$Th 79%</td>
<td>$^{252}$Cf 40%</td>
<td>none</td>
</tr>
<tr>
<td>WG Pu 1” Pb</td>
<td>$^{137}$Cs 70%</td>
<td>$^{252}$Cf 33%</td>
<td>$^{252}$Cf 90%</td>
<td>none</td>
</tr>
</tbody>
</table>
Conclusions

The bottom line
Conclusion

- What are the problems in nuclide identification
  - Ambiguity, Nuisance sources, Inadequate resolution
- What are the problems in a Classifier and an Estimator
  - Classifier – Restricted to ranked list
  - Estimator – Restricted to one solution
- How well do current technologies work
  - Not so swift
- What is to be gained by defining a test bench
  - We can optimize our methods to improve their performance
Learning from our mistakes

Fool me once shame on you,
Fool me twice shame on me.
LLNL’s Template Based Isotopic Identifier

- Produces
  - Optimum fit for single isotope or specified mixtures with arbitrary ratios
  - An “unknown” result in response to novel samples or unexpected mixtures
  - Multiple solutions where more than one possible
  - Significance and Confidence levels for each solution
- Designed for low count spectra (<1000 cts)
- Works with large (2x4x16) NaI detectors
- Uses non-linear Gauss-Newton solver
Verification Result

- Verified by probing algorithm 100 random samples for each template.
  - Samples were drawn to have ~300 counts of source with 334 counts of background
  - Reference 5 minute background provided
- Scored based on false positive and false negative

Un-weighted Results:

- **False Negative:** 134/14300 trials less than 1%
- **False Positive:** 4217/14300 trials ~30%

- Require real world frequency data to compute weighted score
Feature Extraction

Getting the most out of an observation
Channel Decimation

- **Method**
  - Adds groups of neighboring channels

- **Properties**
  - Maintains statistical properties
  - Resulting information loss can cause ambiguity
  - Increases statistical significance of each channel
  - Must strike a balance between information loss and improved significance
  - Radiation spectrum has natural grouping by the square root of the channel energy
Principle Component Analysis

- **Method**
  - Transform input along the basis vector representing the greatest variance (most representative)

- **Mathematics**
  - \( R = PP^T = U^T \Lambda V \)  
    - Eigenvalue decomposition
  - \( W = [U_1 \cdots U_k] \)  
    - Select K largest eigenvalues
  - \( X = W^T O \)  
    - Transform on this basis

- **Properties**
  - Does not preserve the statistics of the observation
  - Good to reduce high dimensional data sets with minimal loss
  - Can reduce noise if it can not be represented in the feature space
Classifiers

What is the best match?
Nearest Neighbor Classifier
Dot Product

- **Purpose**
  - *Compute the nearest template using L2 norm to the observation.*

- **Mathematics**
  \[
  \min \epsilon = \|O - E - kT_i\|_2^2 \quad \rightarrow \quad \max \epsilon = (O - E) \cdot \frac{T_i}{\|T_i\|}
  \]

- **Properties**
  - Shaped based spectral analysis frequently paired with PCA.
  - Computationally inexpensive for each template.
  - Requires many templates to fully span input domain.
  - Does not account for statistical nature of noise.
  - Does not allow for fluctuations in background conditions.
Estimators

How much of each?
Anatomy of An Estimator

MSE
\[ \varepsilon = \frac{1}{2} \| O - Ax \|_2^2 \]

Objective Function
\[ f(x) = \frac{\partial \varepsilon}{\partial x_j} = 0 \quad \forall j \]
Maximum Likelihood of Subgroups

- Estimator using Poisson Statistics and Maximum Likelihood Nonlinear Solver
- Requires Logarithmic Barrier Function (LBF) to impose fully positive constraints
- Computes Likelihood of best fit for Background plus each set of nuclides (all shieldings)
Anatomy of fittoddb (GADRAS)

- Core is Heuristic guided MLR (multiple linear regression)
- Objective Function is $\chi^2$ based on 7 variance estimations
- Breaks the library into 4 classes for subgroup analysis
  - Natural
  - Medical
  - Industrial
  - SNM
- Produces
  - Fitness of SNM
  - Nuclide Identification (only reports “significant contributors”)
  - Significance (reduced $\chi^2$)
Anatomy of fittodb (GADRAS)

- Sample → Downsample
- Background → Downsample

Gain Adjust → Full Library
SNM Library → MLR
Industrial Library → MLR
Medical Library → MLR
Natural Library → MLR

- Reduce to 62 Energy Channels
- Weights based on Fitness
- 143 Isotope/Shield Pairs

SNM Fitness → Isotope ID

PROPRIETARY
Other Techniques

One of these things are not like the others.
Materials Basis Set

- **Purpose**
  - Estimate the shielding located between a known nuclide and the detector.

- **Mathematically**

  \[
  b_{z,i} = -\ln\left(\frac{c_{z,i}}{c_{z,\text{ref}}}\right) \quad U = \begin{bmatrix}
  b_{0,\text{ref}} & b_{0, z1} & \cdots & 1 \\
  b_{1,\text{ref}} & 1 \\
  \vdots & \ddots & \ddots & \vdots \\
  b_{n,\text{ref}} & \cdots & 1
\end{bmatrix} \quad b = U \cdot \rho
  \]

- **Properties**
  - Uses Beer’s Law \((A=\varepsilon/c)\) estimate shielding thickness
  - Works in a log space
  - Assumes that increased shielding decreases the mean counts in a channel
Materials Basis Set

- Primary functions on the photo-peaks
  - Compton scatter breaks assumptions thus is biasing the solution

- Working in a logarithmic space makes mixture analysis difficult.
  - Nuclide signatures add linearly
  - Complexity of estimator will increase as $N^2$ as additional nuclides are included in the mixture
  - Perturbations from Compton Scattering likely to bias mixture solution

- Assumes $\chi^2$ statistics on reconstructed spectra
Deconvolution

- Purpose
  - Compute the energy flux at the surface of the detector from the observation

- Properties
  - Requires relatively large numbers of counts to produce a quality result (10k)
  - Requires extremely well tuned detector model
  - Removes virtually all detector effects
    - Compton Scatter
    - Backscatter peaks
  - Decreases the FWHM of the detector by a factor of 4
  - Allows isolation of peaks within $\frac{1}{2}$ of the FWHM
Nal Deconvolution

- Deconvolution using EM algorithm
- Allows direct evaluation of shielding from Compton scattering or branching ratios
- Removed backscatter peak
- Recovered Compton Scatter in the detector to the photo-peak

Simulated 1C $^{137}$Cs behind 3 cm of Pb
Plastic Deconvolution

- Provides
  - Peaks otherwise not visible can be identified
  - Allows calibration of energy scale

- Deconvolution using EM algorithm
  - 128 bin energy square root energy
  - Gaussian basis

Original Spectrum

--137Cs

--60Co

--60Co
Multi-detector Nuclide Comparison

- **Purpose**
  - Uses multiple detectors to improve identification or match spectra between previous encounters

- **Properties**
  - Simultaneously solve detectors by information sharing or summing
  - Depending on the number of energy channels used can operate with less counts at a particular encounter than possible otherwise
  - Demonstrated in DTS to improve nuclide identification for high speed traffic by using detections from multiple locations
Asymmetric Detector Nuclide Identification/Deconvolution

- **Purpose**
  - Using two detectors with different resolutions and efficiencies to improve identification.

- **Properties**
  - Simultaneously solves identification in both detectors by information sharing
  - Complexity increases at number of detectors squared
  - Pairs small high resolution (HPGe, SiLi, CZT) detector with larger low resolution detector (NaI, Plastic)
  - Creates hybrid detector with resolution and efficiency somewhere between the two
Non-negative Iterative Solvers

- NNLS - Lewson and Hanson
- Logarithmic Barrier Function – method of generalized inequality constraints
- Expectation Maximization – uses probability density function that are positive by design
What do these silly numbers all mean?
Model Confidence (Trust)

- **Purpose**
  - Indicates how frequently a specified model is a correct identification.

- **Mathematics**
  \[ C_{M_i} = \frac{P(O \mid M_i)P(M_i)}{\sum_{M_j} P(O \mid M_j)P(M_j)} \]

- **Properties**
  - Depends on immeasurable quantity \( P(M) \)
  - Requires the sum of all possible solutions that may not be computable in finite time.
  - At best we can compute an empirical estimate of confidence or pseudo-confidence
Nuclide Confidence

- **Purpose**
  - *Indicate how frequently a specified nuclide is a correct identification.*

- **Mathematics**
  \[
  C_x = \sum_{X \subseteq M_i} \frac{P(O \mid M_i)P(M_i)}{\sum_{M_j} P(O \mid M_j)P(M_j)}
  \]

- **Properties**
  - As with Model Confidence, depends on immeasurable quantities. Thus we can at best estimate it.
Significance

- **Purpose**
  - Indicates how frequently a similar observation may be produced from a model.

- **Mathematics**
  \[ P( F(x) > F(O) \mid M) \]

- **Properties**
  - Evaluated by either a null hypothesis test (\( \chi^2 \)) or by likelihood ratios.
  - Used as the objective function in estimators.
  - Well defined for radio-nuclide identification problem.
  - Controls the rate of Type II errors.