New Directions in Radioisotope Spectrum Identification

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OVERVIEW

Recent studies have found the performance of commercial handheld detectors with automatic RIID software to be less than acceptable [14, 15]. Previously, we have explored approaches rooted in speech processing such as cepstral features and information-theoretic measures [18]. Scientific advances are often made when researchers identify mathematical or physical commonalities between different fields and are able to apply mature techniques or algorithms developed in one field to another field which shares some of the same challenges. The authors of this paper have identified similarities between the unsolved problems faced in gamma-spectroscopy for automated radioisotope identification and the challenges of the much larger body of research in speech processing. Our research has led to a probabilistic framework for describing and solving radioisotope identification problems. Many heuristic approaches to classification in current use, including for radioisotope classification, make implicit probabilistic assumptions which are not clear to the users and, if stated explicitly, might not be considered desirable. Our framework leads to a classification approach with demonstrable improvements using standard feature sets on proof-of-concept simulated and field-collected data.

BACKGROUND

Radioisotope identification algorithms based on gamma-ray spectra take an unknown gamma-ray spectrum recorded by a detector as input and attempt to determine which isotopes emitted the observed gamma photons. Approaches can generally be divided into two broad areas. The first focuses on specific regions of interest in the unknown spectrum where gamma photons from certain isotopes would be expected to be seen. This approach is exemplified by peak picking, in which the locations of peaks in the spectrum are used to identify the gamma-ray sources (see, for example Routti and Prussin [9]). In a noisy spectrum, it can be difficult to determine the exact location of the peaks, and many approaches to this problem have been explored [11]. Furthermore, when shielding is present, the photons emitted at the expected peak energy may be shifted down to lower energies, to the point where a peak is not identifiable.

In the second approach, the algorithm attempts to match the full spectrum with templates of spectra from known isotopes. To accomplish this, some measure of similarity must be chosen; the most common choices are correlation coefficients and error measures. For correlation measures, the

correlation coefficient is computed between an unknown spectrum and a library of reference spectra [17].

Many authors have proposed least square error approaches. Salmon [1] and McWilliams, *et al.* [2] used non-weighted least squares procedures to solve for the target strengths of isotopes in an unknown spectrum. The former author mentions that a weighted approach would be more robust but does not pursue the idea. Other researchers have pursued weighted least squares approaches [3, 4, 5, 6, 7, 8, 10]. In particular, Eckhoff [10] describes a nonnegative weighted least squares algorithm, where the weights are determined by variance estimates from the observed spectrum, the template spectrum, and the estimator. If the template set of known spectra is constructed without shielding, however, the usefulness of these approaches is reduced when shielding materials are present. These approaches either assumed simple background subtraction or that the background could be described as a combination of the template sets; no separate background contribution to the weighting was incorporated.

Gamma photons interact with matter via several different processes: Compton scattering, the photoelectric effect, and pair production. We will not give a detailed description of these effects here because they are well documented in the literature (e.g., Knoll [13] or Gilmore and Hemingway [12]). However, in general, the interaction of gamma photons with matter between the source and detector causes the photon to be detected at a different energy than that at which it was emitted. This effect complicates the process of radioisotope identification because the measured spectrum from a given isotope may be significantly different from that which was expected. Therefore it is highly desirable to develop RIID algorithms which are robust to the effects of shielding.

The Multiple Isotope Material Basis Set (MIMBS) method for RIID works on the principle that the effects of any shielding material can be approximately modeled using the effective atomic number. MIMBS uses a small number of basis shielding materials and unshielded reference spectra and attempts to solve, using a least squares approach, simultaneously for the composition of the shielding and the source emitters [16].

MODEL FORMULATION

Automated detection and classification systems can take many forms. Probabilistic modeling is particularly useful from a research point of view as well as in situations where the target platform is intended for use by nontechnical users. Probability is an intuitive concept that enables researchers to examine systematically the effects of various features and variations, and it is also one that can lead directly to intuitive outputs for a wide variety of users. Specifically, a probabilistic problem formulation can give us not just an estimate of the quantity of interest but a meaningful estimate of how likely that estimate is to be correct. Because this confidence estimate is so valuable, many non-probabilistic formulations produce an *ad hoc* number that is labeled as "confidence" but does not have a mathematical relationship to any real question that could be understood by a non-technical user.

In the application being studied under this work, the goal is to detect the presence of one or more radioactive isotopes in an environment where there are many possible environmental sources of radiation as well. The data available are the counts of emissions received at different energy levels:

$$\mathbf{k_u} = [k_u(1), k_u(2), ..., k_u(N)]^{\mathrm{T}} \tag{1}$$

collected over a time interval T_u, where N is the number of channels (energy bins) and $k_u(i)$ is the count in bin i. For this pilot study, we also assume the availability of a reference background spectrum

$$\mathbf{k_r} = [k_r(1), k_r(2), ..., k_r(N)]^{\mathrm{T}} \tag{2}$$

which is taken in over a period T_b in a similar environment but not directed at the object being interrogated. Given a list of possible isotopes which may be present in the unknown spectrum, we model the unknown spectrum as

$$\mathbf{k_u} = \mathbf{k_b} + \sum_{j=1}^{N_c} \mathbf{k}_j \tag{3}$$

where $\mathbf{k_b}$ is the spectrum of received emissions due to the background, and $\mathbf{k_j}$ is the spectrum due to component j in our library of N_c components (this spectrum may be $\mathbf{0}$ if the component is not present). The components may correspond with isotopes or with isotopes under specific conditions (such as a particular shielding setup).

To address this probabilistically, we consider that the question we want to answer is **"Given the sampled spectrum $\mathbf{k_u}$, what is the most likely combination of target components present in the interrogated envronment, and in what strengths?"** We can write this as

$$\hat{\mathbf{c}} = \underset{\mathbf{c}}{\operatorname{argmax}}\, p(\mathbf{c}|\mathbf{k_u}) \tag{4}$$

where

$$\hat{\mathbf{c}} = \{\hat{c}_1, \hat{c}_2, ..., \hat{c}_{N_c}\} \tag{5}$$

are the strengths of the N_c components which may be present in the unknown spectrum at higher levels than in the reference background spectrum (we can assign $c_j = 1$ to the strength of a source at a reference distance and radioactivity, such as 10μC at 1 meter distance). According to Bayes' rule

$$p(\mathbf{c}|\mathbf{k_u}) = \frac{P(\mathbf{k_u}|\mathbf{c})p(\mathbf{c})}{P(\mathbf{k_u})} \tag{6}$$

which involves the prior probability estimates $p(\mathbf{c})$ and $P(\mathbf{k_u})$, which may be environment- or application-dependent. As a result, we may choose to focus on the *maximum likelihood estimate* [20] of $\mathbf{c}$,

$$\hat{\mathbf{c}} = \underset{\mathbf{c}}{\operatorname{argmax}}\, P(\mathbf{k_u}|\mathbf{c}), \tag{7}$$

which is equivalent to asking "**Which combination of component strengths would be most likely to produce the observed channel counts *given that that set of strengths were present in the environment?***" In other words, we ignore the expected (prior) probability of each isotope in the environment. If there are significant differences in these expected probabilities for a given scenario, we may wish to include them in the estimated quantity as in Equation 6, but for many applications the relative probabilities of particular options given the data are so much more differentiated than the prior probabilities that the latter do not significantly affect the classification result.

The channel counts are random variables which we assume to be independent given the target strengths and the background spectrum, so we can write the probability of a given unknown spectrum in Equation 7 as a product of the individual channel counts:

$$P(\mathbf{k_u}|\mathbf{c}) = \prod_{i=1}^{N} P(k_u(i)|\mathbf{c}). \tag{8}$$

We model each component j with an expected spectrum (at some reference target strength)

$$\boldsymbol{\lambda}_j = [\lambda_j(1), \lambda_j(2), ..., \lambda_j(i), ..., \lambda_j(N)]^{\mathrm{T}} \tag{9}$$

and an expected background spectrum (which in practice we will need to estimate)

$$\boldsymbol{\lambda}_b = [\lambda_b(1), \lambda_b(2), ..., \lambda_b(i), ..., \lambda_b(N)]^{\mathrm{T}} \tag{10}$$

Equation 3 can be viewed as a single sampling of an underlying distribution

$$\boldsymbol{\kappa}_u = \boldsymbol{\kappa}_b + \sum_{j=1}^{N_c} \boldsymbol{\kappa}_j \tag{11}$$

where the κs are random variables. The physics tell us that these κs are Poisson-distributed, but if we approximate the Poisson distribution as a normal distribution we can write Equation 11 as

$$\boldsymbol{\kappa}_u \approx \boldsymbol{\lambda}_b + n(\boldsymbol{\lambda}_b) + \sum_{j=1}^{N_c} [c_j\boldsymbol{\lambda}_j + n(c_j\boldsymbol{\lambda}_j)] \tag{12}$$

where $n(\mu, \sigma^2)$ is a normally-distributed random variable with mean μ and variance σ^2 and let $n(\sigma^2) = n(0, \sigma^2)$, and vector arguments to the normal function are interpreted as the diagonal values of a covariance matrix with no non-zero off-diagonal values. We can rewrite this in matrix form as

$$\boldsymbol{\kappa_u} \approx \mathbf{Ac} + \boldsymbol{\lambda}_b + n(\mathbf{Ac} + \boldsymbol{\lambda}_b) \tag{13}$$

where $\mathbf{A}$ is our library of expected spectra; for component j in bin i, $\mathbf{A}(i, j) = \lambda_j(i)$ for $c_j = 1$. However, we do not have $\boldsymbol{\lambda}_b$ itself but $\mathbf{k}_r$, one sample of this distribution.

For sufficiently large values of $k_r(i)$ we may model the distribution of $\boldsymbol{\lambda}_b$ given $\mathbf{k}_r$ as

$$\mathbf{k}_r + n(\mathbf{k}_r), \tag{14}$$

which makes the approximation that the standard deviation of a Poisson distribution with an expected value equal the sample count is not significantly different from the deviation of a distribution with the expected value equal the theoretical background distribution. We can then rewrite Equation 13 as

$$\boldsymbol{\kappa_u} \approx \mathbf{Ac} + \boldsymbol{\lambda}_b + n(\mathbf{k}_u) \tag{15}$$

For small expected counts, this approximation will lead to overestimation of the target strength and an improved model is part of our future work direction. For cases where the assumption holds, we can now further approximate Equation 11 as

$$\boldsymbol{\kappa_u} \approx \mathbf{Ac} + \mathbf{k}_r + n(\mathbf{k}_u + \mathbf{k}_r) \tag{16}$$

where we neglect the variance in the variance term. As a point of reference, note that the variance estimate includes not just the background contribution as in anomaly-detection features such as spectral comparison ratios [19], but also incorporates variance due to the hypothesized target isotopes.

Our goal now is to estimate $\mathbf{c}$ as

$$\hat{\mathbf{c}} = \underset{\mathbf{c}}{\operatorname{argmax}}\, P\left[\mathbf{k_u}|\boldsymbol{\kappa}_u(\mathbf{c})\right], \tag{17}$$

The isoprobability curve of the multivariate normal distribution $\boldsymbol{\kappa}_u$ in this probability space is a hyperellipsoid. By a scaling of axes, we can operate in a space where the isoprobability curve is a hypersphere, which will enable us to solve for $\hat{\mathbf{c}}$ using linear projection. For a scaling vector $\mathbf{s}$ such that

$$s(i) = \left[k_u(i) + k_r(i)\right]^{1/2} \tag{18}$$

we can scale all the vectors in the spectral space, resulting in

$$\boldsymbol{\kappa}_u{}' - \mathbf{k}_r{}' \approx \mathbf{A}'\mathbf{c} + n(\mathbf{I}) \tag{19}$$

where the prime indicates scaling by s: $A'(i,j) = A(i,j)/s(i)$, etc. The linear projection of $\boldsymbol{\kappa}_u{}' - \boldsymbol{\lambda}_b{}'$ onto $\mathbf{A}'$ is the choice of $\hat{\mathbf{c}}$ which maximizes the probability presented in Equation 17. Thus the maximum likelihood estimate for $\mathbf{c}$ is

$$\hat{\boldsymbol{c}} = (\mathbf{A}')^{-1}(\mathbf{k}'_u - \mathbf{k}'_r). \tag{20}$$

To understand the value of the probabilistic approach, consider for comparison a linear projection which does not incorporate such scaling, as seen for example in the MIMBS method[16]. That approach is equivalent to the probabalistic formulation just described, if the variance is assumed to be the same in every channel. This means, for example, that an excess of 16 counts in a particular channel is treated as having the same likelihood whether the expected number of counts due to the background and other isotopes were 1 or 100.

Alarms and confidence reporting

Given the variance model described above, we can estimate the pdf of observed channel counts

$$p(\mathbf{k}_u|\mathbf{k}_r, \mathbf{A}', \hat{\mathbf{c}}) = \frac{1}{(2\pi)^{N/2}\prod_{i=1}^{N} s(i)} exp(f(\mathbf{k}_u, \mathbf{k}_r), \hat{\mathbf{c}}) \tag{21}$$

where

$$f(\mathbf{k}_u, \mathbf{k}_r, \hat{\mathbf{c}}) = -\frac{1}{2}(\mathbf{A}'\mathbf{c} - [\mathbf{k}'_u - \mathbf{k}'_r])^T(\mathbf{A}'\mathbf{c} - [\mathbf{k}'_u - \mathbf{k}'_r]) \tag{22}$$

which we note is a simple function of the distance between the expected target spectrum $\mathbf{A}\hat{\mathbf{c}}$ and the estimated target spectrum $\mathbf{k}_u - \mathbf{k}_r$ in the scaled space. As such, we can use this distance as a measure of fit of the model to the data. More particularly, we have a simple measure of how likely a particular model component is to be present in the data, since we can calculate how much the pdf increases when we add that component to the model:

$$p(\mathbf{k}_u|\mathbf{k}_r, \mathbf{A}', \hat{\mathbf{c}}) - p(\mathbf{k}_u|\mathbf{k}_r, \mathbf{A}'_j, \hat{\mathbf{c}_j}) \tag{23}$$

where ${A'}_j$ and $\hat{\mathbf{c}}_\mathbf{j}$ are, respectively, the expected library and estimated target strengths with the isotope in question removed.

More generally, we can apply this approach to determine the model's confidence in a group of components—for example, representing a particular isotope under a variety of shielding conditions or in a group of SNMs that may be easily confused—to report confidences on a variety of alarm conditions of value in a particular scenario.

In fact, confidence may be a more reliable measure of target presence than target strength. Our preliminary studies indicate that low-strength targets are more easily separable from false alarms along the confidence axis than the estimated target strength axis. As a result, our baseline detection and identification system identifies as present all isotopes above some very nominal target strength that meet a set of empirically-determined confidence thresholds.

RESULTS

In this section, we describe the results of two experiments conducted to evaluate the performance of this approach. The first experiment was a preliminary in-house test involving a small set of source isotopes. This was limited in scope to allow for a detailed analysis of the results. The second experiment was a test administered by SRNL. The results of this second experiment will be described here, but an in-depth analysis will be published at a later date.

The first experiment was performed using only simulated data. We created spectra by embedding Poisson-sampled spectra corresponding with sources between 0 and 5 μC at 1 meter range in field-collected background spectra as before, and with an available reference background collected in a similar environment. Each spectrum contained four of the five isotopes available to us (although the actual number of sources was neither used by nor available to the detection/classification algorithm.) We created 100,000 spectra in this fashion in order to simulate conditions that required very low false alarm rates. Our algorithm consisted of a simultaneous target strength estimation for all targets in the library, as presented in Equation 17. We assumed the availability of a reference background and included the variance effects of such a background.

To examine the effects of the probabilistic formulation on target strength accuracy estimation, we compared performance using a straight linear projection (which minimizes the mean as in MIMBS) to the probabalistic approach described in this report. We found a significant improvement in absolute target strength estimation as summarized in Table 1.

A method of characterizing this system which is more relevant to a field operator's experience is to choose an operating point, as defined by P_D and P_{FA} (respectively the probability of detection of each isotope and the probability of false alarms when there is no target source present), and identify the minimum target strengths at which this operating point can be achieved. We looked at the operating points corresponding to zero observed false alarms, which means that our operating point has a false alarm rate of 0.005% or lower. At that level, we looked at the minimum target strengths required to produce a capture rate of 90% or greater, and found they ranged from 1 μC for ^{133}Ba and ^{60}Co up to 2.5 μC for ^{228}Th.

For the second experiment, the data was created by SRNL and it consisted of a large number of high-quality gamma-ray spectra that included various distances, shielding and combination of radioisotopes. The data set consisted of 446 measured and 830 simulated spectra and included 45 measured background spectra and 147 simulated background spectra. Table 2 shows the breakdown

Target	MSE min	Probabilistic
^{60}Co	0.0433	0.0195
^{228}Th	0.0411	0.0355
^{133}Ba	0.0190	0.0193
^{241}Am	0.0308	0.0268
^{152}Eu	0.0248	0.0238
Mean	0.0318	0.0250

Table 1: Mean target-strength errors for the standard linear projection (MSE minimization) and the probabilistic approach. The probabilistic approach results in a 21% improvement in target strength estimation (from 0.0318 down to 0.0250).

of data into that collected and that simulated by GADRAS, as well as breakdown into number of actual targets present in the data.

Test Segment	**One Isotope**	**Two Isotopes**	**Three Isotopes**	**Backgrounds**	**Total**
Simulated	443	125	115	147	830
Measured	254	105	42	45	446
Total	**697**	**230**	**157**	**192**	**1276**

Table 2: Breakdown of test spectra

Each test spectrum was associated with a statistically independent reference background in order to simulate real-world measurement conditions. A collection of 34 isotopes, mostly derived from ANSI 42.34, were used as gamma-ray sources. Each isotope was categorized as Special Nuclear Material (SNM), Medical, Industrial, or Naturally Occurring. The categorization of isotopes for this project differed from ANSI 42.34 in that ^{241}Am and ^{238}U were categorized as SNM in this experiment.

Many of the isotopes included in this experiment produce daughter isotopes in their natural decay processes, so the algorithm was modified in the following way to take advantage of that fact. First, target strengths were estimated for a template set that included the target isotopes as well as their daughters. Then a modified template set was created that eliminated all of the daughters whose parent isotopes did not alarm. In this way, the daughter templates were used to provide a better fit when their parents were present.

Various levels of shielding could exist between the gamma-ray source and the detector, the shield materials used were aluminum, iron, and lead, and they could be up to a maximum thickness of one inch. The reference library contained expected spectra for a variety of shielding scenarios, and the estimated target strengths for a particular isotope were created by combining the estimates from all shielding scenarios.

The algorithm received the test spectra, associated reference backgrounds, and calibration information as input. As output, the algorithm reported a maximum of three detected isotopes, a confidence score for each, and a flag indicating if an SNM was present or not. The output was scored according to the following procedure. A true positive was worth 10 points, the first false positive was worth -5 points, and additional false positive were worth -2 points. A true positive SNM flag

was worth 3 points while a false positive SNM flag was worth -3 points. Note that in this test, the definition of a false alarm is slightly different as the operations scenario assumed a previous detection phase and thus it is assumed there is some target present and therefore a much higher false alarm rate is acceptable. The scoring system is summarized in Table 3. The reported confidence was not used in the quantitative scoring.

Trial Result	**Score Assigned**
True Positive	10
First False Positive	-5
Additional False Positives	-2
True Positive SNM Present	3
False Positive	-3

Table 3: Summary of the scoring methodology

The results as described by the points scored are presented in Table 4. The results are broken down into simulated and measured data because different thresholds were used for each. According to the scoring system, the algorithm had nearly the same performance on the simulated and measured data.

Data Type	**Score**	**Possible**	% Correct
Simulated	4297	6062	71%
Measured	7958	10894	73%
Total	12255	16956	72%

Table 4: Points scored

A common way to evaluate the performance of a classification algorithm is by examining its capture rate and false alarm rate. The capture rate is defined as the percentage of the isotopes present that were correctly identified. The false alarm rate is defined as the percentage of trials in which the algorithm reported an isotope that was not actually present. The capture and false alarm rates for this test are shown in Table 5. We note that the capture rates for the simulated and measured data are similar while the false alarm rate for the measured data is significantly higher than for the simulated data. Preliminary analysis indicates strong correlations between the particular isotopes present and the isotopes that false alarmed; these correlations are due to specific mismatches between the simulated spectra and the received spectra and we see obvious directions for significant near-term improvement. We consider the overall capture rate of 75% to be good performance, considering that some of the isotopes in this test were under heavy shielding.

NEXT STEPS

The work presented in this document describes approaches to radioisotope detection and identification which have found success in other areas. The probabilistic problem formulation was successful in our

Data Type	Capture Rate	False Alarm Rate
Simulated	72%	1.0%
Measured	76%	12%
Total	75%	4.7%

Table 5: Capture and false alarm rates

limited tests, and has the most straightforward implementation in an environment when multiple sources are potentially present. We introduced a means of using this formulation to provide an intuitively meaningful measure of result confidence. We noted but tabled several opportunities for improvement in the preliminary study which we intend to return to, in particular taking advantage of the correlation between adjacent energy bins and the divergence of low-count bin distributions from the normal distribution.

Also of primary interest for future work is further study of and response to the physics underlying the variation among spectra that nominally have the same source isotopes present. We observed great divergence between simulated and observed spectra, and we are pursuing further understanding of this difference with a goal of incorporation into the search space over which we are optimizing, thus creating a more robust algorithm. We also intend to address differences due to the physics of nonstationary backgrounds.

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