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# Benchmarking Algorithm for Radio Nuclide Identification (BARNI) Literature Review

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February 4, 2019

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This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Nuclear Smuggling Detection and Deterrence Program  
Science and Engineering Team

# **Benchmarking Algorithm for RadioNuclide Identification (BARNI) Literature Review**

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01/30/2019

Office of Defense Nuclear Nonproliferation  
National Nuclear Security Administration  
U.S. Department of Energy



This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344.

LLNL-SR-767242.

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## **Executive Summary**

This is a literature review of published radioisotope identification (ID) methods, and an attempt at systematic organization of the approaches for solving this problem. In addition, there is an overview of the related open and closed source software, and patents related to radioisotope identification. This document is also part of the development plan for BARNI (Benchmarking Algorithm for RadioNuclide Identification) software, since it is meant to be a comparison tool, a summary of radiation ID performance evaluations is also included.

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## **Acronyms and Abbreviations**

BARNI	Benchmark Algorithm for RadioNuclide Identification
DOE	Department of Energy
FLD	Fisher's Linear Discriminant
ICA	Independent Component Analysis
ID	Identification
ML-EM	Maximum Likelihood Expectation Maximization
MEM	Maximum Entropy Method
NSDD	Nuclear Smuggling Detection and Deterrence
NNMF	Non-Negative Matrix Factorization
PCA	Principal Component Analysis
SVM	Support Vector Machines



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## Introduction

The following is a literature review of published radioisotope identification (ID) methods, open-source software, commercial products and related patents. The motivation for this work is to characterize the landscape of the available technologies and minimize any unnecessary duplication of efforts as part of the development of the BARNI (Benchmark Algorithm for RadioNuclide Identification) software. For completeness, this work also includes a review of reports that evaluate the performance of radionuclide ID algorithms.

## Published Methods

The process of determining the correct set of nuclides which contribute to a gamma-ray spectrum cannot be accomplished by a single “method”. Identification is a multistep process, and individual publications often focus on one of the steps in this process. Approaches to radionuclide identification can be placed in two broad categories: (1) peak search and match and (2) template matching. The first approach consists of extracting energy lines from a gamma-ray spectrum and matching them to a radionuclide library. In the second approach, the entire spectrum, or some rotation of the spectrum, is matched against a library of spectral “templates”.

The **peak search and match approach** can be broadly broken into the following triad:

- 1) **Peak search:** The photopeaks in the spectrum are located, and typically reported as “lines” at discrete energies. Sometimes the search includes Compton edges, which not only provide secondary confirmation but are also useful in estimating shielding.
- 2) **Feature extraction/design:** Although not strictly necessary, this step serves the purpose of a dimensionality reduction which alleviates the problems of many different discrete line solutions originating from the peak search. Most commonly a feature group is defined by a range of energies that encompass all plausible extracted locations from a peak and includes any associated information about that peak (e.g. area).
- 3) **Classification:** The results from the previous steps are matched against a known nuclide library, and the mixture of correct nuclides is identified. A well-designed classifier can overcome the shortcoming of the results fed to it by the previous steps, and may additionally leverage any prior probabilities of identifying a specific set of radionuclides.

**Template matching** has different steps, but in some ways are analogous to those above:

- 1) **Template library:** Produce a representative library of gamma-ray spectra for different radionuclides under various shielding configurations, including dynamic template generation (e.g. account for scattering).
- 2) **Dimensionality reduction:** There may be an intermediate step here that rotates the resulting data (e.g. Principal Component Analysis) from spectral space into some other constellation of features which are then used for the search.
- 3) **Mixture search:** Solve the combinatorial optimization problem of finding the right mixture of radionuclide contributing to the sample spectrum. The most robust and clever mixture selection algorithm will fail if the underlying template library is not representative of the detection system.

Both the peak search and classification can be automated, computed entirely by an algorithm, or performed manually through expert analysis. Furthermore, it is conceivable to automated one step without the other. For example, an expert could use a graphical interface to manually select location of each peak, and an automated classification scheme would match these choices against predefined nuclide library. Conversely, an expert could use any of the openly available peak finding tools and then perform the rest of the assignment of manually searching gamma-ray emission library [1].

## Peak Search

If measured spectra were a smooth continuous curve, then the list of peaks could by definition be obtained by taking the derivative of the entire spectrum. However, discrete Poisson fluctuations in the underlying data necessitate a smoothing procedure before any number of derivatives is taken [2]. A wide variety of smoothing methods have been applied for gamma-ray spectroscopy from simple moving average [3] to more complex piecewise polynomials such as B-splines [4], or Savitzky-Golay filter [5] [6]. Fourier transforms have been employed since the early days of automated peak search [7], and more recently wavelet analysis has been investigated as a solution to finding peaks in noisy data [8] [9] [10].

Regardless of the implementation details, all these aforementioned methods require parameters to be tuned in order to function optimally. The right balance has to be achieved between smoothing away noise, while preserving features of interest in a spectrum, namely the peaks. This balancing act gets more complicated with low-count data, where real features of interest are difficult to discern from the underlying background.

An alternative approach is a class of so-called “deconvolution” algorithms, which attempt inversely solve for the incident gamma-ray flux [11] [12] [13]. Deconvolution is strictly speaking a misnomer, since the measure pulse height spectrum can be represented as the Fredholm equation of the first kind:

$$P(H) = \int R(H,E)S(E) dE$$

where  $R(H,E)$  is the response function for pulse amplitude  $H$  for a given incident energy  $E$  [14]. The goal of the deconvolution algorithms is to recover the incident energy distribution  $S(E)$ . Examples of deconvolution techniques include Maximum Likelihood Expectation Maximization (ML-EM), Maximum Entropy Method (MEM) and linear regularization [15].

Deconvolution requires at least some approximation for  $R(H,E)$  but can yield a more robust peak search with less dependence on scenario specific “tuning” as compared with the derivative methods. Instead, there is the necessary burden on the user to provide even a crude model of the specific detector system. This model for detector response can attempt to approximate physical reality to a varying degree, from simple Gaussian kernel, and semi-empirical models [16] to full detector response matrix developed from a detailed and computationally expensive Monte Carlo simulations [17]. Nominally the performance of the overall algorithm should scale with the details captured by the detector response model provided by the user.

## **Feature Extraction and Design**

A feature is some measurable characteristic of a class and is typically represented as a numerical value. For radionuclide identification, an obvious feature would be counts under a peak at some discrete energy corresponding to a characteristic gamma-ray emission energy. Features that are well chosen and designed will maximize the potential for discriminating among numerous classes (i.e. radionuclides) of interest. A set of features that describe a class is called a feature vector, and large examples of which are ultimately used by the classifier for training and testing.

If the space of possible radionuclides for identification is large, especially factoring in additional variables such as shielding, then numerous features may be necessary for the classifier to distinguish among various radionuclides. However, more accurate classification cannot be achieved by simply adding on more features ad infinitum, as the classifier performance begins to actually deteriorate as the dimensionality of the feature space increases. This so-called “curse of dimensionality” is the result of feature space becoming sparser, leading to problems such as overfitting. However, some of these negative side-effects can be avoided or minimized through the use of a sufficiently large and representative training set, or a prudent choice of a classifier algorithm.

The problem with high dimensionality is especially acute for radionuclide identification. The continuous energy space in gamma-ray spectra presents the peak search algorithm with infinite line energies to extract. These estimated energies will necessarily deviate from expected

gamma-ray emission energies due to imprecision of the peak center extraction, presence of shielding, count rate, calibration errors, and incident spectrum itself (e.g. presence of other near peaks). It would be difficult to assemble a training set sufficiently large to cover the space of solution directly from peak search, and it is therefore more practical to group various solution into features before feeding them into the classifier.

This dimensionality reduction step is a familiar process for anyone applying machine learning for classification problems, it is also the least directly covered aspect of radionuclide identification in published literature. Properly engineered features necessitate domain knowledge and in-depth understanding of the problem space. As a result, this step can be rather expensive, and could be considered the “secret sauce” that makes a particular implementation stand out.

One statistical procedure that is used generally for dimensionality reduction in feature design and can be applied to problems in gamma-ray spectroscopy is Principal Component Analysis (PCA). This technique can be applied to transform the spectral space into a principal component space where the first few of these uncorrelated components account for most of variation in the original (energy) space. The mechanics of PCA is the eigenvalue decomposition of the covariance or correlation matrix of underlying data, but in gamma-ray spectroscopy it is the pre-processing centering and normalization of the data that makes the difference in producing principal components that can maximally discriminate among radionuclides [18] [19]. Alternative approaches to decomposition related to PCA that have been applied to analysis of gamma-ray spectra are Independent Component Analysis (ICA) [20], Non-Negative Matrix Factorization (NNMF) [21] and Fisher’s Linear Discriminant (FLD) [22] [23].

## **Classification**

Classification is the process of selecting the correct solution (i.e. radionuclide mixture) based on the results of the peak search and subsequent extracted features. This step necessitates some form of nuclide library [24] to perform the matching, and the libraries size and scope can greatly impact the overall performance by dramatically changing the space of possible solutions. The size of the nuclide library has to be sufficient to cover the problem domain, but not so large as to make the classification task unwieldy. Any algorithm will struggle to find the correct solution, especially within a reasonable amount of time, if the space of possible solutions is infinitely large.

Classifier algorithms are used for a wide area of applications, from sorting emails to medical diagnosis, which vastly exceeds their application for radionuclide identification. As a result, there are a plethora of openly available toolkits that one can leverage directly for radionuclide identification and perform the necessary calculations. In contrast, peak search and feature extraction and design require more domain specific knowledge and are generally not readily

available outside of the gamma-ray spectroscopy community. Classifier algorithms that have been applied to radionuclide identification include:

- 1) **Expert systems:** These are essentially hard coded decision trees that are typically found in commercially available RIIDs. The resulting procedural code is meant to emulate the radionuclide selections that would be made by an expert gamma-ray spectroscopist [25].
- 2) **Neural networks:** As with the aforementioned classifier algorithms, neural networks are used in a wide area of pattern recognition problems. In gamma-ray spectroscopy it has been applied to identify mixture of many radionuclides using the entire spectrum of a low to medium energy resolution detector systems [26] [27] [28] [29]. The neural network can also be used on a reduced feature space [30]. One downside of neural networks is that the decision-making process is opaque, and this may preclude it from application that require the path to the final solution to be audited.
- 3) **Naïve Bayes:** The posterior probability is calculated for each radionuclide where the maximum points to the correct solution [31] [32] [33]. Reasonable conditional probabilities, or likelihoods, have to be estimated from a training set, and any custom model can be developed for this purpose [34]. The prior probabilities are more subjective and should be adjusted depending on operating environment and problem space.
- 4) **Nearest neighbor:** This approach involves calculating a distance metric between feature vectors, for example the Mahalanobis distance [18] [19], in order to find most similar samples. Classification can be derived directly from the proximity to one of the classes in the training data. A variant of this type of algorithm, k-nearest neighbors, can be used to calculate the relative density of each sample in an unlabeled dataset, which can be applied for anomaly detection.
- 5) **Support vector machines:** This method constructs an optimal hyperplane (or hyperplanes) decision boundary, the shape of which is dependent on the chosen kernel (e.g. linear, polynomial, sigmoid). SVM has been applied for radionuclide identification, following peak extraction procedure [35] [36], and using the entire spectra to discriminate among a few classes [37].

The classifier algorithms can help sort the most likely radionuclides that contribute to the sample spectrum, but to find the most likely radionuclide mixture requires the following search optimization strategies

## **Template Matching**

Template matching requires a separate class of algorithms that can search the space of possible radionuclides for the right mixtures which contributes to the spectrum. These types of algorithms fall into two broad categories:

- 1) **Heuristic:** A strategy-based approach that can start from either the full set of possible nuclides and eliminate them on the way to a solution (strip down) [38] [39] [40] [41] or start with background and add nuclides until a solution is found (buildup). The removal or addition of candidate radionuclide is followed by an optimization step (e.g. non-linear least squares regression, gradient decent) to determine the proportions of new set of potential radionuclides. This approach can be efficient at finding the optimal solution, provided that certain conditions are met, and the problem size is not too large. There is also a path dependence, that can change the ultimate outcome (i.e. final solution depends on the initial guess).
- 2) **Systematic** (branch bounds/all subset regression): Considers multiple possible solutions at each decision node, therefore alleviating the problem of path dependence in heuristic methods [39] [42]. Unlike the heuristic approach, which can contain expert provided fallback strategies, this is a more mathematically rigorous approach for solving the combinatorial optimization.

Full detector response information is required for this approach in order to generate the necessary templates [43]. Models are often used since a data-driven approach is not feasible, and these models have to be very accurate for the method to be successful [44]. Slight shifts in spectral shape are especially acute at high energy resolutions, therefore this technique is preferred for low to moderate energy resolution detection systems.

## Open Source Tools

Open source tools are programs for which source code is published and available at no charge provided the user complies with any licensing requirements. For our purposes it will be instructive to distinguish between generic tools, those that have wide multidisciplinary application, and the much smaller universe of radionuclide identification software.

### Generic (Multidisciplinary)

The following tools encompass various methods used in radionuclide identification, and could be pieced together to make a complete identification software suite:

- SciPy [45]: The signal processing part of this python library (scipy.signal) has the smoothing and filtering functions used in peak search, it also includes some derivative and wavelet transformation based peak finding functions. The optimization and root finding packages (scipy.optimize) contain useful least squares solvers.
- PeakUtils [46]: Finding and fitting peaks in 1D data, and higher level wrapper for some scipy.signal methods with additional functionality, such as baseline subtraction.



- Octave [47]: Open source alternative to Matlab, with similar signal processing capabilities as SciPy.
- Scikit-learn [48]: Collection of machine learning tools in python, including all the dimensionality reduction, regression, and classification packages.
- TensorFlow [49]: Popular library for implementing high performance neural networks on both CPUs and GPUs.
- Geant4 [50] : Toolkit for simulating particle interaction through matter, which is useful for detector response modeling.

## Radionuclide Identification Specific

Gamma-ray spectra analysis tools are rarely openly published, and none provide fully automated radionuclide identification – in contrast with the goals of the BARNI project. The few tools that are published are typically packaged as Graphical User Interfaces (GUIs) and are therefore not readily extendable for use directly with detector systems. Instead, these provide assisted analysis for expert gamma-ray spectroscopists.

- InterSpec [51]: Peak-based interactive nuclide identification application and can estimate nuclide activities and shielding. Automatic nuclide identification is not performed, candidate peaks have to be highlighted by the user.
- GammaSpy [52]: GUI wrapper around the non-linear curve fitting routines in SciPy for peak fitting and finding.
- RASE [53] [54]: An acronym for Replicative Assessment of Spectrometric Equipment, this software is used for evaluating the performance of radiation detectors and radionuclide identification algorithms.

## Closed-Source and Commercial Products

As with the open source radionuclide identification counterparts, these closed-source and commercial products are for the most part locked down GUIs that require some manual input for identification:

- GADRAS [55]: Contains many functionalities ranging from modeling detector response, radiation transport and template matcher for radionuclide identification.
- Radio-Nuclide Analysis Kit (RNAK) [56]: Template matching radionuclide identification tool which provides physical properties of the mixtures, summary of nuclide probabilities and source classification.
- PeakEasy [56], GammaVision [57], GENIE 2000 [58], SODIGAM [59]: Gamma-ray spectra visualization tools with peak search and find algorithms. These tools are grouped together because they all have similar functionality, mainly the user manually selects



regions of interest that encompass a peak of interest which can then be labeled with assistance of a built-in library.

We omit listing any RIIDs, such as Rad-ID and identiFINDER, which run hardware dependent non-portable firmware for identification.

## **Patents**

The patents directly relating to radionuclide identification include areas cover variations on: principal component analysis [60], region of interest [61], support vector machines [63], shielding estimation [63] [64], template matching (branch and bound) [42].

## **Evaluations**

BARNI is intended to be used as part of evaluation of other radioisotope identification algorithms and detector systems, therefore it is appropriate to include a summary of previously published reports and articles on the subject. One of the many issues with scoring identification performance is that unlike detection it is not a simple binary decision process, because multiple nuclides could contribute to as single spectrum. A common way to visualize the performance of a classification algorithm is through the construction of a confusion matrix, where each row is the predicted nuclide and the columns are the truth, or actual nuclides present. The F-score, the harmonic mean of precision and recall, can then be used to summarize these results into a single value. These scores can be modified with appropriate weighting factors which reflect the importance of identifying specific nuclides of interest [65].

Using an appropriate scoring metric is only a part of the challenge of comparing radionuclide identification algorithms. Performance of the same algorithm can vary with the change in the selection of nuclides used for training and testing [66]. Defining appropriate categories of errors for identification is also a challenge [67], as reported performance can change depending on the chosen definition of category error. For this reason, pure algorithm requires that there are enough common elements shared between the algorithms to make the comparison fair and meaningful [68].

The availability of relevant and representative spectral data is another challenge for both testing and training radionuclide identification algorithms [69]. Complicating matters are other factors that affect the final spectrum, such as calibration, threshold, pile-up rejection, which are not inherently tied to the measured radionuclide. To control for these factors the relevant sources are often modeled, which produces synthetic spectra that can cover the threat space of interest [70] [71]. These simulations results have to be validated and verified to ensure adherence to physical reality. The physics of photon transport is well understood, and so is the

discrete gamma-ray emission from relevant nuclides. The challenge is often with including other details in the model, such as surrounding materials and details of detector response, which complicate matching measured and simulated spectra.

Rather than testing stand-alone algorithms, the performance of commercially available instrumentation is often compared [72] [73] [74] [75] [76]. The advantage in those cases is that the algorithm is already coupled to the appropriate detector, and presumably the commercial vendor took all the necessary steps to tune instrument performance to the appropriate threat space. In addition, performance criteria for these instruments is already defined by ANSI standard N42.34. Beyond the algorithm itself there are other factors that affect overall performance, such as detector resolution, calibration, material, geometry, and extrinsic factors like count rate [77] [78] [79] [80].

## **Conclusions**

This literature review has attempted to systematically organize the various algorithms and methods employed for the problem of radionuclide identification. Solutions to this problem can be broken down into two broad categories, peak search and template matching, each employing a unique set of approaches and methods. We hope that this document can serve as a guide for researchers in this field in helping sort out the myriad of relevant publications, which are often titled by one method used to solve a subset of the larger problem. This is especially relevant since the proliferation of openly available tools has made it easier to apply powerful methods to this problem, but it remains difficult to quantify the objective performance gains achieved by them. The review of the evaluation literature enumerates the various obstacles in obtaining objective measures of identification performance across different algorithms.

Researchers have a generous pool of open source tools which can tackle the various subset problems of radionuclide identification, but only a handful of software suites that deal with the problem in its totality, and none of them automatically provide identification from input spectra. The closed-source tools that do exist have a limited audience and are often unavailable for those without connections to government institutions or employment at private companies. Therefore, there exists a gap for a fully automated and flexible identification software like BARNI, which could serve as a benchmark for the wider community.

While the final choice of the BARNI implementation will be derived from the project's requirements, this review will provide the basis for choosing the most appropriate methods, leveraging knowledge from this literature search.

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