Interagency Technical Nuclear Forensics Technical Review
SAND2018-7991PE

An Expert Test Bed For Nuclear Forensics Group Inclusion/Exclusion

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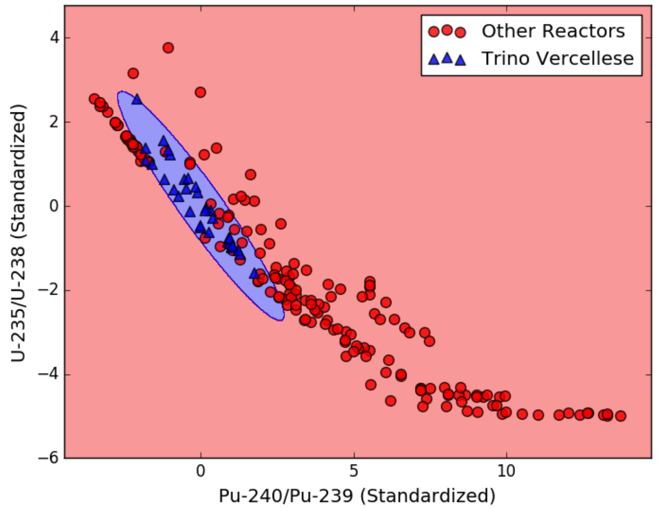
Project Name: Multivariate Algorithms Enabling Group Inclusion/Exclusion of TNF Data
Project Numbers: 16.003, 17.003
Sandia National Laboratories
Funding Agency: NTNFC-TA

Sandia National Laboratories

Multivariate Algorithms Enabling Group Inclusion/Exclusion of TNF Data

Objective: The project is focused on developing mathematically rigorous algorithms and software tools to enable the linking of questioned nuclear materials to their potential processes, location, or fabrication facility.

Relevance: This project will enable the rapid, accurate, and credible identification of the origins of questioned nuclear materials, addressing a key NTNFC objective.



Approach: Use one-class classification methods to statistically compare the multivariate features (e.g., isotopic and trace element measurements) for a questioned nuclear material to the features for materials originating from different, known groups.

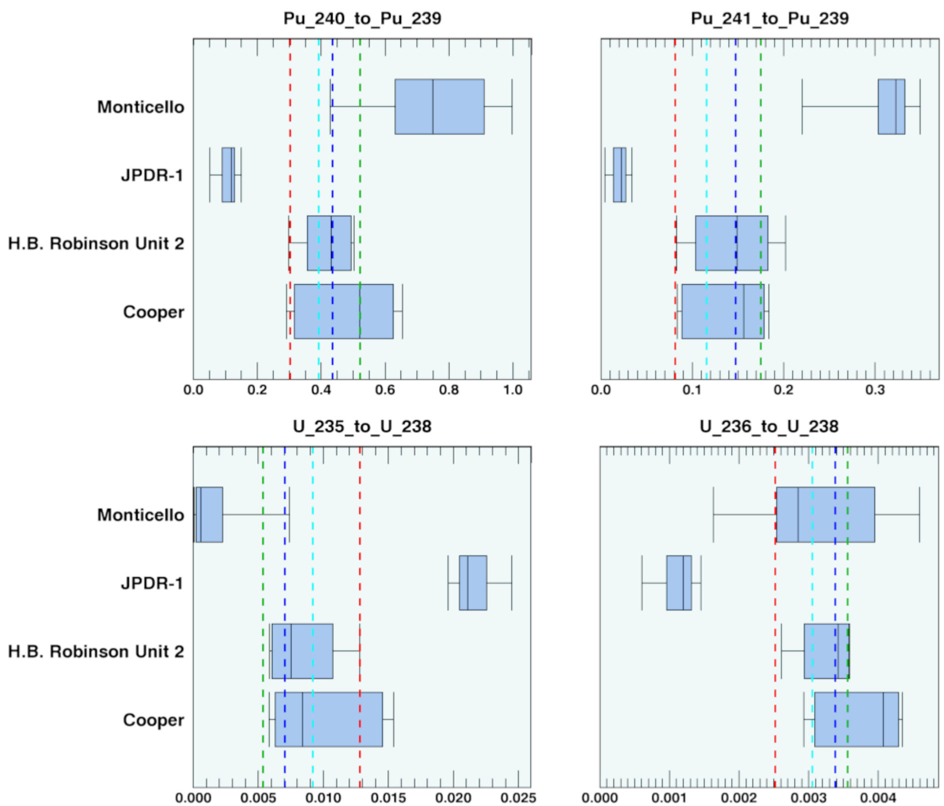
Personnel Support: 4 technical staff members (1 analytical chemist, 3 statisticians)

Accomplishments/Results:

- Developed GUI-based Dynamic Analysis Environment (DAE) software package to facilitate group inclusion/exclusion method testing, evaluation and comparison.
- One journal publication (Computer Physics Communications, 210, 60-71, 2017).
- Developed Python-based expert test bed.
- One conference talk (American Chemical Society, April 2017).
- Completion of uncertainty analysis study.
- Completion of ensemble classifier study.

Overview

Sandia National Laboratories supports both pre/post detonation nuclear forensics including Pu/U Signatures projects, multivariate algorithms enabling group inclusion/exclusion classification, and analyses of NUDET signals.



Sample # Color Key:
1
2
3
4

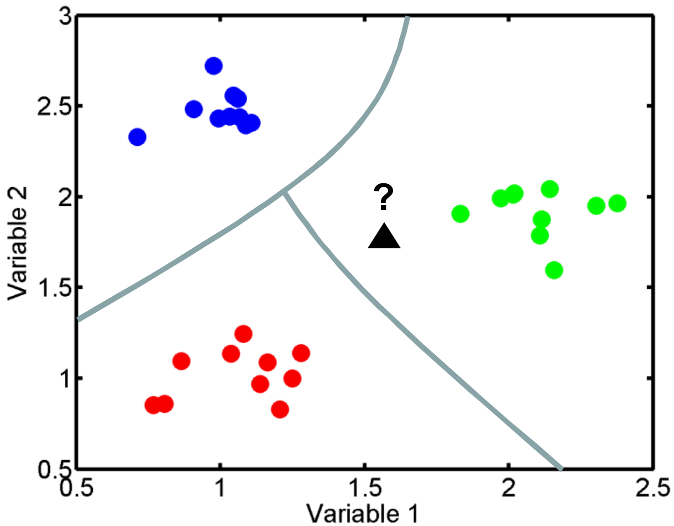
Boxplot visualization tool incorporated in Dynamic Analysis Environment (DAE)* helps analyst compare questioned materials with known groups of nuclear materials, facilitating group inclusion/exclusion. In this example, the four questioned samples most closely resemble the H.B. Robinson Unit 2 reactor.

*C. Stork, M. Clopeck, D. Stuart, “Improved Dynamic Analysis Environment for Nuclear Forensic Analyses,” SNL, 2016.

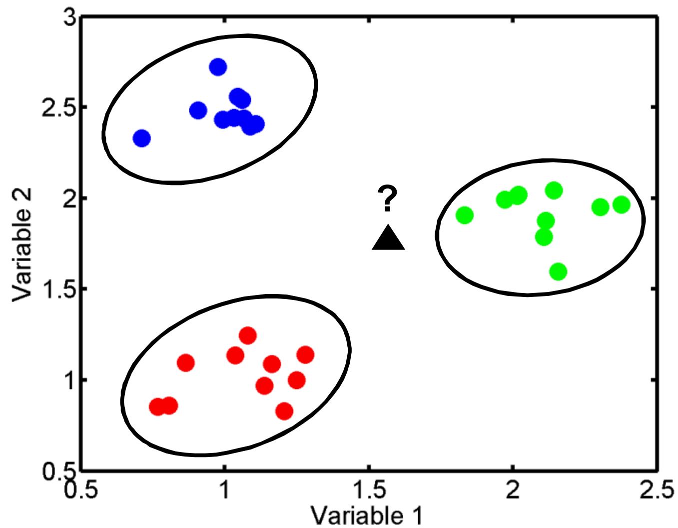
Research/Project Description

Goal: Develop defensible, statistically rigorous tools for nuclear forensics group inclusion/exclusion.
Approach: Employ one-class classification methods to enable both group inclusion and exclusion for questioned nuclear materials.
Relevance: Answer questions regarding how, where, and by whom material was produced.
Recent/Current Work: (1) Expert test bed, (2) ensemble learning, (3) uncertainty analysis.

Discriminant multi-class methods forcibly assign questioned material to known group.



One-class methods allow for exclusion of questioned material from all known groups.



Technical Approach: Expert Test Bed

- Existing software tools predominantly address the discriminant multi-class problem. One-class tools, however, are needed for nuclear material group inclusion/exclusion.
- Developing one-class tools consistent with the Python scikit-learn interface to facilitate group inclusion/exclusion method testing, evaluation and comparison. Benefits include:
  - Tools can be freely distributed and installed on multiple operating systems (Windows, Mac/OS X, Linux).
  - Can leverage scikit-learn modules for data preprocessing, training/test data partitioning, model training and parameter optimization, and model performance evaluation (accuracy, sensitivity, specificity, ROC).

Technical Approach: Expert Test Bed

- One-class methods currently implemented in expert test bed:
  - Hotelling's T^2 Full Rank Covariance: Takes data correlation into account.
  - Principal Component Analysis (PCA): Extracts new set of features that optimally describe variation or major trends in a given data set.
  - Probabilistic Fusion: Statistical approach for fusing the outputs of multiple classification methods or variables.
  - Support Vector Machines (SVM): Constructs boundary around class that encompasses almost all points in the data set with minimum radius.
  - Recently integrated methods include Minimum Covariance Determinant (MCD), Isolation Forest, and Kernel Density Estimation (KDE).
- Demonstrate and evaluate performance of one-class methods using Spent Fuel Isotopic Composition (SFCOMPO) database.

Spent Fuel Isotopic Composition (SFCOMPO) Database

- Open source international database of isotopic compositions for spent nuclear fuels (SNFs) obtained through post-irradiation experiments.
  - Data from 14 reactors in 4 countries
  - Includes U, Pu, Am, Cm and several fission products (Nd, Cs, Sr).
  - 7 boiling water reactors (BWRs) and 7 pressurized water reactors (PWRs).

Gundremmingen/Germany

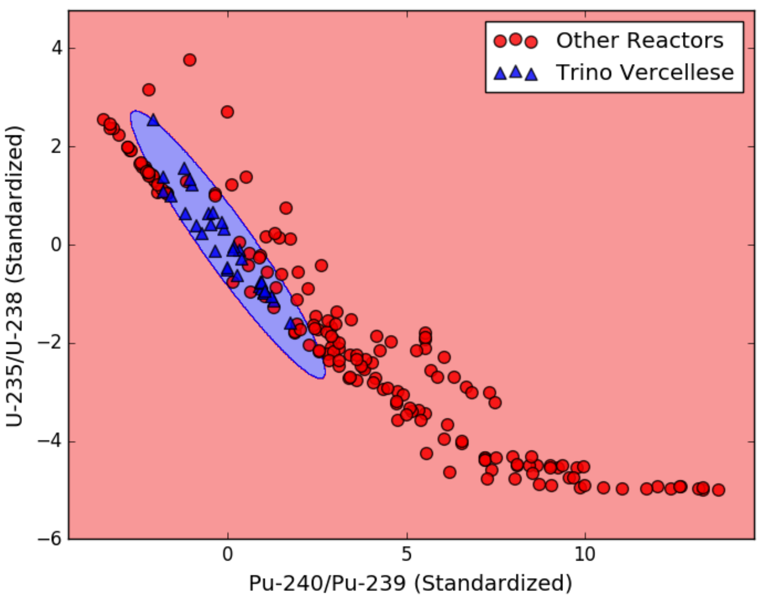
Tsuruga Plant/Japan

Calvert Cliffs No. 1/USA

Technical Approach: Expert Test Bed

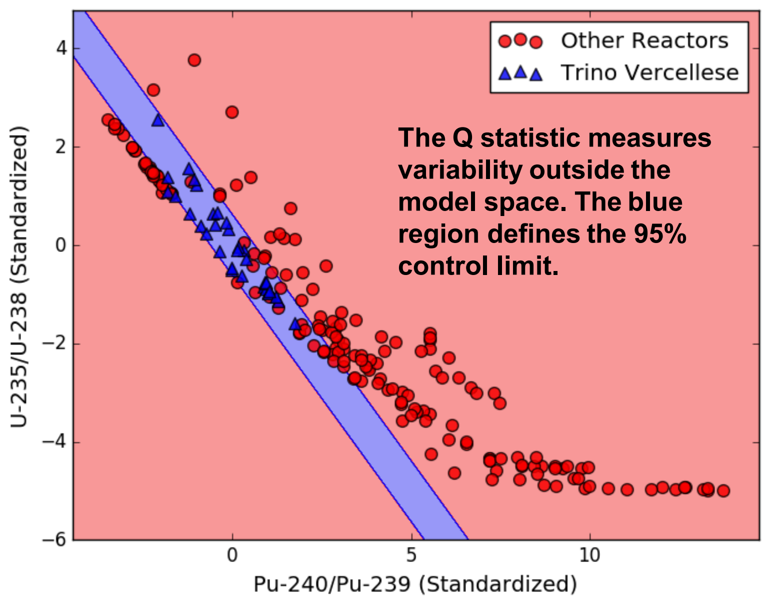
- Models constructed using SNF data from Trino Vercellese:
  - Decision boundaries differentiating Trino Vercellese materials (blue regions) from non-Trino Vercellese materials (red regions) are shown.

Hotelling's T^2 Full Rank Covariance



Models correlations between the two variables. The blue ellipse defines the 95% control limit.

PCA (1 PC), Q Statistic



PCA defines new coordinate system that optimally captures data variance.

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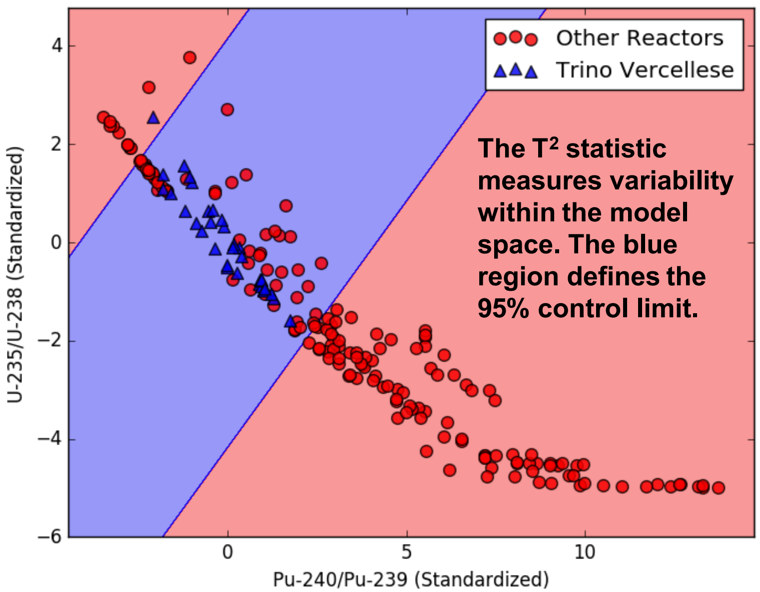
PCA (1 PC), T^2 Statistic



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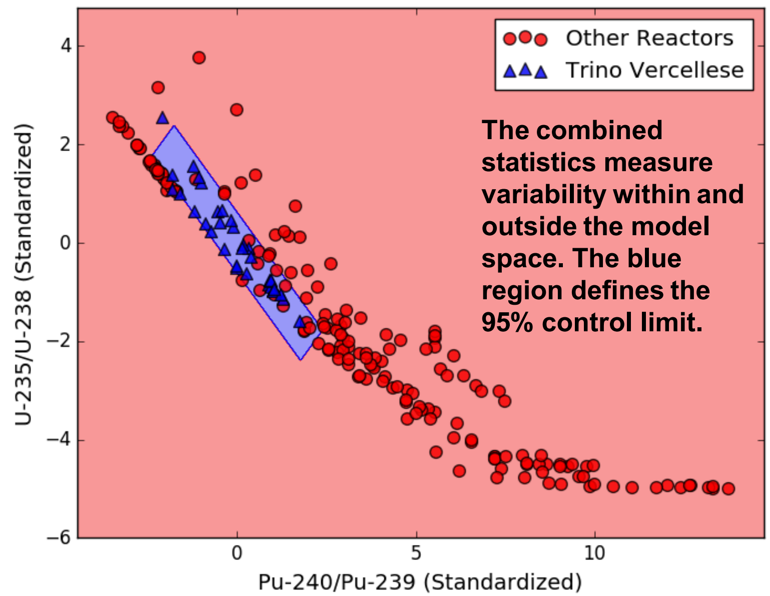
PCA (1 PC), Combined Q and T^2 Statistics



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Technical Approach: Expert Test Bed

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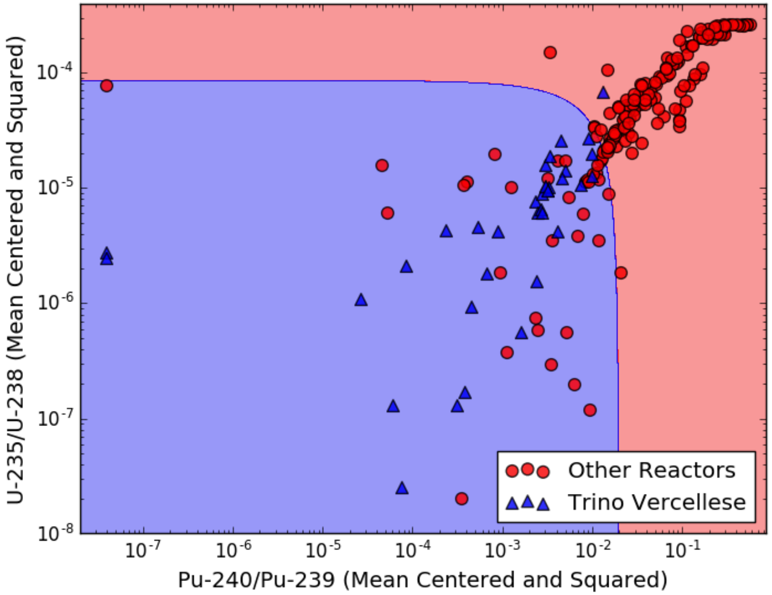
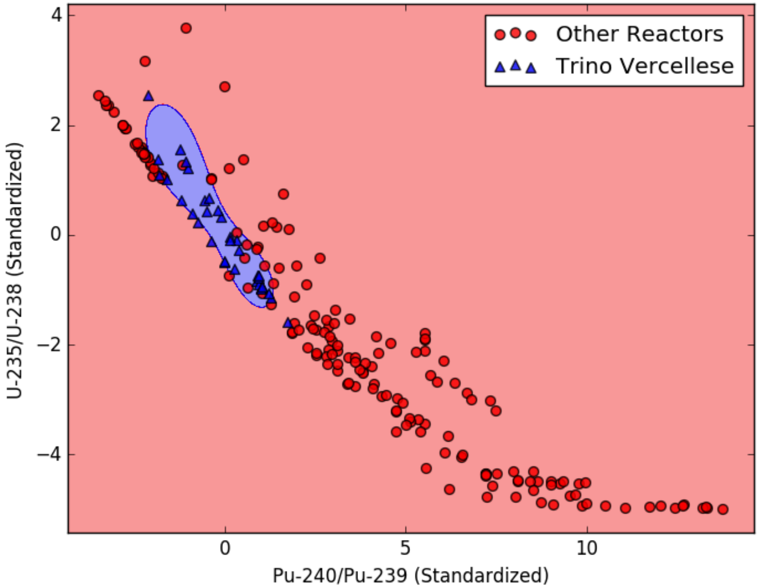
Probabilistic Fusion



One-sided decision boundary is generated. The blue region defines the 95% control limit.

One-Class SVM



One-class SVM is a non-parametric method and its decision boundary cannot be defined in terms of a statistical confidence limit.

Technical Approach: Expert Test Bed

Summary of properties of one-class methods included in expert test bed*:

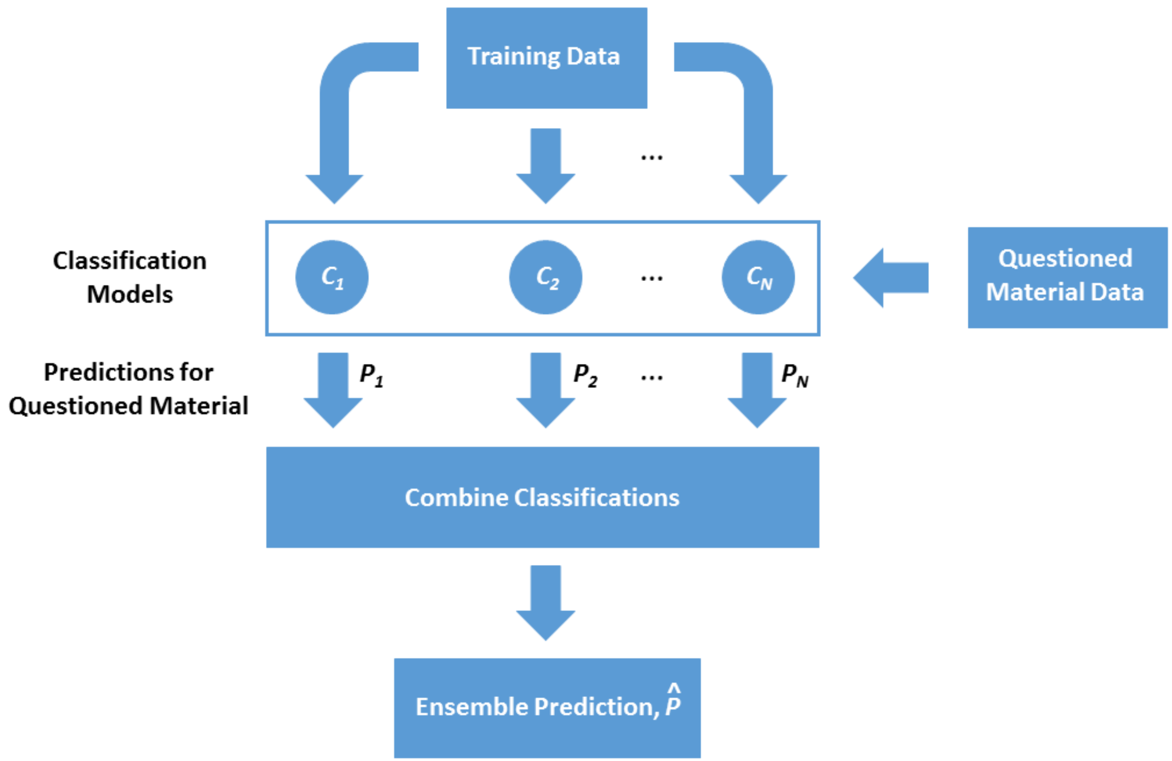
Method	Parametric/ Nonparametric	Structure of Class Boundaries	Estimate of Degree of Certainty	Amount of Training Data Required	Robust to Outliers	Data Sets Method is Appropriate for
1. PCA	Parametric	Linear	Yes	Low	No	Multivariate Normal
2. Hotelling's T^2 Full Rank	Parametric	Hyperellipsoidal	Yes	Low	No	
3. MCD	Parametric	Hyperellipsoidal	Yes	Low	Yes	Elliptically Symmetric
4. Probabilistic Fusion	Parametric	Variable	Yes	Medium	No	Marginal distributions of each variable can be specified
5. One-Class SVM	Nonparametric	Up to Highly Nonlinear	No	Medium	No	Form of class-conditional densities unknown
6. KDE	Nonparametric	Up to Highly Nonlinear	Yes	High	No	
7. Isolation Forest	Nonparametric	Up to Highly Nonlinear	No	Medium	Yes	

*C. Stork, "Properties of one-class classification methods and guidelines for method selection in nuclear forensics," SNL, 2018, in preparation.

Technical Approach: Ensemble Learning

Ensemble learning uses a collection of multiple, individually trained classification models to predict the group membership of a questioned material.

- Motivation for using ensemble learning is that accuracy of combined classifier can exceed accuracy of any individual model (reduce variance and/or bias).



Ensemble methods used:

- Majority vote – Class allocation decided based on what majority of base classifiers predict.
- Bagging – Averages predictions over set of bootstrap samples.
- Boosting – Algorithm for fitting adaptive basis function models, where more weight is placed on observations that are difficult to classify.
- Stacking – Combines predictions from multiple, different classification methods.

Technical Approach: Ensemble Learning

Compared performance of individual classifiers and ensemble methods using SFCOMPO*:

- For individual classifiers, Hotelling's T^2 method performed very well.
- Bagging showed results that were marginally better than individual classifiers.
- Overall, ensemble methods did not significantly improve on the individual classifiers due to the small number of observations in SFCOMPO.

Average statistics for individual classifiers

	Accuracy	Precision	Sensitivity	Specificity	NPV
SVM	0.94	0.77	0.40	0.98	0.95
NORM	0.78	NA	0.23	0.82	0.93
KNN_1	0.42	0.19	0.82	0.41	0.92
KNN_3	0.40	0.19	0.87	0.37	0.93
KNN_5	0.38	0.19	0.90	0.36	0.92
PCA/Q	0.62	0.29	0.88	0.59	0.99
PCA/T^2	0.26	0.17	1.00	0.21	0.92
PCA/C	0.63	0.29	0.88	0.61	0.99
T^2	0.98	0.90	0.99	0.98	1.00
Tree	0.89	0.45	0.38	0.92	0.95

Average statistics for ensemble methods

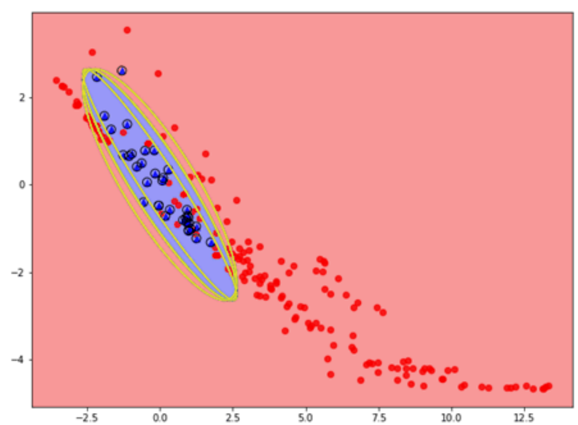
	Accuracy	Precision	Sensitivity	Specificity	NPV
Stacking	0.85	0.66	0.92	0.99	0.99
Tree Boost	0.92	NA	0.36	0.97	0.95
Bag SVM	0.94	NA	0.33	0.99	0.94
BagNORM	0.79	NA	0.20	0.83	0.92
Bag KNN	0.93	0.19	0.96	0.27	0.99
Bag PCA/Q	0.68	0.35	0.99	0.66	1.00
BagPCA/T^2	0.27	0.16	1.00	0.21	NA
Bag PCA/C	0.68	0.35	0.99	0.66	1.00
Bag T^2	0.99	0.92	0.96	0.99	0.99
RandFores	0.93	NA	0.18	1.00	0.93

*D. Ries, A. Foss, N. Martin, "Ensemble methods for one class classification in nuclear forensics," SNL, 2018.

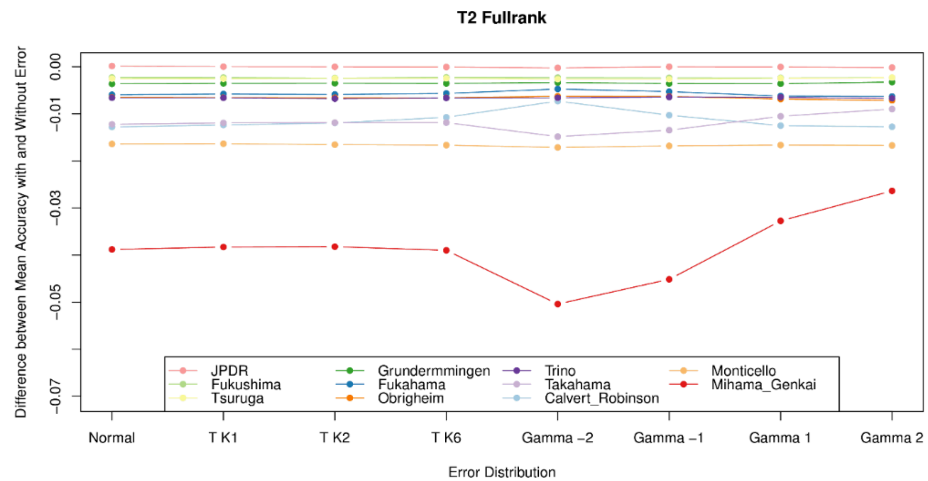
Technical Approach: Uncertainty Analysis

- Completed statistical study investigating and quantifying impact of uncertainty in input variables on uncertainty in the group inclusion/exclusion model*.
- Used uncertainty information on isotopic and trace element measurements for SFCOMPO to design Monte Carlo simulation, whose aim was to quantify impact of uncertainty under various distributional assumptions on model performance.
- Overall, found that impact of uncertainty in input variables due to measurement uncertainty is small in SFCOMPO data set (due to small magnitude of uncertainty in isotopic measurements).

Impact of measurement error on decision boundary for Trino Vercellese reactor



Difference between mean accuracy with and w/o error



*N. Martin, A. Foss, "The Impact of Uncertainty in Input Variables on the Uncertainty in Group Inclusion/Exclusion Models," SNL, 2018.

Results / Accomplishments

Dynamic Analysis Environment (DAE) Package for Nuclear Forensics

- Developed fully functioning software package for nuclear forensics data visualization and group inclusion/exclusion analysis.
- One peer-reviewed journal article documenting DAE package:
  - C.L. Stork, C.C. Ummel, D.S. Stuart, S. Bodily, B.L. Goldblum, “Dynamic Analysis Environment for Nuclear Forensics,” Computer Physics Communications 210 (2017) 60-71.

Expert Test Bed for Nuclear Forensics Group Inclusion/Exclusion

- Seven one-class methods integrated in expert test bed.
- Tools validated using SFCOMPO database.
- One conference presentation:
  - C.L. Stork, “Assessment of One-Class Supervised Pattern Recognition Methods for Nuclear Material Group Inclusion/Exclusion,” 253rd American Chemical Society National Meeting, San Francisco, CA (2017).

Ensemble Methods for Nuclear Forensics

- Completed statistical study comparing performance of individual one-class classifiers and ensemble methods for SFCOMPO.
- Technical report documenting comparison study near completion.

Uncertainty Analysis

- Completed Monte Carlo simulation study investigating and quantifying impact of uncertainty in input variables on uncertainty in the group inclusion/exclusion model for SFCOMPO.
- Technical report documenting simulation study completed.

Future Plans

- Start moving tools and advances developed within DAE and expert test bed into production ready environment to support nuclear forensics analysis. Vision is to create environment that is:
  - User friendly and highly interactive.
  - Freely distributable.
  - Installable on multiple operating systems (Windows, MAC/OS X, Linux).
  - Installable on unclassified and sensitive systems.
- FY18 tasks include requirements document for production ready environment, nonfunctioning mockup of proposed environment, and effort timeline for fully functional environment.
- Successful planning for production ready environment will require input from potential users and stakeholders.