

Todo list

Cite inverse stuff, possibly adjoint?	1
Workflow for determining SNF quantities of interest	2
find MS technique and citation	3
assumes previous section on fuel cycle sim	3
cite and discuss	4
cite hungarian guy, viz guy, dayman paper	4
insert ML schematic	5
insert example diagnostic plot?	5
cite dayaman	5
intro, alg math, explain distance metrics	6
intro, alg math, explain regularization	6
add schematics from pres...or diff pics with the math?	7
cite	9
add deets and citations	9
show table of training set space	9
show table of test set space	9
either explain or cite cross validation next	9
Discuss understanding confidence intervals in predictions.	12
add label	12
other classification tasks?	12
or burnup?	12
add label when this section is done	12

general knowledge or citation?	12
the algorithm validation section	12
should this be introduced in the background?	12
ROC curves, confidence intervals on error, confusion matrix if nec- essary	13
the algorithm comparison section	13

My Awesome Title

by

Arrielle C. Opotowsky

A dissertation submitted in partial fulfillment of
the requirements for the degree of

Doctor of Philosophy

(Engineering Physics)

at the

UNIVERSITY OF WISCONSIN-MADISON

2017

Date of final oral examination: 01/01/2100

The dissertation is approved by the following members of the Final Oral Committee:

Jane Doeverything, Professor, Electrical Engineering

John Dosomethings, Associate Professor, Electrical Engineering

© Copyright by Arrielle C. Opotowsky 2017
All Rights Reserved

Please insert your dedication here.

ACKNOWLEDGMENTS

It is customary for authors of academic books to include in their prefaces statements such as this: "I am indebted to ... for their invaluable help; however, any errors which remain are my sole responsibility." Occasionally an author will go further. Rather than say that if there are any mistakes then he is responsible for them, he will say that there will inevitably be some mistakes and he is responsible for them....

Although the shouldering of all responsibility is usually a social ritual, the admission that errors exist is not — it is often a sincere avowal of belief. But this appears to present a living and everyday example of a situation which philosophers have commonly dismissed as absurd; that it is sometimes rational to hold logically incompatible beliefs.

— DAVID C. MAKINSON (1965)

Above is the famous "preface paradox," which illustrates how to use the `wbepi` environment for epigraphs at the beginning of chapters. You probably also want to thank the Academy.

CONTENTS

Contents iii

List of Tables v

List of Figures vi

Abstract vii

1 Introduction 1

1.1 *Motivation* 1

1.2 *Methodology* 5

1.3 *Goals* 5

2 Literature Review 6

2.1 *Nuclear Forensics* 6

2.2 *Machine Learning* 6

2.3 *Fuel Cycle Simulation* 8

2.4 *Applying Statistical Methods to Nuclear Forensics Analysis* 8

3 Demonstration 9

3.1 *Introduction* 9

3.2 *Experimental Components* 9

3.3 *Comparison to Other Work* 10

3.4 *Expanding the Training Set* 10

4 Methodology 11

4.1 *Experimental Design* 11

4.2 *Posting here for now* 12

4.3 *Validation* 12

References 14

LIST OF TABLES

LIST OF FIGURES

ABSTRACT

FIXME: basically a placeholder; do not believe

I did some research, read a bunch of papers, published a couple myself, (pick one):

1. ran some experiments and made some graphs,
2. proved some theorems

and now I have a job. I've assembled this document in the last couple of months so you will let me leave. Thanks!

1 INTRODUCTION

Fill me in, yo.

1.1 Motivation

In the event of a nuclear incident, such as the retrieval of stolen nuclear material or the detonation of a dirty bomb, it is necessary to learn as much as possible about the source of the materials in a timely manner. In the case of non-detonated special nuclear material, knowing the reactor parameters that produced it can point investigators in the right direction in order to determine the chain of custody of the interdicted material. Determining these parameters (e.g., reactor type, cooling time, burnup) requires first characterizing and calculating certain isotopic ratios, chemical compounds, or trace elements. Both radiological methods (e.g., gamma spectroscopy) and ionization methods (e.g., mass spectroscopy) measure these quantities. Although both measurement techniques have a multitude of techniques within them and thus varying strengths and weaknesses, the main tradeoff is between time/cost and amount of information gained.

The results of these analytic techniques are then compared against existing databases to obtain the desired reactor parameters. These databases are highly multidimensional, and furthermore, are rife with missing data entries and inconsistent uncertainties. Direct comparison between measurement results and a database therefore may not yield accurate results. Thus, computational techniques have been developed by nuclear engineers to calculate the parameters relevant to nuclear forensics analysis. Another approach with the uniqueness of requiring minimal domain knowledge is the use of statistical methods via machine learning algorithms to predict these characteristics or values. These algorithms can create a model using the database entries that enables "filling between the lines" of its entries.

Cite
inverse
stuff,
possibly
ad-
joint?

Additionally, having a machine-learned model may overcome the above challenges of multidimensionality, missing data, and irregular uncertainty.

Needs in Nuclear Forensics

The process of nuclear forensics includes the analysis and interpretation of nuclear material to determine its history, whether that be intercepted spent nuclear fuel, uranium ore concentrate, or the debris from an exploded nuclear device. After the technical portion is complete, intelligence data can be used to aid in material attribution; this is the overall goal of nuclear forensics.

This study focuses on non-detonated materials, specifically, spent nuclear fuel. It is important to determine if some intercepted material is from a commercial fuel cycle or if it is meant for weapons production (and where the material was obtained from).

: measure material, use isotope content and/or isotope ratios to determine things like reactor type, fuel type and enrichment at beginning of irradiation, cooling time, burnup. (Classification, Characterization, Interpretation (Analysis), Reconstruction (Attribution) - from the New Nuclear Forensics book) (Char methods to get isotopic ratios or use S/ML, Interp examples) After the material characteristics are measured, they are matched in a forensics database that includes some or all this information for pre-existing/pre-measured SNF. These databases are kept by individual countries, and a given database will have widely varying uncertainty depending where the material was measured as well as missing data in some fields. Therefore, matching can be difficult.

Workflow
for
deter-
mining
SNF
quanti-
ties of
interest

A lofty goal for the forensics community would be to develop methods that provide instantaneous information that is reliable enough to guide an investigation (e.g., within 24 hours). Fast measurements to provide isotopic ratios to calculate the above-mentioned fuel parameters of interest would provide this via some form of a handheld detector that measures

gamma spectra. However, while this nondestructive analysis is rapid, it is also difficult to evaluate because of the presence of overlapping peaks. Thus, gamma spectra give less information at a higher uncertainty than the near-perfect results of some destructive mass spectroscopy techniques, like TIMS. Additionally, within gamma spectroscopy techniques (e.g., field vs. lab detectors), uncertainties can vary significantly because of the detector response, environment, storage, electronics, etc. However, using a well-trained machine-learned model may be able to overcome these inherent issues with gamma spectra. The current and future work of this study is designed with this in mind.

find
MS
tech-
nique
and
citation

Contribution of Statistical Methods

While different machine learning algorithms and parameters will be investigated, it is first important to determine if statistical methods can overcome the inherent database deficiencies. Thus, this paper focuses on probing the amount of information required to obtain realistic results. This can be best understood as the analogous real-world scenario. Although mass spectroscopy techniques provide extremely accurate isotopic information, they are time-consuming and more expensive. And although gamma spectroscopy can give extremely fast results cheaply, it only measures certain radiological signals and is influenced by many environmental factors, storage, and self-attenuation.

In the simulation and machine learning paradigm, we need to determine what exactly is needed to train a machine-learned model. Of interest to an entity trying to create a weapon is partially irradiated fuel if they have plutonium separations capabilities or any radioactive substance in the case of a dirty bomb. Addressing the former, we used a set of simulations of spent nuclear fuel at different burnups and cooling times.

assumes
previ-
ous
section
on fuel
cycle
sim

Can the algorithm overcome the deficiencies of gamma detection and still provide useful results? Or does it need more information, e.g., exact

isotopics? Thus, ultimately, the goal is to answer the question *How does the ability to determine forensic-relevant spent nuclear fuel attributes degrade as less information is available?*.

But first, we must establish some baseline expectations of reactor parameter prediction and algorithms to use. This work is based off previous work on the subject (cite Dayman) regarding machine learning performance with respect to information reduction, and expands upon it by also evaluating a more advanced machine learning algorithm: support vector regression. Below is a more in depth discussion of nuclear forensics and how machine learning can contribute to this research area. After that, an experimental design is outlined. Lastly, the results are presented and discussed.

Given imperfect data with varying amounts of uncertainty as well as the required comparison to highly multidimensional databases with missing entries, many have begun considering computational approaches to nuclear forensics problems, such as the INDEPTH

Another approach utilizes artificial intelligence to solve nuclear forensics problems, such as implementing searching algorithms for database comparison and machine learning for determining spent fuel characteristics. A variety of statistical and machine learning tools have been used to characterize spent fuel by predicting categories or labels (reactor type, fuel type) as well as predicting values (burnup, initial enrichment, or cooling time) The former uses classification algorithms and the latter uses regression algorithms. Many algorithms can be applied to both cases.

A typical (supervised) machine learning workflow would take a set of training data with labels or values inserted into some statistical learner, calculate some objective, minimize or maximize that objective, and provide some model based on that output. Then a test set (with known values) is provided to the model so that its performance can be evaluated and finalized. After model finalization, a user can provide a single instance

cite
and
discuss

cite
hun-
garian
guy,
viz
guy,
day-
man
paper

and a value can be predicted from that.

To obtain reliable models, one must 1. choose/create a training set carefully and 2. study the impact of various algorithm parameters on the error. Many algorithms are developed on an assumption that the training set will be independent and identically distributed (i.i.d.). [Aside: there are ways to handle skewed data sets] This is important so that the model does not overvalue or overfit a certain area in the training space. Additionally, algorithm performance (or error) can be optimized with respect to training set size, number of features, or algorithm parameters (regularization terms, etc). These are known as diagnostic plots. When plotting the training and testing error with respect to the number of instances, this is known as a learning curve. When plotting these errors with respect to the number or features or algorithm parameters, this is known as a validation curve.

Algorithm choice is usually based on what is being predicted and intuition regarding strengths and weaknesses. For the sake of comparison (i.e. weak validation), some machine learning approaches here are based on previous work while also extending to a more complex model via an algorithm that is known to handle highly dimensional data sets well. Thus, this paper investigates three regression algorithms: nearest neighbor, ridge, and support vectors.

insert
ML
schematic

insert
exam-
ple
diag-
nostic
plot?

cite
daya-
man

1.2 Methodology

Talk about workflow here. Might need separate tex file. Prob should keep pretty simple since everything is discussed later in the demonstration part of the prelim.

1.3 Goals

I have many goals.

2 LITERATURE REVIEW

Fill me in, yo.

2.1 Nuclear Forensics

Need to figure out what to put here and what goes in intro.

2.2 Machine Learning

Something Introductory

Doopdedoop poopdepoop I'm an intro or something

Classification and Regression Algorithms

Blah blah I know it's only regression right now

Nearest Neighbor Regression

Nearest neighbor regression calculates a value based on the instance that is closest to it. The metrics for distance differ, but in this study, Euclidian distance was used. There is no learning in this regression, per se, the training set populates a space and the testing set is compared directly to that.

intro,
alg
math,
explain
dis-
tance
metrics

Ridge Regression

intro,
alg
math,
explain
regular-
ization

Ridge regression utilizes normal linear least squares regression, but with a parameter that penalizes correct answers to prevent overfitting, which is referred to as regularization.

Support Vector Regression

Support vector regression (SVR) is an extension of the popular classification algorithm, support vector machine (SVM). This algorithm was chosen because of its ability to handle highly dimensional data well, which in this study is approximately 300 features.

SVM classifies two classes by determining an optimal hyperplane, given by $wx+b$, between them. As seen in Figure ?, the algorithm evaluates the quality of the line that separates two classes by maximizing the width of the margin given the constraints surrounding the line. Some problems are not linearly separable, and thus a penalty term is introduced to allow for misclassifications. As shown in Figure ?, the algorithm then simultaneously minimizes the misclassifications while maximizing the margin.

This can be extended easily to multidimensional analysis via what is called the *kernel trick*. First, using a nonlinear kernel function maps the data into higher dimensional feature space. Then the algorithm can find a linear separation in this space, as shown in Figure ?. Further, this can be upgraded from classification to SVR by doing similar math but instead minimizing the margin, as shown in Figure ?.

The kernel chosen for this study is the Gaussian radial basis function, shown below. This has two tuneable parameters, gamma and C. Gamma influences the width of influence of individual training instances, and strongly affects the fitting of the model. Low values correspond to underfitting because the instances have too large of a radius (low influence) and high values correspond to overfitting because the instances have a small

add
schematic
ics
from
pres...or
diff
pics
with
the
math?

radius (high influence).

The C parameter also affects the fitting of the model by allowing more or less support vectors, corresponding to more or less misclassification. A lower C smooths the surface of the model by allowing more misclassifications, whereas a higher C classifies more training examples by allowing fewer misclassifications. Too low and too high of a C can cause under- and overfitting, respectively.

Since there is a tradeoff of fitting strength provided by both parameters, it is common to run the algorithm on a logarithmic grid from 10^{-3} to 10^3 for each parameter. If plotted on a heatmap of accuracies given gamma and C , there will be a diagonal of ideal combinations that emerges. The lowest of these is usually chosen.

Beep

2.3 Fuel Cycle Simulation

Boop

2.4 Applying Statistical Methods to Nuclear Forensics Analysis

Bop

3 DEMONSTRATION

Fill me in, yo.

3.1 Introduction

Need to figure out what to put here and what goes in intro. Also workflow details repeated if it's in the intro?

3.2 Experimental Components

This work begins by simulating the training and test sets described in ref (cite Dayman). As with the previous work, this will be done using SCALE 6.2 . Specifically, the ARP module of the activation and depletion code ORIGIN was used.

The parameters of the training set are defined as follows. A smaller burnup than is typical for spent fuel from a commercial reactor is used in the previous work likely because stolen fuel pins for weapons use would not likely be at the end of their lifetime, as the plutonium of interest has decreased by then. A truly i.i.d. training set would go beyond this, but this is purely for demonstration with a single use case in mind.

The previous work also used an external test set, designed to have values in between the trained values of burnup. This is implemented in this study but it is expected that cross-validation will better indicate the model performance. More specifically, using k-fold cross-validation is a common method to use in the application of machine learning to create more confidence in the resulting model. detector response function and iso ID here's some awesome success with only isotopes

cite

add
deets
and ci-
tations

show
table of
train-
ing set
space

show
table of
test set
space

either
explain
or cite
cross
vali-
dation
next

3.3 Comparison to Other Work

Information Reduction

This study evaluates the impact of randomly introduced error of varying amounts on the ability of the algorithms to correctly predict the burnup. Thus, first investigated are the three algorithms with no error introduced, and next with the random errors applied uniformly to each nuclide vector. Since error in a nuclide vector is not random, in fact it is systematic and dependent on a number of known sources of uncertainty, the next study will introduce error by limiting the nuclides to only those that can be measured with a gamma spectrometer (future work).

3.4 Expanding the Training Set

BeepBop

4 METHODOLOGY

This is the main methodology intro.

4.1 Experimental Design

Introduction

blah

Algorithm Evaluation

Additionally, machine learning algorithms are heavily dependent on the inputs and parameters given to them, such as training set sizes, learning rates, regularization, etc. To evaluate the performance or tweak the model from an algorithm, diagnostic plots will be used. Learning and validation curves will indicate how the models are performing, initially both with respect to the testing error and the cross validation error. As previously mentioned, these two errors are to be compared to the training error to understand the prediction and generalization strength with respect to training set size and the algorithm parameters governing model complexity.

The learning curves were obtained as follows. For a given (randomly chosen) training set size between 15 and 100% of the total data set, several training and prediction rounds were performed. The repetition for obtaining the testing error is the same value as the k in k -fold cross validation. The testing error scenario averages the values of the obtained errors whereas the k -fold cross-validation performs this automatically. The validation curves were obtained as follows. For a given parameter, the value of the parameter is varied and k training and prediction phases are completed, and their errors averaged. Again, for k -fold cross-validation,

these errors are already averaged. The learning curves help determine if we are over- or under-training. The validation curves help determine the optimal way to be robust to over- and under-fitting.

Comparing Algorithms

Maybe can delete this if I already discuss it in the above section. Options for comparison of algorithms: Comparing classification of 2 classes on same ROC plot with multiple ML systems, Scatter plots, Pairwise t-tests.

4.2 Posting here for now

1. Learning curve 2. Validation curve 3. Random error curve

Want to show the difference between test/train error plots and CV/-train error plots. Determine some argument that prefers the latter. For the above categories in the validation section, can show plots directly next to each other (for 1, 2, 3) to hopefully show that cross validation provides better generalizability.

4.3 Validation

As previously mentioned in the demonstration section, the validation was carried out as a comparison of accuracies of the predicted classes (reactor type,) and values (enrichment amount) to the classes and values in the predetermined test data set (discussed in).

However, because it is difficult to ensure consistently representative testing data, the accuracy of a learned model should not depend on only one testing set . The learned model's accuracy can be better evaluated as discussed in by using cross validation . Other additional evaluation

Discuss understanding confidence intervals in predictions.

add label

other classification tasks?

or burnup?

methods will be discussed here as well.

In addition to evaluating a single learned model, it may be beneficial to compare models. As discussed in , there are three methods that will be used: comparison of Receiving Operator Characteristic (ROC) curves, scatter plots, and pairwise t -tests.

the
algo-
rithm
com-
parison
section

ROC
curves,
confi-
dence

REFERENCES

Dayman, Kenneth, and Steven Biegalski. 2013. Feasibility of fuel cycle characterization using multiple nuclide signatures. *Journal of Radioanalytical and Nuclear Chemistry* 296:195–201.