

Evaluating Statistical Methods for Nuclear Forensics Analysis

Preliminary Examination

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Outline



1 Introduction

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2 Literature Review

Nuclear Forensics

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Algorithms for Prediction

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ML Model Validation

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Research Overview



How does the ability to determine forensic-relevant spent nuclear fuel attributes using machine learning techniques degrade as less information is available?

Determine

The inverse problem: given end measurements, calculate the model parameters that created them

Information

Nuclide vectors, measurements of isotope ratios

Forensic-relevant Attributes

Reactor type, enrichment, cooling time, burnup

Machine Learning Techniques

Creating statistical models (not physical)

Degrade

Model prediction performance

Less Information

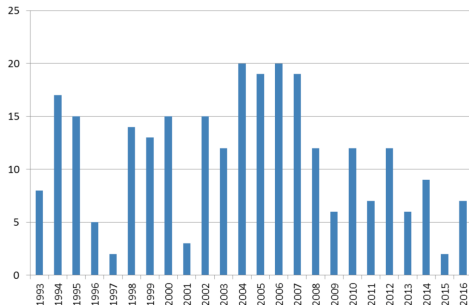
Error in nuclide vectors, fewer measurements, etc

Figure 1: Definitions of terms within the main research question



Nuclear Security and Forensics

Incidents related to trafficking or malicious use, 1993–2016



- FY2016 DHS DNDO budget : 0.3 bill
- FY2016 DOE NNSA nonpro budget : 1.6 bill

Figure 2: 24 years of incidents: HEU (12), Pu (2), Pu-Be neutron sources (4) [Obtained from: <https://www.iaea.org/sites/default/files/17/12/itdb-factsheet-2017.pdf>]



Needs in Nuclear Forensics

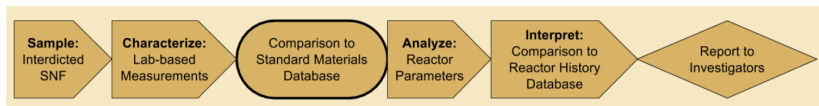


Figure 3: Typical technical nuclear forensics workflow

Material-specific:

- Measurement needs
- Measurement techniques
- Forensic signatures

Challenges:

- Rapid characterization
- Forensics databases
 - Multidimensional
 - Inconsistent uncertainties
 - International cooperation



Computational Methods

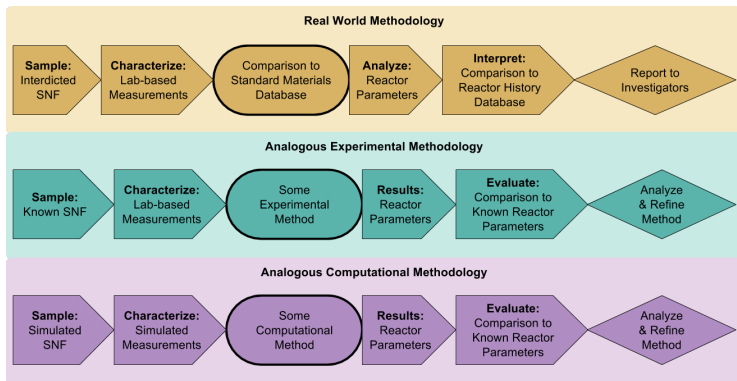


Figure 4: Nuclear forensics research: physical, experimental, and computational

Computational Methods

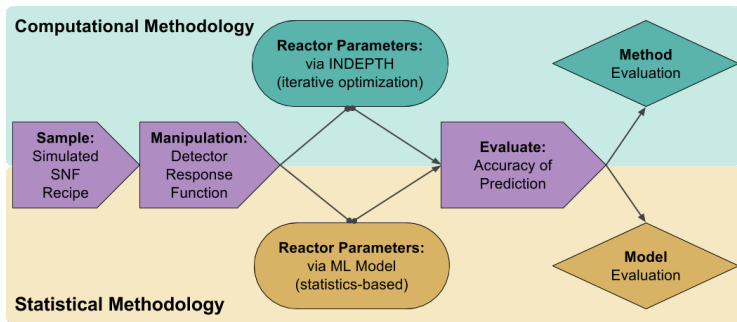


Figure 5: Comparison of two different computational approaches



Statistical Methods

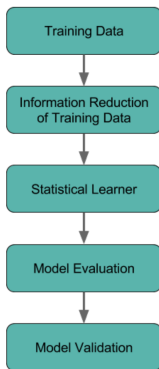


Figure 6: Workflow of a methodology using statistical models

- Training data: large set of SNF measurements
 - Labels (e.g., burnup)
 - Features (e.g., nuclide concs)
 - Instances (individual SNF recipe)
- Statistical learner
 - Machine learning algorithms
 - Algorithm parameters
 - Predict label of new instance
- Model evaluation
 - Diagnostic curves
 - Learning curves
 - Validation curves
 - Prediction error
 - Bias versus variance
 - Generalizability

Statistical Methods



	TRAINING DATA	TESTING DATA
Physical Motivation		
Ideal World	<i>Lab-Measured Mass Spectra</i>	<i>Lab-Measured Mass Spectra</i>
Real World	<i>Lab-Measured Gamma Spectra</i>	<i>Field-Measured Gamma Spectra</i>
Computational Representation		
Ideal World	<i>Simulation-Created Isotopics</i>	<i>Simulation-Created Isotopics</i>
Real World	<i>DRF-Derived Gamma Spectra</i>	<i>DRF-Derived Gamma Spectra</i>

Figure 7: Illustration of data set modularity

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Nuclear Forensics Investigations



Post-detonation

- Collection: debris, swipe samples
- Characterization: rapid analysis of isotope ratios
- Goals
 - Inverse problem: reconstruct weapon design/yield
 - Safety: informing disaster response
- Data evaluation



Nuclear Forensics Investigations

Post-detonation

- Collection: debris, swipe samples
- Characterization: rapid analysis of isotope ratios
- Goals
 - Inverse problem: reconstruct weapon design/yield
 - Safety: informing disaster response
- Data evaluation

Pre-detonation

- Collection: depends on intercepted material
- Characterization: non-destructive and destructive
- Goals:
 - Inverse problem: material chain of custody
 - Safety: material handling and security
- Data evaluation



Nuclear Forensics as an Inverse Problem

Use Bayes' Framework:

$$P(M|D) = \frac{P(D|M)P(M)}{P(D)}$$

M : **M**odel parameters

D : Measured **D**ata

Physical System	Bayes Representation	Calculated from:	
Model Parameterization	Prior Probability : P(M)	Model Space	Simulation <i>Input</i> : Rxtr Parameters
Forward Problem	Marginal Likelihood : P(D)	Data Space	Simulation <i>Output</i> : SNF Recipes
	Likelihood : P(D M)	Both	<i>Output</i> + <i>Input</i> = (Statistical) Model
Inverse Problem	Posterior Probability : P(M D)	Both	(Statistical) Model : <i>Output</i> -> <i>Input</i>

Table 1: Mapping the study of a physical system its Bayesian representation



Machine Learning

ML Tasks	Supervised	Unsupervised
Variable Types		
Discrete	Classification	Clustering
Continuous	Regression	Dimensionality Reduction

Figure 8: Table depicting the different machine learning algorithms depending on the task



Supervised Regression

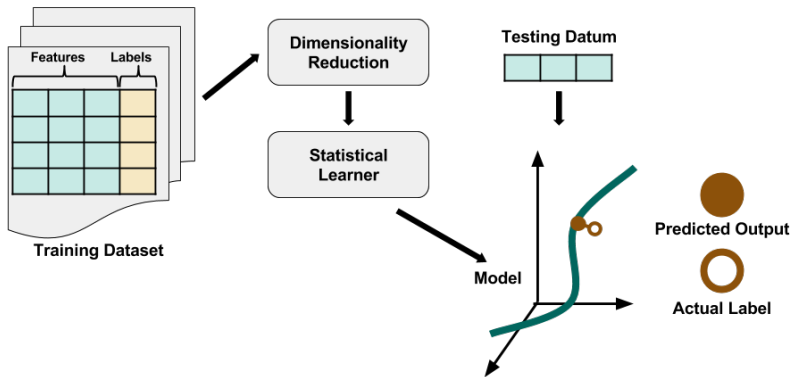


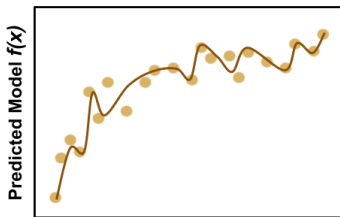
Figure 9: Schematic of a representative training and predicting workflow



Linear Models

Objective: minimize error over all training data wrt their labels

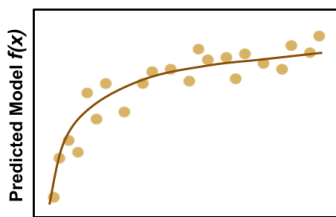
$$F(\mathbf{X}) = \beta_0 + \sum_{j=1}^P x_j \beta_j$$



Input Feature (x), $\lambda = 0$

Smoothing model using regularization by varying λ

$$F(\mathbf{X}) = \beta_0 + \sum_{j=1}^P x_j \beta_j + \lambda \sum_{j=1}^P \beta_j^2$$



Input Feature (x), $\lambda > 0$

Figure 10: How regularization might affect the generalizability of an ML model



Nearest Neighbor Methods

Objective: minimum distance between test sample and training instance(s)

$$Y(\mathbf{x}) = \frac{1}{k} \sum_{x_i \in N_k(\mathbf{x})} y_i$$

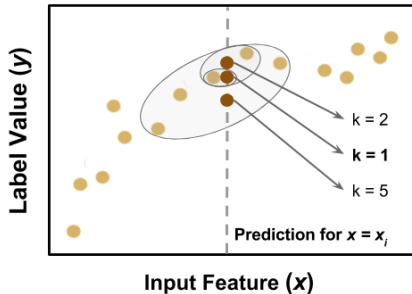


Figure 11: Illustration of the regularization effects by choosing k



Support Vector Machines and Regression

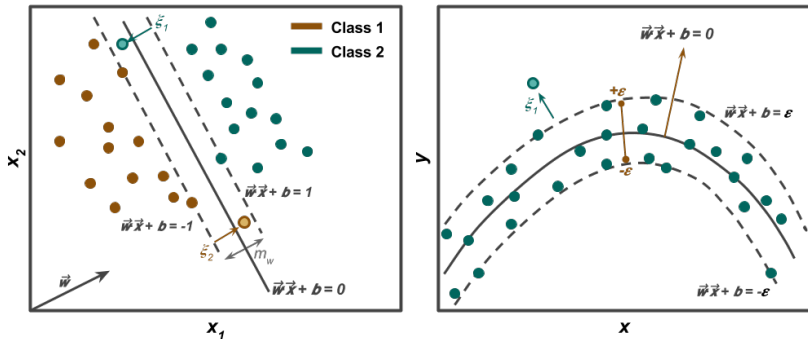


Figure 12: Classification with SVM and regression with SVR

Support Vector Regression with Many Dimensions



Objective: minimize margin width and outliers

$$\min \frac{1}{2} \|w\|^2 + C \sum_i \xi_i$$

$$\text{subject to : } |y_i - (w\phi(x_i) + b)| \leq \varepsilon + \xi_i$$

$$\text{where : } w = \sum_i \alpha_i y_i \phi(x_i)$$

$$\text{and : } K(x_i, x_j) = \phi(x_i)\phi(x_j) = e^{\gamma \|x_i - x_j\|^2}$$

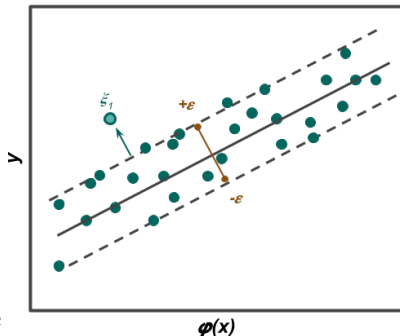


Figure 13: Diagram showing the use of the kernel trick with SVR

Model Smoothing



- ① Regularization (reduce weights of features)
- ② Dimensionality Reduction (delete features)
 - Manual : some metric
 - Manual : domain knowledge
 - Manual & Statistical : factor analysis
 - Statistical : principal components analysis (PCA)
 - Statistical : independent components analysis (ICA)



Types of Error

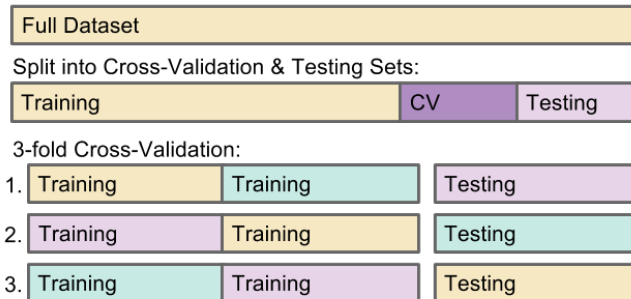


Figure 14: Diagram explaining the concept of k -fold cross-validation



Error Metrics

$$\text{Mean Squared Error (MSE)} : \frac{\sum_{i=1}^n (y_i - f(x_i))^2}{n}$$

$$\text{Mean Absolute Error (MAE)} : \frac{\sum_{i=1}^n |y_i - f(x_i)|}{n}$$

$$\text{Mean Absolute Percentage Error (MAPE)} : \frac{\sum_{i=1}^n \frac{|y_i - f(x_i)|}{y_i}}{n}$$

$$\text{Coefficient of Determination, } R^2 : \frac{\sum_{i=1}^n (f(x_i) - \bar{y})^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$$

Sources of Error

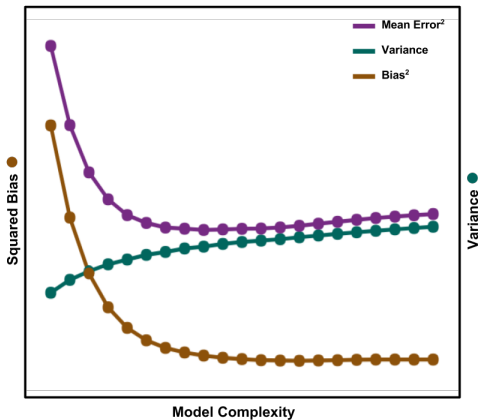
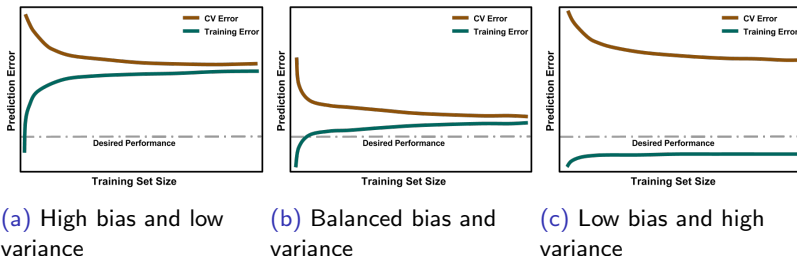


Figure 15: Bias and variance comprise the prediction error



Training Set Size: Learning Curves



(a) High bias and low variance

(b) Balanced bias and variance

(c) Low bias and high variance

Figure 16: Learning curves for three training scenarios with respect to training set size



Model Complexity: Validation Curves

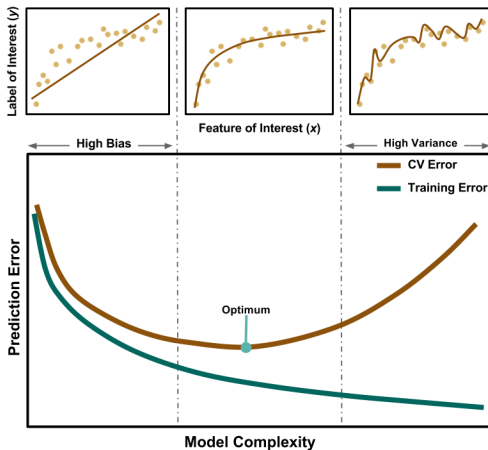


Figure 17: Validation curve showing different fitness of models with respect to model complexity



Model Comparison

$$Posterior = \frac{Likelihood * Prior}{Marginal Likelihood}$$

Probabilities	Calculation Method	Example
P(D M) Likelihood	MLE or ML model prediction w/ CV	Given [M] : BWR, burnup = x GWd/MTU Then [D] : Pu-239 concentration = y %
P(M) Prior	Histogram of simulation inputs	Given [D] : No direct information Then [M] : BWR, burnup = x GWd/MTU
P(D) Marginal L.	Histogram of simulation outputs	Given [M] : No direct information Then [D] : Pu-239 concentration = y %
P(M D) Posterior	Indirectly, from 3 probabilities above	Given [D] : Pu-239 concentration = y % Then [M] : BWR, burnup = x GWd/MTU

Table 2: Table showing how each component of the model comparison framework will be computed

Computational Tools



- Training Data : SNF recipes from SCALE/ORIGEN-ARP [11, 13]
- Information Reduction
 - Gamma energies: ORIGEN
 - Computational gamma spectra: GADRAS [2]
- Statistics Toolkit : scikit-learn (python) [12]

Pre-detonation Materials of Interest



- UOC
- UOX powder
- SNF
- Reprocessed SNF
- Separated Pu
- Anything radioactive from the fuel cycle



Statistical Methods Employed

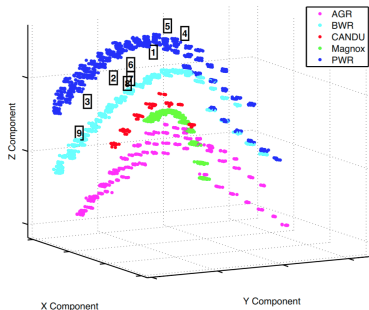


Figure 18: Unsupervised clustering for visualization separating reactor types [4]

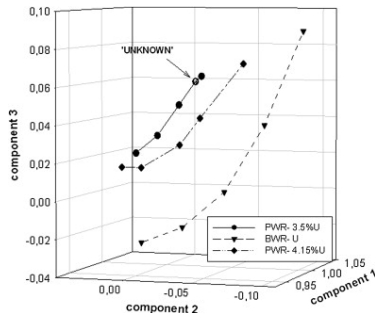


Figure 19: Factor analysis employed to determine provenance of unknown plutonium [8]

Statistical Methods Employed

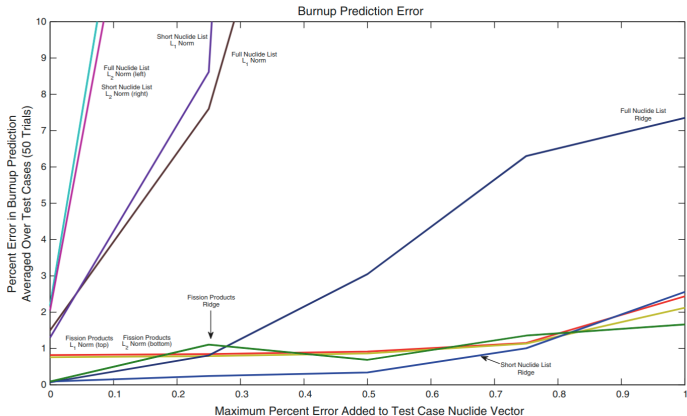


Figure 20: Burnup prediction error with respect to random nuclide error, using nearest neighbor & ridge regression methods [1]



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Proposed Experiment Methodology

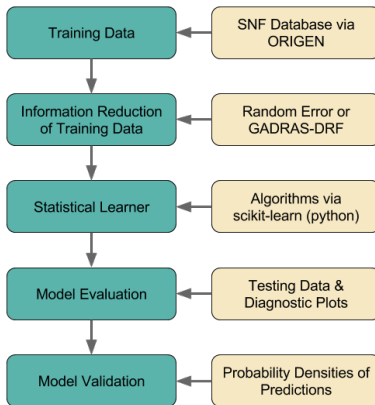


Figure 21: Workflow of the experiments with tools used for each step



Training Set

ORIGEN Rxtr	Rxtr Type	Enrichment
CE14x14	PWR	2.8
CE16x16	PWR	2.8
W14x14	PWR	2.8
W15x15	PWR	2.8
W17x17	PWR	2.8
S14x14	PWR	2.8
VVER440	PWR	3.60
VVER440_3.82	PWR	3.82
VVER440_4.25	PWR	4.25
VVER440_4.38	PWR	4.38
VVER1000	PWR	2.8
GE7x7-0	BWR	2.9
GE8x8-1	BWR	2.9
GE9x9-2	BWR	2.9
GE10x10-8	BWR	2.9
Abb8x8-1	BWR	2.9
Atrium9x9-9	BWR	2.9
SVEA64-1	BWR	2.9
SVEA100	BWR	2.9
CANDU28	PHWR	0.711
CANDU37	PHWR	0.711

Table 3: ORIGEN simulations [1]

	PWR	BWR	PHWR
Power Density [MW/MTU]	32	23	22
Burnup [MWd/MTU]	600–17700	600–12300	600–12300
Cooling Time	{1m, 7d, 30d, 1y}		

Table 4: Range of burnups and cooling times simulated for the training set [1]



Independent Testing Set

Reactor	Type	Enrichment	Cooling Time	Burnup
CANDU28	PHWR	0.711	{1m, 7d, 30d, 1y}	{1400, 5000, 11000}
CANDU28	PHWR	0.711	{3m, 9d, 2y}	{5000, 6120}
CE16x16	PWR	2.8	{1m, 7d, 30d, 1y}	{1700, 8700, 17000}
CE16x16	PWR	2.8	{3m, 9d, 2y}	{8700, 9150}
CE16x16	PWR	3.1	{7d, 9d}	{8700, 9150}
GE7x7-0	BWR	2.9	{1m, 7d, 30d, 1y}	{2000, 7200, 10800}
GE7x7-0	BWR	2.9	{3m, 9d, 2y}	{7200, 8800}
GE7x7-0	BWR	3.2	{7d, 9d}	{7200, 8800}

Table 5: Separate testing set used in previous work [1]

Initial Results



Algorithm	Error Origin	MAPE	RMSE [MWd/MTU]
Nearest Neighbor Regression	Testing Set	9.82	812.43
	5-fold Cross-Validation	2.24	421.41
Ridge Regression	Testing Set	15.68	1049.66
	5-fold Cross-Validation	0.08	13.08
Support Vector Regression	Testing Set	12.28	769.97
	5-fold Cross-Validation	2.08	188.07

Table 6: MAPE and RMSE for both CV and testing sets



Information Reduction

Demonstrated : Random error

Introduced $0\% < E_{max} < 10\%$

Each nuclide receives $[1 - E_{max}, 1 + E_{max}]$ error

Not Demonstrated : Systematic error

Gamma energies (ORIGEN), radionuclides only

Gamma spectra (GADRAS), reduced radionuclide observation

ML Model Prediction with Reduced Information

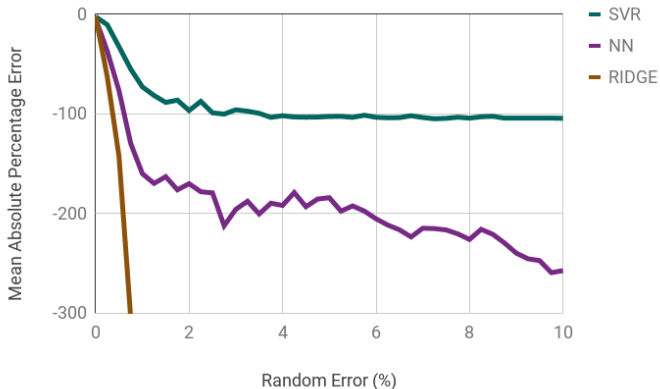


Figure 22: Negative MAPE for three algorithms given increasing random nuclide error



Algorithm Parameters

Algorithm	Parameter	Value
Nearest Neighbor Regression	n -neighbors	1
	Weights	uniform
	Distance Metric	L2: Euclidian Distance
Ridge Regression	Regularization, α	1.0
	Normalization	False
	Stopping Tolerance	0.001
Support Vector Regression	Kernel	Radial Basis Function
	Gamma, γ	0.001
	C	1000
	Epsilon, ϵ	0.1
	Stopping Tolerance	0.001

Table 7: Parameters chosen for demonstration; C and γ are not the default values



Learning Curves : Linear Model

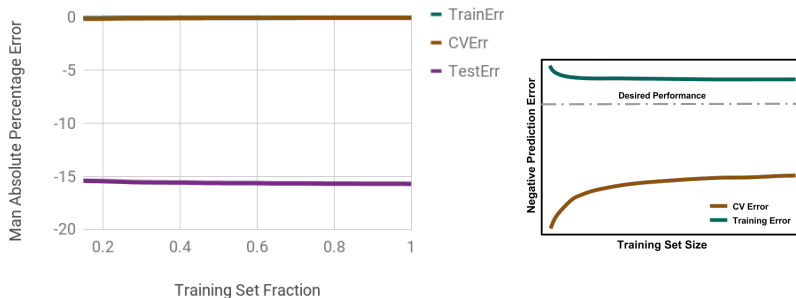


Figure 23: Learning curve and comparison schematic for ridge regression;
 $\alpha = 1.0$



Learning Curves : k -Nearest Neighbors

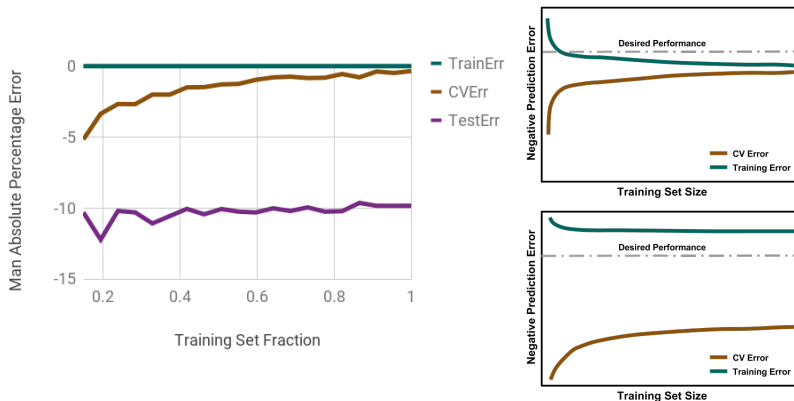


Figure 24: Learning curve and comparison schematic for k -NN regression; $k = 1$



Learning Curves: Support Vectors

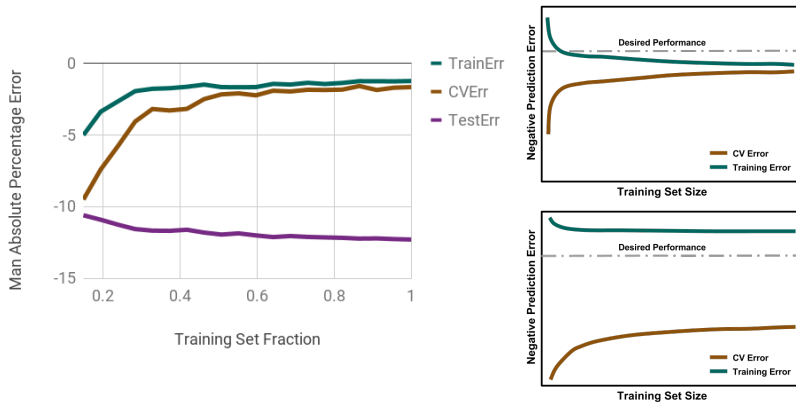


Figure 25: Learning curve and comparison schematic for SVR; $\gamma = 10^{-3}$ and $C = 10^3$



Validation Curves : Linear Model

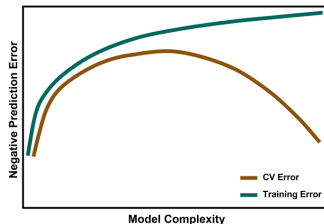
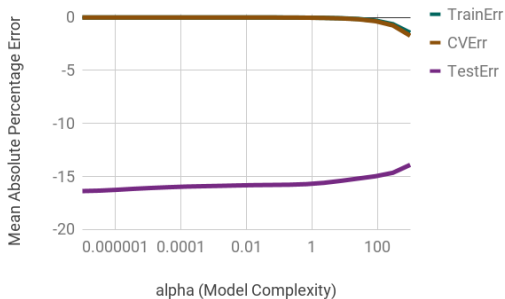


Figure 26: Validation curve and comparison schematic for ridge regression;
TrainingSetSize = 2313



Validation Curves : k -Nearest Neighbors

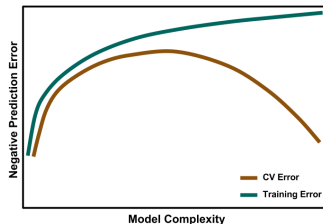
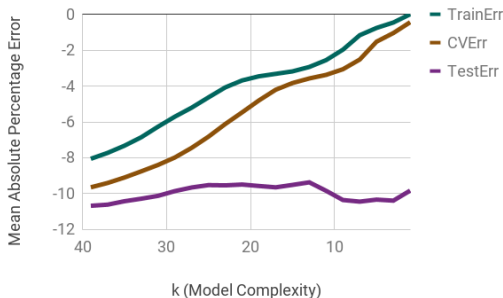


Figure 27: Validation curve and comparison schematic for k -NN regression;
 $TrainingSetSize = 2313$



Validation Curves : Support Vectors

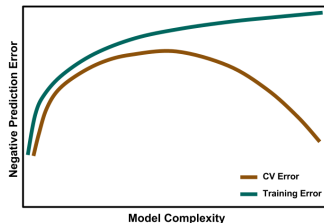
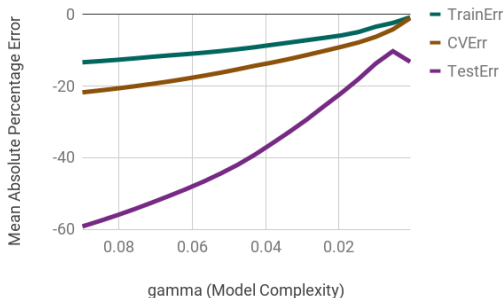


Figure 28: Validation curve and comparison schematic for SVR;
 $TrainingSetSize = 2313$ and $C = 10^3$

Note: Default γ would be $\frac{1}{2000} = 0.0005$

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Research Proposal Preparations

- 1 Training set considerations
- 2 Finalizing set of algorithms
- 3 Computational resources

Reactor Type	U-235 Enrichment (%U-235)	Cooling Times	Burnup (MWd/te)
Advanced Gas Reactor (AGR)	1, 1.5, 2, 2.5, 3, 3.5, 4	1, 5, 10, 15, 20, 30, 40 years	1000, 5000, 10000, 15000, 20000, 25000, 30000, 35000, 40000, 45000
Boiling Water Reactor (BWR)	2, 2.5, 3, 3.5, 4	1, 5, 10, 15, 20, 30, 40 years	5000, 10000, 15000, 20000, 25000, 30000, 35000, 40000, 45000, 50000, 55000
Canada Deuterium Uranium (CANDU)	0.711, 1.2	0, 1, 2, 10, 15, 20, 30, 40 years	5000, 10000, 15000, 20000, 25000, 30000
Magnesium Non-Oxidizing (Magnox)	0.711	0, 16, 90, 115, 280, 365 days 2, 3, 4, 5, 10, 15, 20, 30, 40, 50, 60 years	500, 1000, 2000, 3000, 4000, 5000, 6000, 7000, 8000, 9000, 10000, 10000, 10000, 12000, 13000, 14000, 15000
Pressurized Water Reactor (PWR)	2, 2.5, 3, 3.5, 4, 4.5	1, 5, 10, 15, 20, 30, 40 years	5000, 10000, 15000, 20000, 25000, 30000, 35000, 40000, 45000, 50000, 55000

Table 8: Example of a training data set based on comparison to the SFCOMPO database [4, 6]



Statistical Learning with Direct Isotopics

Goals : Understand limits of simplest scenario

- ① Usefulness of statistical methods for reactor parameter prediction
- ② Best performing methods

Variables

- ① the complexity of the ML algorithm used,
- ② feature reduction, and
- ③ different subsets of the decision space.



Statistical Learning with Direct Isotopics

Qualitative Hypotheses

- Complex algorithm will provide best behavior
- Manual preprocessing (feature reduction): speed, accuracy
- Reduction of decision space should help: PWR vs. BWR?

Risk Mitigation

- New algorithms: tree-based, neural nets, Bayesian MLE
- Statistical preprocessing: PCA, ICA
- New materials: Pu, UOC, Post-detonation (urban canyon [3])

Statistical Learning with Gamma Spectra



Goals : Understand limits of real-world scenario

- ① Level of reduction in reactor parameter prediction
- ② Best performing methods

Variables

- ① the complexity of the ML algorithm used,
- ② feature reduction (implicit), and
- ③ quality of training and/or testing data set.

Statistical Learning with Gamma Spectra



Qualitative Hypotheses

- Complex algorithm will provide best behavior
- Indirect isotopics = implicit feature reduction: less accurate
- Higher quality gamma spectra will yield better results

Risk Mitigation

- New algorithms: tree-based, neural nets, Bayesian MLE
- Further manual or statistical preprocessing
- Add isotope identification step

Statistical Learning with Reprocessed Fuel



Goals : Probe prediction performance in reprocessing scenario

- ① Experiment with both direct and indirect isotopics
- ② Fresh evaluation of preprocessing
- ③ Best performing methods for materials with multiple sources

Variables

- ① the complexity of the ML algorithm used,
- ② quality of training data set, and
- ③ type of preprocessing for feature reduction.

Statistical Learning with Reprocessed Fuel



Qualitative Hypotheses

- Complex algorithm will provide best behavior
- Reduced information will provide less accurate results
- ICA may outperform PCA, but factor analysis may outperform components analysis [7, 9, 10, 15, 14, 4, 5]

Risk Mitigation

- New algorithms: tree-based, neural nets, Bayesian MLE
- Manual preprocessing
- Results may be interesting even if prediction fails
- Ensemble methods or other creative solutions [15, 14]



Probability Distribution Functions

$$P(\mathbf{m}|\mathbf{d}) = C * P(\mathbf{d}|\mathbf{m}) * P(\mathbf{m})$$

\mathbf{d} : training data set

\mathbf{m} : model parameters

C : constant from marginal likelihood

$P(\mathbf{m})$: prior probability distribution

$P(\mathbf{d}|\mathbf{m})$: likelihood distribution function

$P(\mathbf{m}|\mathbf{d})$: posterior probability distribution

Typically, (cumulative) probability distributions are integrated probability density functions:

$$P(\mathbf{d}|\mathbf{m}) = \int_{\mathbf{d}, \mathbf{m}} \rho(\mathbf{d}|\mathbf{m}) d\mathbf{m}$$



Estimating Density Functions

MLE is the CV error because the results are reported as:
 $\mu \pm \sigma$ [12]

MLE is not this simple for other methods that do not employ CV [16, 17]

Probabilities	Calculation Method
P(D M) Likelihood	MLE or ML model prediction w/ CV
P(M) Prior	Histogram of simulation inputs
P(D) Marginal L.	Histogram of simulation outputs
P(M D) Posterior	Indirectly, from 3 probabilities above

Table 9: The density functions that represent each probability are estimated from histograms or the ML model

Note: This implies the posterior is now only dependent on the likelihood.



Posterior Odds

Posterior odds = probability of ML model i being correct

- ① Calculate $MLE_i = P_i(m|d)$ for statistical model i
- ② Calculate $MLE_j = P_j(m|d)$ for statistical model j
- ③ Ratio of MLE_i to MLE_j to get Bayes' factor: $B_{ij} = \frac{P_i(d|m)}{P_j(d|m)}$
- ④ Take ratio of both Bayes' relations to get posterior odds:

$$\frac{P_i(m|d)}{P_j(m|d)} = B_{ij} \frac{P_i(m)}{P_j(m)}$$

$ \ln B_{ij} $	Probability	Likelihood Strength
< 1.0	< 0.750	Inconclusive
1.0	0.750	Weak
2.5	0.923	Moderate
5.0	0.993	Strong

Table 10: Model comparison using the Bayes' factor to describe the likelihood strength [16, 17]



Outline

1 Introduction

- Motivation
- Methodology

2 Literature Review

- Nuclear Forensics
- Statistical Models
 - Algorithms for Prediction
 - ML Model Assessment
 - ML Model Validation
- Computational Tools
- Previous Work

3 Demonstration

- Training Data
- Reactor Parameter Prediction
- ML Model Validation

4 Research Proposal

- Experiment 1
- Experiment 2
- Experiment 3
- Method Comparison

5 Summary



Summary

Pre-detonation nuclear forensics analysis on SNF

- Demonstrated:
 - Simulation of training data set
 - Information reduction of training set
 - Burnup prediction using three statistical models: ridge, k -nearest neighbor, and support vector regression
 - ML model optimization via diagnostic curves
 - Plan for ML model comparison
- Simplifications:
 - Only predicted burnup (missing rxtr type, enrichment, cooling time)
 - Borrowed training set
 - No statistical feature reduction
 - No physically based information reduction
- Three experiments:
 - Nuclide concentrations
 - Gamma energies/spectra
 - Reprocessed SNF



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