Evaluating Statistical Methods for Nuclear Forensics Analysis

Preliminary Examination

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Outline

Research Overview

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

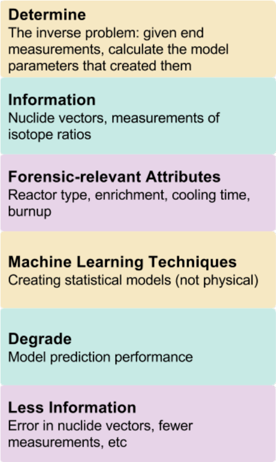


Figure 1: Definitions of terms within the main research question

Nuclear Security and Forensics

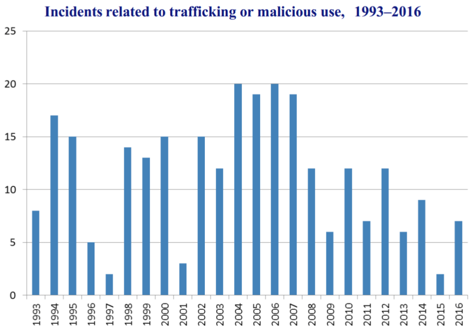


Figure 2: 24 years of incidents: HEU (12), Pu (2), Pu-Be neutron sources (4) [Obtained from: https://www.iaea.org/sites/default/files/17/12/itdb-factsheet-2017.pdf]

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

Needs in Nuclear Forensics

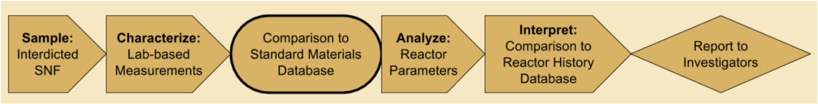


Figure 3: Typical techincal nuclear forensics workflow

Material-specific:

- Measurement needs
- Measurement techniques
- Forensic signatures

Challenges:

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

Computational Methods

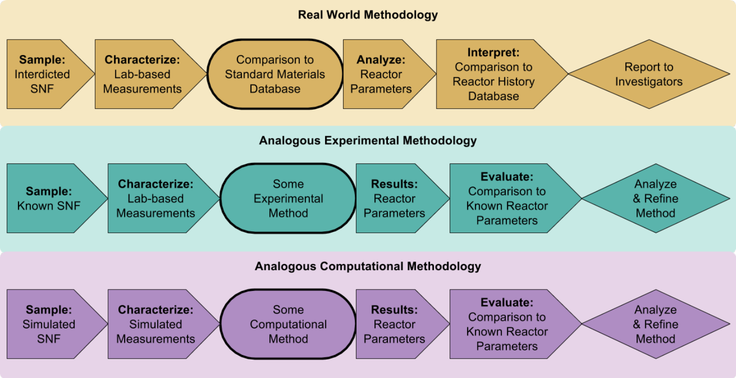


Figure 4: Nuclear forensics research: physical, experimental, and computational

Computational Methods

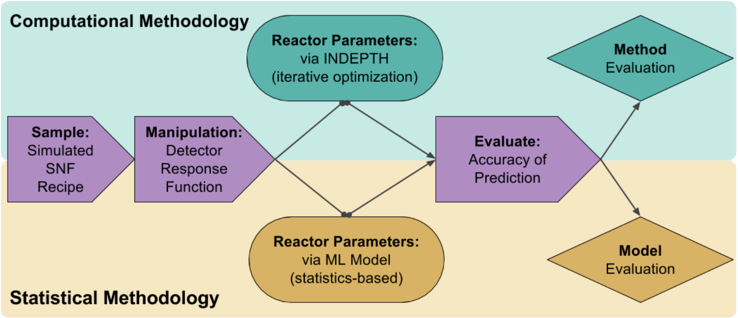


Figure 5: Comparison of two different computational approaches

Statistical Methods

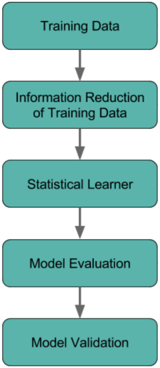


Figure 6: Workflow of a methodology using statistical models

- 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

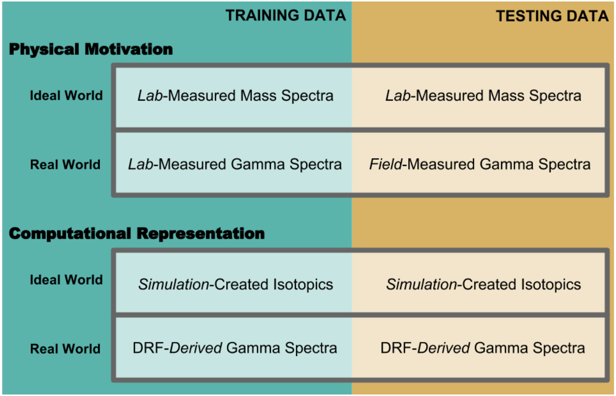


Figure 7: Illustration of data set modularity

Outline

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 *Input* : Rxtr Parameters
Forward Problem	Marginal Likelihood : P(D)	Data Space	Simulation *Output* : SNF Recipes
	Likelihood : P(D|M)	Both	*Output* + *Input* = (Statistical) Model
Inverse Problem	Posterior Probability : P(M|D)	Both	(Statistical) Model : *Output->Input*

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

Machine Learning

machine vs. statistical (domain knowledge-¿none)
supervised and unsupervised
clustering, dimensionality reduction
classification, regression – discrete and continuous variables

Supervised Regression

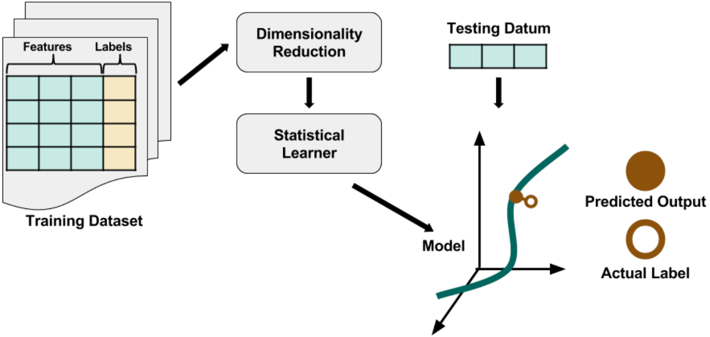


Figure 8: Schematic of a representative prediction workflow

Linear Models

Objective: minimize error over all training data wrt their labels
$F(\boldsymbol{X}) = \beta_0 + \sum_{j=1}^{p} x_j \beta_j$

Smoothing model using regularization by varying λ
$F(\boldsymbol{X}) = \beta_0 + \sum_{j=1}^{p} x_j \beta_j + \lambda \sum_{j=1}^{p} \beta_j^2$

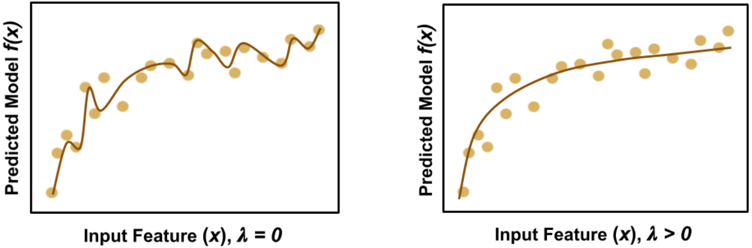


Figure 9: How regularization might affect the generalizability of an ML model

Nearest Neighbor Methods

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

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

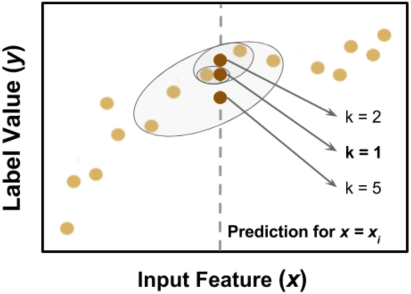


Figure 10: Illustration of the regularization effects by choosing k

Support Vector Machines and Regression

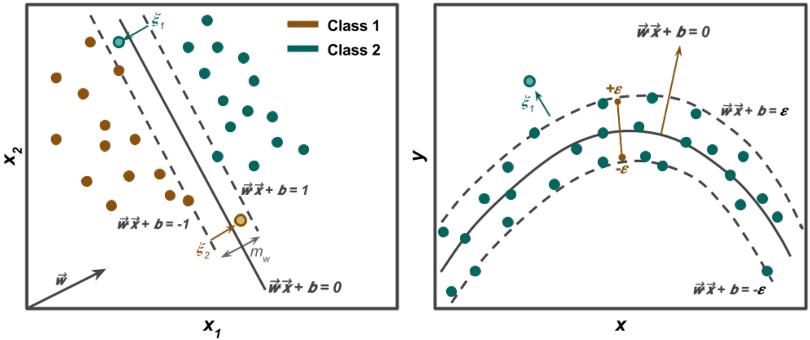


Figure 11: Classification with SVM and regression with SVR

Support Vector Regression with Many Dimensions

Objective: minimize margin width and outliers

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

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

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

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

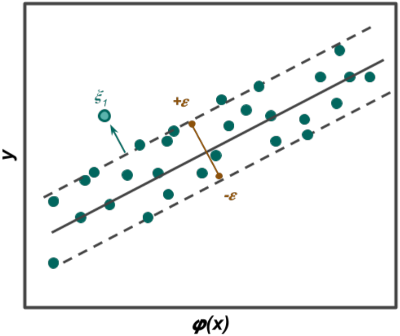


Figure 12: Diagram showing the use of the kernel trick with SVR

Dimensionality Reduction

- Manual via domain knowledge or some measure
- PCA
- Factor Analysis
- ICA

Types of Error

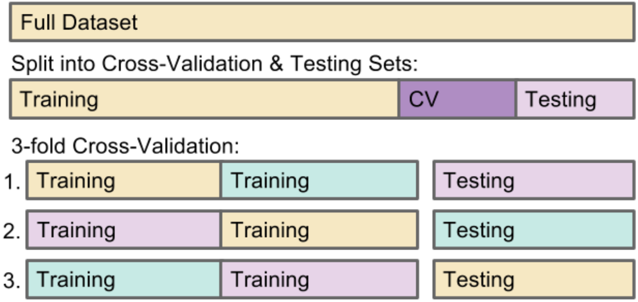


Figure 13: Diagram explaining the concept of *k*-fold cross-validation

Error Metrics

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

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

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

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

Sources of Error

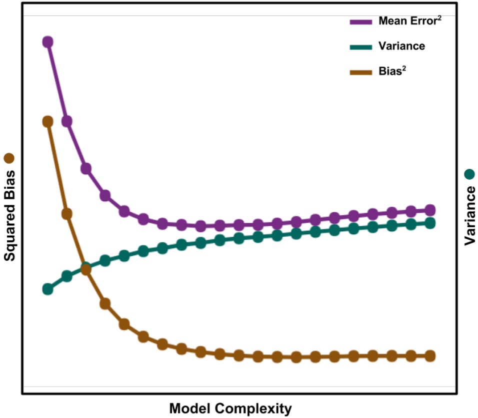
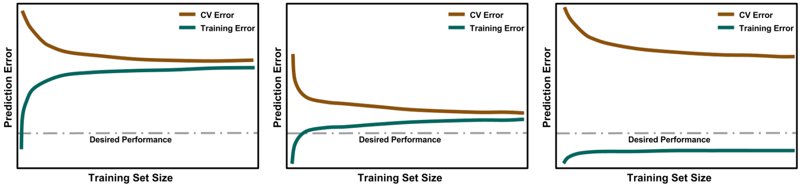


Figure 14: Bias and variance comprise the prediction error

Training Set Size: Learning Curves



(a) High bias and low variance

(b) Balanced bias and variance

(c) Low bias and high variance

Figure 15: Learning curves for three training scenarios with respect to training set size

Model Complexity: Validation Curves

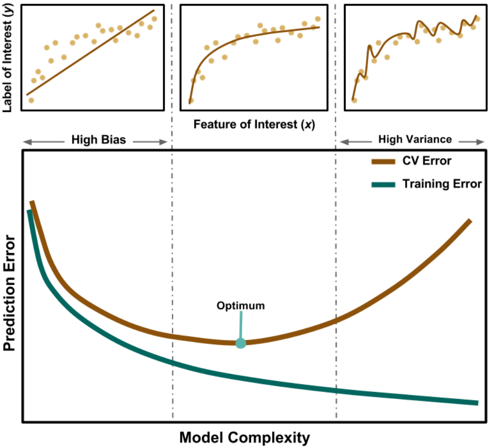


Figure 16: Validation curve showing different fitness of models with respect to model complexity

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

Statistical Methods Employed

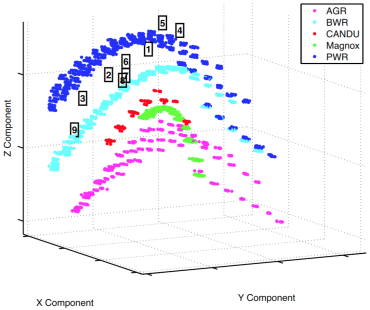


Figure 17: Unsupervised clustering for visualization separating reactor types [4]

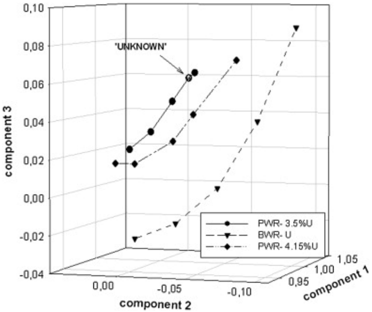


Figure 18: Factor analysis employed to determine provenance of unknown plutonium [8]

Statistical Methods Employed

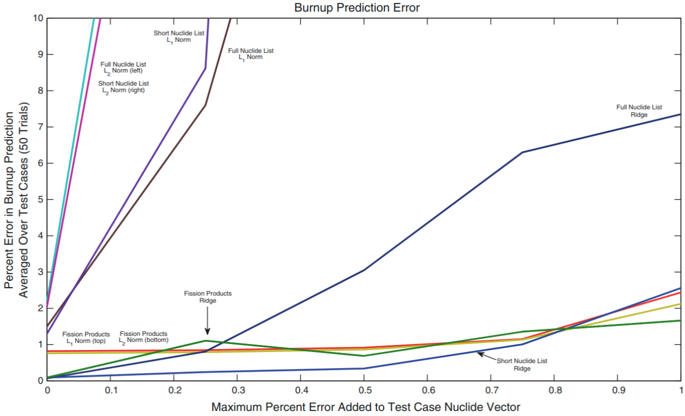


Figure 19: Burnup prediction error with respect to random nuclide error, using nearest neighbor & ridge regression methods [1]

Outline

Proposed Experiment Methodology

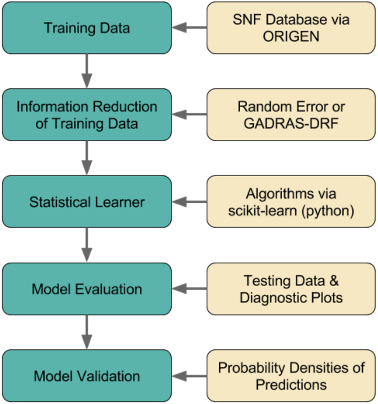


Figure 20: Workflow of the experiments with tools used for each step

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

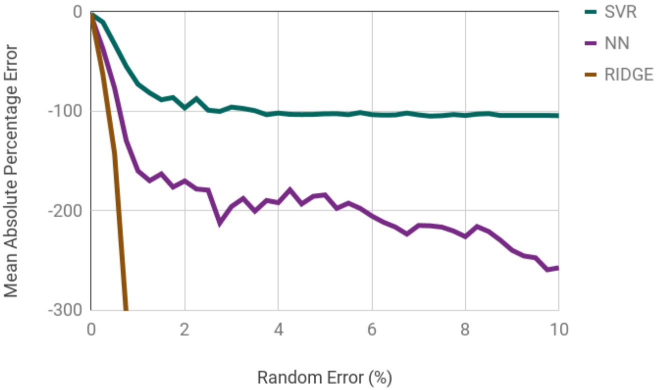


Figure 21: Negative MAPE for three algorithms given increasing random nuclide error

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

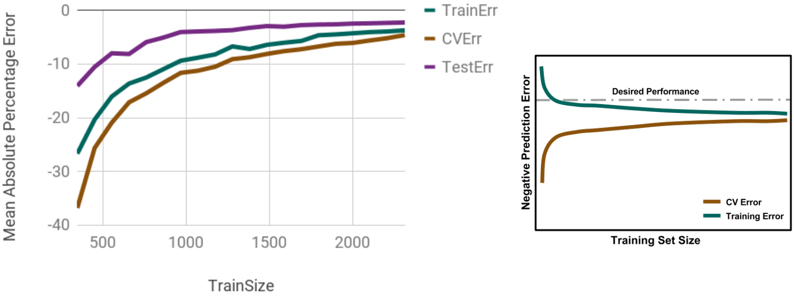


Figure 22: Learning curve and comparison schematic for SVR

Learning Curves

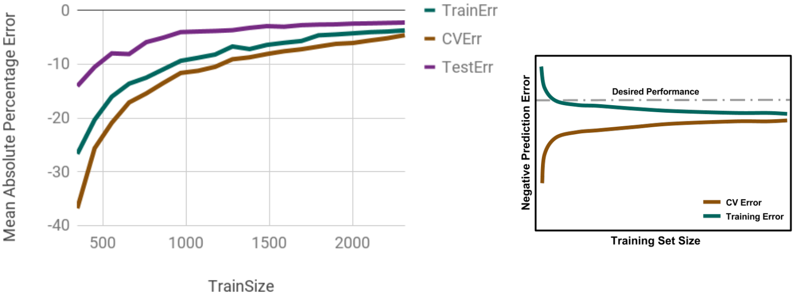


Figure 23: Learning curve and comparison schematic for NN Regression

Validation Curves

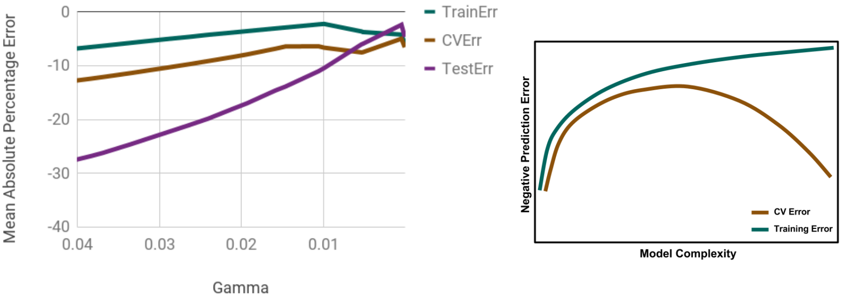
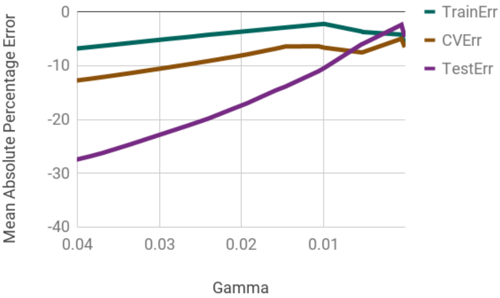


Figure 24: Validation curve and comparison schematic for SVR

Validation Curves



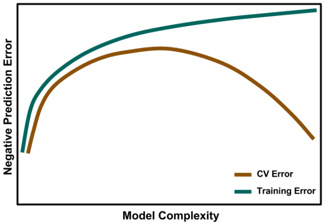


Figure 25: Validation curve and comparison schematic for NN Regression

Outline

Research Proposal Preparations

Previous Work -¿ SFCOMPO-based
Finalizing set of algorithms
computational resources

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 performace 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 Distributions

Include uncertainty for measures of confidence, posterior probs become prob distribs
C : constant given by marginal likelihood
$\boldsymbol{d}$: training data set
$\boldsymbol{m}$: model parameters
$P(\boldsymbol{d}|\boldsymbol{m})$: likelihood distribution function
$P(\boldsymbol{m})$: prior probability distribution
$P(\boldsymbol{m}|\boldsymbol{d})$: posterior probability distribution

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

Integrate over prob densities to get prob distrib
$\boldsymbol{m}$: range of predicted model parameters
$\boldsymbol{d}$ is a set of nuclide vectors

$$\rho(\boldsymbol{x}) = \prod_i \rho(x_i)$$

$$P(\boldsymbol{m}) = \int_{\boldsymbol{m}} \rho(\boldsymbol{d}) d\boldsymbol{d}$$

Likelihood distribution function:

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

But, we infer them...

Estimating Density Functions

estimate rho, have a 'sense' or try different

prior probability distributions are given by the model space, e.g., reactor parameters as predicted from the ML models. [17] Note: This implies the posterior is now only dependent on the likelihood.

likelihood function: the training phase provides the maximum likelihood distribution through the use of CV, since the results are reported as a mean error with a standard deviation (which can be converted to accuracy for likelihood) [12]

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

Posterior Odds

citations plz

calc a non-normalized posterior probability distribution, $P(m_i|d)$ then do it for a model obtained from a different algorithm, $P(m_j|d)$

relative posterior probability distribution : *posterior odds* $B_{ij} = \frac{\rho(d|m_i)}{\rho(d|m_j)}$: *Bayes factor*.

$$\frac{P(m_i|d)}{P(m_j|d)} = B_{ij}\frac{P(m_i)}{P(m_j)}$$

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

Table 8: Model comparison using likelihood strength

posterior probabilities calculated from $|InB_{ij}|$

Summarize:

Given a mean-squared error and its standard deviation from using CV with any alg, get MLE

compare two models : MLE_i to MLE_j

Outline

Summary

Summarize

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