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?

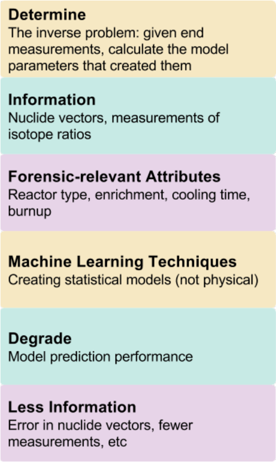

Figure 1: Definitions of terms within the main research question

Nuclear Security and Forensics

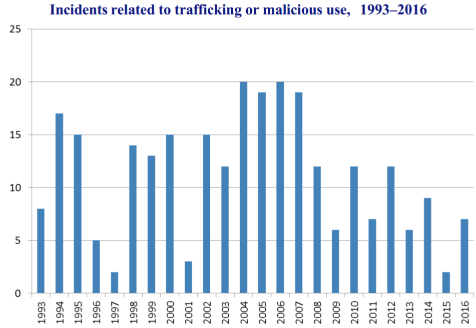

Figure 2: 24 years of incidents: HEU (12), Pu (2), Pu-Be neutron sources (4) [Obtained from: https://www.iaea.org/sites/default/files/17/12/itdb-factsheet-2017.pdf]

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

Needs in Nuclear Forensics

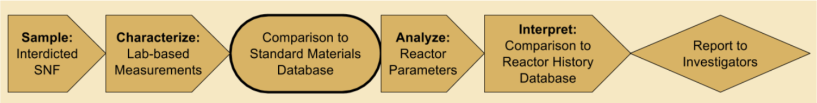

Figure 3: Typical techincal nuclear forensics workflow

Material-specific:

- Measurement needs
- Measurement techniques
- Forensic signatures

Challenges:

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

Computational Methods

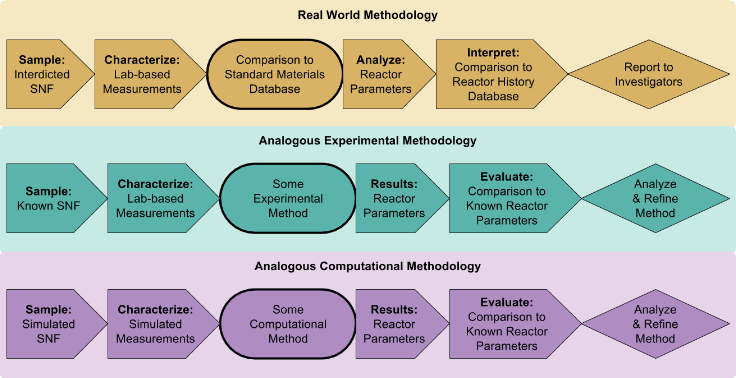

Figure 4: Nuclear forensics research: physical, experimental, and computational

Computational Methods

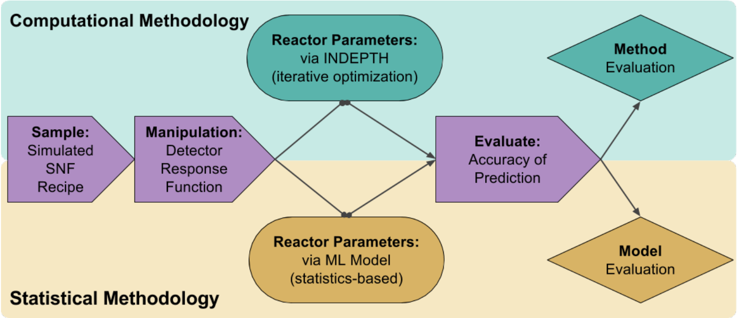

Figure 5: Comparison of two different computational approaches

Statistical Methods

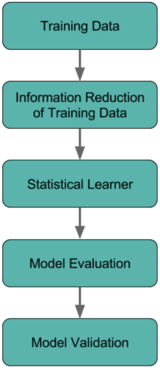

Figure 6: Workflow of a methodology using statistical models

- 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

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

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

Necessary to determine the quality of prediction
Use Bayes' Framework:

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

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

Machine Learning

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

Supervised Regression

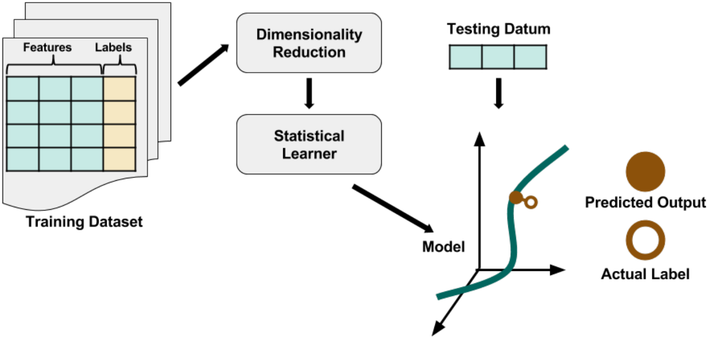

Figure 8: Schematic of a representative prediction workflow

Linear Models

Objective: minimize error over all training data wrt their labels

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

Regularization using λ

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

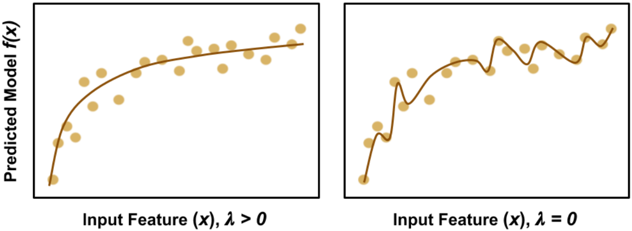

Figure 9: How regularization might affect the generalizability of an ML model

Nearest Neighbor Methods

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

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

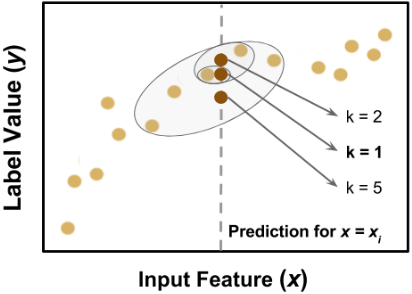

Figure 10: Illustration of the regularization effects by choosing k

Support Vector Machines

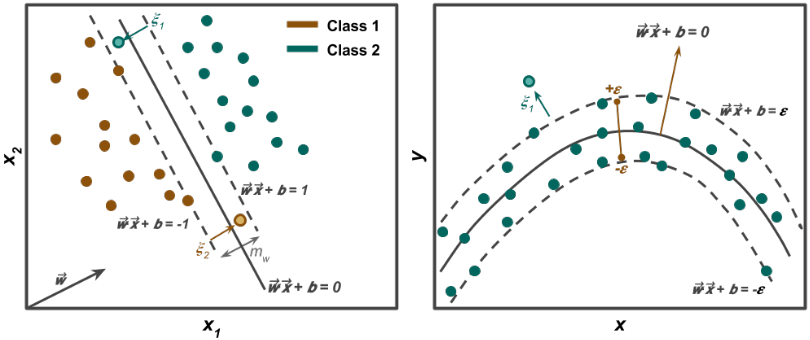

Figure 11: Classification with SVM and regression with SVR

Support Vector Regression with Many Dimensions

Objective: minimize margin width and outliers

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

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

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

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

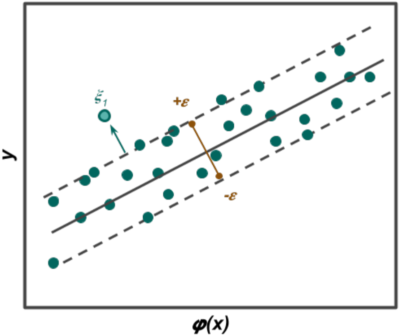

Figure 12: Diagram showing the use of the kernel trick with SVR

Dimensionality Reduction

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

Sources of Error

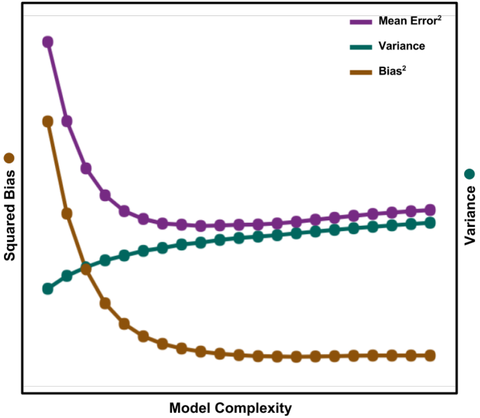

Figure 13: Bias and variance comprise the prediction error

Types of Error

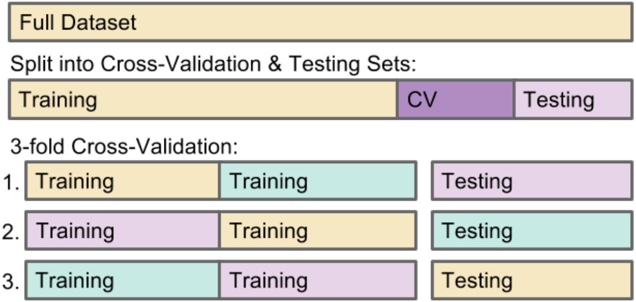

Figure 14: Diagram explaining the concept of k-fold cross-validation

Error Metrics

L1, L2: absolute error and squared error
Others: r2 score, percent error
Used for model prediction error and optimization of algs in obj funcs

Training Set Size: Learning Curves

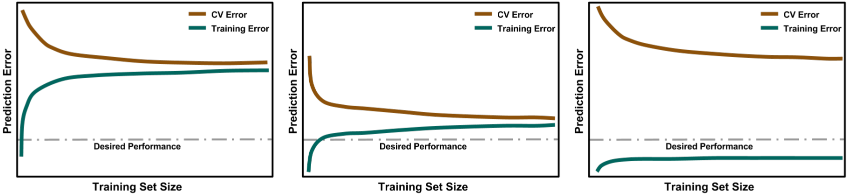

Figure 15: Learning curves for three training scenarios: high bias, balanced bias and variance, and high variance

Model Complexity: Validation Curves

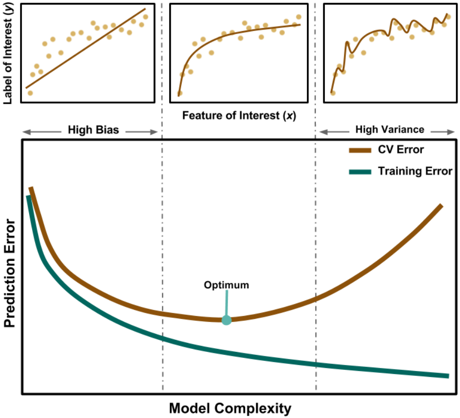

Figure 16: Validation curve showing different fitness of models

Model Comparison

Probabilities	Calculation Method and Example
P(D|M) Prior	*Given:* M = BWR U-oxide with burnup = ***x*** GWd/MTU *This is true:* D = nuclide vector with Pu-239 = ***y***% *With:* ***z***% probability *Calc'd from:* ORIGEN simulations in training set
P(M) Likelihood	*Given:* No direct information on D *This is true:* M = BWR U-oxide with burnup = ***x*** GWd/MTU *With:* ***z***% probability *Calc'd from:* Machine-learned model prediction
P(D) Marginal L.	*Given:* No direct information on M *This is true:* D = nuclide vector with Pu-239 = ***y***% *With:* ***z***% probability *Calc'd from:* Summation of training set instances
P(M|D) Posterior	*Given:* D = nuclide vector with Pu-239 = ***y***% *This is true:* M = BWR U-Ox with burnup = ***x*** GWd/MTU *With:* ***z***% probability *Calc'd from:* All quantities above

Table 1: Bayes

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

Computational Tools

cite stuff

- Training Data : SCALE/ORIGEN-ARP
- Statistics Toolkit : scikit-learn (python)
- Information Reduction
  - Gamma energies: ORIGEN
  - Computational gamma spectra: GADRAS

Pre-detonation Materials of Interest

- UOC
- UOX powder
- SNF
- Reprocessed SNF

Statistical Methods Employed

get images
Factor Analysis
SFCOMPO extension
Dayman paper on prediction ability wrt info reduction

Outline

Proposed Experiment Methodology

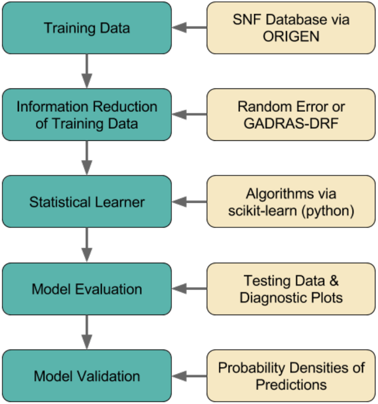

Figure 17: Workflow of the experiments with tools used for each step

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

Independent Testing Set

Reactor	Type	Enrichment	Cooling Time
CANDU28	PHWR	0.711	{1m, 7d, 30d, 1y}
CANDU28	PHWR	0.711	{3m, 9d, 2y}
CE16x16	PWR	2.8	{1m, 7d, 30d, 1y}
CE16x16	PWR	2.8	{3m, 9d, 2y}
CE16x16	PWR	3.1	{7d, 9d}
GE7x7-0	BWR	2.9	{1m, 7d, 30d, 1y}
GE7x7-0	BWR	2.9	{3m, 9d, 2y}
GE7x7-0	BWR	3.2	{7d, 9d}

Information Reduction

Random error here
gamma not implemented here

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 5: caption

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: caption

ML Model Prediction with Reduced Information

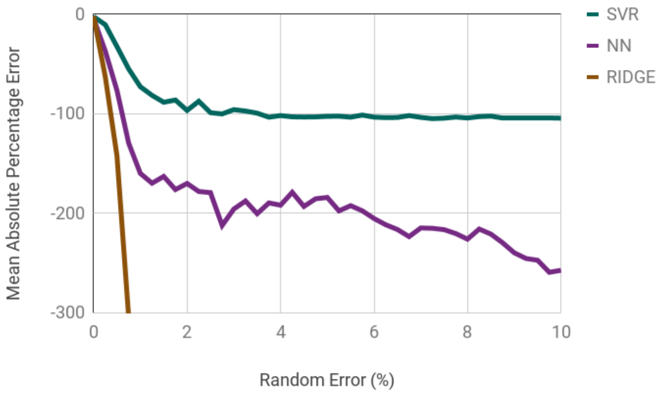

Figure 18: caption

SVR Learning Curve

add in example LCs for comparison add in NN or Ridge LC (They look the same)

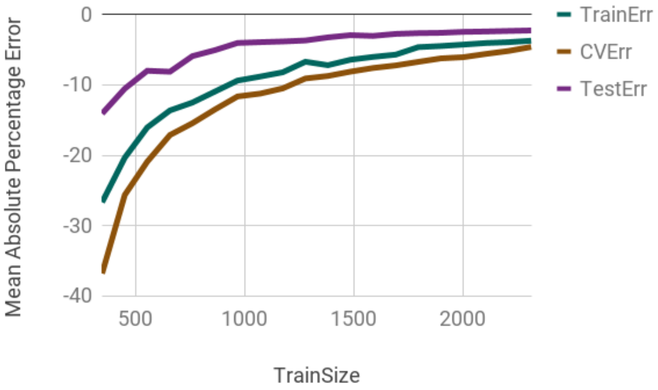

Table 7: caption

SVR Validation Curve

add in example VCs for comparison add in NN or Ridge VC (They look the same)

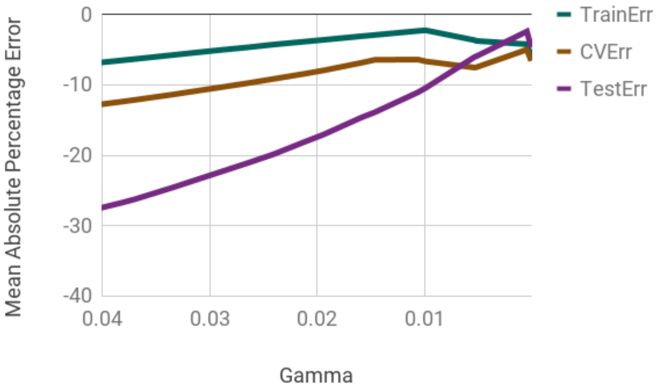

Table 8: caption

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 [1])

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 [4, 5, 6, 8, 7, 2, 3]

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 [8, 7]

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. [**?**] 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) [**?**]
MLE is not this simple for other methods that do not employ CV [**?**, **?**]

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 9: Model comparison using likelihood strength

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

Summarize:

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

compare two models : MLE to MLE

Outline

Summary

Summarize

References I

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