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Single Channel Design Based on Artificial Intelligence for Molten Salt Reactors

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Part I - Methodology

- Motivation
- Validation
- Assumptions/Approximations/Simplifications
- Step 1: Reactor Database Generation
- Step 2: Training a Predictive (Machine Learning) Model
- Step 3: Design Optimization

Motivation/Aim for This Study

Aim:

To introduce an efficient, novel, robust, accelerated and reliable design recommendation approach based on machine learning methods in predicting performance metrics of any design

Why:

- parametric studies ignore interdependence of variables
- obligation to use a reactor physics code for any neutron transport calculation
- possibility to converge to a local instead of global optima
- concerns on the parameters of the optimizers due to the indeterminacy of these parameters prior to evaluations

How:

- Phase I: Single Channel Validation
- Phase II: Full Core Implementation

Computational Steps

Main steps:

i. generation of a reactor database
ii. training a predictive machine learning model and
iii. design optimization

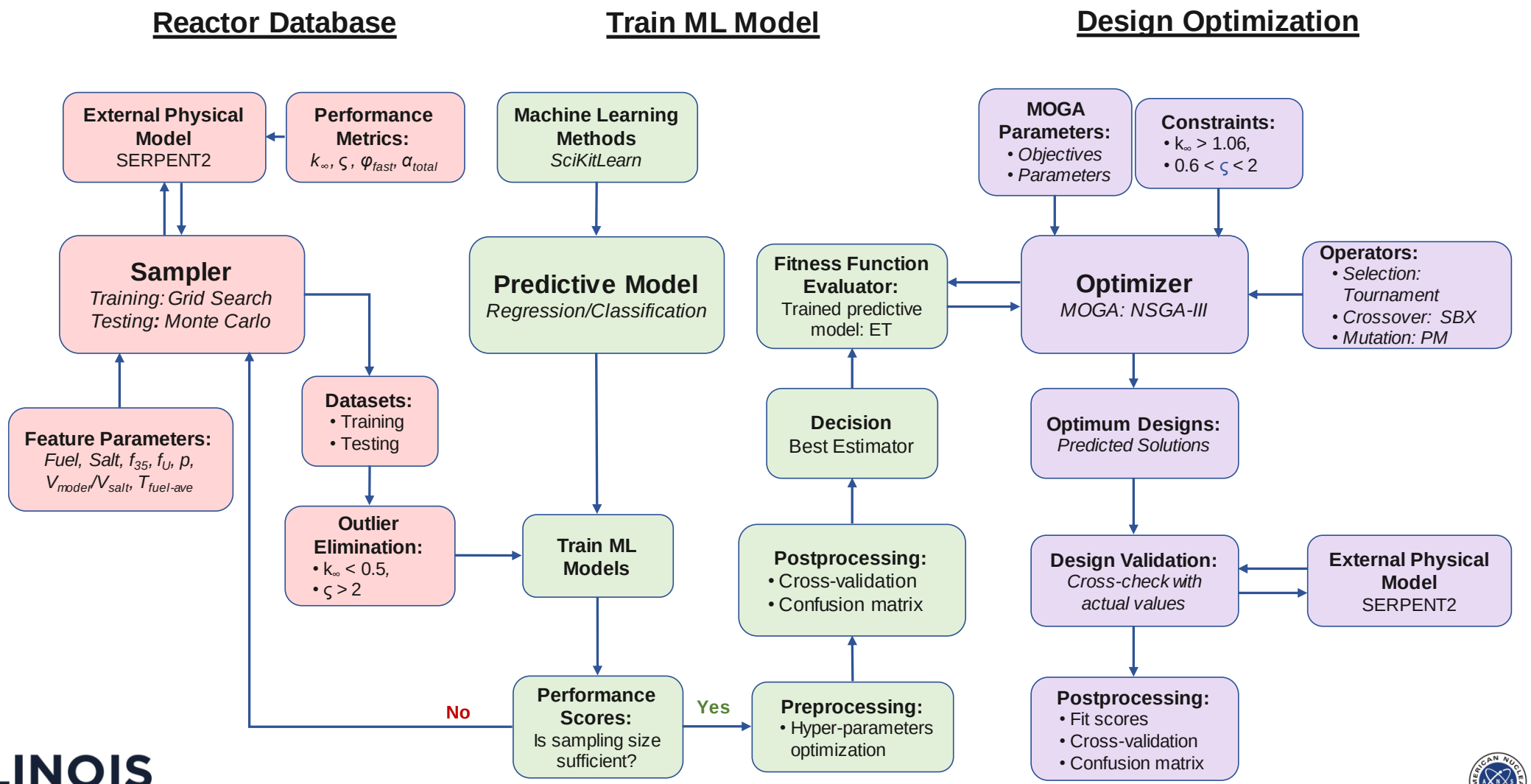
A python tool was prepared to:

i. produce training and testing datasets for an interested design space,
ii. examine performance scores of ML methods and train a predictive model
iii. find optimal designs by predicting performance metrics within the design space

The tool couples to:

i. a reactor physics code which computes key performance metrics
ii. an optimization method to search for optimum designs and
iii. miscellaneous utilities for the regression and classification analyses, the quantification of the quality of predictions and preprocessing.

Computational Flowchart of Python Tool



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Programs/Codes in Python Tool

- Language: Python 3.7
- Reactor model: *Monte Carlo Technique (Serpent 2)*
  - Criticality calculations: Serpent 2, Version 2.1.31
  - Computational standard deviation of k_{inf} < 100 pcm
  - Neutron data library: ENDF/B-VII.0
- Target reactor design: *Molten Salt Reactor*
- Sampling strategy: *Grid Sampling Approach*
- Prediction of performance metrics: *Machine Learning Methods*
- Training methods: *Regression and Classification*
  - From Scikit-learn tools
- Optimization: *Multi-Objective Genetic Algorithm – NSGA-III*

Validation: Single Fuel-Salt Channel

Feature Parameters:

i. Fuel types: U, U-Th, U-Pu
   - ✓ Th as ^{232}Th
   - ✓ Pu as weapons-grade Pu

ii. Salt types: LiF-BeF_2, NaF-BeF_2, NaCl

iii. ^{235}U fissile content (ε): 5 to 20 wt. % in U

iv. U content:
   - ✓ 100 wt. % for U type
   - ✓ 10 to 90 wt. % in U-Th and U-Pu

v. Pitch (p): 1 to 16 cm

vi. V_{moder}/V_{salt} (ξ) : 0.274 to 10.46
   - ✓ minimum value: 0.274 for $p=D_f$
   - ✓ maximum value: 10.46 for $p=3D_f$

vii. T_{ave}: 900 to 1200 K

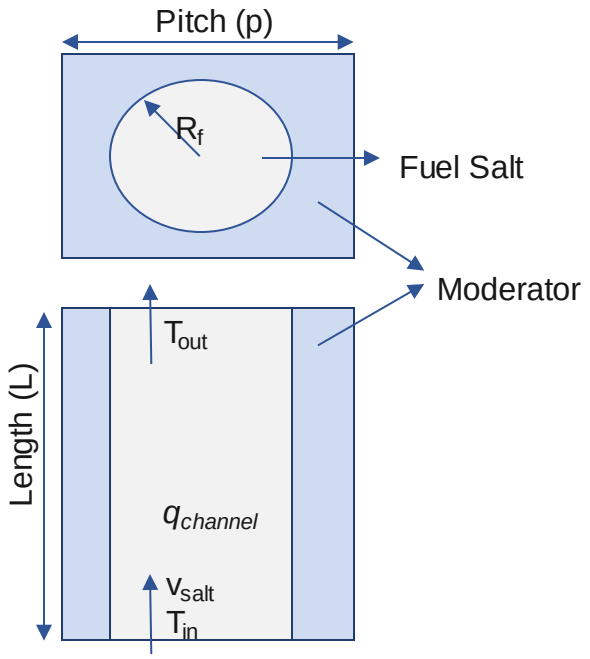
Performance Metrics:

i. Infinite multiplication factor (k_∞),

ii. Conversion ratio (ς),

iii. Fast flux (φ_{fast}) incident on moderator

iv. Total feedback coefficient (α_{total})



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Assumptions/Approximations/Simplifications

- The α_{total} is a vital metric but non-urgent matter once the k_∞ is precisely predicted, the α_{total} can be predicted promptly and accurately with the following equation

$$\alpha_{total} = \partial\rho/\partial T \approx \Delta\rho/\Delta T \text{ where } \rho = 1\text{-}1/k$$

- Unit cell approximation with square lattice is a basic but effective geometry structure for periodicity
- Fuel-salt is assumed to be stationary, by neglecting the thermal-hydraulic effects
- Calculations for fresh fuel
- The total heat generation rate per unit channel length, expressed as average temperature difference between inlet and outlet temperatures, T_{ave}

$$T_{ave} = (T_{in} + T_{out})/2$$

- The base temperature 900 K for feedback calculations

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Step 1: Reactor Database Generation

- Grid sampling strategy, the simplest exploration approach to explore an uncertain domain, construct an N-dimensional grid where each dimension is represented by one variable
- Neutron transport calculation is conducted at each node of the grid
- Sample size in training dataset: 285000 designs
- Sample size in testing dataset: 8000 designs with Monte Carlo method
- Equally divided steps in grid sampling strategy
- Learning curve for sampling size determination

Variable	Distribution	Lower/Upper Values	Step
Fuel Type	Discrete	U, U-Th, U-Pu	3
Salt Type	Discrete	LiF-BeF_2, NaF-BeF_2, NaCl	3
f^{35}	Continuous	1-20 wt.%	10
f^{U}	Continuous	10-90 wt.%	9
p	Continuous	1-16 cm	10
ξ	Continuous	0.274-10.46	10
T^{ave}	Continuous	900-1200	5

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Step 2: Training a Predictive Model

- Machine learning methods: Regressor/Classifiers
- Multi-target multi-output method in regression while multi-label multi-output method in classification
- MinMaxScaler scaler for standardization of datasets
- GridSearchCV technique for the optimization of hyper-parameters of estimators

Method	Estimator
Ensemble	RandomForest (RF), Bagging (B), AdaBoost (AB), ExtraTrees (ET), GradientBoosting (GB)
Linear	ElasticNet (EN), Perceptron (P), Ridge (R), Lasso (L), LassoLars (LL), StochasticGradientDescent (SGD), Logistic (Log)
Naive Bayes	GaussianNB (GNB), BernoulliNB (BNB)
Neighbor-Based	KNeighbors (KN)
Support Vector	SupportVector (SV)
Neural Network	MultiLayerPerceptron (MLP)
Decision Tree	DecisionTree (DT)
Semi-Supervised	LabelPropagation (LP)

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Step 2: Training a Predictive Model

Classification labels:

- ς value (conversion ratio) determines reactor type
- EALF value (energy corresponding to average lethargy of neutrons causing fission) determines reactor spectrum
- k_∞ determines criticality
- α_{total} determines reactivity feedback

Reactor Type	Reactor Spectrum	Criticality	Reactivity Feedback
Breeder (≥1)	Thermal (<1 eV)	Subcritical (<1)	Positive (≥0)
Burner (<1)	Fast (≥1 eV)	Supercritical (≥1)	Negative (<0)

Step 3: Design Optimization

- Choice of Optimizer:
  - Linear, non-linear, gradient-based methods are not working due to discrete values in feature parameters like fuel-type and salt-type
  - Only evolutionary algorithms such as GA, Pattern Search
  - Non-dominated Sorting Genetic Algorithms (NSGAIII) from the pymoo tool
- Operators:
  - Selection: Tournament,
  - Crossover: Simulated Binary (SBX),
  - Mutation: Polynomial (PM)
- Objectives: Performance metrics
- Variables of Fitness Function: Feature parameters
- Fitness Function Evaluator: The trained estimator in Step 2

Step 3: Design Optimization

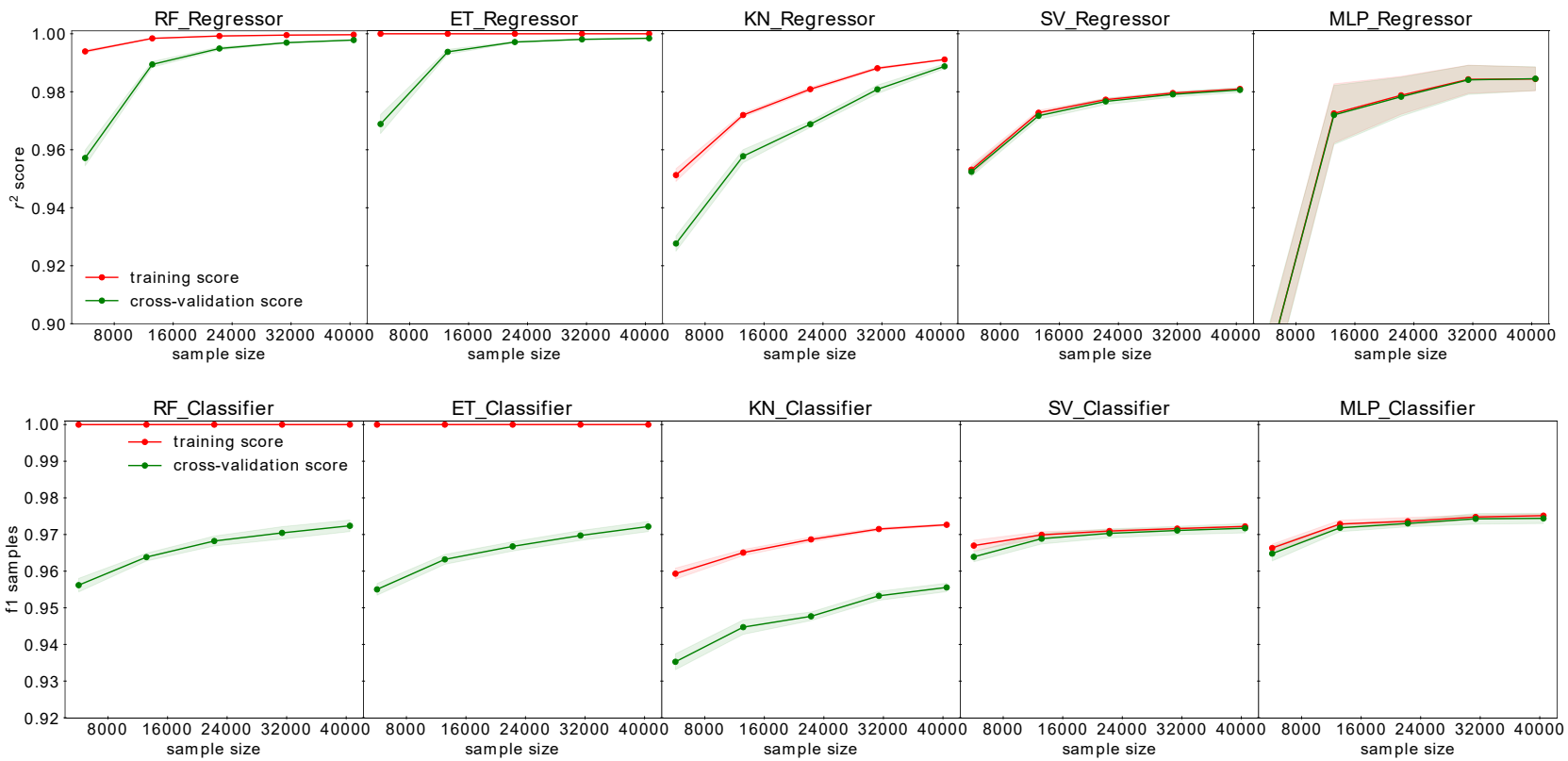
- Constraints:
  - $k_\infty > 1.06$,
  - $\varsigma > 0.6$,
  - $\varphi_{fast} < 50$ (# per source neutron)
- Parameters of Optimizer:
  - Population: 150,
  - Number of generations: 5000,
  - Other parameters are set to defaults
- Cross-check with their actual values:
  - Serpent simulations for optimum solutions
  - Acceptance criterion for the prediction: less than 5% relative error
- Search for a set of optimum solutions for each fuel-salt couple

Part II - Results

- Sampling Size Determination
- Training a Predictive Model: Preselection
- Training a Predictive Model: Finalization
  - Hyper-Parameter Optimization
  - Cross-validation and Confusion Matrix
- Design Optimization

Step 1: Sampling Size Determination

- R^2 scores for regression and f1 samples for classification
- Performance scores approach a constant value
- About 40000 samples for each fuel-salt couple.
- For nine fuel-salt couples, about 300,000 samples for the training dataset.



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Step 2: Preselection

- Linear (i.e., SGD, R, and Log) and Naive Bayes methods yield lower fit_score and higher errors with respect to non-linear methods such as ensemble, SVM and NN.
- Some estimators have similar results as they use the same base estimator

- Based on their scores/errors and methods, RF, ET, KN, SV and MLP are the candidate estimators
  - ✓ higher than 0.90 R2 score for regressors
  - ✓ higher than 0.93 ROC_AUC score for classifiers

Regressors

	RF	ET	KN	SV	MLP	DT	GB	B	AB	SGD	R	EN	L	LL
fit_score	1.00	1.00	0.99	0.96	0.99	1.00	0.97	1.00	0.78	0.54	0.73	0.70	0.69	0.55
EVR	0.90	0.98	0.97	0.98	0.95	0.90	0.89	0.90	0.54	0.38	0.37	0.46	0.25	0.38
MAE	1.27	0.35	0.57	0.54	0.87	1.28	1.72	1.27	3.36	4.77	4.78	4.60	4.77	4.77
MSE	7.60	0.62	1.61	1.45	2.97	7.71	12.99	7.60	38.85	82.73	82.94	77.95	81.94	82.95
R^2	0.90	0.98	0.97	0.98	0.95	0.90	0.89	0.90	0.00	0.23	0.22	0.35	0.07	0.23

Classifiers

	RF	ET	KN	SV	MLP	DT	B	LP	GB	AB	SGD	R	GNB	BNB	P	Log
fit_score	1.00	1.00	0.91	0.90	0.90	1.00	0.98	0.90	0.88	0.84	0.61	0.65	0.64	0.55	0.45	0.68
AP	0.90	0.93	0.92	0.95	0.96	0.90	0.90	0.96	0.91	0.90	0.80	0.69	0.78	0.52	0.77	0.81
HL	0.05	0.04	0.04	0.03	0.04	0.05	0.05	0.04	0.05	0.06	0.17	0.18	0.13	0.18	0.22	0.17
LRAPS	0.94	0.95	0.95	0.96	0.96	0.94	0.94	0.95	0.94	0.93	0.81	0.81	0.86	0.82	0.77	0.82
LRL	0.09	0.07	0.07	0.06	0.06	0.09	0.09	0.06	0.08	0.09	0.27	0.28	0.21	0.27	0.34	0.27
ROC_AUC	0.92	0.94	0.94	0.96	0.95	0.92	0.92	0.92	0.93	0.93	0.79	0.70	0.87	0.60	0.75	0.77

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Step 2: Preselection

- RF, ET, KN, SV and MLP estimators predict performance metrics remarkably good, with a high accuracy
- Without hyper-parameter optimization, these five estimators provide
  - ✓ R2 scores up to 98% for regression
  - ✓ ROC_AUC score up to 96% for classification.
- To further improve the scores:
  - ➢ optimization of hyper-parameters
  - ➢ outlier elimination: $k_{\infty} < 0.5$ and $\varsigma > 2.0$

Regressors

	RF	ET	KN	SV	MLP	DT	GB	B	AB	SGD	R	EN	L	LL
fit_score	1.00	1.00	0.99	0.96	0.99	1.00	0.97	1.00	0.78	0.54	0.73	0.70	0.69	0.55
EVR	0.90	0.98	0.97	0.98	0.95	0.90	0.89	0.90	0.54	0.38	0.37	0.46	0.25	0.38
MAE	1.27	0.35	0.57	0.54	0.87	1.28	1.72	1.27	3.36	4.77	4.78	4.60	4.77	4.77
MSE	7.60	0.62	1.61	1.45	2.97	7.71	12.99	7.60	38.85	82.73	82.94	77.95	81.94	82.95
R^2	0.90	0.98	0.97	0.98	0.95	0.90	0.89	0.90	0.00	0.23	0.22	0.35	0.07	0.23

Classifiers

	RF	ET	KN	SV	MLP	DT	B	LP	GB	AB	SGD	R	GNB	BNB	P	Log
fit_score	1.00	1.00	0.91	0.90	0.90	1.00	0.98	0.90	0.88	0.84	0.61	0.65	0.64	0.55	0.45	0.68
AP	0.90	0.93	0.92	0.95	0.96	0.90	0.90	0.96	0.91	0.90	0.80	0.69	0.78	0.52	0.77	0.81
HL	0.05	0.04	0.04	0.03	0.04	0.05	0.05	0.04	0.05	0.06	0.17	0.18	0.13	0.18	0.22	0.17
LRAPS	0.94	0.95	0.95	0.96	0.96	0.94	0.94	0.95	0.94	0.93	0.81	0.81	0.86	0.82	0.77	0.82
LRL	0.09	0.07	0.07	0.06	0.06	0.09	0.09	0.06	0.08	0.09	0.27	0.28	0.21	0.27	0.34	0.27
ROC_AUC	0.92	0.94	0.94	0.96	0.95	0.92	0.92	0.92	0.93	0.93	0.79	0.70	0.87	0.60	0.75	0.77

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Step 2: Final Scores

- With optimal hyper-parameters and outlier elimination:
  - ✓ scores of MLP significantly improves
  - ✓ a slight enhancement in the scores of other regressors
  - ✓ no notable difference in the scores of the classifiers
  - ✓ training and R2 scores increase by 4% in regression
  - ✓ a small fraction (< 5%) of incorrectly predicted labels and a high precision (> 95%) in classification
- To find the right estimator, we investigated the cross-validation plots and confusion matrices

Regressors

Regressors	Random Forest	Extra Tree	K-Neighbors	Neural Network	SVR
training_score	1.00	1.00	1.00	1.00	0.97
exp_var_err	0.94	0.99	0.99	1.00	0.96
mean_abs_err	1.07	0.28	0.41	0.23	0.37
mean_sqrt_err	5.52	0.41	0.83	0.24	0.44
r2_score	0.94	0.99	0.98	1.00	0.96

Classifiers

Classifiers	Random Forest	Extra Tree	K-Neighbors	Neural Network	SVC
training_score	0.93	1.00	1.00	0.90	0.89
precision_score	0.92	0.94	0.95	0.97	0.96
hamming_loss	0.04	0.04	0.04	0.03	0.03
label_ranking_average_precision_score	0.95	0.96	0.96	0.97	0.96
label_ranking_loss	0.07	0.06	0.06	0.05	0.05
roc_auc_score	0.94	0.95	0.96	0.96	0.95

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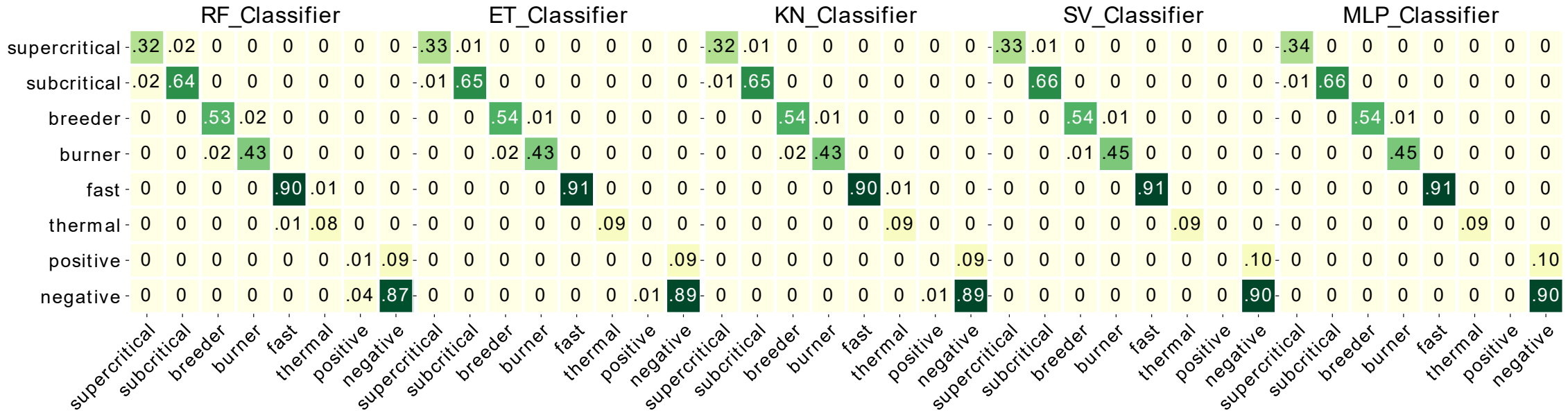
Step 2: Cross-validation and Confusion Matrix



- Performance scores of estimators are very close each other.
- All labels are classified by less than 4% error except for the feedback label which has an error of about 10%.
  - This mislabeling originates from the feedback coefficient very close to zero.

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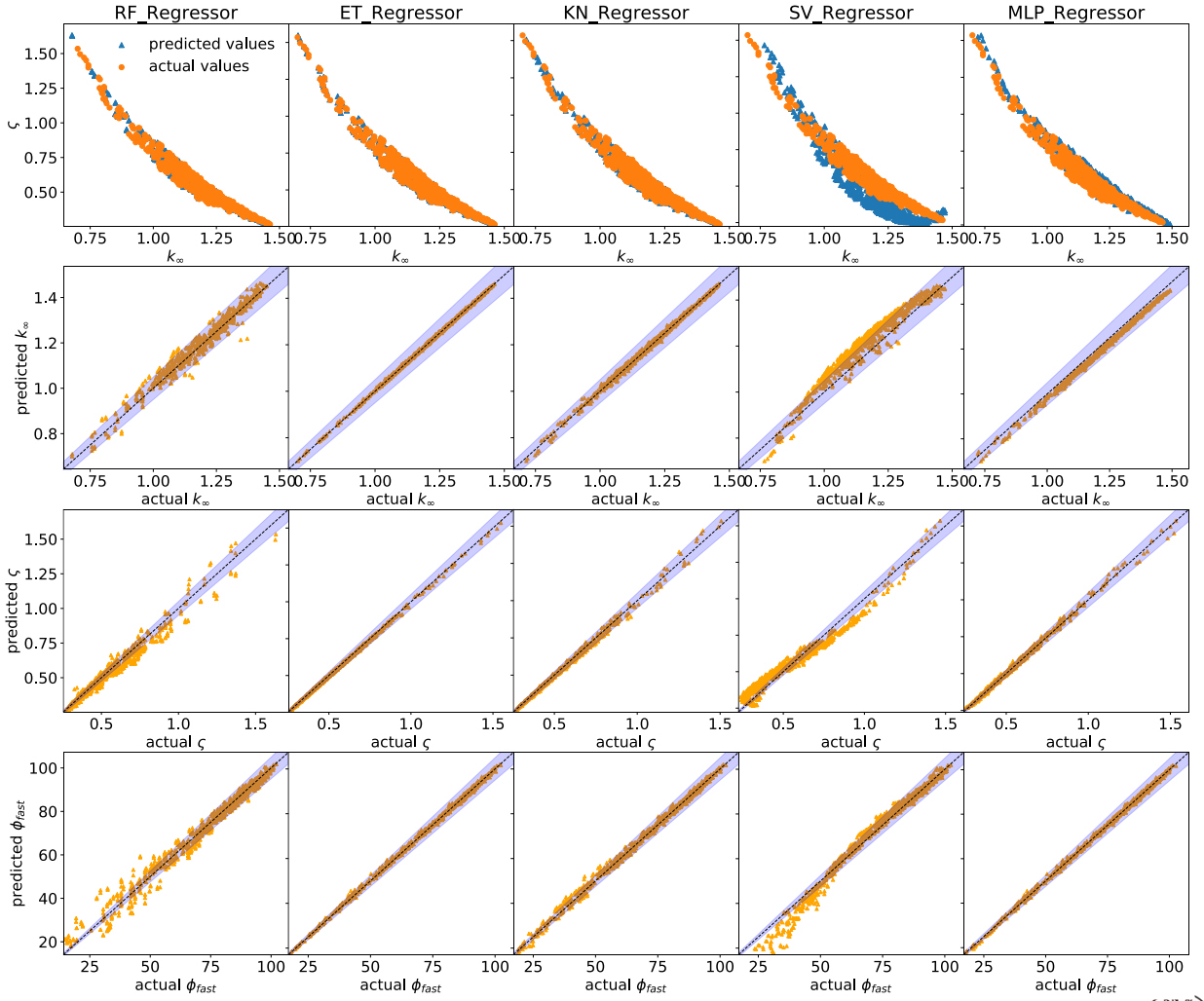
Step 2: Cross-validation and Confusion Matrix

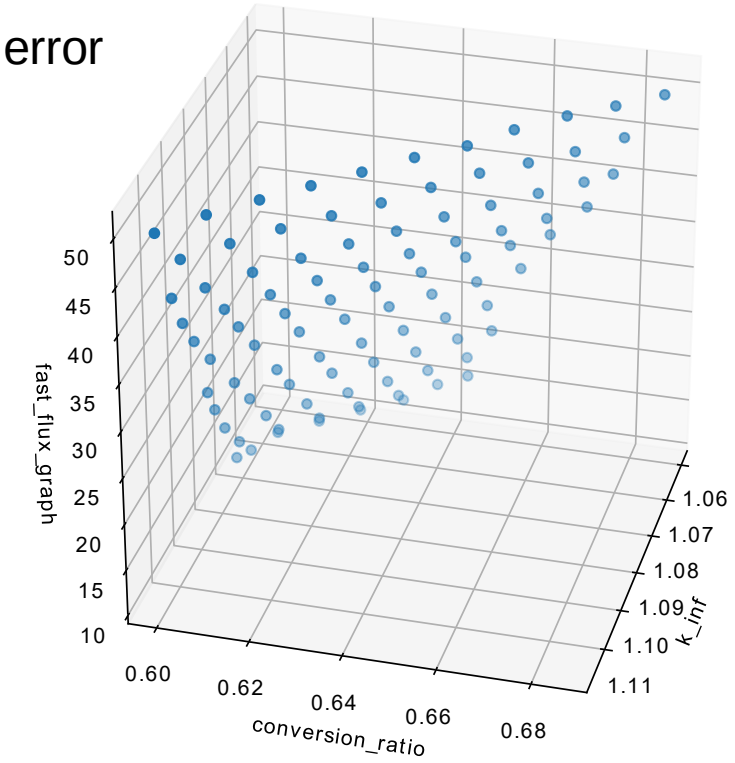
- Despite their high performances, SVR and RF are not eligible
- ET and MLP predict each performance metric very well
  - ✓ All performance metrics predicted by less than 5% relative error
  - ✓ No need to further improvement
- MLP as good as ET, but with considerably higher uptime
- ET was concluded as one of the final estimators and was used in optimization step as it totally satisfies the acceptance criterion

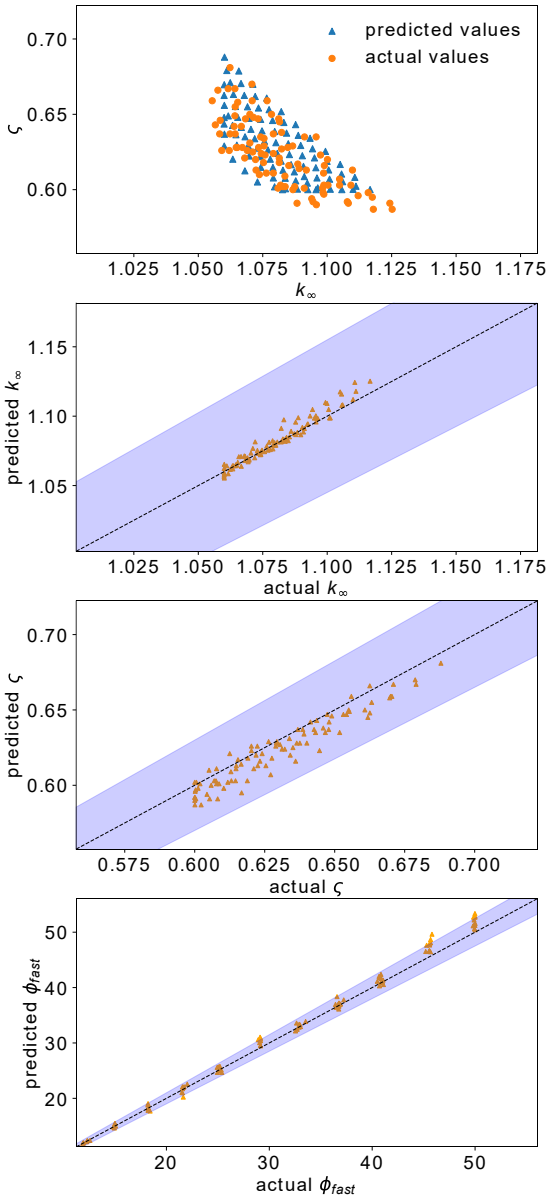


Step 3: Design Optimization

- Fuel-salt couple: (U-Th)F_4 - NaF-BeF_2
- Well distributed solution set
- All optimum solutions satisfy the acceptance criterion, staying within the gray area
- All labels are predicted with no error

	supercritical	subcritical	breeder	burner	fast	thermal	positive	negative
supercritical	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
subcritical	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
breeder	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
burner	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00
fast	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
thermal	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
positive	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
negative	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.99





Step 3: Design Optimization

- Optimum designs based on the constraints on the performance metrics:
  - ✓ have an explicit relation with fuel type rather than salt type
  - ✓ require a particular ^{235}U enrichment and U content depending on fuel type
  - ✓ favor a T_{ave} > 1100 K and ξ = 0.274
- The best fuel-salt options:
  - ✓ for the highest negative feedback coefficient: UF_4-PuF_3-LiF-BeF_2
  - ✓ for the longest graphite lifetime, the highest ς and a sufficiently high α_{total}: (U-Pu)Cl_3-NaCl

Fuel Type	Salt Type	f_{35} [wt.%]	f_U [wt.%]	p [cm]	T_{ave} [K]	ξ	k_∞ (pcm)	ς (milli)	φ_{fast} [# per source neutron]	α_{total} [pcm/K]
U	LiF-BeF2	14.47	100	5.73	1200	0.274	1.0600(+60)	0.661(-6)	18.6(-0.5)	-3.9
U	NaF-BeF2	14.88	100	7.18	1125	0.274	1.0600(-120)	0.638(+6)	19.0(-0.9)	-4.0
U	NaCl	14.28	100	1.00	1176	0.274	1.0604(-20)	0.692(0)	12.6(0)	-3.0
U-Th	LiF-BeF2	19.10	86.7	5.50	1123	0.276	1.0601(-70)	0.665(-7)	17.1(-0.2)	-4.3
U-Th	NaF-BeF2	20.00	86.8	5.98	1125	0.275	1.0600(+30)	0.643(-11)	16.0(-0.2)	-2.8
U-Th	NaCl	18.48	86.2	1.00	1199	0.274	1.0600(+140)	0.696(-1)	14.4(0)	-2.8
U-Pu	LiF-BeF2	5.00	90.0	4.40	1198	0.274	1.0600(-20)	0.732(+3)	16.0(0.2)	-4.5
U-Pu	NaF-BeF2	5.00	89.3	4.37	1125	0.275	1.0600(+460)	0.723(+15)	13.6(0.3)	-3.3
U-Pu	NaCl	5.00	90.0	1.00	1193	0.274	1.2192(+10)	0.753(+1)	13.0(0)	-3.4

Step 3: Design Optimization

- Very small difference from the actual values (values within round brackets)
- α_{total} values are comparable with literature values
- All calculations were done in a single processor less than 60 minutes including validation simulations with the actual values.
- Solutions free from the GA parameters like population size

Fuel Type	Salt Type	f_{35} [wt.%]	f_U [wt.%]	p [cm]	T_{ave} [K]	ξ	k_∞ (pcm)	ς (milli)	φ_{fast} [# per source neutron]	α_{total} [pcm/K]
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U-Th	NaCl	18.48	86.2	1.00	1199	0.274	1.0600(+140)	0.696(-1)	14.4(0)	-2.8
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U-Pu	NaCl	5.00	90.0	1.00	1193	0.274	1.2192(+10)	0.753(+1)	13.0(0)	-3.4

Key Achievements and Drawbacks in the Research

- Integration of the ML-enabled technique into the reactor core design process for the prediction of performance metrics
- Facilitation of the reactor design process in a very short time (within minutes) compared to other methods
- Without using any reactor physics code, evaluation of performance metrics with very high accuracy
- Independent from number of feature parameters and performance metrics
- Makes multi-purpose reactor designs available by providing more flexibility in fuel management, prolonged reactor life-time and so forth

- The only concern is the optimization constraints on the performance metrics
- Quality of training dataset containing out-of-interest values (outliers)
- The only difficulty is to generate a high-quality reactor database.

Concluding Remarks

- The highest scores: ensemble, support vector, neural network and decision tree methods
- The lowest scores: linear methods
- RF, ET, KN, MLP and SV showed outstanding performance among ML methods
- No significant improvement on the fit scores of the estimators by the hyper-parameters optimization except for NN
- All the performance metrics predicted and classified with very high accuracy.

- The common properties of the optimum designs implies:
  - ✓ a particular ^{235}U fraction (f_{35}) in U
  - ✓ a certain fraction of U content (f_U) associated with fuel type but not salt type,
  - ✓ T_{ave} higher than 1100 K and
  - ✓ a moderator-to-salt ratio of 0.274.
- All the optimum designs were classified as supercritical reactor, burner type, fast spectrum and negative flag in feedback coefficient.
- Based on the best fuel-salt options are (U-Pu)Cl_3-NaCl and UF_4-PuF_3-LiF-BeF_2

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Future Work

- As a second phase of the ongoing study, a full-core (or small scale or assembly) design of MSR
- A more sophisticated sampling strategy instead of grid sampling technique used in generating the reactor database
- Integrating the Moltres software with the python tool for thermal-hydraulic feedbacks

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Thank you for your attention!

Any questions?