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Risk Modeling and Optimization Using Machine Learning Algorithms for PSA Applications

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According to the latest reports from the International Atomic Energy Agency, the global nuclear power plant (NPP) fleet is aging, requiring enhanced risk estimation and safety management tools. Additionally, international organizations are promoting the use of artificial intelligence to improve NPP operation and safety, as highlighted by the U.S. Nuclear Regulatory Commission in its Strategic Plan for 2023-2027. This context presents an opportunity to incorporate artificial intelligence and machine learning techniques into risk-informed applications. This work presents a methodology that integrates a metamodel for predicting Core Damage Frequency (CDF) with an optimization method using genetic algorithms to reduce CDF, thereby enhancing plant safety. The proposed metamodel predicts CDF using reliability parameters related to component failure modes and test intervals (TI) of standby equipment as explanatory variables. Traditionally, TIs are set as fixed values grouped by periodicity (e.g., weekly, monthly, yearly). This study introduces additional levels—higher and lower than standard values—to assess their impact on NPP risk, using a Fractional Factorial Design to efficiently generate a representative dataset. Several metamodels were trained and evaluated, with the best-performing one selected to replace conventional Probabilistic Safety Assessment (PSA) models. The genetic algorithm was then implemented to find the optimal combination of TI values, minimizing the mean CDF. The use of the metamodel drastically reduces computational effort compared to resolving large event and fault trees, which is needed to speed up the genetic algorithm's computational time. The results demonstrate that this methodology enhances NPP safety by providing a powerful tool for risk management. Future developments could include analyzing the impact of maintenance on reliability parameters, and consequently, on the CDF.

Keywords: Probabilistic Safety Assessment (PSA), Core Damage Frequency (CDF), machine learning, metamodel, optimization.

1. Introduction

For several years now, member countries of the European Union (EU) have been dedicating part of their efforts to achieving decarbonization as soon as possible. In January 2022, the EU classified nuclear energy and natural gas as transitional activities under strict conditions to reach a net-zero emissions scenario. This classification requires nuclear power plants (NPPs) to meet the highest standards of reliability and safety (European Comission, 2022).

Additionally, according to the 2023 report by the International Atomic Energy Agency (IAEA), many operational nuclear reactors have exceeded 30 years of service (IAEA, 2023). Specifically, 73% of reactors have been operating for over 30 years, and 25% have surpassed 40 years, indicating that they have been licensed for extended operational life beyond their original design, known as Long-Term Operation (LTO). In Spain, the National Integrated Plan of Energy and Climate (PNIEC) establishes the gradual shutdown of NPPs by 2035 (Ministry for the Ecological Transition and the Demographic Challenge, 2020). However, by this date, all NPPs in Spain will have exceeded their design life and will need to request authorization to operate longer, entering the LTO phase.

During this phase, some critical reactor safety elements may have experienced significant degradation, making it even more important to accurately predict their reliability and associated risks to ensure a safe LTO.

One of the most effective tools used in NPPs to estimate risk levels is Probabilistic Safety Assessment (PSA). In the industry, specific software tools like RiskSpectrum or CAFTA are fundamental for implementing PSA. However, these commercial programs have significant limitations in modeling flexibility, as they do not explicitly account for dependencies between failure rate models and aging, the effectiveness of maintenance and asset management policies, or the impact of surveillance on the availability of safety equipment.

In this context, the use of advanced computational techniques can help improve PSA accuracy. In fact, the United States Nuclear Regulatory Commission (US NRC), in its 2023–2027 Strategic Plan, recognized the need for artificial intelligence (AI) and machine learning techniques in risk-informed applications (U.S.NRC, 2023).

Different surrogate models have been proposed before (Asensio et al., 2023). This paper focuses on the use of machine learning algorithms to develop a metamodel capable of predicting the Core Damage Frequency (CDF), which can replace commercial PSA software and address its limitations. The proposed approach aims to integrate the effects of surveillance and maintenance programs, as well as their relationship with aging, into the model. To achieve this, the models developed in this study are trained using 54,000 simulations derived from a PSA code, encompassing 1,055 variables, including failure rate parameters and test intervals for standby equipment (TI).

2. Probabilistic Safety Assessment (PSA)

PSA is a technique used to quantitatively evaluate the risk associated with a facility. In the context of NPPs, this risk is defined as the probability of a specific accident occurring, weighted by the consequences resulting from that accident (IAEA, 2001). To quantify risk, PSA combines Event Trees (ET) and Fault Trees (FT). ETs describe the possible outcomes of an initiating event (an occurrence that could endanger the plant if not properly managed), considering the success-failure relationships of the critical systems involved. On the other hand, FTs estimate the probability of failure of a specific system based on the likelihood of basic events (BE) occurring. This approach has proven suitable for analyzing facilities whose safety depends on multiple and redundant safety systems, as is the case with NPPs (Martorell et al., 2018). In the nuclear industry, PSA is divided into three levels:

- Level 1: Estimates the frequency of accidents that result in core damage, known as Core Damage Frequency (CDF).
- Level 2: Calculates the frequency of radioactive material release to the environment for each accident identified in Level 1. This frequency is referred to as the Large Early Release Frequency.
- Level 3: Assesses the consequences of these accidents in terms of harm to the public and the environment.

Currently, all NPPs in Spain have Level 1 and Level 2 PSA, but the scope of this work focuses solely on Level 1. The procedure followed in a Level 1 PSA allows identifying the most probable accident sequences and the failures that contribute most to the risk. The information obtained is used to reduce the risk at the facility through design improvements, additional training for operators, or adjustments to the testing frequency of the most critical components, among other measures. However, PSA for Spanish NPPs are updated every five years, incorporating modifications and significant operational experiences since the last update.

As can be inferred, this approach limits the ability to continuously monitor the impact of aging, degradation, and maintenance policies on safety. This results in a static perspective that may not adequately reflect risks as plants approach LTO, where aging requires stricter consideration. To address these limitations, it is essential to develop a metamodel that explicitly integrates the effects of surveillance and maintenance programs and their relationship to equipment aging. If a model with these characteristics can be validated, it could replace the standard PSA model, providing a more dynamic and accurate risk assessment.

3. Methodology

The stages of the proposed methodology are briefly described below. To aid comprehension, Figure 1 presents a diagram summarizing the process.

- *Stage 1. Modeling of reliability parameters*
  Reconstructing the distribution function for each parameter enables the sampling of potential values through Monte Carlo simulation. These sampled values are used to estimate the CDF values required for building the models (Stage 3).

- *Stage 2. Analysis of test groups and Design of Experiments (DoE).*
  Initially, only those groups with a significant impact on plant risk are selected. Subsequently, groups of components sharing the same testing strategy—tested at intervals of equal duration—are identified. To develop a model applicable not only to current test intervals (TIs) but also to a broader range, variability is introduced through a DoE approach.

- *Stage 3. Development of a machine learning model for CDF estimation.*
  Several metamodels (ElasticNet, LightGBM, MARS, and XGBoost) are developed. These utilize data generated from the simulation of reliability parameters (ρ, λ, and γ) and the DoE for TIs to predict the CDF. The algorithms implemented by the metamodels are presented in Section 4.

- *Stage 4. Selection and analysis of performance metrics.*
  To select the best final model, three performance metrics are considered to evaluate the models' performance.

  a) Coefficient of determination (R^2) is commonly interpreted as the proportion of the variance that is explained by the regression model.

$$R^2 = 1 - \frac{\sum_{i=1}^{I}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{I}(y_i - \bar{y}_i)^2} \quad (1)$$

  where y_i is the observed response variable value, $\hat{y}_i$ the predicted value, and $\bar{y}_i$ the mean of y_i.

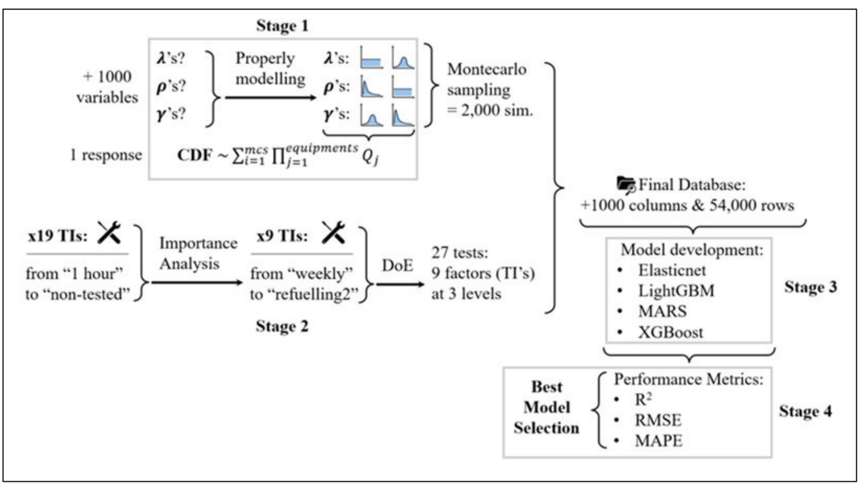

Figure 1. Four-step based methodology scheme.

b) Root Mean Square Error (RMSE) measures the error between model's estimation and the true value.

$$RMSE = \sqrt{\frac{1}{I}\sum_{i=1}^{I}(y_i - \hat{y}_i)^2} \quad (2)$$

c) Mean Absolute Percentage Error (MAPE) measures the error as a ratio defined by the following formula:

$$MAPE = \frac{100}{I}\sum_{i=1}^{I}\left|\frac{y_i - \hat{y}_i}{y_i}\right| \quad (3)$$

4. Metamodels

The following sections briefly describe the different metamodels implemented.

4.1. ElasticNet

ElasticNet is a linear regression method that combines Ridge and Lasso regularization terms in the cost function. This approach balances Ridge's ability to handle multicollinearity with Lasso's feature selection advantages. The cost function is expressed as:

$$\min_{\beta_j}\left[\frac{1}{2I}\sum_{i=1}^{I}(y_i - \hat{y}_i)^2 + \lambda_1\sum_{j=1}^{J}\beta_j^2 + \lambda_2\sum_{j=1}^{J}\|\beta_j\|\right] \quad (4)$$

where λ_1 and λ_2 are the penalization parameters for Ridge and Lasso, respectively. If ($\lambda_1 > 0,\ \lambda_2 = 0$) the method reduces to Ridge regression. On the other hand, when ($\lambda_1 = 0$, $\lambda_2 > 0$) it corresponds to Lasso regression. When both parameters are greater than zero, the ElasticNet method is applied (Bai et al., 2023).

4.2. Multivariate Adaptative Regression Splines (MARS)

MARS model (Friedman, 1991) is a non-parametric regression model that extends the linear models and it modeling non-linearities and interactions between independent variables, $\boldsymbol{x}$. MARS can be expressed as:

$$\hat{y}_i(x_i) = \beta_0 + \sum_{n=1}^{N}\beta_n \cdot h_n(x_i) \quad (5)$$

The functions $h_n(x_i)$ serve as basis that apply transformations based on the value of the input variables, x_i. The model construction follows a forward iterative process, where two basis functions are generated for each selected knot, t_{ij}:

$$h_1(x_i) = \begin{cases} x_{ij} - t_{ij}, & x_{ij} > t_{ij} \\ 0, & x_{ij} \le t_{ij} \end{cases}$$

$$h_2(x_i) = \begin{cases} 0, & x_{ij} > t_{ij} \\ t_{ij} - x_{ij}, & x_{ij} \le t_{ij} \end{cases} \quad (6)$$

These functions are then incorporated to the original model:

$$\hat{y}_i(x_i) = \beta_0 + \beta_1 h_1(x_i) + \beta_2 h_2(x_i) \quad (7)$$

This procedure allows splines to be interpreted as regression lines that operate within different ranges of predictor variables. A linear regression model is fitted to each segment of the dataset, and the process is repeated until the desire number of functions $h_n(x_i)$ is reached, leading to a final pruning phase (a backward variable elimination process).

4.3. Extreme Gradient Boosting (XGBoost)

XGBoost is one of the most widely used boosting tree algorithms for gradient boosting machines (Friedman, 2001). At each step of the algorithm, it generates a weak learner and integrates it into the final model. By employing an additive approach, XGBoost combines multiple functions to predict the response variable as follows:

$$\hat{y}_i(x_i) = \sum_{m=1}^{M} f_m(x_i) \quad (8)$$

where f_m represents a regression tree and $f_m(x_i)$ denotes the scoring given by the m-th tree to the i-th observation.

The objective function consists of two components: the loss function l, which measures the model's accuracy, and the regularization term Ω, which controls its complexity:

$$OF = \sum_{i=1}^{I} l(y_i, \hat{y}_i) + \sum_{m=1}^{M}\Omega(f_m) \quad (9)$$

being Ω evaluated as:

$$\Omega(f_m) = \gamma K + \frac{1}{2}\lambda\|w\|_2 \quad (10)$$

In Eq. (10), γ and λ are parameters that regulate the penalization applied to the number of leaves K and the magnitude of the weights w, respectively (Chen & Guestrin, 2016).

4.4. Light Gradient Boosting (LightGBM)

LightGBM operates similarly to XGBoost, as both optimize trees using gradient descent (Ke et al., 2017). However, LightGBM preprocesses data by converting continuous variables into discrete ones (histogram-based algorithm), reducing computational cost.

Unlike level-wise tree algorithms, LightGBM follows a leaf-wise strategy, expanding the leaf with the highest loss function value instead of growing all branches evenly. This approach enhances predictive accuracy in high-variability regions and achieves lower loss levels with the same number of leaves.

5. Application Case

This section focuses on the specific challenges encountered during the project. The primary goal is to demonstrate how the theoretical component (methodology) was effectively translated into practical results (data generation and analysis).

The following provides a detailed explanation of the application of the procedure described in Section 3.

5.1. *Stage 1: Modeling of reliability parameters*

The first step in the work focuses on modeling the reliability parameters of NPP's equipment to calculate their unavailability. This involves identifying the statistical distributions used by commercial software to represent these parameters. The parameters for these distributions, such as scale, shape, mean, and spread, are obtained from the software

With this information, it becomes feasible to calculate the unavailability associated with different failure scenarios, such as failures during demand, operation, or standby.

By combining the unavailability for individual components within the plant, it is possible to estimate CDF. This is achieved by referencing the Level 1 PSA, which provides the minimal cut set structures for evaluating how combinations of component unavailability contribute to the overall risk.

5.2. *Stage 2: Analysis of test groups and Design of Experiments (DoE).*

To develop a machine learning model capable of predicting the CDF not only for the current TIs, but also for a wide range of them, a DoE approach has been used. First, it is necessary to prioritize the different TI groups to determine the required number of experiments and how to structure the design.

Based on an importance analysis using the Fussell-Vesely (FV) metric (Van der Borst & Schoonaker, 2001) the BEs with the greatest impact on plant safety were selected. This process reduced the number of BEs from 3,941 to 595. Then, only BEs classified as standby failures (the only type of unavailability dependent on TIs) were retained, further reducing the count from 595 to 150. Finally, the different TIs applied to these 150 BEs were identified and grouped, resulting in 9 TI groups.

Applying a Fractional Factorial Design (FFD) is feasible with 9 TIs, offering a specialized methodology within the DoE framework that significantly reduces the number of required tests. Specifically, a Taguchi L_{27} orthogonal array design was employed, allowing the study of the 9 TI groups across three levels for each group using only 27 experiments.

Table 1 summarizes the values at which each TI group will be tested.

Table 1. TI groups with the highest impact on risk and values (hours) of corresponding levels.

Factor (TI)	Levels (hr)		
	1	2	3
Weekly	48	168	288
Monthly	360	720	1,440
Tower replenish	720	1,252	2,160
Quarterly	720	2,160	4,320
RX	2,160	4,616	6,570
9 Months	4,320	6,570	8,760
Yearly	4,320	8,760	13.080
Refuelling	8,760	13,140	17,520
Refuelling2	13,140	26,280	39,420

After determining the TI combinations for each experiment, 2,000 simulations were conducted for each of the 27 combinations using the Monte Carlo method. These simulations are essential to account for the variability in the distributions of failure rate parameters, resulting in a total of 54,000 observations.

5.3. *Stage 3: Development of a machine learning model for CDF estimation*

Once the required dataset was generated, the machine learning models presented in Section 4 —Elastic Net, Light GBM, MARS, and XGBoost— were implemented.

From the total 54,000 observations, 80% (43,200) were used to train the models, while the remaining 20% (10,800) was used as a test set to evaluate the models' performance on new data. For both the training and validation sets, the 27 tests from the FFD were sampled proportionally to ensure equal representation, a process known as stratified sampling.

5.4. *Stage 4: Selection and analysis of performance metrics*

The results for the three performance metrics (R^2, RMSE, and MAPE) considered during the validation of the different models are presented in Table 2. These metrics were calculated using the test set.

Table 2. R^2, RMSE and MAPE for the four metamodels.

Model	R^2	RMSE (hr^{-1})	MAPE (%)
MARS	0.943	$2.167E^{-6}$	16.1
XGBoost	0.914	$2.755E^{-6}$	9.8
LightGBM	0.877	$3.293E^{-6}$	12.3
ElasticNet	0.615	$6.014E^{-6}$	28.3

Based on the information about model performance, two candidates stand out clearly above the rest. On one hand, the MARS model achieved the best results in terms of R^2 (0.943) and RMSE ($2.167E^{-6}$). On the other hand, comparing its MAPE (16.1%) with that of the tree-based models (XGBoost and LightGBM) suggests that its predictions may be less accurate, especially compared to XGBoost, which achieved the best MAPE result (9.8%) while also ranking as the second-best model in the other metrics.

From a risk prediction perspective, it is important to use a "conservative" model—one that tends to overestimate rather than underestimate risk. To evaluate the conservatism of the models the percentage of observations where the predicted value falls below the actual value is calculated for all four models. This percentage is also obtained for the 95th and 99th percentiles of the CDF, as they represent the highest risk scenarios. The results are presented in Table 3.

Table 3. Percentage of underestimated predictions for the CDF's total, 95th and 99th percentile.

Model	Underestimated predictions (%)		
	Total	Perc.95	Perc.99
MARS	45.34	62.04	62.04
XGBoost	49.91	63.52	71.30
LightGBM	45.03	67.59	74.08
ElasticNet	51.69	80.37	86.11

The behaviour of the models is similar, showing a decrease in conservatism as the CDF value increases. Among the four models, MARS appears to be the least affected by this trend, with the percentage of underestimated predictions stabilizing around 62%. Also considering its R^2 and RMSE values, the finally selected model is the MARS.

5.5. *TI optimization*

This section aims to demonstrate the application of the validated machine learning model beyond predicting the CDF. In this application, the metamodel is combined with a genetic algorithm (GA) to optimize TIs under risk criterion. The optimization problem is formulated as follows:

Objective Function: $Minimize\ CDF_{mean}(TI_i)$

Variables: TI_i

being i the subscript indicating the TI group. These variables are defined as integers and are subject to the following constraints.

Constraints:
$Lower\ Bound = L_{low_i},\ Upper\ Bound = L_{upp_i}$

where the values of L_{low_i} and L_{upp_i} correspond to the minimum and maximum values of the TI shown in Table 1.

The algorithm implemented to find the combination of TI values that minimize the CDF mean is a GA. This type of optimization method is widely recognized and has been successfully applied in similar contexts (Choi et al., 2024). Figure 2 shows a diagram of the GA algorithm.

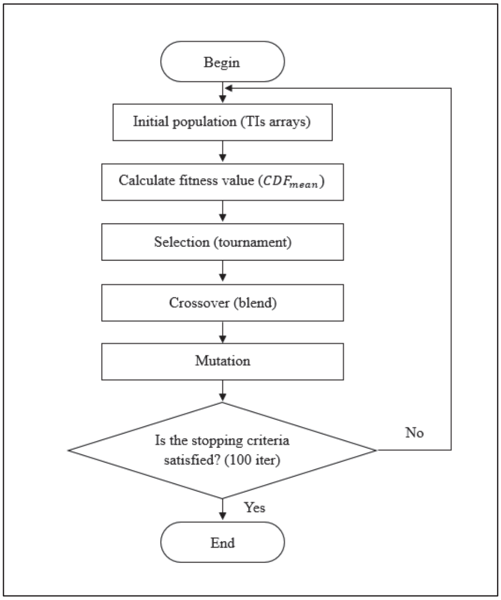

Fig. 2. Flow diagram of the GA stages.

To ensure a good performance from the GA the selection of its parameters has been realized using the methodology proposed in (Kucukkoc et al., 2013) based on response surface design.

Table 4. GA's parameters tested and their values.

Parameters	Values tested		
Population size	20	60	100
Crossover probability	0.1	0.5	0.9
Mutation probability	0.05	0.15	0.25
Elitism	2	4	8

These values were tested until completing the 81 unique combinations. Finally, all the solutions obtained were compared, and the one with the lowest mean CDF was selected (see Table 5).

Table 5. GA's parameters leading to the lowest mean CDF.

Population size	Crossover probability	Mutation probability	Elitism
60	0.9	0.25	2

The optimized TI values obtained using the GA and the initial values are presented in Table 6.

Table 6. TI values before and after the implementation of the GA.

TI	Value (hr)	
	Original	GA
Weekly	168	170
Monthly	720	980
Tower replenish	1252	1685
Quarterly	2160	2013
RX	4616	2160
9 Months	6570	6549
Yearly	8760	8141
Refuelling	13140	14458
Refuelling2	26280	29046

Using the optimized TI values the mean CDF decreases from $9.716E^{-6}$ (using the original TIs) to $8.680E^{-6}$, achieving a reduction of approximately 10.66%.

6. Conclusions

The main goal of this study was to develop a machine learning model capable of predicting the CDF while accounting for the effect of TIs. This approach can be used, for example, to optimize of TIs using the risk as criterion.

To achieve this, the methodology involved modeling reliability parameters and using the structure of minimal cut sets to compute the CDF. A FFD was applied to the TIs, defining the experiments needed to generate the dataset for training and validating the metamodels. Once the best-performing model was identified, a GA was used to determine the optimal combination of TI values that minimizes the mean CDF.

The results indicate that the MARS model is the most suitable for this purpose, achieving the highest R^2 (0.943) and demonstrating reliable predictive performance.

The inclusion of additional levels for TIs expands the range of operating conditions under which the safety of NPPs is assessed. This enhancement enables effective reduction of the mean CDF by optimizing TIs value, achieving an improvement of 10.66%.

Looking ahead, future work could focus on developing models that incorporate aging effects (APSA) and allow for continuous updates of reliability parameters, enabling a dynamic safety assessment framework (living PSA).

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