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Known as the fourth industrial revolution, digitization is an ongoing trend in all fields, in which various industries are integrating information technologies to support and improve their businesses. Nuclear technology industries have also increased their interest in data-driven methods by leveraging the potential of pattern recognition to identify anomalies and to take actions more rapidly, in areas such as health and monitoring, radiation detection, and optimization. By acknowledging the practicality and popularity of these methods, it is imperative to understand the benefits and barriers of implementing such methodologies to create better research plans and identify project risks and opportunities. This dissertation discusses different technologies and their integration and challenges within the nuclear industry. It is recognized that concepts of complexity and emergent behavior, as well as the importance of such properties as a distinctive aspect of nuclear and radiological engineering problems in which holistic approaches are crucial to innovation. Overall, the development and application of learning-based methods can be promising in the nuclear industry and many related tasks as long as expert knowledge is considered in the desired application to ensure a robust application of such methods. Cross-discipline studies and the creation of benchmarks are highly suggested for future practices.

Understanding the Application and Benefits of Learning-based Methods in Nuclear Science and Engineering

by

Mario Enrique Gómez Fernández

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I understand that my dissertation will become part of the permanent collection of Oregon State University libraries. My signature below authorizes release of my dissertation to any reader upon request.

Mario Enrique Gómez Fernández , Author

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I would like to dedicate this thesis to my aunt Alicia Mariela Fernández Arbizú, my family and friend in Guatemala, whose energy has always been by my side encouraging me to do my very best. My motivation has always come from my deepest love of my parents, Mario Enrique Gómez Ayala and Patricia Elena Fernández Arbizú, my sister, Luz Angelina Gómez Fernández and my passion towards challenging ideas.

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Chapter 1: General Introduction

This dissertation encompasses four self-contained papers corresponding to the relevant phases of the presented research. The first being a state of the art or review paper published in Nuclear Engineering and Design. As a review paper, it sets the scene to the domain of nuclear, radiological, and automation science to give an overview of some of the different areas where learning-based methods are being applied. It is the basis of the rest of this thesis, as the following chapters build on each of the different subsections of the review paper. The second paper, also published in Nuclear Engineering and Design, looks into the application of neural networks to predict the behavior of a prototype of a nuclear reactor system. The third paper was submitted for publication in Nuclear Instruments and Methods in Physics Research Section A. It focuses on the application to gamma spectra classification using convolutional neural networks in combination with an explainability method to understand the rationale of the decision of the algorithm. All of them also note the future work that needs to be done to develop trust among practitioners in the field as it considers many areas where modern technologies are being applied. I, Mario Enrique Gómez Fernández, am the principal investigator and first author of the work that is presented herein.

Chapter 2: A Status of Research and Development of Artificial Intelligence in Nuclear and Radiological Sciences: A Review

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Abstract

Nuclear technology industries have increased their interest in using data-driven methods to improve safety, reliability, and availability of assets. To do so, it is important to understand the fundamentals between the disciplines to effectively develop and deploy such systems. This survey presents an overview of the fundamentals of artificial intelligence and the state of development of learning-based methods in nuclear science and engineering to identify the risks and opportunities of applying such methods to nuclear applications. This paper focuses on applications related to three key subareas related to safety and decision-making. These are reactor health and monitoring, radiation detection, and optimization. The principles of learning-based methods in these applications are explained and recent studies are explored. Furthermore, as these methods have become more practical during the past decade, it is foreseen that the popularity of learning-based methods in nuclear science and technology will increase; consequently, understanding the benefits and barriers of implementing such methodologies can help create better research plans, and identify project risks and opportunities.

2.1 Introduction

Over the past decades, many industries have integrated information technologies to support the design and innovation of products and services. While the field of nuclear science and engineering is not known as a highly innovative industry, there has been increasing interest in modernizing the instrumentation in existing and new nuclear reactor technologies[1] as well as emergent technologies, such as nuclear robotics. The International Atomic Energy Agency (IAEA) has suggested that it *"is necessary to address obsolescence issues, to introduce new beneficial functionality, and to improve overall performance of the plant and staff"* [2] and to *"enhance and detect subtle variation that could remain unnoticed"* [3], including the use of artificial intelligence (AI)[4] to support decisions. For instance, in nuclear power plants (NPP) there are approximately 1,200 different alarms for a 3-loop pressurized water reactor (PWR).

In the early days, the field of AI focused on solving problems that were intellectually difficult for humans and problems that could be easily described by simple mathematical rules[5], such as chess. Unfortunately, for tasks in uncertain real-world environments,

the development of a set of rules is not practical and becomes infeasible. The subfield of AI, known as machine learning, has the particular characteristic of deriving relationships or set of rules from data, which allows machines to solve more complex problems and deal with uncertainty. Subsequently, its application in engineering as a fast-estimator tool or fast optimization has become an area of research. In the nuclear industry, the interest in developing a computer-aided system to reduce information load in operations tasks has been at the forefront since the 1980s[6], and in radionuclide detection since the 1990s[7]. While many applications of learning-based methods have been proposed, understanding both the potential benefits and challenges that arise from these methods will help individuals to better formulate the problem and collect representative data for a robust implementation.

While the field of AI has seen remarkable achievements over the past decade, robustness and ethics in AI is of increasingly concern to the scientific community because of emerging applications of AI in high-stakes applications[8], such as surgical assistants[9], autonomous driving[10], power grid stability[11], or autonomous weaponry[12], because of the possible risk imposed to humans lives. Therefore, the purpose of this paper is to: (1) provide an introduction to the fundamentals of artificial intelligence (AI), (2) explore the evolution of different technologies and their integration and challenges within the nuclear science domain, and (3) provide recommendations for more robust implementation in academia and beyond. Furthermore, due to the nature of the paper, more emphasis is placed on concepts and scope of methods while the technical details are left to the references. By providing the reader with this review, it will ease the researcher to better allocate resources and investigative capabilities for future studies.

The reminder of this paper is organized as follow. Section 2.2 provides a brief overview of the field of artificial intelligence and explores some of the concepts and historical achievements of machine learning methods, particularly neural networks, as they are widely applied in the nuclear domain. Section 2.3 presents an overview of different applications of machine learning in the nuclear and radiological engineering domain, focusing on identifying the potential benefits and challenges in this specific area. Section 2.4 discusses and provides suggestions on further research, as well as some of the challenges for a successful deployment of such methods in the nuclear industry. Finally, section 2.5 provides a summary, conclusion, and recommendations.

2.2 Fundamentals of Artificial Intelligence

The literature on the subject of artificial intelligence (AI) is rather vast and can be overwhelming for non-AI researchers. To better understand the advances in the field, however, it is important to understand the fundamentals as they will guide nuclear and radiological scientists and engineers to better define the objectives for a successful and robust implementation. As one of the newer fields in science and engineering, the term artificial intelligence was coined in the mid-50s at the Dartmouth Summer Research Project on AI. Historically, four schools of thought have been followed as noted by[13]:

- Think Humanly: the philosophy of fundamentally understanding how humans think (e.g., human reasoning)
- Act Humanly: the philosophy of making machines perform tasks than can be perceived as performed by a human (e.g., [14])
- Think Rationally: governed by the field of logic or laws of thought, where problems are described and solved in a logical manner (e.g., solving a problem using principles vs practice)
- Act Rationally: the philosophy of achieving the best/expected outcome, based on the exogenous and endogenous factors over time

These four schools of thought have formed the basis of the overall goal of AI of: building machines that can learn and think like people. Nonetheless, early ambitions diminished over time as the magnitude, difficulty, and lack of understanding of human reasoning was acknowledged[15]. Thus, it is practical to use reductionism by isolating specific aspects that comprise AI. As one of the most important papers in the history of AI, which the authors highly encourage reading, "Steps Towards Artificial Intelligence"[16] notes five major subfields that fundamentally constitute the AI domain: planning, pattern recognition, credit assignment, and inference; each focusing in solving a different type of problem. *The search problem:* given a well-defined problem, a computer must have ways to find a solution other than an exhaustive search. *The planning problem:* given a complex problem where limitations exists (e.g., time, cost, constraints, and multiple solutions are possible), a machine must have ways to select only a few for full analysis. *The pattern recognition problem*: given a problem, a machine must classify it based on extracting features that are invariant to common distortion into the problem's different categories. *The credit assignment problem:* uses the analogy of reinforcement to encour-

age desired behavior, through which a system *"learns"* by stimulation via reward. *The inductive inference problem:* given a specific domain; a machine must have methods that can be used to construct a general statement based on unrecorded information.

Following the combination of these concepts, AI is focused on solving four fundamental problems[17] to try to model human traits:

1. General problem-solver: modeling *"reasoning"* by modeling the human cognitive process
2. Game-playing machine: modeling *"strategy"* through strategy games
3. Question and answering machines: modeling *"comprehension"* through natural language and text
4. Other applications: modeling *"decision making"* through heuristics, combinatorial, and searching problems

Subsequently, when a machine is able to answer all fundamental question, then it can be considered to be *"intelligent"*. The latter has been an ongoing debate[15] and it is beyond the scope of this study. Nevertheless, within the last decade AI systems have been able to play Jeopardy, recognize objects in photos, describe the photos, and recognize your voice and commands in a "human-like" way. Before discussing implementations in nuclear science, let us present the most popular machine learning methods that have and continue to be used for pattern recognition problems.

2.2.1 Popular machine learning methods

There are several AI methods that can be encountered in the literature, the "old-fashioned AI" [18], more modern AI[13], and machine learning methods [19, 20, 21], each having its own strengths and weaknesses. Generally, most machine learning methods try to find an empirical model f that learns from a training data matrix $D \in R^{n \times d}$ obtained from a system, where d is the number of concerned variables and n is the number of training data samples. Machine learning combines the pattern-recognition, credit assignment, and inductive inference problem, where in supervised learning, the updates aim to reduce an error and improve the algorithm's pattern recognition capabilities by modifying parameters, and for unsupervised learning, the updates work toward matching an expected value based on the presented data[22]. There are five popular algorithms that can be found in nuclear and radiological science applications; these are decision trees (DT), artificial

neural networks (ANNs), nearest neighbor (NN), support vector machine (SVM), and Naïve Bayes (NB), because of their flexibility for pattern recognition problems, see Table 2.1. Two more are also presented, evolutionary algorithms (EA) and fuzzy logic, as they are found in nuclear- and radiological-related problems as standalone algorithms or in combination with neural networks (i.e., neuro-fuzzy or neuro-evolutionary), in some of the literature.

1. Decision trees are some of the simplest, yet powerful, methods in machine learning and work by partitioning the input space into local simple models in each of the resulting regions. While many optimal partition strategies exist, the most commonly used are based on the GINI index (see CART[23]), entropy, or information gain (see C4.5 and ID3[24, 25]).
2. Artificial neural networks are some of many biologically-inspired techniques that enables a computer to learn from observational data. It is inspired by the biological structure of the brain, where the artificial counterpart reproduces a similar functionality[26]. They work by presenting data to the network via the "input layer," which communicates to one or more "hidden layers" where the processing is done via a system of weighted "connections." The development and success of the error back-propagation algorithms, gives the network the ability to use a loss function to find a learning rule that decides under which circumstances the weighted connections need to be modified such that the desired value and the actual output value are close [27]. ANNs are the dominant learning-based algorithm used in nuclear and radiological science[28] because of their ability to deal with nonlinear, inconsistent, and noisy data [29, 30].
3. k-Nearest Neighbor is an intuitive classification technique that classifies a data instance according to the majority class of its k nearest neighbors. This algorithm requires a distance metric such as Euclidean distance.
4. Support vector machine is a powerful non-parametric method whose principal idea is to construct a decision boundary that maximizes the distance to example points, referred to as maximum margin separator. Furthermore, SVMs have the ability to embed the data into a higher dimensional space using the original set. By transforming the data into a higher dimensional space, a linear separator is found. This linear separator is nonlinear when transformed back into the original space. This is the so-called *kernel trick*. For further details see [31, 32, 33]
5. Naïve Bayes is formulated based on Bayes theorem $P(y|x) = \frac{P(x|y)P(y)}{P(x)}$, where the

prior probability ($P(y)$) is estimated using the training set, and the class-conditional probability $P(x|y)$ is estimated assuming that the input variables are conditionally independent (i.e., $P(y|x) = \frac{P(y)\prod_{i-1}^{N} P(x_i|y)}{P(x)}$).

6. Evolutionary learning techniques are popular because of their nature-inspired concept of simulating the evolutionary process. These holistic approaches do not guarantee a best solution; however, they generate or approximate a good enough (local optimum) solution to complex problems in a reasonable amount of time. Generally, the central common feature of all evolutionary methods is that they start off with an arbitrary initial solution, iteratively produce new solutions by a (simple) rule, evaluate the newly generated solutions by a penalty or fitness function, and report the best solution found during the search process. Presumably the goal of generating solutions is to create more, and varied, solution conjectures to enhance diversity and quality. For further details see [34, 35, 36].
7. Fuzzy logic is a technique derived from the so-called principle of incompatibility[37] which correlates imprecision and uncertainty to the complexity of a complex system. Introduced in 1965[38], fuzzy set theory and fuzzy logic revolves around the idea that given two sets, an object can belong to a set with a degree of membership. This deviates from the classical set theory and classical logic where an object either belongs to one set or not. Fuzzy logic approaches are efficient when applied in fields where imprecision and uncertainty is high and are less efficient when precision is apparent[39]. For details on the evolution of fuzzy logic see[40]

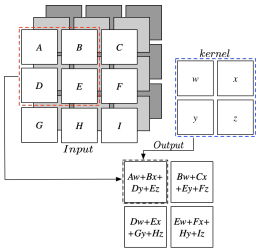
2.2.2 Beyond classical ANNs

In the new millennium, multi-layered ANNs have demonstrated remarkable performance when data is plentiful because they have outperformed other alternative machine learning methods (e.g., SVM) through improved representation learning via many hidden layers and improved optimization algorithms that facilitate training. ANNs have been mathematically substantiated to be universal function approximators[41, 42, 43] (i.e., according to the universal approximation theorem), there exists a neural network with at least one hidden layer with a finite number of units that can approximate any function at any desired degree of accuracy. Additionally, training speed also saw a breakthrough with the utilization of graphical processing units (GPUs), which excel at fast matrix and

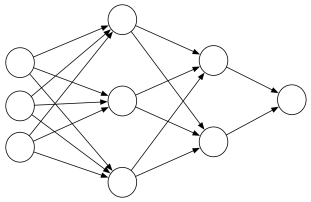
vector multiplications required not only for image processing but can also be used for ANN training. GPU hardware reported an increase in speed by a factor of 20[44] or more based on the specifications, and better computational scalability[45] than central processing units (CPUs). Deep learning (DL) models have rapidly evolved to become the state-of-the-art technology in machine learning tasks such as object recognition, speech recognition, adversarial games, and controls. The two most popular deep learning structures are *convolutional neural networks* for object detection in images and *recurrent neural networks* and *Long Short Term Memory* for sequential information with time dependencies. Although these require higher levels of understanding to appropriately tune them, the application of these structures has been rather limited in nuclear sciences, but some examples are detecting steel cracks underwater using video[46] or isotope detection[47] using convolutional structures.

Convolutional Neural Networks

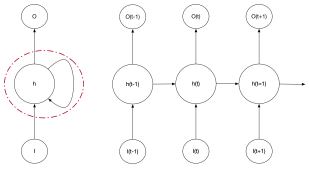
Convolutional neural networks, more commonly known as CNNs or ConvNets, were firstly introduced in [48, 49, 50] by means of mimicking the vision process of mammals, and later implemented for handwritten number recognition[51]. Currently, CNNs are the dominant structure for object recognition tasks and it can be comparable to human-level performance[52, 53, 54]. The novelty of the approach was the use of convolution layers to significantly reduce the number of parameters that needed to be optimized, as shown in Figure 2.1a, which both reduces the memory required and increases the model efficiency. The convolution layer consist of three different stages: convolution, activation, and pooling. First, a convolution is a mathematical operation of two functions of real value arguments that form a new function [55]. Secondly, each entry is then transformed by a nonlinear activation function to extract features. At the pooling stage, the pooling function replaces the output of the network with a statistical summary of the nearby outputs. The key concept from this stage, is to make the representation invariant to small transformations of the inputs. Thus, after the feature extraction stage the $m \times n$ image is divided into a $m \times n$ disjoint and take the max (or other function) feature activation over these regions to obtain the *"convolved features"* that can then be used for classification.



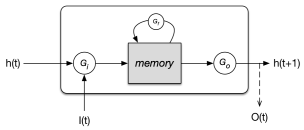
(a) 2-D convolution representation, where the blue dotted box represents the filter or kernel that is multiplied by the red dotted box, resulting in the new image.



(b) A typical feedforward neural network representation or two hidden layer and one output layer.



(c) A recurrent network structure representation with the unfolded equivalent. The red dotted line represents the section where more elaborated units are placed, such as the shown in 2.1d.



(d) Conceptual visualization of gated units, where G_i is the input gate, G_o is the output gate, and G_f is the forget gate.

Figure 2.1: Popular deep learning structures

Recurrent Neural Networks

Recurrent neural networks (RNNs) have been the preferred choice for tackling memory tasks with time dependencies. However, when long-time dependencies are required to be learned, RNNs suffer from the vanishing gradient problem [56], for which memory structures have been proposed in the form of gated units. Gated recurrent neural networks are based on the idea of hybrid-designed gates that create pathways through time whose derivatives neither vanish nor explode [55]. This is achieved by using three types of control gates: the write control that determines the input to the memory state (with linear activation), the forget gate that controls how much of the stored memory value is transferred to the next time step, and the output gate which regulates the output of the memory cell. The most popular gated type units used are the gated recurrent unit (GRU)[57] and the Long Short Term Memory(LSTM)[58], and these are regarded as the state-of-the-art for sequential data such as speech recognition and translation[59].

2.2.3 Comparison of popular algorithms

While it is unrealistic to expect that the data collection or generation is going to be perfect, data availability is one of the major factors that determines which method is suitable for a successful application. A selection criteria is presented in Table 2.1[60, 61] with the following criteria explanations:

- Mixed data: the ability to handle different types of data (i.e., continuous, discrete, etc.)
- Missing Values: sensitivity to unrecorded data
- Irrelevant inputs: sensitivity to values that do not contain relevant information to the application
- Outlier: robust to unusual or inconsistent values
- Data dimensionality: ability to handle increasing features in data sets
- Monotonic transformations: sensitivity to monotonic transformations
- Interpretable: ability to understand the rationale behind the decision/classification of the algorithm [62]

Table 2.1: Sensitivity evaluation of popular machine learning methods

Criterion	DT	ANNs	NN	SVM	NB
Mixed data	yes	no	no	no	yes
Missing Values	yes	no	some	no	yes
Outlier	yes	yes	yes	yes	no
Monotone transformations	yes	some	no	yes	no
Data dimensionality	yes	yes	no	no	yes
Irrelevant inputs	some	no	no	yes	no
Interpretable	yes	no	no	yes	yes

2.3 Intelligence Augmentation: A Nuclear and Radiological Challenge

The civil uses of nuclear technology have a number of different applications with various benefits to the general public. Medical applications include the use of nuclear materials to diagnose, monitor, and treat many different human conditions; industrial applications are numerous and are characterized by being non-intrusive including sterilization, radiography, smoke detectors, and food safety among others; academic applications include the use of nuclear material for laboratory practices, and research and development; and energy applications include to produce electricity, heat water, and work in conjunction with other energy sources. While it is common to characterize physical systems employing first principles, which can be very accurate when the underlying laws are well known, empirical methods can be used to develop approximate mathematical models when the laws are not well understood [63], which, if used correctly, can be very useful.

This section presents the performance and flexibility or machine learning methods in nuclear technologies, with a focus on nuclear reactor health monitoring, gamma spectroscopy and optimization, and their support to both technical and economic objectives shown in Table 2.2; ultimately, enhancing safety, reliability, and availability of the equipment. The collective problems in this section are of different types: (1) regression refers to the prediction of continuous values, (2) classification to the prediction of a category or class, or (3) combinatorial and exploratory. In nuclear engineering, researchers have identified the potential use of pattern recognition in various tasks in nuclear reactors [64, 65, 66, 67]. In radiation detection, research takes advantage not only of the pattern recognition to analyze the reactor detectors' signals for anomalies, but also to analyze and categorize gamma and neutron spectrums for transportation, security, and environ-

mental monitoring. Lastly, optimization applications use available data for the discovery of more, and varied, solutions in a timely manner.

Table 2.2: Nuclear Science Objectives

Technical	Economical
• Reduce radiation exposure to personnel • Enhance equipment reliability • Avoid actuation of safety systems • Assist with correct and timely decision making • Enhance safety margins	• Optimize the maintenance schedule • Improve plant availability • Avoid escalation of minor problems into major event • Support power uprate and life extension

2.3.1 Plants health and management approaches

In nuclear power plants (NPPs), there are a wide variety of tasks that have been studied using learning-based methods, particularly the development of neural network structures for parameters prediction and classification using sensor data to perform monitoring, diagnosis, prognosis, controls, planning, and other tasks that can benefit from pattern recognition. Degradation, ageing, and transients can happen over a short or long period of time; thus, it is feasible to extract a unique set of patterns or fingerprints for the operators to perform a root cause analysis in a timely manner. The primary goal of such applications is to provide a quick and accurate insight such that additional time can help derive the optimal procedure/strategy to be implemented to correct the situation via artificial anticipators or fast first estimation tools, therefore increasing the safety of the plant and components.

In NPPs, learning-based methods have been studied for instrument calibration monitoring, equipment monitoring, reactor core monitoring, loose part monitoring, transient identification, reactor controls, and others. The task of monitoring and diagnosis systems consists of detecting the departure of a process from normal conditions to characterize the new process/state based on temporal trends [68]. Conventionally, a fault threshold level for each plant parameter is set and an alarm is given when the signal exceeds

the threshold level (i.e., if-then rules derived from model-based approaches[69, 70, 71]). However, minor abnormal conditions may not be detectable until they reach a critical threshold[72, 73], which is where computer-aided systems can prove to be worthwhile. Plant health and management capabilities are not unique to the nuclear industry, as other complex engineered systems are also interested in such features [74, 75, 76, 77, 78], which translates to better performance and help conserve the asset in optimal conditions. The economic impact of the development of advanced systems can have a potential savings of $48 billion USD over a 40-year life span of a typical power plant as shown in [79]; roughly $1 billion USD per year, when optimal operation is maintained.

Research in the monitoring domain using simulators and codes has been extensive [80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 72, 90, 73] because of the potential economic impact. Nevertheless, for the success of intelligent aided systems in the nuclear industry, the use of real or prototypical systems is also encouraged as such systems will be subject to the problem of verification and validation (V&V) [91]. Some examples of machine learning studies using real plant information are: the Tennessee Valley Authority Sequoyah NPP [92] to determine the variables that affect the heat rate and thermal performance, Watts Bar NPP [93] for operating status recognition, High Flux Isotope Reactor operated at Oak Ridge National Laboratory [94] for sensor calibration systems and sensor fault detection systems, experimental Breeder Reactor [95], prototypical Small Light Water [96] for plant wide behaviour analysis, and Narora Atomic Power Station [97] to identify eight particular initiating events. Although there have been some real setting applications, the use of real NPPs information for performance studies has been rather limited due to the highly regulated industry and intellectual property protection concerns [64, 30, 98].

Other applications where machine learning methods can be encountered are: the prediction of the behavior of systems components such as heat exchangers[99, 100, 101, 102], power peaking factor estimations[103, 102], key safety parameter estimation[104, 105, 106], aging and degradation[107, 108], uncertainty propagation[109], severe accidents classification[110, 28, 111], functional failures of passive systems [112], research reactors [113], and more recently crack detection in internal reactor components[46]. All of these problems are well suited, with the advantage that more data can be generated or made available to researchers.

2.3.1.1 Flow regime identification

Other related areas to reactor safety is the identification of flow regimes. Several methodologies for flow identification seem to be subjective based on visual observations[114], with some being more objective [115, 116]. The use of learning-based methods to predict flow regime identification based on nonintrusive instrumentation has been explored mainly using feed forward neural networks[117, 118, 119, 120, 121, 122, 123, 124, 125, 126], including some deep learning approaches[127, 128]. Proper flow regime identification can accelerate the design analysis and operation of engineering systems as correct hydrodynamic and kinematic mechanism can be modeled. Additionally, nonintrusive techniques can be used for the detection of wears, leakages, or unwanted events while operating.

2.3.2 Radiation protection

As one of the fundamental pillars of nuclear safety, intelligence augmentation also extends to its application in radiation protection-related tasks. In spectroscopy, the goal is to find a pattern or structure, full peaks in most cases, and differential count rates by analyzing the distribution of counts over a spectrum. Efficient and accurate characterization and identification of radionuclides is of great importance as it can help with illicit transportation of radioactive materials, or contaminants in the field, which are traditionally determined using gamma spectroscopy. There is a wide variety of application for spectroscopy ranging from the analysis of the instrumentation, the spectrum itself, its meaning, and its derived features. Radionuclide identification using learning-based methods based on gamma and neutron spectroscopy is of interest as such approaches do not require templates or peak libraries calculated in advance[129]. Moreover, they can help discern subtle patterns in large multivariate data sets to reduce false negatives [130], calibration drifts [131], data uncertainties[132], and peak overlapping [133, 134]. Other applications with limiting research include nuclear stability and decay[135], SVM for anomaly detection from thermoluminescent dosimeter (TLDs) glow curves[136], radiation signals encryption[137], radiation therapy[138], among others. However, because of the large use of spectroscopy in the field, the scope of this section will be focused on this particular application. While the interest has been extensive, and many different learning-based algorithms have been used, neural networks are the dominant method.

In gamma spectroscopy, research related to the identification of isotopes for hand-held instrumentation [47, 139] based on ANSI N42.34 standard isotope selection[140], independent isotope classification [141, 142, 143, 144, 145], mixture of elements[7, 47, 146, 141], and specific activity of naturally occurring radioactive materials (NORMs)[147, 148] have been carried out. Similarly, neutron spectroscopy analysis has been a subject of research using Bonner sphere systems[149, 150, 151], and neutron dose estimation[152] using neural networks have been reported. The identification of radionuclides can also be extended to other specific subfields such as special nuclear materials detection and environmental monitoring where detection is more difficult. In other specific areas such as optimization, one of the key principles of radiation protection, via machine learning approaches can lead to the discovery of solutions that typical deterministic approaches are not able to provide or for which the exploration can be too costly.

2.3.2.1 Special nuclear material

Illicit nuclear material trafficking is one of the applications where substantial efforts have gone into devising strategies for inspection. The use of gamma spectroscopy is also extended to nonproliferation and nuclear security applications. However, special nuclear material (SNM) identification presents additional challenges, such as data collection time, background level, and attenuation or distorted shielded spectrums, where scientists have applied machine learning methods to improve on such challenges. Clustering methods for radioxenon classification [153], neural networks for shielded plutonium [154], uranium ore compound classification[155, 156], spent fuel pool classification to ease nuclear forensics [157], and general SNM detection using: fuzzy logic systems [158, 159, 160, 161], evolutionary algorithms [162, 163], Gaussian process[164], naïve bayes[165, 166], are some of the different tasks for which learning-based methods have been considered. The Gamma Detector Response and Analysis Software (GADRAS)[167, 168] has been used as a training data generator in some of the presented work for both gamma and neutron spectrums.

2.3.2.2 Environmental monitoring

Environmental monitoring is achieved mainly from the detection of gamma radiation, as it is the most penetrating radiation either natural or anthropogenic. Other situations include the environmental application of gamma spectroscopy for geological, geochemical, and environmental mapping, allowing the interpretation of regional features, such as atmospheric radon levels; human-made contamination around nuclear facilities to determine a baseline for accidental releases; mining and other industrial activities [3, 169]. However, environmental systems present a particular barrier that their dynamics are complex, nonlinear, and affected by many exogenous stressors; therefore, the development of simulation models, risk mapping, spatial predictions, representative data collection and analysis[170] are ongoing challenges, where models obtained through empirical data are typically better suited than those from analytical equations[171, 172]. Some noticeable studies are, legacy site Ra-226 contamination characterization[173] and distribution[174]; and remediation monitoring[175], which can serve as a first estimation tool to provide rapid insights of the activity, depth, and distribution of the contamination. Estimation of an ambient dose rate risk map using various machine learning methods[176], spatial prediction of fallout at the Chernobyl site [177], suitability of neural networks for uranium activity ratio in environmental spectra[178], and bio-availability and bio-accumulation of NORMs in aquatic species through produced water from the gas and oil industry [179, 180], are some of the areas that have shown promise for the potential benefit of learning based methods. Other technologies such as the Internet of Things (IoT) are also being explored in the field of environmental monitoring [181, 182].

2.3.3 Optimization

Designing and analyzing engineering systems can be a very complex process, of which energy systems are an exceptional example. Optimization can be defined as the *"act of obtaining the best result under the given circumstances"*[183]. The highly iterative process in an interdisciplinary environment leads to multiple suboptimal designs or decisions until one is determined to be the best performing one (i.e., meeting the requirements imposed as well as being cost-effective, efficient, reliable, and durable[184]). In practical engineering, optimization problems are expressed as an analytical function that includes decision

variables and constraints, such that traditional optimization tools can be used (e.g., first or second order optimization algorithms). However, in some cases analytical formulations are not feasible or too simplistic to capture the complexity, for which nontraditional or modern optimization methods are of particular interest.

In nuclear and radiological engineering, many processes can be optimized by using a well-studied, and justifiable, machine learning method. Bio-inspired methods, such as neural networks, evolutionary algorithms, and particle swarms, among others, are very popular in the optimization domain as their working mechanism allows them to generate more, and varied, solutions to enhance diversity and quality. Combinatorial types of problems can easily take advantage of these methods; for instance, in fuel loading management [185, 186, 187, 188, 189, 190, 191], optimal maintenance scheduling[192], dry cask loading[193, 194, 195], packing and waste handling[196], or dose optimization [197, 171].

2.3.3.1 Robotics and controls

Although the scope of this paper is on learning based methods, robotics and controls are complementary, as optimization is at the core of control theory and machine learning methods are also being evaluated[198]. The desire to provide autonomy (i.e., ability for self-governance in the performance of functions[199]) to machines has been one of the fundamentals of the field of artificial intelligence as it can eliminate or reduce human roles from low level tasks. Optimization and controls are conceptually different, where the goal of controls is to produce a desired output given feedback from the systems controllers[184], (i.e., the output is known). Robotics in the nuclear industry can be beneficial by substantially reducing the time that an individual has to spend in a radiation area and remotely handling material that is considered hazardous, or when the conditions of the environment or structural integrity are unknown. For instance, [200] identifies three key areas where autonomous controls can be beneficial: (1) detection and progression limitation of off-normal events, (2) detection and response to degraded or failure conditions[201], and lastly, (3) potentially unattended operation with limited human interaction[202]. Others include, reactor temperature or power control[203, 204, 205, 206], coordinated control strategies development using fuzzy logic and neural networks in a multi-unit small modular reactor [207, 208], inspection [209], hazardous material search

and radiation mapping using robots[210, 211, 212], and computer vision for radwaste management[213]. Robotics and controls present some particular challenges as they require special design considerations, material selection, operational constraints, processes knowledge, etc. With high-stake controls, it is of paramount importance that the probability of taking or advising the wrong solution path is minimal, which is part of the *robust artificial intelligence* presented in recent years [8].[1]

2.3.4 Suitability of popular algorithms in nuclear and radiological problems

This section presents a general analysis based on the commonly collected data for each of the different applications and is summarized in Table 2.3. Please note that more than one algorithm among the popular algorithms can be applied for a specific task, which is also reported in the literature. Other factors such as training speeds/cost, accuracy, model complexity, interpretability, etc., become part of the selection process and are beyond the scope of this review. Table 2.1, along with literature (i.e., section 2.3), is used to provide an overall assessment of the suitability of the algorithms that have been presented.

Moreover, it is worth noting that most, if not all, existing engineered systems of relevance here consists of the human, measurement of physical phenomena, purposeful design of small to large engineered devices and systems (D&S) and other than unanticipated events, operation of devices and systems as designed, constructed and intended. On the basis thereof, both phenomena and function of D&S many times have been created with inherent *complexity* (i.e., with multiple variables/parameters not only interacting within the D&S but via human-machine interaction). The current state of understanding of complexity is limited and rudimentary not only because those who acknowledge complexity are scattered across disciplines, but there is no emerging consensus on characterizing it. The emerging application of learning-based approaches, across the sub-disciplines and applications noted herein is an attempt to characterize the complex interactions of phenomena and D&S via an algorithmic approach that relies on coded sampling of limited channels/streams of data generated by measure or functional 'gauges' of the D&S. What is evident in the applications described here is that phenomena and D&S with say ap-

[1]For a more detailed review on nuclear robotics, see [214], and radiation effects on electronics, see [215, 216].

proximately 10-50 variables and parameters approximately defined complexity and that characterization of such a problem is limited to non-existent.

Further, learning-based methods of relevance and complexity level herein implied are largely known or recognized as substantiating the bulk of any characteristic distribution of recurring phenomena or function. In other words, these methods do not work well for outliers. Characterizing rare occurrences, such as "black swan" events, are not well-suited for these methods. Thus, as noted by [**tokuhiro2019**, 217], learning-based methods are able to decipher many familiar, coded "if–then–when" instances at a systematic level as inspected and then predict the likely next occurrence. Therefore, at this time, prescriptive and systematic approaches and methods to complexity, other than accessible cases of applicability as cited here, do not yet exist.

Table 2.3: Algorithm selection scheme for nuclear and radiological data criteria

Plant health and management: Data collected for this application consist mainly of NPP's sensor data or synthetic data (simulators or codes), which mainly represents continuous data collected over a long period of time from different sensors, i.e., large datasets. Noise has to be considered when applied to NPP data collection	
DT	Suitable; better suited for categorical features, larger trees are hard to interpret, small changes in input data can result in low accuracy (misclassification).
ANNs	Suitable; require hyperparameter search (time consuming), data-hungry, not interpretable.
NN	Unsuitable; Very sensitive to the definition of neighborhood, does not perform well in high dimensions, computationally expensive for large data sets.
SVM	Somewhat suitable; requires tuning hyperparameters (time consuming), not suitable for extremely large data sets.
NB	Unsuitable, conditional independence assumptions between variables are usually not suitable for monitoring applications operating on time series

Table 2.3 (continued)

Flow Regime Identification: Data used in flow regime identification has mainly consisted of visual representation for both vertical and horizontal flow regimes. This data includes variations in bubbles shapes, locations, deformations, diameters, etc.	
DT	Unsuitable; it requires very large trees, sensitive to input variations.
ANNs	Suitable; mainly CNNs, same requirements as above.
NN	Unsuitable; does not perform well for high dimensional data.
SVM	Somewhat suitable; sensitive to variations, transitions between regimes will affect its performance (i.e., hard to know which kernel function works best).
NB	Suitable; feature engineering is required, conditional independence assumption may be too strong.
Spectrometry: Data collected for this application is measured information and synthetic information. Typically the raw data is uses, i.e., all channels with no preprocessing	
DT	Somewhat suitable; small changes in input data can result in misclassification (e.g., decalibrated samples).
ANNs	Suitable; RNNs should be considered for temporal spectrometry. Same challenges as above.
NN	Somewhat suitable if the nuclides of interest are strong gamma emitters and peaks do not overlap; it does not scale well, other algorithms might achieve better classification performance.
SVM	Suitable if the data set is not large (e.g., number of channels matter); irrelevant information can result in misclassification (e.g., background for field work).
NB	Suitable; conditional independence assumption may be unsuitable and other algorithms might achieve better accuracy.
Optimization, Robotics and Controls: The data collected for these applications varies depending on the task (i.e., exploratory, vision, learning-based controls, etc.). Large data sets, noisy, incomplete and highly uncertain data can be found in this area. Synthetic data-based problems are presented which can remove some data related issues. Combinations of algorithms are also common (e.g., neuro-evolution).	

Table 2.3 (continued)

DT	Unsuitable; missing information, data variation affects the performance.
ANNs	Suitable for most applications, especially for reinforcement learning (controls).
NN	Not suitable for large, uncertain, and noisy datasets.
SVM	Suitable; however, keep in mind scalability and hyperparameter tuning.
NB	Likely unsuitable due to conditional independence assumption; more general Bayesian networks might be more suitable.

2.4 Discussion and suggestions

In many industries, the rapid growth of information is creating a dependence and reliance on advanced algorithms to analyze and make decisions, or partial decisions, gradually reducing human involvement. Unlike the nuclear industry, nonnuclear power systems have made digital upgrades to their systems, whose lessons learned can be an advantage for more effective modernization[2]. While automating and modernizing technology is part of its evolution, [218] notes that underloading the mind can be just as harmful as overloading because new issues arise not only by the levels of automation defined for the domain, but also the result from the interface between the user and automation[219]. Failure to acknowledge the challenges can lead to the following: misuse or the over-reliance on automation; disuse or the under-utilization of automation; and abuse or inappropriate application of automation[220]. Thus, fostering experts' understanding of the benefits of developing learning-based solutions can help avoid potential issues. Moreover, a lack of proper evaluation method has previously been identified in [221], resulting in additional challenges and an impediment to the progress and improvement in research and practice in the application of learning-based methods in engineering.

2.4.1 Ethics

The aspiration to apply and deploy intelligent systems to improve processes is a co-evolution between developers, users, and technology. Unfortunately, such human-machine symbiosis is coupled with ethical issues, which are not always anticipated by developers or the common users. While data and algorithms are ethically neutral (i.e., they don't

have a built-in perspective on what is right/wrong or good/bad), the use of data and learning-based algorithms can represent a risk (e.g. trusting black box models). [222] provides a philosophical discussion of how developers tend to evaluate the performance of the tools based on accomplishing what they were designed for, and after the technology matures, these norms become of second nature (i.e., ethics derived from their human developers). Other prominent ethical issues in the AI domain that are inherently carried over to other domains are: undesirable uses of AI[223], loss of accountability[224, 225], and machine ethics[226]. All of these constitute an active, and rapidly evolving, area of research that continues as the adoption of AI methods increases.

Because AI methods have not been extensively used, and AI-based autonomy is still in early research stage in nuclear science and engineering, ethical issues are not commonly mentioned. Based on the state of the technology, the goal of intelligent systems in nuclear sciences must be to inform and provide users with the appropriate inputs to ***formulate, conform, and perform*** the most effective actions, and *not* the replacement of any human input. A human counterpart has the expertise to ensure that trade-offs are fully understood before taking proper decisions, while taking advantage of the superior data processing from computers. Thus, learning-based systems should be a supplement to, rather than a substitute for, traditional methods to enhance decision making. This holistic approach should serve as a guide to the development of robust intelligent augmentation systems through the most effective implementation of learning algorithms toward the desired task, heeding the different objectives shown in Table 2.2, Table 2.1 and Section 2.2. Further consideration beyond the technological advantages and ethical issues are legal and social implications and the development of guidelines and standards (with a recent publication being [227]).

2.4.2 Collaborative and open access research

As information technologies continue to advance, so is the way research is being conducted and shared; particularly in the fields of AI/ML. The concept of FAIR (Findability, Accessibility, Interoperability, and Reusability) [228] is now a reality that all researchers must consider. Open platforms, such as GitHub Inc., allow research to be shared such that reproducing others' work is simple, and improvements on the current state of the research can be made. Thus, increasing FAIR and focusing on new ideas will avoid un-

necessary time expenditure in reproducing results or duplicating research. Moving the research process into a more collaborative and inclusive process will encourage more discussion and interaction with other peers, companies, and developers, during (and after) the research cycle. This process, in principle, increases the quality of the contributions made and accelerates innovation. While sharing information is one way of facilitating research, information technologies include other research enhancers such as the Internet of Things/IoT (see Section 2.3.2.2) and cloud computing[2], which allow for users with limited resources to access services at lower costs, such as intensive multi-physics simulations [232].

2.5 Conclusion

This study presents a review of various applications of machine learning to the field of nuclear science and associated engineering. It is the authors' intent that this review helps provide researchers with a background and guidance to understand the benefits of new technologies as applied to the nuclear science domain to enable and accelerate the scientific and technological outcomes of learning-based approaches. Furthermore, it is crucial that the primary goal for the development and implementation of machine learning algorithms is to provide fast estimation for better informed decisions for the users (human in the loop), as well as assuring interpretability and reproducibility of the models. Lastly, to accelerate innovation the use modern research accelerators that allow for active (virtual) discussion and collaborations is encouraged. Ultimately, the goal is a safe and effective application of learning-based method in nuclear science.

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[2][229, 230, 231] note some of the current trends and challenges and opportunities regarding to cloud-based computing and IoT as related industry and research applications.

of the author(s) and do not necessarily represent the views of the Department of Energy or Oregon State University.

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Chapter 3: Nuclear Energy System's Behaviour and Desicion Making using Machine Learning

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Abstract

Early versions of artificial neural networks' ability to "learn" from data based on multivariable statistics and optimization demanded high computational performance as multiple training iterations are necessary to find an optimal local minimum. The rapid advancements in computational performance, storage capacity, and big data management have allowed machine-learning techniques to improve in the areas of learning speed, nonlinear data handling, and complex features identification. Machine-learning techniques have proven successful and been used in the areas of autonomous machines, speech recognition, and natural language processing. Though the application of artificial intelligence in the nuclear engineering domain has been limited, it has accurately predicted desired outcomes in some instances and has proven to be a worthwhile area of research. The objectives of this study are to create neural networks topologies to use Oregon State University's Multi-Application Small Light Water Reactor integrated test facility's data and evaluate its capability of predicting the system's behavior during various core power inputs and a loss of flow accident. This study uses data from multiple sensors, focusing primarily on the reactor pressure vessel and its internal components. As a result, the artificial neural networks are able to predict the behavior of the system with good accuracy in each scenario. Its ability to provide technical data can help decision makers to take actions more rapidly, identify safety issues, or provide an intelligent system with the potential of using pattern recognition for reactor accident identification and classification. Overall, the development and application of neural networks can be promising in the nuclear industry and any product processes that can benefit from utilizing a quick data analysis tool.

3.1 Introduction

There has been significant scientific interest in understanding and imitating natural and biological process, particularly neural biology. One of the first neural methodologies was first achieved with the creation of the perceptron capable of reproducing some of the Boolean operators [1]. Later in the mid 80's there was a lot of effort "to find a powerful synaptic modification rule that will allow an arbitrarily connected neural network to develop an internal structure that is appropriate for a particular task" [2]; in other words, a

self-organizing method that can be used in machines to learn a task without being explicitly programmed. The application of neural methods has been found useful in addressing problems that usually require the recognition of complex patterns or complex classification decisions. In the domain of computers science, there has been a rapid improvement of self-organizing methods along with advancements in data storage, parallel computing, and processing speeds, which have made possible for these methods to succeed in the development of new products and technologies. In the engineering domain, particularly in nuclear engineering, the application of machine learning methods, e.g. neural networks, utilizing full-scale facilities or real components' data has been rather limited. In early applications researchers have used neural networks to assess the heat rate variation using the thermal performance data from the Tennessee Valley Authority Sequoyah nuclear power plant, where a small artificial neural network was used to determine the variables that affect the heat rate and thermal performance of the plant by looking at the partial derivative of the different input patterns [3]. Others have developed monitoring systems based on auto-associative neural networks and their application as sensor calibration systems and sensor fault detection systems [4] using the High Flux Isotope Reactor operated at Oak Ridge National Laboratory and an experimental Breeder Reactor [5]. During the mid-1990's a group of scientists explored the application of neural networks in the area of multiple-failures detection with the objective to develop an operator support system that can support operators during severe accidents in a nuclear power plant, referred as Computerized Accident Management System [6]. In nuclear operations the inclusion of redundant, independent and diverse systems is necessary to ensure adequate defense-in-depth; however, the increase in systems lead to more complex human-machine interactions. Neural networks have also been trained with data from a simulator, and the results proved to be very satisfactory at modeling multiple sensor failures and component failure identification [7]. Other areas outside of nuclear surveillance and diagnostics have also shown interest in the application of neural networks; for instance, in two-phase flow the use of neural methods as a method to predict two-phase mixture density [8] or flow regime identification [9]. More recently, researchers have applied advanced optimization algorithms for the prediction of the behavior of systems components such as a printed circuit heat exchanger [10, 11], power peaking factor estimations [12], key safety parameter estimation[13] and functional failures of passive systems [14]. The reduction in computational cost and the availability of data facilitates further the use of such methods where

predicting more complex tasks is desired. In this research the application of neural methods using two transient events from a prototypic test facility is presented, where noise and uncertainty are present as an inherently natural phenomenon of a realistic problem.

3.2 Materials and Methods

3.2.1 Multi-Application Small Light Water Reactor

The Multi-Application Small Light Water Reactor (MASLWR) is an integral pressurized test facility developed by Idaho National Engineering and Environmental Laboratory, Oregon State University and NEXANT-Bechtel [15], with the conceptual design shown in Figure 3.1. The MASLWR module includes a self-contained vessel, steam generator and containment system that rely on natural circulation for its normal operation. The test facility is scaled at 1:3 length scale, 1:254 volume scale and 1:1 time scale, and it is designed for full pressure (11.4 MPa) and full temperature (590 K) prototype operation and is constructed of all stainless steel components[15]. The purpose of this facility is to study the behavior of a small light water reactor concept design that uses natural circulation for both steady-state and transient operation. The MASLWR concept was the predecessor to the NuScale small modular reactor design.

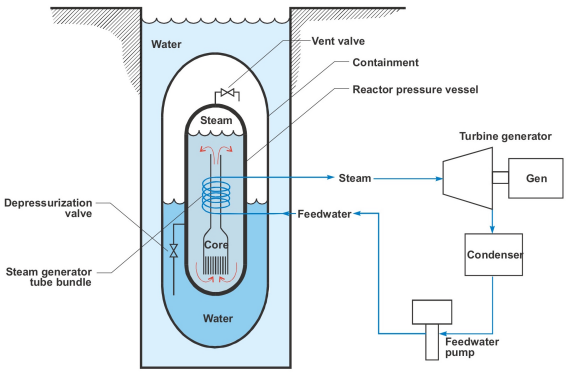


Figure 3.1: MASLWR's Conceptual Design

The data used in this study has been collected for the International Atomic Energy Agency as an International Collaborative Standard Problem (ICSP). Two different data sets were used to train two different neural networks. The first, ICSP-3, characterize

the steady-state (S.S.) natural circulation in the primary side during various core power inputs [16]. The test procedure was to increase the power inputs of the heaters stepwise from 10% to 80% full power in the core by 10% increments and had a total duration of 6,348 seconds (∼1.76 hrs). The second, ICSP-2, characterizes the activation of safety systems of the MASLWR test facility, and the long-term cooling of the facility to determine the progression of a loss-of-feedwater transient (LOFW). For this test, first, the facility was brought to steady state at 75% core power, 8.62 MPa and the main feed water running in the steam generator, then, the main feed water was shut off, the core was set to decay power, and a blow-down procedure was conducted until the High Pressure Containment (HPC) and Reactor Pressure Vessel (RPV) were at equal pressures [17]. This transient had a total duration of 16,483 seconds (∼4.58 hrs).

3.2.2 Data

Data recorded from 58 different sensors was used as labeled data for the supervised learning process, with the purpose of capturing the behavior inside of prototype's RPV. Given that the data collected in the test facility inherently contains noise and uncertainty, the use of a neural network along with the backpropagation algorithm is suitable as this algorithm is robust to noise [18]. However, the main challenge of the application of such method to this particular application is to find the suitable parameters that are to represent the problem, also known as feature selection. The selection of the features has been based on the sensors that are mainly controlled by the test facility's operator. Table 3.2 and Table 3.1 show the sensors used as inputs and outputs.

Table 3.1: MASLWR instrumentation used as output parameters

Sensor Label	**Description**
TF-[611-615]	Thermocouples Inside the Outer Coil Pipe of the Steam Generator Inlet
TF-[621-625]	Thermocouples Inside the Middle Coil Pipe of the Steam Generator Inlet
TF-[631-634]	Thermocouples Inside the Inner Coil Pipe of the Steam Generator Inlet
TF-[701-706]	Steam Generator Liquid Temperature
PT-602	Main Steam Pressure
FVM-602-T	Main Steam Temperature
FVM-602-P	Main Steam Pressure
FVM-602-M	Main Steam Pressure Volumetric Flow Rate
TH-[141-146]	Core Heater Rod Temperatures
TF-132	Primary Water Temperature inside Chimney below Steam Generator Coils
DP-101	Pressure Loss in the Core
DP-102	Pressure Loss between Core Tope and Cone
DP-103	Pressure Loss in the Riser cone
DP-104	Pressure Loss in the Chimney
DP-105	Pressure Loss across the Steam Generator
DP-106	Pressure Loss in the annulus below Steam Generator

Moreover, given the different scales in the data, the entire set had to be normalized, using Equation 3.1, to a $[0, 1]$ range to improve learning and avoid the saturation regions of the sigmoid function.

$$X' = (X_{max} - X_{min}) \frac{X - X_{min}}{X_{max} - X_{min}} + X_{min} \tag{3.1}$$

The implementation of other normalizing techniques can also be used as long as it scales within the output range of the selected activation function.

Table 3.2: MASLWR instrumentation used as input parameters

Sensor Label	**Description**
TF-[121-124]	Core Inlet Temperatures
KW-[101-102]	Power to the core heater rod bundles
TF-[101-106]	Center of Core Thermocouple Rod, six thermocouples spaced 6' apart, measuring water temperatures
TF-111	Primary Water Temperature at top of Chimney
KW-301	Power to Pressurizer
TF-501	Feed Water Temperature
FMM-501	Main Feedwater Volumetric Flow Rate
FCM-511	Feed Water Supply in the Steam Generator Outer Coil Mass Flow Rate
FCM-521	Feed Water Supply in the Steam Generator Middle Coil Mass Flow Rate
FCM-531	Feed Water Supply in the Steam Generator Inner Coil Mass Flow Rate
PT-511	Feed Water Pressure in the Steam Generator Outer Coil Mass Flow Rate
PT-521	Feed Water Pressure in the Steam Generator Middle Coil Mass Flow Rate
PT-531	Feed Water Pressure in the Steam Generator Inner Coil Mass Flow Rate

3.2.3 Neural Networks [1]

Firstly introduced in [21], neural networks are biologically-inspired techniques, which enables a computer to learn from observational data. McCulloch and Pitts stated that "*The nervous system is a net of neurons, each having a soma and an axion. Their adjunctions, or synapses, are always between the axon of the neuron and the soma of another. At any instant, a neuron has some threshold, which excitation must exceed to initiate an impulse. This is determined by the neuron, not by the excitation. From the point of excitation, the impulse is propagated to all parts of the neuron*" [21]. To mimic a biological neuron, its artificial counterpart reproduces a similar functionality. As shown in Figure 3.2, the network receives a series of data points or input vector $(x_1,\dots,x_i)$, whose contribution to the 'impulse' is determined by the synaptic weights associated with each neuron (w_i), and the activation function will use the weighted sum of input signals $(\sum w_i x_i)$ to emit an output signal, whose value will determine if its 'impulse' is propagated to the rest of the network. This output will then become an input of the next layer and so on.

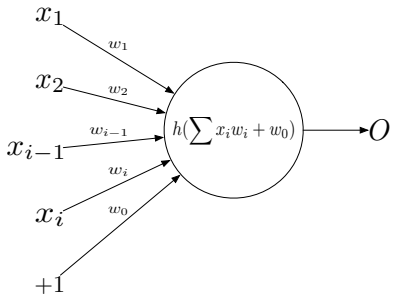


Figure 3.2: Artificial neuron representation

Neural networks are constructed using this principle to include multiple layers with many neurons to increase their representation capabilities as shown in Figure 3.3. Consequently, when building neural networks, there are a few fundamental properties that need to be considered:

1. Activation function

2. Optimization algorithm

[1] If the reader is interested in further details see [19] [20].

3. Structure or architecture of the network (known as model selection)

For the first property, the logistic or sigmoid function (Equation 3.2) is used as it is one of the most commonly used activation functions.

$$a(x) = \frac{1}{1 + e^{-x}} \tag{3.2}$$

To describe what is known as the forward pass, the first the input vector is presented to the network and is then multiplied by the synaptic weights, as described previously. Let us defined it as:

$$c_j = w_j^T x + b \tag{3.3}$$

where b represent the bias term, w_j is the weight matrix of the j^{th} layer. Then the activation function decides whether to propagate the value by applying the activation function

$$h(c_j) = a(c_j) \tag{3.4}$$

After the activation function is applied, the result will then become the new input (x) for Equation 3.3 and the cycle repeats for as many j^{th} layers were chosen and the output layer is reached. Taking the following general forward pass formula:

$$f_p(x) = a_j(w_j^T a_{j-1}(w_{j-1}^T a_{j-2}(...a_1(w_1^T x + b)) + b_{j-1}) + b_j \tag{3.5}$$

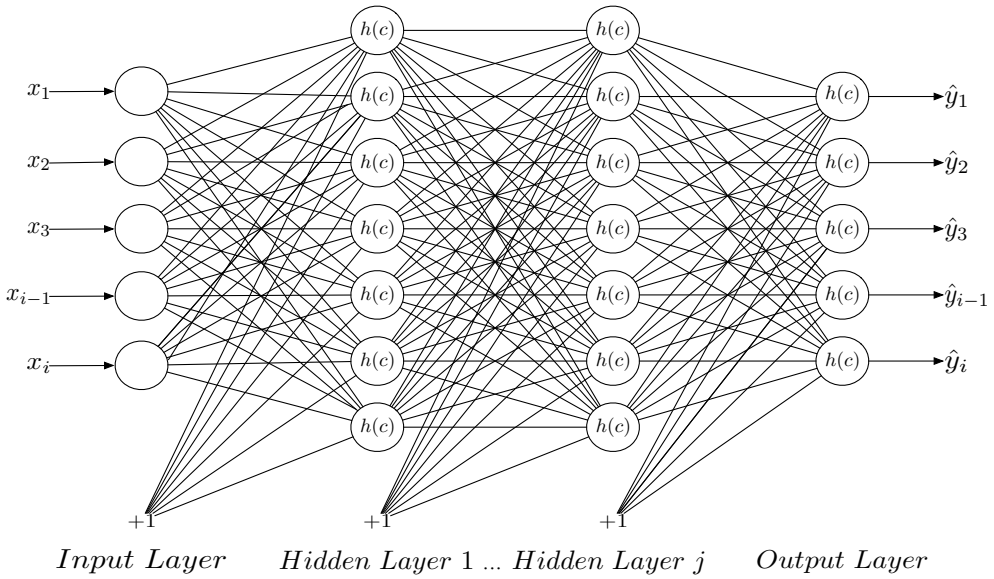


Figure 3.3: Neural network representation

In the next couple section the selection of the structure and optimization algorithm is explained for the optimal design of a neural network.

3.2.3.1 Backpropagation Algorithm

The novel development and success of the backpropagation algorithm is greatly attributed to the ability to use an error function as a corrective factor for the connection strength (synaptic strength or weight), which allows the neurons to learn many layers of non-linear feature detection, such as recognizing handwritten zip codes [22]. Its primary objective is to find a learning rule that decides under which circumstances the hidden units should be active by a measure of the weights that when applied in a neural network the desired value and the actual output value are close [2]. This is achieved by minimizing an objective function, in this case, the mean square error (MSE) function,

$$E_n = \frac{1}{2}\sum_n (\hat{y}_j - y_j)^2 \tag{3.6}$$

and,

$$\hat{y}_j = h_j(w_j^T x + b_j) \tag{3.7}$$

where $\hat{y}_j$ is the predicted value for a particular input set and y_j is the desired output value. Then the gradient of this function with respect to the weights can be expressed as,

$$\frac{\partial E_n}{\partial w_j} = \frac{\partial E_n}{\partial h_j}\frac{\partial h_j}{\partial w_j} \tag{3.8}$$

Which indicates by what amount the error will increase or decrease if the value of w_j is to change by a small amount. After some mathematical manipulation, we obtain the following general backpropagaion formula

$$\nabla E = w_{j-1}\delta_j * h(c_{j-1}) * (1 - h(c_{j-1})) \tag{3.9}$$

where δ_j is the error from higher up units. Then, it can be used to form the gradient of the error function that is used for optimization.

For this study, a regularized mean square error was used to further control over-fitting

$$E_n = \frac{1}{2}\sum_i (\hat{y}_{ji} - y_{ji})^2 + \frac{\lambda}{2}w^2 \tag{3.10}$$

where λ is the penalization term or regularization coefficient that controls the complexity of the model by driving some of the weights to zero, or decreasing the importance or influence of a feature, also known as weight decay [23].

3.2.3.2 Conjugate Gradient Method

The conjugate gradient method (CG) or the Fletcher-Powell method is a state-of-the-art algorithm for optimization problems as it is able to converge rapidly and handle large amounts of data [24]. It has many advantages over the typical steepest descent, as it is a more robust and mathematical intense method that will converge as long as the function to be minimized is continuous and differentiable. The method starts similarly to the Cauchy's method or steepest descent in which minimization of the error gradient is desired by moving in the negative direction of the gradient:

$$d_o = -g_o \tag{3.11}$$

Then new values of w are calculated using the gradient direction by an amount of α_n

$$w_{n+1} = w_n + \alpha_n d_n \tag{3.12}$$

Where α_n can be calculated by a line search $min_\alpha F(\alpha d_n)$, and it is the optimal step size in the direction d_n. Once the new values of w are obtained the gradient is then updated by evaluating the gradient with respect to the new values of w

$$g_{n+1} = g(w_{n+1}) \tag{3.13}$$

Followed by the generation of a new direction

$$d_{n+1} = -g_{n+1} + \beta_z d_n \tag{3.14}$$

Where, $\beta_z = \frac{g_{z+1}^T g_{z+1}}{g_z^T g_z}$ in the Fletcher-Reeves algorithm; however, in this study a slight variation of the non-linear version of CG algorithm has been used called the Polak-Ribiere algorithm. This algorithm is similar to the Fletcher-Reeves algorithm, with the only difference being the way β_z is calculated (see [24])

$$\beta_z = \frac{g_{z+1}^T (g_{z+1} - g_z)}{g_z^T g_z} \tag{3.15}$$

Overall, the elegance of this algorithm is that in order to generate a new direction d, only three vectors need to be stored (the previous and current gradients and the previous direction) which makes efficient use of computer memory.

3.2.3.3 Structure

One of the principal issues regarding neural networks is the lack of an approach to determine the proper size of the neural network, where the usual approach is to try and keep the best [25]. Consequently, a K-fold cross validation (CV) technique was used to determine the optimal size of each of the hidden layers in each of the networks, such that each of the models' configuration is trained and tested 10 different times (K=10), and the model that minimizes the average cost function of the test set is selected[2]. Figure

[2]This process has been parallelized

3.4 shows the different neural network structures used and Table 3.3 [3] shows the configuration ranges in each structure, totaling a number of 28 models tested. Moreover, this ensures that the size of the neural network is optimized and computational power is efficiently used.

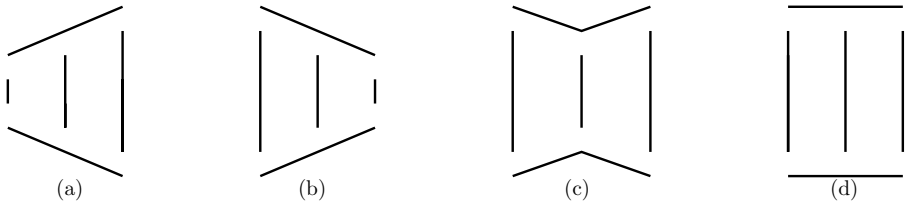


Figure 3.4: Neural Network structures

Table 3.3: Ranges of number of units in each of the different structure presented in Figure 3.4

Structure	Layer 1	Layer 2	Layer 3
(a)	[20:10:80]	[30:10:90]	[40:10:100]
(b)	[40:10:100]	[30:10:90]	[20:10:80]
(c)	[20:10:80]	[10:5:40]	[20:10:80]
(d)	[20:10:80]	[20:10:80]	[20:10:80]

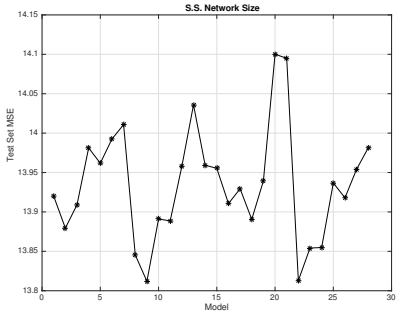
3.3 Results

3.3.1 Neural Network Optimization

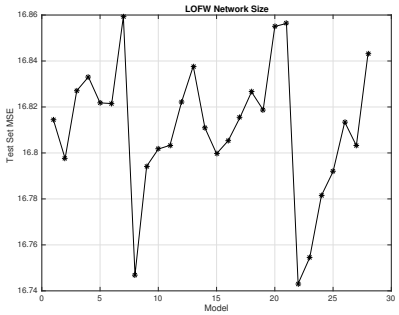
For the supervised learning process the data has been divided in a 70 to 30 ratio, i.e. training set (∼70%) and test set (∼30%). Each of the different networks has been optimized to use the ideal size and the regularization parameter to control over-fitting. Figure 3.5 shows an interesting pattern, where both neural networks have a preference towards structures 3.4.b and 3.4.d of medium size. Increasing the complexity also increases the

[3]The numbers shown in the table represent the initial number of units, number units incremented by each model, and final number of units

MSE of the test set, making the model less accurate. Table 3.4 summarizes the results of the optimal size and regularization parameters for each of the networks.



(a) Steady state behavior neural network



(b) Loss of feedwater behavior neural network

Figure 3.5: Mean MSE as a function of structure

Table 3.4: Neural network sizes and regularization parameter

Network ID	Hidden Layer 1	Hidden Layer 2	Hidden Layer 3	λ
Network 1	30	30	30	5E-3
Network 2	40	30	20	5E-4

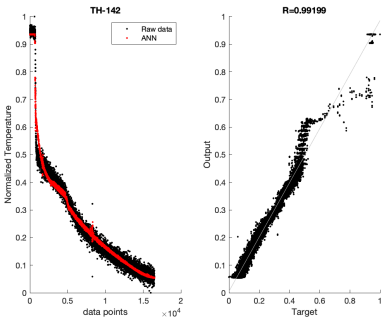
3.3.2 Predictions

Despite the fact that neural networks are known to have a "black box" characteristic and lack of physical representation, the results achieved in this study show the ability of neural methods to successfully learn from the data regardless of the complexity of the data. To illustrate the results obtained, a number of sensors and its predictions were selected in each of the networks along with a linear correlation coefficient to show the linearity between the data and the neural network predictions. Figures 3.6a, 3.6c, 3.6e, 3.6g, 3.6i, 3.6k, 3.6m, show the learned behavior under a LOFW event. It can be observed that there is good agreement between the predicted data and the real data, as the network learned the average of most of the sensors data. The temperature patterns

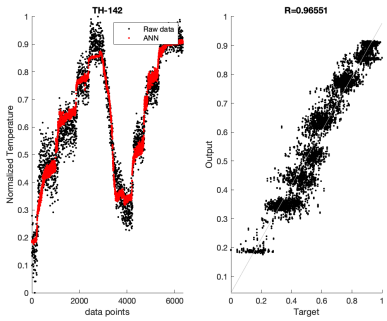
in this data set are similar since the prototype is set to a decay mode and the neural network is able to fit the behaviors very well. It is worth pointing out that Figures 3.6g and 3.6i show quite some noise and the network seems to identify and leans towards the greatest concentration of data (Figure 3.6g), or learns an average (Figure 3.6i) as the real data varies substantially. Similarly, Figures 3.6b, 3.6d, 3.6f, 3.6h, 3.6j, 3.6l, 3.6n, show the learned steady-state behavior under a various core power. Again, good agreement is shown between the data and the prediction. In this data set, the event produces more challenging patterns and not all the sensors have similar patterns, in fact, they are quite different from one another. Again noise in the data is expected, but it can also affect the network's perdition capability. For instance, in Figure 3.6h the unnormalized differential pressure sensor fluctuates between 501.16 Pa and 503.28 Pa and the network is not able to fully adapt to the sensors behavior; nonetheless, the network does lean towards the greatest concentration of data, identifying a linear pattern for this sensor.

3.4 Discussion

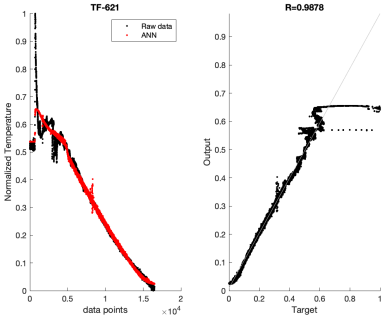
In the study of complex systems there are a wide variety of different properties that determine the behavior of the overall system and researchers usually pursue the use of physical representation to explain the physical phenomena. The test facility used here clearly shows the difficulty of analyzing a system as a whole since some of the data show a wide variety of patterns that no model can fully adapt. Neural networks can mimic most highly non-linear relations, making this method popular among researchers. However, their success depends on the characteristics of the chosen model, which vary based on trial-and-error, in addition to other limitations [26], such as the availability, quantity and quality of data that can be obtained from test facilities or share with other institutions. Data is the most important element in the application of machine learning, which can represent an issue in the nuclear industry as most the data is restricted. Parallel computing has also significantly accelerate parameter tunning, i.e. regularization and structure, and continues to improve with the use of GPU; nonetheless, it is still a challenge in neural networks as there is no given technique to quickly define these parameters that best suits the problem. Overall, the expressiveness of neural networks has produced satisfactory results, as many in the literature, for proof-of-concept in this application. It is highly encouraged in this research to further investigate this application in the



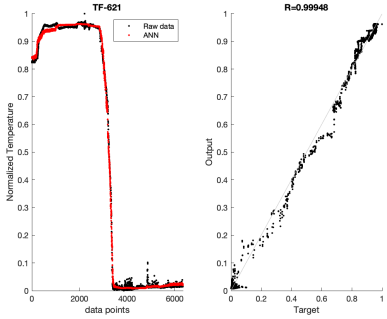
(a) LOFW-Core Heater Temperature



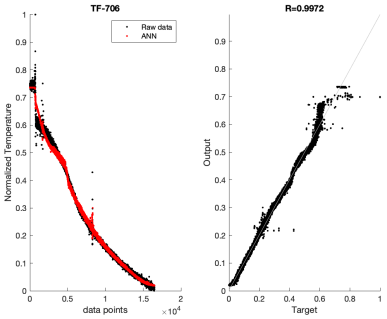
(b) S.S.-Core Heater Temperature



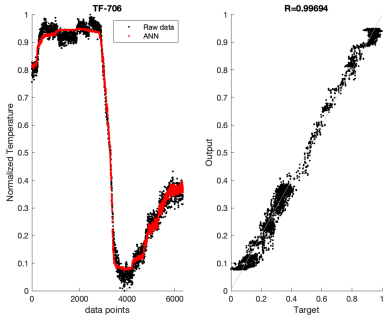
(c) LOFW-Middle Coil Steam Generator Temperature



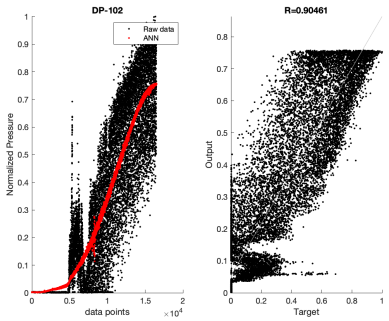
(d) S.S.-Middle Coil Steam Generator Temperature



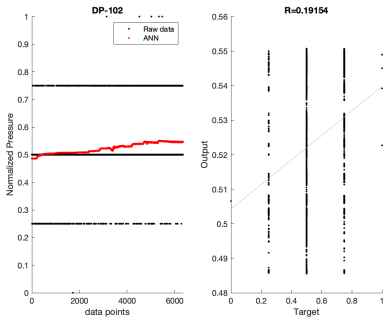
(e) LOFW-Steam Generator Liquid Temperature



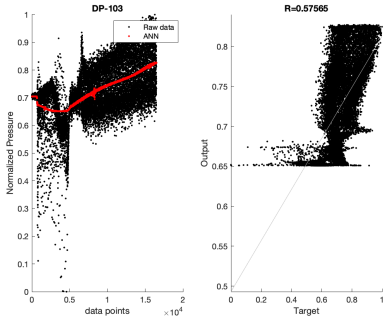
(f) S.S.-Steam Generator Liquid Temperature



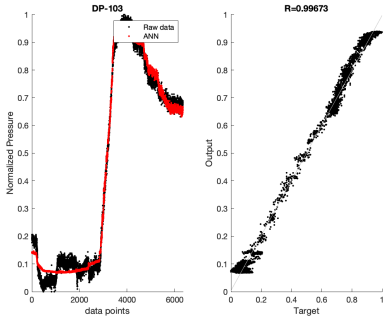
(g) LOFW-Pressure Drop between Core and Cone



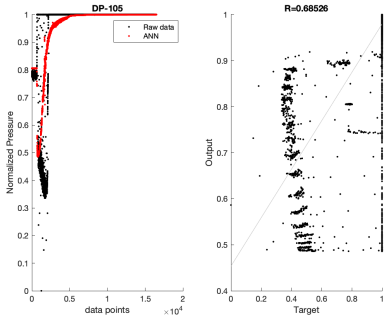
(h) S.S.-Pressure Drop between Core and Cone



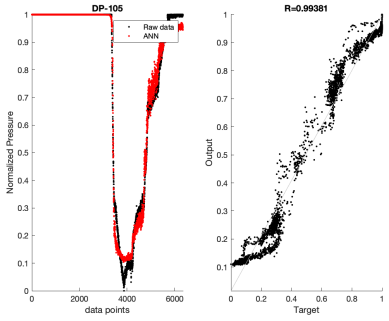
(i) LOFW-Pressure Drop in Riser Cone



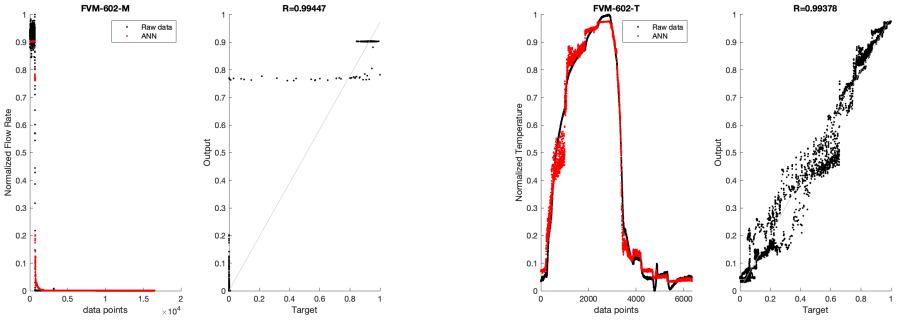
(j) S.S.-Pressure Drop in Riser Cone



(k) LOFW-Pressure Drop across the Steam Generator



(l) S.S.-Pressure Drop across the Steam Generator



(m) LOFW-Steam Volumetric Flow Rate (n) S.S.-Steam Volumetric Flow Rate

Figure 3.6: Neural Networks Results

test facility to validate the functionality, speed and accuracy of the predictions using additional transients, with the ultimate goal of integrating a systems as an operational enhancement tool to support decision-making.

3.5 Conclusion

The application of machine learning and other artificial intelligence techniques have been considered for many day-to-day applications in different industries. The purpose this study was to explore the application of machine learning methods, particularly neural networks, in the nuclear engineering domain for systems behavior predictions using the MASLWR test facility. The prototypical test facility was designed to assess the operation of an integrated small modular nuclear reactor at full pressure and temperature, and also, to assess the passive safety systems under different events. Despite the lack of physical representation in neural networks, the results obtained show their capability to use multiple sensors data to predict the behavior of the facility given various core powers and during a loss-of-feedwater event. Good agreement has been shown between the prediction and the raw data obtained from the facility without postprocessing of the data. Moreover, in cases where there was a lot of variance in the data, the neural network leaned toward greater concentration of data which it considered as the expected value. However, there are sensors where prediction is more difficult and can be further investigated. Though there is still a need to further explore the use of neural methods

in the nuclear engineering domain, the neural networks have successfully captured the behavior of most sensors inside the prototype.

Acknowledgements

The first author will like to extend his appreciation to the MASLWR team at Oregon State University for their extensive work in collecting the data and the guidance and support from NuScale Power‘s lead engineers. This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

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Chapter 4: Isotope Identification using Deep Learning: An Explanation

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Abstract

The exceptional performance of machine learning methods has led to their adaptation in many different domains. In the nuclear industry, it has been proposed that machine learning methods have the potential to revolutionize nuclear safety and radiation detection by leveraging that they can be used to augment human and device capabilities. While many application focus on the accuracy of the learning algorithm's prediction, it has been shown in practice that these algorithms are prone to learn characteristics that are not descriptive or relevant. Hence, this paper focuses on understanding the reasoning behind the classification using saliency vectors. Visual representations of the network's learned regions of interest are used to demonstrate whether domain-specific characteristics are being identified, which allows for the end-user to evaluate the performance based on domain knowledge. The results obtained show that focusing on a human-centered approach, will ultimately, increase the transparency and trust of deep learning algorithm's decision.

4.1 Introduction

The utilization of radiation detection devices has had a wide range of applications, and a successful technological evolution [1]. The task of isotope identification through gamma-ray spectroscopy is a mature field that has been partially automated by incorporating full spectrum identification algorithms which typically include a defined library of isotopes. In spectroscopy, the goal is to find a pattern, full energy peaks in most cases, and differential count rates by analyzing the distribution of counts over a spectrum. However, it is rather challenging to perform spectroscopy outside laboratories, where the environment is not well controlled. For example, applying spectroscopy to applications such as nuclear threat detection is very challenging because of (1) device limitations, (2) changing environmental conditions, and/or (3) variability in isotope location (e.g., sources in motion). Additional challenges such as detection time limitations, shielding, unknown backgrounds, calibration, maintenance, and timely decision-making are also commonly present [2]. The use of machine learning (ML) for this task aims to reduce false positives and false negatives in isotope identification by leveraging pattern recognition to identify characteristics or deviation in spectra information[3]. While various neural network

models have reported good accuracy in gamma spectroscopy tasks, there is a trade-off between accuracy and explainability that is commonly left out [4]. If accuracy is the only metric of performance, then black-box models will be trustworthy; however, for sensitive or high stakes applications, understanding the logic behind classifications or actions becomes important[5] because of the possible risk imposed to society (e.g., [6, 7, 8, 9, 10, 11]). Explainable AI (XAI) is a very active area of research that seeks to understand the decision behind learning algorithms [12, 13, 14], and has to be considered as an optimization driver such that domain knowledge is used to evaluate performance. With a prudent attitude toward research on unintended consequences, this study explores how and why a prediction is being made in a way that is comprehensive or intuitive for a domain expert to evaluate the quality of the model.

The remainder of this paper is organized as follows. Section 4.2 introduces the software utilized to generate the data for this study, and the concepts of convolutional neural networks and saliency. Section 4.3 presents the need for explainability by showing that the creation steps of a convolutional neural network tasked to classify radionuclides provides a level of intuition, but no reason behind the classification. Section 4.4, present the model's classification explanation associated with the prediction (i.e, the network's regions of interest (ROI)) in a form of saliency vectors. Section 4.5 shows a ROI comparison between a shallow and convolution network and their differences between model accuracy and its ability to show a physical characteristic associated with the classification. Moreover, suggestions on further research and challenges are presented. Finally, section 4.6 provides a summary and conclusions.

4.2 Materials and methodology

4.2.1 GADRAS-DRF

Gamma Detector Response and Analysis Software – Detector Response Function (GADRAS-DRF) is a software program developed by Sandia National Laboratories (SNL) that computes the response of gamma or neutron detectors to radiation. It contains a suite of capabilities related to radiation detection, such as plotting and viewing measures and computed spectra, spectra analysis to identify isotopes, and estimating source energy distributions [15]. Its primary function is the simulation of gamma-ray and neutron de-

Table 4.1: Radioactive library[1]

^{241}Am	^{137}Cs	^{40}K	^{232}Th
^{133}Ba	^{67}Ga	^{99m}Tc	^{235}U
^{57}Co	^{131}I	^{201}Tl	^{238}U
^{60}Co	^{192}Ir	^{226}Ra	^{239}Pu

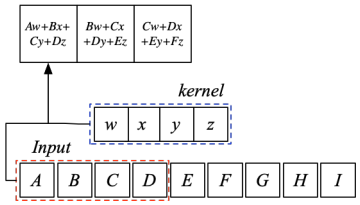
tector signals to radiation sources which derives spectrum features; such as photopeaks and the Compton continuum, from first-principles calculations based on interaction cross-sections. The software is used in this study to simulate the response of a common NaI(Tl) (3"X3") detector using different activity levels to simulate different conditions. The data generated is normalized using Equation 4.1 [16]. For the purpose of this study, the isotopes listed in the American National Standards Institute (ANSI) [17], and shown in Table 4.1, are used with activities ranging from 1E-5 to 1E-3 Curies (3.7E5 to 3.7E7 Becquerels). The data, and associated identification or ID, serve as input to the deep learning model.

$$X' = log(\frac{X+1}{X_{max}}) \tag{4.1}$$

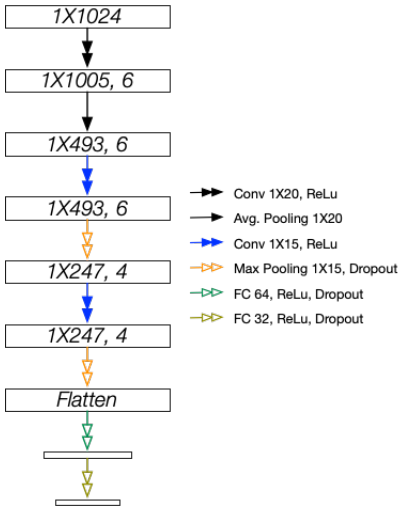
4.2.2 Convolutional Neural Networks

While Convolutional Neural Networks (CNNs) are well known nowadays, a conceptual introduction will be presented. CNNs were firstly introduced in [19, 20] as the analog of mimicking the vision process of mammals, and had its first success by being able to recognize handwritten numbers[21] without feature engineering. A *convolution layer* consist of three different stages: convolution, activation, and pooling. First, a convolution is a mathematical operation on two functions of real value arguments that form a new function [22]. The convolution operation is denoted with an $\circledast$, where the operation $O = k \circledast I$ as applied to the data is interpreted as the feature vector O, resulting from the convolution of the I vector and the kernel k, where k is also referred as a filter. This layer reduces the amount of parameters needed to be optimized, as shown in figure 4.1a, which both decreases the memory required and increases the model efficiency.

[1]See [18] for details on categorization and purpose of each radionuclide



(a) 1-D Convolution representation



(b) IsotopeID structure

Figure 4.1: Convolutional Neural Network used in this study, where: 4.1a is an illustration of the convolution operation; and 4.1b is the network structure that shows the dimensions of the data followed by the number of filters used at each of the layers

Subsequently, each of the convolutions are then transformed by a non-linear activation function to extract features, i.e. for each k, transform using $f = \sigma(W * k + b)$, where σ is the activation function of choice. This stage is typically known as the *detection stage*. Finally, the transformed data passes through a pooling function that changes the output of the layer. At the pooling stage, the pooling function replaces the output of the network with statistical summary of the nearby outputs. The key concept from the pooling stage, is to help the representation to be invariant to small transformations of the inputs, i.e. the network will be robust to small changes. The "convolved features" following the feature extraction stage can then be used for classification by the currently known Feed-forward Neural Network (FFNN)[2]. The general network structure used in this research is shown in figure 4.1b. A softmax function is applied in the decision layer. Additionally, the convolution layers are removed to create an FFNN for comparison purposes.

[2]The details of the FFNN can be found in various different textbooks such as[23, 24, 22, 25]

4.2.3 Saliency

The concept of saliency was introduced in the computer vision to better understand the importance of pixels of a given image. An explanation on the principle of saliency presented in [26] and a similar example is described in this section. Given a vector V_0, a class c, and a model with the class score function $S_c(I)$, where we want to rank the values in V_0 based on their influence on the score $S_c(V_0)$. Let us consider a linear score model for the class c

$$S_c(V) = w_c^T(V) + b_c$$

where V is vector, w_c is the weight vector and b_c the bias of the model. For this simple example, the magnitude of the elements of w defines the region of interest in V for the class c. However, because convoutional neural networks are not linear functions with respect to V, we can approximate the score function with a linear function in the neighbourhood of V_0 by computing the first-order Taylor expansion:

$$S_c(V) \approx w_c^T(V) + b_c$$

where w_c is the derivative of S_c with respect to the vector V at the point V_0

$$w = \frac{\partial S_c(V)}{\partial V}$$

This means that the magnitude of the derivative indicates which values affect the class score the most. Saliency vectors will be referred as *attentions* in this work and some examples are shown in figure 4.4 bellow their respective spectrum.

4.2.4 Sanity checks

While many different explainability methods have been proposed (e.g., [27, 28, 29]), limitations are also known. To evaluate the robustness of an explainability method for a

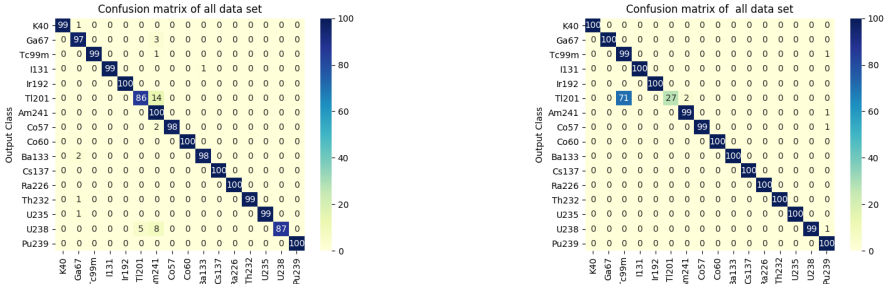
particular application, two sanity checks described in [30] have been carried out. These include: randomly initiating all the weights, and retraining with permuted the labels (i.e., ^{137}Cs labeled as ^{241}Am). The purpose is to show that the trained model is sensitive to randomization, i.e., all explanations must be different.

4.3 An explainability problem

Different feed-forward [31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46] and convolutional neural network models[47, 48, 49] have been reported in the literature for radionuclide identification, which have shown high accuracy for the task under different conditions. However, as it has been shown in practice, neural networks are prone to learn characteristics that are not descriptive or relevant of the object or task [28]. While a promising application, their black-box nature can impede the deployment of such methods in a highly regulated industry. Therefore, explainability methods can be used to enhance the transparency of these algorithms by showing that domain knowledge is being reflected. To demonstrate this, the network depicted in figure 4.1b is developed and the inner working of the algorithm is shown and explained.

4.3.1 Accuracy

In principle, the learning algorithm will achieve remarkable accuracy as each of the spectra (patterns) are different from each other. Creating a confusion matrix for the network using all the data (see figure 4.2a) shows that the model is very accurate and is able to distinguish most the spectra. The high accuracy obtained is aligned with the literature. However, confusion matrices only show the classification and misclassification instances, but do not provide any reasoning as to what is characteristic of the class being chosen. As noted in [50], for the solution to be explainable, each element constituent of the solution needs to be understood. Mathematically, the steps of the models are conceptually simple; however, they might not be as intuitive as the use of visualization tools.



(a) Convolutional neural network (b) Feedforward neural network

Figure 4.2: Radionuclide classifier confusion matrices

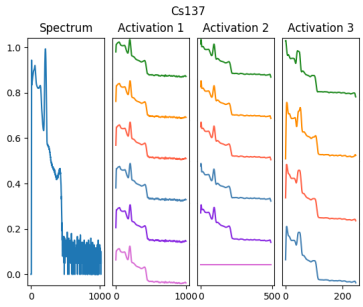
4.3.2 Visualization of internal layers

Visualization of the internal functions of a neural network is a method that has been used to understand the features that are extracted from the data[51]. As stated by [52], "gaining some insight into the function of the intermediate layers, one can find more suitable model architectures". The same can be done for the spectra data as shown in figure 4.3a[3], where one can be observe the convolved spectra after each of the activation functions. At each convolution layer it searches to isolate important features. The last four spectra are the features that were derived and used for classification process, in this case for ^{137}Cs. While it certainly gives an intuition of how the data is being transformed, it does not provide the rationale to its decision. The derived features appear to be less noisy spectra, yet no highlighted characteristic.

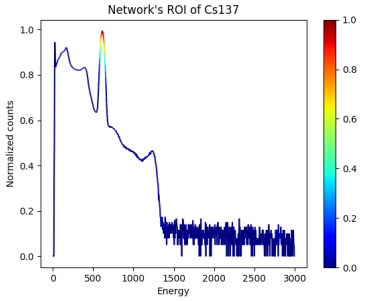
4.4 An explainable approach

Utilizing explanability methods, such as saliency, can help users judge their classification by context rather by accuracy alone. These explanations are important identify potential problems in the classification and ensure that domain knowledge is reflected in the algorithm [12]. For instance, figure 4.4a shows the spectrum and its respective attentions and 4.3b a heat vector representation of the spectrum classification of ^{137}Cs. In other words, attentions are the region of interest determined by the neural network and are to

[3]Please refer to the supplemental material for the visualization and explanation results for each of the different isotopes

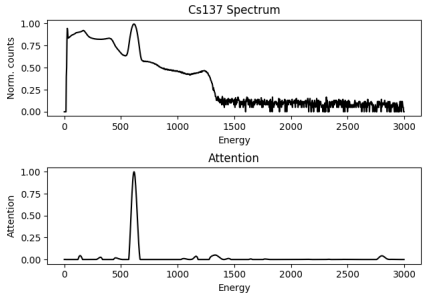


(a) Activation operations on the ^{137}Cs spectrum

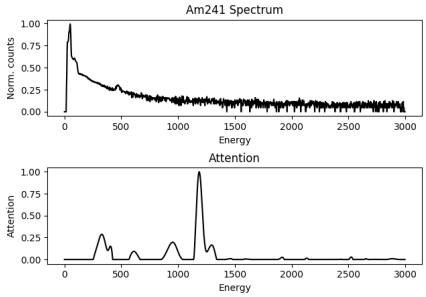


(b) ^{137}Cs heat vector

Figure 4.3: Inner layer and heat vector visualization of the ^{137}Cs spectrum



(a) ^{137}Cs spectrum and attentions



(b) ^{239}Pu spectrum and attentions

Figure 4.4: Regions of interest identified by the network

be compared with the characteristic peak, i.e., of 662 keV for ^{137}Cs, which is accurate for this class. However, this is not always the case. As shown in figure 4.4b, it's ability to give an explanation about which ^{241}Am peaks are characteristic of the radionuclides[3]. Low resolution devices are not suited for the detection of low energy gammas, or radionuclides with overlapping peaks that an only identified with higher resolution devices as such information is not presented to the algorithm; consequently, it cannot be expressed that a deep learning algorithm enhance low resolution devices without demonstrating that at minimum a relevant characteristic is identified. The classification of complex spectra is related to the differences in patterns as compared to the rest of the spectrum, but not necessarily to a characteristic peak(s).

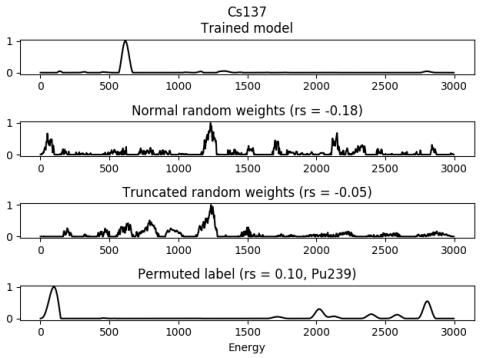


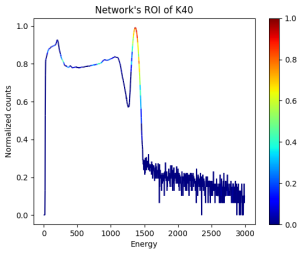
Figure 4.5: Sanity checks results of the trained model, weights and label randomization followed by spearman rank correlation (rs)

4.4.1 Sanity Checks

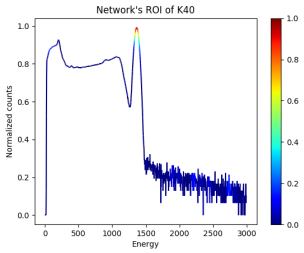
As described in section 4.2.3, the sanity checks are included for illustration and transparency purposes. Shown in figure 4.5 are the attentions of the trained model, two different weights randomization and label randomization. Spearman rank correlations are obtained based on the trained model and are used to show that the model is indeed sensitive to this test. The label randomization is particularly important as changing the labels forces the model to memorize a wrong relationship between the input and the label.

4.5 Discussion

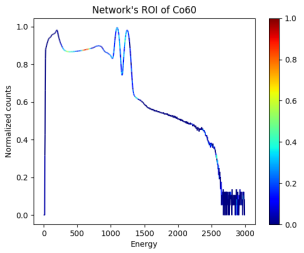
Some of the most exciting aspects of deep learning are to understand how the algorithms work and how the decisions are made, especially if visualization tools are used to facilitate the end user's job. For further comparison and discussion purposes, a shallow network is created by removing the convolution layers and visualizing their saliency vector. Both models' classification accuracy are shown in figure 4.2a and 4.2b. They are accurate and potentially suitable to classify the radionuclides in table 4.1; however, the heat vectors in figure 4.6, show that the ROIs from each model prioritize different areas in the spectrum[3]. As shown in 4.6c and 4.6d, CNN's find ROIs that are closer to characteristic peak(s). Better agreement is shown from the convolution layers as they are intended to extract features from the raw data and fit a function based on those features as opposed to



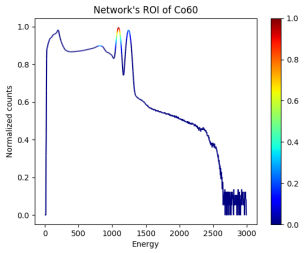
(a) ^{40}K ROI using FFNNs



(b) ^{40}K ROI using CNNs



(c) ^{60}Co ROI using FFNNs



(d) ^{60}Co ROI using CNNs

Figure 4.6: Networks comparisons of regions of interest

simply fit a function to the spectra. The algorithm presented is only able to correlate to some known peaks of strong gamma-emitters in table 4.1, and more research is suggested for more complex spectra, i.e., decay chains and mixtures. Mentioned in [53, 54, 55, 56, 57], demanding the user to understand the logic of learning-based models can help reduce the odds of negative consequences. To the best of our knowledge, this is the first attempt at showing that saliency vectors can serve as tools to highlight and relate an area of interest to a physical characteristic of the given information (i.e., energy peaks). Such demonstrations have a significant impact in the nuclear industry because radiation practitioners can justify that domain knowledge is being captured by the algorithm, and consequently, understand it. To that extent, deep learning as applied to radiation devices are yet to be fully explored, specifically when logic is needed. Finally, cross-discipline research and development of benchmarks are key to design and ensure the intended use of machine learning technologies and gain acceptance among the community.

4.6 Conclusions

This study builds upon the literature for task of isotope classification and explainable artificial intelligence. It is demonstrated that while different neural network models can achieve high accuracy, their specific properties (e.g., convolution) provide some advantage to the characterization of the spectra. The method of saliency for explanations is used to evaluate the rationale behind the classification and to test if it is correlated to the isotope's characteristic peak(s), i.e., context accuracy. The results, processes, and limitations presented in this paper show a more transparent and human-centered approach for the identification of isotopes task, which is of particular importance in a highly regulated industry. Lastly, it is emphasized that for the effective application of deep learning in a nuclear and radiation related fields, cross-discipline studies must be encouraged.

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Chapter 5: General Summary and Conclusions

The application of machine learning and other artificial intelligence techniques have been considered for many day-to-day applications in different industries. These changes are taking place in the industrial world and will shape the future of the nuclear industry. The manuscripts presented herein show the application of learning-based methods in various applications related to nuclear science. First, it presented an overview of the state-of-the-art application of artificial intelligence in three different subareas of nuclear science; it shows that while there have been many advances in the technology, there are multiple areas of improvement. Additionally, it discusses the importance of concepts such as FAIR and MAD to the development and deployment of learning-based methods. It highlighted that the primary goal for the development and implementation of machine learning algorithms is to provide fast estimation for better-informed decisions for the users (human in the loop), as well as assuring the interpretability and reproducibility of the models. A case study on the implementation of a popular method, neural networks, as a fast tool to predict the behavior of a nuclear reactor concept is shown. While a highly complex task, good agreement has been shown between the prediction and the raw data obtained from the facility without postprocessing of the data (i.e., mapping controls to reactive sensors). A lack of physical representation is, however, acknowledged and suggested for further research before any real deployment is considered. This is followed by a concept that looks into using expert-knowledge to evaluate the use of neural networks for gamma spectroscopy classification. The explanation method of saliency is used to evaluate the decision of the classifier by correlating it to its characteristic peak(s). It is demonstrated that while different neural network models can achieve high accuracy, their specific properties (e.g., convolution) provide some advantage to the characterization of the spectra. Ultimately, presenting a more transparent and human-centered approach to the development of neural networks in isotope classification. Overall, as more research, cross-discipline training, and information become available, the implementation of AI to perform different tasks in the nuclear industry is certainly possible in the near future. It is a matter of understanding the benefits of new technologies, regulatory acceptance, and

collaboration, until more innovative approaches, are available within the domain.