Uncertainty Quantification Methods for Neural Networks Pattern Recognition

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***Abstract*—On-line monitoring techniques have attracted increasing attention as a promising strategy for improving safety, maintaining availability and reducing the cost of operation and maintenance. In particular, pattern recognition tools such as Artificial neural networks are today largely adopted for sensor validation, plant component monitoring, system control, and fault-diagnostics based on the data acquired during operation. However, classic artificial neural networks do not provide an error context for the model response, whose robustness remains thus difficult to estimate. Indeed, experimental data generally exhibit a time/space-varying behaviour and are hence characterized by an intrinsic level of uncertainty that unavoidably affects the performance of the tools adopted and undermine the accuracy of the analysis. For this reason, the propagation of the uncertainty and the quantification of the so called margins of uncertainty in output are crucial in making risk-informed decision.**

The current study presents a comparison between two different approaches for the quantification of uncertainty in artificial neural networks. The first technique presented is based on the error estimation by a series association scheme, the second approach couples Bayesian model selection technique and model averaging into a unified framework. The efficiency of these two approaches are analysed in terms of their computational cost and predictive performance, through their application to a nuclear power plant fault diagnosis system.

I. Introduction

The attractiveness of nuclear energy in the market and among the public is generally challenged by the operation and maintenance costs (equal to 73% of the total nuclear power generation cost in contrast with 15% of the cost of electricity generation from fossil sources [1]), and most especially, the concern regarding the system safety and reliability. Hence, the challenges for the growth of the nuclear sector involve the enhancement of safety, the preservation of availability and the reduction of the costs associated with the operation and maintenance of the plants. Subsequently, the acquisition of data during the normal operation of the installations and the use of such information to evaluate the health of the ongoing processes would provide powerful tools for tackling these issues. Indeed, it would limit the reliance on operators judgement for diagnosis and prognosis (on which common practice currently relies) and promote the adoption of condition-based maintenance strategies and automate testing activities. For this reason, much focus has been paid in the last decade on the development of efficient on-line techniques for equipment and plant condition monitoring, able to anticipate, identify and resolve the occurrence of malfunctions and ensure the continuous availability of the plant.

On-line monitoring relies on the acquisition of data while the plant is operating (i.e. through the use of sensors) on one hand, and on the adoption of effective computational methodologies that ensure real-time response on the other. Both these aspects raise reasonable questions about the impact of the input and model uncertainty on the analysis accuracy: measured data possess an intrinsic level of uncertainty, due to their evolutionary nature, i.e. time-space variability, and unavoidable measurement imprecision or even errors. Similarly, a further contribution to the overall uncertainty of the analysis is ascribable to the use of mathematical models that, due to the restrictions imposed by the real-time requirements of this kind of analysis, must be low computational demanding even at the cost of higher model errors. In light of this, the quantification of the uncertainty in output and hence the robustness of the tools adopted for the analysis play a role as crucial as the primary diagnostic analysis itself. In other words, any robust on-line monitoring methodology should characterize the output of interest with margins of uncertainty in order to provide a fully risk-informed decision support.

The present study focuses on the use of Artificial Neural Networks (ANNs) as a pattern recognition tool for fault diagnosis. This latter can be interpreted as a mapping from the measurement space into the decision space: the first stage consists of the measurement of the data significant for the detection of the fault; then the important features are extracted and classified into one or more classes in order to identify the

type of fault occurred [2]. The adoption of ANNs is motivated by the satisfactory results obtained in previous studies, which have highlighted the efficiency of such technique for nuclear power plant transient diagnosis [3] [4]. This is mainly due to their capability of capturing non-linear relationships between the input and output space as well as the dependencies between variables. Furthermore, ANNs have been demonstrated to endure noise, ensuring that the disturbances in the measurement signal, if within the acceptable level, do not prevent the recognition and classification process. The current literature offers several studies about the performance of ANNs for fault diagnosis, in particular in the field of nuclear industry. Nevertheless, in spite of the large attention recently dedicated to ANNs by the research community as well as the industry, in most applications the output of the ANN is simply assumed to be reliable and only limited literature is available on the estimation of the uncertainty associated with the network response.

The current research compares two possible approaches for the quantification of the uncertainty affecting the model output. The first relies on an error estimation strategy, referred to as Error Estimation by Series Association (EESA), which is shortly described in Section II-C1. The second approach is based on a Bayesian model selection technique described in Section II-C2. Finally, the two methodologies are applied and compared through their application to a case-study described in Section III.

II. Theoretical Background

The following sections aim to provide a general overview of the theoretical background of the proposed research. First the structure and operating principles of ANNs are briefly introduced in Section II-A while an overview of their application for fault diagnosis is provided in Section II-B. Finally, Sections II-C1 and II-C2 briefly describe the methods adopted and their application to the ANN implemented.

A. Artificial Neural Networks

The first studies on the implementation of computational methods aiming to reproduce the behaviour of human neural networks date back to the mid 20^{th} century. Since then, ANNs have gained increasing interest and are used today for a wide variety of applications, from cutting-edge reverse-engineering research to popular mobile apps.

Reasonably, the terminology used for ANNs recalls that of biological neural networks, which the approach aims to imitate: the structure of an ANN consists mainly of artificial *neurons* which have the task to process the incoming signal; such neurons are indeed organized in *layers* and linked to each other through connections imitating the axons of a biological brain. The overall task of such structure is to process the input fed into the network, passing the signal from the first (commonly referred as *input layer*) to the last (*output layer*) through all the intermediate layers (*hidden layers*). During this process the initial signal is modified, thanks to the interaction among the neurons of the network. Indeed, each connection (represented in Fig.**??** as arrows) is associated with a weight that multiplies each signal (coming as an input of the model or from a preceding neuron) before being sent to the corresponding neuron. Here, all the incoming input (modified according to the corresponding weights) are summed together. The overall input signal resulting from such arithmetic addition is then transmuted to the neuron output through the use of the so called *transfer* (or *activation*) *function*.

The basic structure of an ANN is then quite simple, while a crucial role in the processing of the input is played by the connection weights. These are assigned throughout the so-called *training* of the network. This latter is performed adopting tailored algorithms (the most common being the *backpropagation algorithm* [5] and its variations [6], [7]) that provide the updating of the weights according to the available data. In other words, given a training dataset containing both the input and the corresponding outputs of a process to be modelled, the training procedure aims to identify the values of the connections weights that ensure the most accurate reproduction of the initial process by the ANN [8]. In order to test the effectiveness of the ANN models implemented, the available data are generally split in two subsets: one, commonly referred to as *training dataset*, contains the data adopted for the only purpose of updating the connection weights of the designed network structure; the second is instead associated with the *validation* process, which consists of evaluating the performance of the ANN obtained from the training process on a still unused set of data.

B. Fault Diagnosis with ANNs

ANNs capability of capturing the behaviour of a system at a low computational cost, makes this method particularly attractive for applications involving complex processes, for which other modelling approaches would imply high computational time. This is the case of nuclear power plants, for which the use of ANNs has been investigated in relation to various areas such as sensor validation [9], system control [10], and fault-diagnosis [3] [11] [4] [12] [13] [14] [15].

This study focuses in particular on fault diagnosis, understood as the detection of the fault and its classification. These tasks are commonly carried out through pattern recognition: during the normal operation of the plant, the monitoring instruments define an unique set of readings that indicates a normal state of the plant or system; conversely, in the case of disturbances, the set of instrument readings undergoes a transition defining patterns that can be interpreted as symptoms of an abnormal status of the system [16]. Such patterns defined by the transient not only highlight the possible occurrence of a fault but can also reveal the specific fault type and extent of the fault. Hence, given an adequate dataset containing the transient data associated with specific faults, an ANN can be trained to recognize the various conditions or states of a complex system and hence detect and identify the state of the system in real-time (typically in a few milliseconds). This ensures an effective on-line monitoring of the processes and an early detection of possible malfunctions.

In summary, an ANN designed for fault diagnosis purposes (referred to as *advisor* or *primary* network in the present study) provides in output a specific diagnosis for a certain symptom highlighted by a set of instruments readings. Nevertheless, the ANN represents only an approximate model of the true process (or system) under study and the accuracy of its performance for input data lying outside the initial available dataset remains unknown. In other words, the overall accuracy of the diagnosis depends both on how much the new input differs from the initial data the network was trained with but also on how well the ANN actually models the true system.

C. Prediction Uncertainty for ANNs

The ANN training process allows to capture the underline relationship existing between a set of input factors and an output and hence to use the implemented model for further predictions. The main limitation of this approach is associated with the *black box* nature of ANNs: this implies the impossibility of having any insight on the internal behaviour of the network and on the physical mechanism that controls the processes. This lack of transparency, together with ANN stochastic nature, anavoidably raises questions on the credibility of point predictions for real-world applications, which have generally to face uncertainty in the data or variability in the underlying system. In order to overcome this drawback, several numerical quantification techniques aiming to characterize the uncertainty affecting the network prediction have been proposed in the literature. According to Kasiviswanathan et al. [17], these can be generally classified in four categories [18]: probabilistic based methods (including Bayesian neural netowrks [19]), error prediction techniques (i.e. based on the analysis model error in reproducing observed data [18]), resampling techniques [20] and fuzzy based method [21]. All the mentioned strategies require the introduction of several assumptions, for example related to the prior distributions of the uncertain input parameters or data to be propagated or to the membership function of the uncertain quantities, on the validity of which depends the accuracy of the analysis. Moreover, most of the mentioned techniques imply the need for sampling, increasing the computational costs of the overall analysis which is a crucial aspect for the on-line monitoring application analyzed in the current study. In light of this, two techniques, both with low computational demand and no assumption on the initial uncertainties, have been selected in this study.

1) Error Estimation by Series Association: The EESA method [22] aims to quantify simultaneously the ANNs errors caused by both the modeling and the input dissimilarity. This task is accomplished implementing, alongside the aforementioned advisor ANN, an error predictor network to assess generalization errors. Such secondary network is trained to estimate the error affecting the output of the primary ANN: while the advisor ANN provides in output the diagnosis of the system state, the error prediction ANN output consists of an estimate of the error associated with such diagnosis. The two networks are identically designed (in terms of number of layers and weight connections) but differs for the number of input: given n input for the advisor network, the error prediction network will have a number of input variables equal to n+1. Indeed, the training set for the secondary ANN can be derived from the initial training input of the advisor ANN with the addition of the advisor ANN output and, for verification purposes, the value of the error understood as the difference between the output provided by the advisor and the true value available from the dataset. In light of this, the error predictor network designed by using the EESA approach can reveal the abnormal behaviour of the primary ANN as well as verify the quality of the advisor network training, since the output of the diagnostic network is incorporated together with inputs to estimate errors. Fig.1 provides the graphical representation of the EESA approach.
The EESA method has already been applied in the field of fault diagnosis and has been shown to achieve satisfactory results in the case of transients at various severity levels and degraded noise conditions [22].

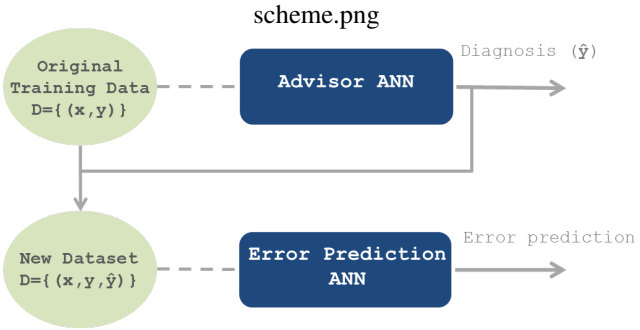

Fig. 1. Architecture of EESA approach

2) Bayesian Model Selection: The second approach, suggested by Oparaji et al. [23], relies on a Bayesian model averaging approach and allows to estimate the model parameter uncertainty at a low-computational cost. It focuses on the inner variability of the training process and aims to exploit such feature in order to obtain robust ANN response [24]. Indeed, networks with identical structures and trained adopting the same dataset result in different models (i.e. ANNs with identical structure but different weights). This is mainly due to the random initialization of the weights in the training process and leads to the implementation of ANNs characterized by different performance and hence output accuracy. In order to maximize the accuracy of the model response, it is common practice to select the best ANN among those trained on the same dataset on the basis of its performance on the validation set. Nevertheless, there is no guarantee that the best-performing ANN on the validation dataset would provide the best results also on new and unseen data; moreover, the criterion behind the identification of the best ANNs relies on the comparison of the R^2 values associated to the trained ANNs: such approach is recognized to have major limitations, such as the impossibility of determining whether the prediction computed is biased or whether the regression model is

adequate. In other word, a good model can be associated with a lower R^2 value than a model that does not fit the data of interest.

In order to address these issues, the approach adopted introduces a model selection procedure based on Bayesian statistics. Given a set of ANNs sharing an identical structure, the method can be roughly summarised in the following steps:

- Computation of the Bayesian posterior probability associated with each network given the specific training dataset adopted.
- Selection of the best ANN on the basis of the probability previously computed (i.e. identification of the ANN of the initial set with the higher posterior probability given the training dataset).
- Estimation of the adjustment factor through model averaging technique.
- Computation of the expected value and variance of the robust prediction on the basis of the previously identified adjustment factor.

An overview of the algorithm is provided in Fig.II-C2.

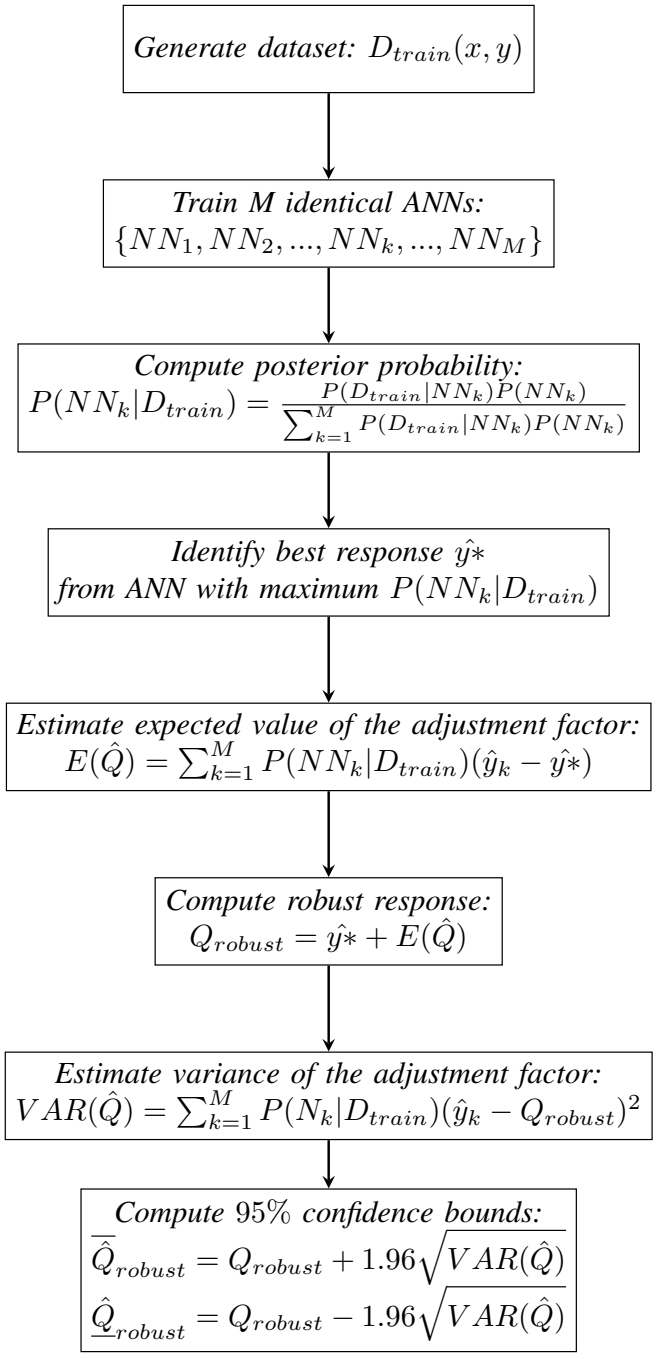

Fig. 2. Flow Chart for Bayesian model selection approach

III. Application

The failure of the cooling system of pressurized water reactors due to the occurrence of break in the water circuit, generally known as loss of coolant accident (LOCA), is the design basis accident of most nuclear facilities. This is due to the potential severity of this failure mode that can compromise the correct heat removal from the reactor that, if not effectively tackled, can lead to core damages. In light of this, the continuous monitoring of the cooling process, as well as the rapid detection and diagnosis of eventual breaks, are essential to ensure the fast and effective action of the operator, limiting the potential damage to the system as well as to the surrounding environment and population around. Thanks to the capabilities of ANNs in terms of pattern recognition and non-linear regression, such technique appears particularly appealing for this kind of applications.

The current study focuses on the application of ANNs to the detection and diagnosis of LOCAs and investigates possible approaches for the quantification of the uncertainty affecting the results of such diagnosis. Section III-A gives and overview of the simulation setting and model adopted, while Section III-B proposes a careful comparison between the results obtained by the two approaches highlighting the advantages and drawbacks of both.

A. Case Study

The simulation case study was referred from from Santhosh et al. [11] and consits of the primary heat transport system of a 220MWe pressurised heavy water reactor, whose design has a double containment with a vapour suppression pool. The main aim of the containment is to limit the release of radioactivity under normal and accident conditions, both at the ground level and through the stack. The accident scenario contemplated by design is a loss of coolant accident (LOCA) involving a double ended guillotine rupture of the reactor inlet header. In case of such accident, the vapour suppression pool is designed to limit the peak pressure and temperature in the containment, allowing the complete condensation of the incoming steam and limiting the leakage of fission products to the surrouning environment. In addition to this, several strategies (e.g.dissolving, trapping, entraining mechanisms) are in place to perform the removal of the fission products that reach the pool. All the instrumentation and control parameters are continuously displayed in the reactor control room.

The aim of the analysis is to identify the severity of the LOCA events on the basis of selected instrument signals: for this purpose, the main task of the implemented ANN is to recognize the pattern drawn by the input signals in time and to provide, on the basis of this information, the severity of the break in output. This is quantified in terms of break size, expressed in comparison with the double-ended rupture of the largest pipe in the reactor coolant system. For instance, a 200% break indicates the free discharge of the primary coolant from both the broken ends of the main pipe (this is generally considered the worst accident that can occur in a water circuit). The dataset available covers a range of break sizes equal to 20%, 60%, 100% and 200%.

The model adopted in the current study refers to a multilayer neural network for the detection and diagnosis of LOCAs, namely the failure of the cooling system of a pressurized water reactor. The dataset available for the training and validation of the network was referred from Santhosh et al. [11] and consists of the sampling of 37 signals from instrument readings which hence represent the input of the ANN implemented. Also the ANN architecture adopted in the current study corresponds to that suggested by Santhosh et al. [11] and consists of a fully connected multilayer network trained adopting the well-known LevenbergMarquardt algorithm, which has been demonstrated to outperform the classic backpropagation algorithm as well as quasi-Newton algorithms in pattern recognition applications [25], [26]. The available dataset was split into three subsets, one dedicated to training containing 70% of the overall data and the other two used for test and validation, overall including 30% of the initial data.

B. Results

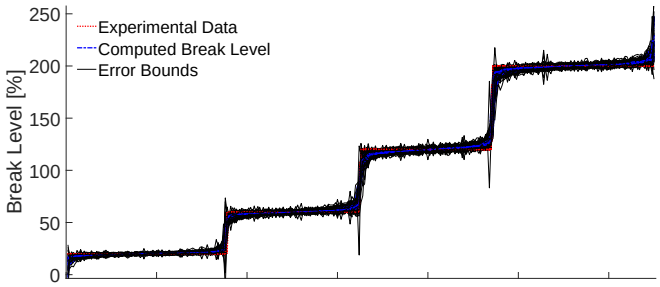

Fig. 3. Results for the EESA Approach

The EESA method has been applied to 50 identical ANNs in order to take into account the output variability due to the random initialization of the weights in the training process. The results obtained are shown in Fig.3: the output of the primary ANN captures the general trend of the experimental data. Nevertheless, the error bounds identified with the EESA method present in all cases analyzed, evident fluctuations and include the true experimental data only 62.8% of times for the best-performing network, and less than 45% for the worst-performing network.

The Bayesian model selection approach has been applied to four ANN sets characterized by a different number of networks (i.e. 50, 25, 10 and 5 networks), in order to estimate the impact of such parameter on the overall performance and to link this latter to the required computational time. As shown in Table I, the 95% confidence bounds obtained with the Bayesian model selection approach include the true value of the output for all the validation data analyzed when considering a set of 50 networks (Fig.4). The accuracy of the results decreases slightly when adopting sets with a lower number of networks, but remaining over 90% for sets of 25 (Fig.5) and 10 ANNs (Fig.6). The results related to the application of the Bayesian approach to a set of only 5 networks, shown in Fig.7, present an accuracy of 62.5%, thus similar to that previously obtained in the best case of the EESA approach. Similarly, the

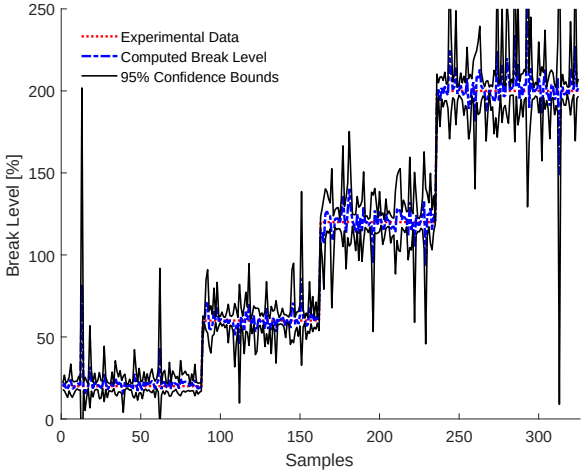

Fig. 4. Results for the Bayesian Averaging approach with 50 NNs and 95% confidence bounds

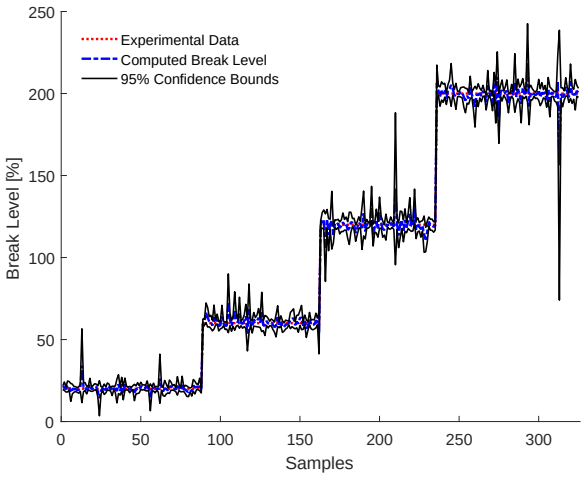

Fig. 5. Results for the Bayesian Averaging approach with 25 NNs and 95% confidence bounds

computational time required for the Bayesian approach using 5 networks is of the same order of magnitude of that required

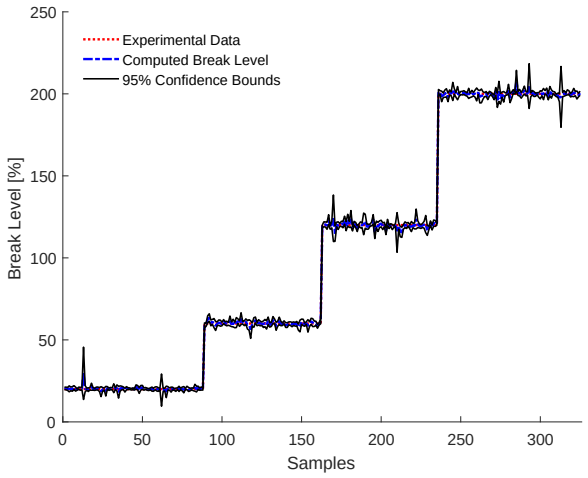

Fig. 6. Results for the Bayesian Averaging approach with 10 NNs and 95% confidence bounds

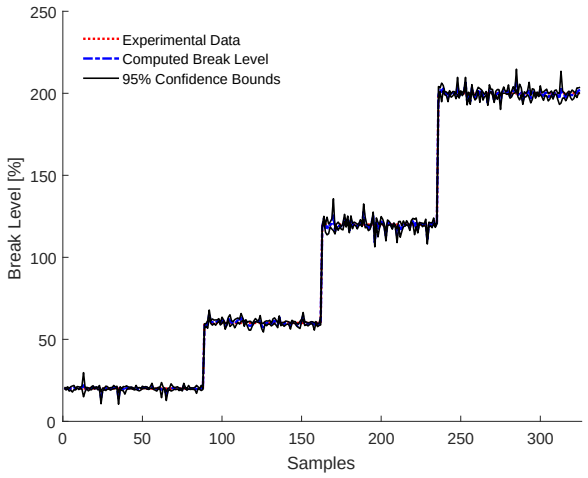

Fig. 7. Results for the Bayesian Averaging approach with 5 NNs and 95% confidence bounds

by the EESA approach, as shown in Table I. Conversely, the computational time increases for the 10-network and 25-network sets, reaching a value of 0.7672 s, hence ten times higher than that required by the EESA method, for the set of 50 networks (hence for a 100% accuracy). Nevertheless, the computational power remains under 1s in all cases considered and could be easily reduced implementing a parallel computing approach since the Bayesian model selection method is highly parallelizable.

In order to take into account the capability of generalization of the two approaches, a leave-out validation procedure has been implemented. In more details, the training of the networks was carried out on the initial database excluding the data associated with 60% break size. The models obtained were then applied on the remaining data, including the 60% break size data previously omitted. The results of such validation are presented in Table II and highlight a greater performance drop for the Bayesian model selection approach: only the ANNs with 50 and 25 networks provide and output accuracy over 90% (the first being very close to 100%) while the use of only 5 networks reduces the performance to an accuracy of 35.7%. Nevertheless, these results appear to be fairly better than those obtained with the EESA approach, whose accuracy remains under 25% for the leave-out validation implemented. On a different note, it is worth to highlight that the mean square error (MSE), calculated for the advisor network for both the approaches implemented as shown in Table II, reaches its maximum value for the best-performing network of the 50-network set. This does not necessarily suggest the unsuitability of such indicator for classifying the performance of the network, but does highlight how the computation of confidence bounds by the Bayesian model selection approach ensures reasonably accurate results even when the best-performing network in the set is characterized by a quite high mean square error.

TABLE I
COMPARISON BETWEEN THE TWO APPROACHES

Approach	Accuracy	Computational Time
EESA (over 50 trials)	[44.6%, 62.8%]	[0.0281s, 0.0759s]
Bayesian Averaging (50NNs)	100%	0.7672s
Bayesian Averaging (25NNs)	96.6%	0.3399s
Bayesian Averaging (10NNs)	90.8%	0.1262s
Bayesian Averaging (5NNs)	62.5%	0.0757s

IV. DISCUSSION

The comparison between the approaches implemented has focused on two main aspects: the accuracy of the prediction and the accuracy of the computed uncertainty bounds. Fig.8 9 10 and 11 show the trend of the relative error associated with the model response for each section of the output domain, i.e. break sizes equal to 20%, 60%, 120% and 200% respectively. The comparison involves the four Bayesian averaging models implemented adopting sets of 5, 10, 25 and 50 networks respectively, as well as the best advisor network included in the EESA implementation and selected on the basis of the mean square error value. The overall accuracy of the prediction seems to be characterized by a similar trend for the 60%, 120% and 200% break level, with 80% of the output samples being associated with a relative error lower than 1%. This value decrease to about 50% of the sample in the case of 20% break size, that is also associated with higher minimum relative error values in comparison to the rest of the domain. This suggests a higher level of difficulty associated with the prediction of small breaks that could be ascribed to the smoother transients to which the system is subject. Besides the common features, it is possible to identify dissimilarities betwen the performance of the different models: generally, the Bayesian model averaging approach using a set of 50 networks outperforms the other models consideres, with a more consistent trend associated with less sparse values of the relative error. This generally

TABLE II
COMPARISON BETWEEN THE TWO APPROACHES FOR LEAVE-OUT VALIDATION

Approach (leave-out 60%)	**Accuracy**	**MSE**
EESA (over 50 trials)	[9.67%,23.9%]	[0.010, 0.048]
Bayesian Averaging (50 NNs)	99.7%	0.317
Bayesian Averaging (25 NNs)	93.0%	0.012
Bayesian Averaging (10 NNs)	65.4%	0.016
Bayesian Averaging (5 NNs)	35.7%	0.019

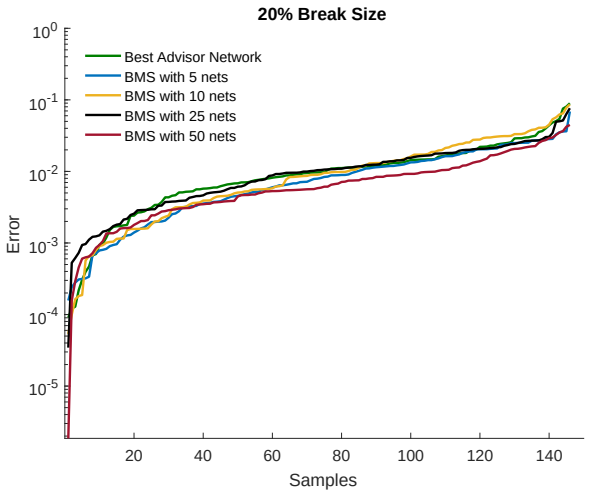

Fig. 8. Relative error associated with the different models implemented for break size 20%

implies lower maxima of the error but, on the other hand, higher minima. Nevertheless, the results show in Fig.9 do not fully respect this trend: the best advisor network from the EESA set seem to provide a slighly higher accuracy. On the other hand, the results of the four Bayesian averaging models suggest the increase of the prediction accuracy along with the size of the ANN set, as expected. Finally, it is worth to highlight that no selection has been made on the networks included in the ANN sets for the model averaging approach. On the contrary, the construction of ANN sets including selected networks is expected to result in higher accuracy and to lead such approach to outperform the best traditional ANN. Considering the performance of the tested models in terms of the uncertainty bounds reliability, the Bayesian model averaging approach seem to largely outperform the EESA approach, achieving an acuracy of 100% for the 50 nets set, as highlighted in section III-B. Nevertheless, this comes at the cost of a higher predicted uncertainty: as shown in Fig. 7 6 5 and 4, increasing the number of networks in the sets the variability of the response increases, widening the computed uncertainty bounds which, if too large, can potentially invalidate the value of the information provided.
Further research should aim to further increase the robustness of the model response provided, imposing a performance selection criteria on the networks adopted for the Bayesian

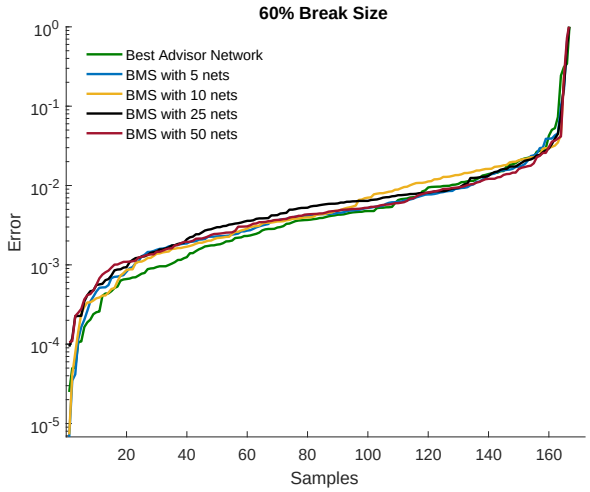

Fig. 9. Relative error associated with the different models implemented for break size 60%

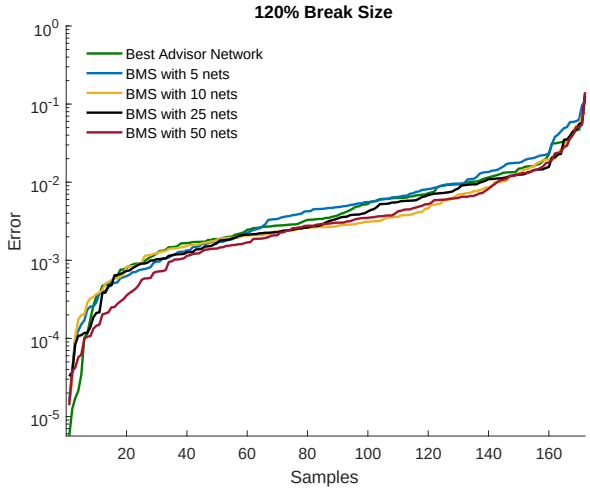

Fig. 10. Relative error associated with the different models implemented for break size 120%

model averaging approach, and to reduce the width of the uncertainty bound maintining high level of accuracy.

V. CONCLUSIONS

This study focuses on the use of ANNs for the on-line detection and diagnosis of LOCAs in a nuclear reactor. Two different approaches for the quantification of the uncertainty affecting the output of the ANN diagnostic model are implemented and compared in order to identify the best strategy to enhance the robustness of the diagnostic tool developed. The first method, known as Error Estimation by Series Association, allows to predict the error associated with the output of the primary ANN through the use of a secondary ANN specifically trained for such task. The results indicate that the confidence bounds identified with the EESA method include the true value of the output (i.e. the true break size) only for a number of cases between 44% and 63%, percentages that

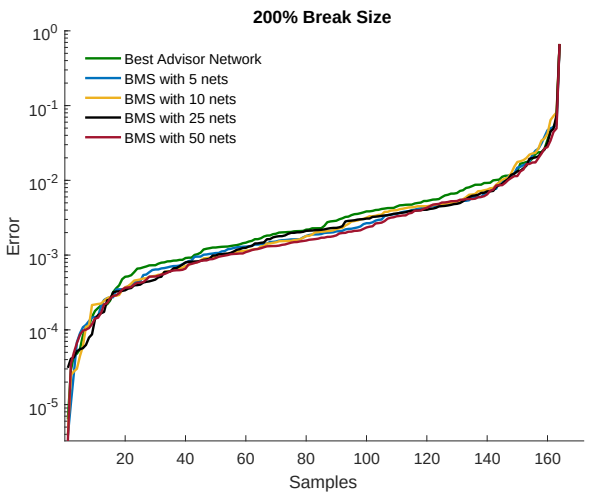

Fig. 11. Relative error associated with the different models implemented for break size 200%

drop dramatically when considering unseen data (i.e. in the case of leave-out validation). On the other hand, the method based on the use of a Bayesian model selection technique (hence training a set of ANNs sharing the same structure) ensures a better performance, with values of the accuracy equal to 100% when using 50 networks and comparable to the EESA results when using only 5 networks. Moreover, when considering unseen data, the drop of accuracy for the Bayesian model selection approach results quite limited. Nevertheless, the second approach results slightly more demanding than the EESA method in terms of computational time, even if this drawback could be easily overcome adopting parallel computing techniques.

ACKNOWLEDGMENT

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