



MOX–Report No. 9/2008

**Quantifying Uncertainties in the Estimation of Safety
Parameters by Using Bootstrapped Artificial Neural
Networks**

PIERCESARE SECCHI, ENRICO ZIO, FRANCESCO DI MAIO

MOX, Dipartimento di Matematica “F. Brioschi”
Politecnico di Milano, Via Bonardi 29 - 20133 Milano (Italy)

mox@mate.polimi.it

<http://mox.polimi.it>

QUANTIFYING UNCERTAINTIES IN THE ESTIMATION OF SAFETY PARAMETERS BY USING BOOTSTRAPPED ARTIFICIAL NEURAL NETWORKS

Piercesare Secchi⁽¹⁾, Enrico Zio⁽²⁾, Francesco Di Maio⁽²⁾

(1) MOX, Department of Mathematics, Polytechnic of Milan

(2) Department of Energy, Polytechnic of Milan

Via Ponzio 34/3, 20133 Milano, Italy

enrico.zio@polimi.it

ABSTRACT

For licensing purposes, safety cases of Nuclear Power Plants (NPPs) must be presented at the Regulatory Authority with the necessary confidence on the models used to describe the plant safety behavior. In principle, this requires the repetition of a large number of model runs to account for the uncertainties inherent in the model description of the true plant behavior. The present paper propounds the use of bootstrapped Artificial Neural Networks (ANNs) for performing the numerous model output calculations needed for estimating safety margins with appropriate confidence intervals. Account is given both to the uncertainties inherent in the plant model and to those introduced by the ANN regression models used for performing the repeated safety parameter evaluations. The proposed framework of analysis is first illustrated with reference to a simple analytical model and then to the estimation of the safety margin on the maximum fuel cladding temperature reached during a complete group

distribution header blockage scenario in a RBMK-1500 nuclear reactor.

The results are compared with those obtained by a traditional parametric approach.

NOTATION AND ACRONYMS

NPP	Nuclear Power Plant
ANN	Artificial Neural Network
RBMK	Reaktor Bolshoi Moshchnosty Kanalny
BE	Best-Estimate
OS	Order Statistics
GDH	Group Distribution Header
FC	Fuel Channel
MCC	Main Circulation Circuit
MCP	Main Circulation Pump
DS	Drum Separator
D	Finite set of input/output data examples for training the ANN
D^*	Finite set of input/output data examples for testing the ANN
\bar{x}	Input vector
X	Input domain
B	Number of bootstrapped networks
$\mu_y(\bar{x})$	Unknown nonlinear deterministic function
$\varepsilon(\bar{x})$	Gaussian white noise
$f(\bar{x}; \bar{w}^*)$	Regression function
\bar{w}^*	Set of synaptic weights
\bar{x}_i	i^{th} input vector
\hat{y}_i^*	i^{th} network output corresponding to \bar{x}_i
n_p	Number of data examples (patterns) for training the ANN
n_t	Number of data examples (patterns) for testing the ANN
$\sigma_f(\bar{x})$	Standard deviation of the distribution of the regression function $f(\bar{x}; \bar{w}^*)$
D_b	b^{th} bootstrapped data sample
$\hat{y}_b^*(\bar{x})$	b^{th} bootstrapped regression function
$y_{i,ANN}$	i^{th} bootstrapped neural network estimate (average of the B regression functions)
$y_{i,BE}$	i^{th} BE code output
$\sigma_{i,boot}^*$	Regression error of $\hat{y}_{i,ANN}$
$\hat{y}_{ANN}^*(\bar{x})$	bootstrapped neural network estimate augmented with σ_{boot}^*
$Errr(\bar{x})$	Prediction error of the regression function
$\sigma_{boot}^*(\bar{x})$	Estimate of the standard deviation of the distribution of the regression function
ε_{bias}	Estimate of the standard bias error of the regression function
\bar{x}_0	Input parameters nominal values vector
$E[\bar{x}]$	Input parameters expected values
\bar{y}_0	Output parameters nominal values vector
$f(\cdot)$	Model function implemented in the BE code
$[L_j, U_j]$	Predefined safety interval for the j^{th} output safety parameter y_j
Ψ	Safety envelope
\bar{x}_k	k^{th} independent input vector
\bar{y}_k	k^{th} independent output vector
γ	Coverage value for the safety parameter distribution

β	Confidence value
α	Confidence level of confidence intervals
m	Number of output values from the N runs that lie beyond the extent γ
r	r^{th} element of ordered statistics
G	Number of simulation batches
N	Number of estimates
g	Index of the g^{th} sample batch
$\hat{y}_{n,ANN}^{(g)}$	n^{th} ANN estimate of the g^{th} sample batch
${}_{\gamma}\hat{y}^{(g)}$	g^{th} estimate of the γ -percentile of the safety parameter distribution
$\sigma_{boot}^{*(g)}$	Regression error of ${}_{\gamma}\hat{y}^{(g)}$
\hat{Y}	Sample of G γ -percentile estimates
${}_{\gamma}y_{\delta}$	Unknown true δ -percentile of the γ -percentile safety parameter distribution
${}_{\gamma}\hat{y}_{\delta}$	Estimated δ -percentile of the γ -percentile safety parameter distribution
${}_{\gamma}\hat{y}^{[r]}$	r^{th} element of the sample \hat{Y}
${}_{\gamma}\hat{y}^{[s]}$	s^{th} element of the sample \hat{Y}
$I(c, j, k)$	Regularized Incomplete Beta Function for non-singular cases
M	Safety Margin
\hat{y}	General temperature estimate
y_{ref}	Reference pellet cladding temperature
$\hat{y}_i^{(g)}$	i^{th} ANN estimate for the g^{th} sample batch
${}_{0.95}\hat{y}_{\delta}$	Estimated δ^{th} percentile of the distribution of the 95^{th} percentile of the safety parameter
${}_{0.95}\hat{y}^{(g)}$	g^{th} element of the sample of the 95^{th} percentile estimates \hat{Y}
${}_{0.95}\hat{y}^{[75]}$	75^{th} element of the ordered sample of the 95^{th} percentile estimates \hat{Y}
${}_{0.95}\hat{y}^{[4]}$	4^{th} element of the ordered sample of the 95^{th} percentile estimates \hat{Y}
${}_{0.95}\hat{y}^{[147]}$	147^{th} element of the ordered sample of the 95^{th} percentile estimates \hat{Y}

1 INTRODUCTION

Conservative calculations have been traditionally performed for the verification of the safety of a Nuclear Power Plant (NPP), in terms of the values reached by selected safety parameters in comparison to predefined thresholds. The differences between the conservatively computed safety parameter values and the predefined safety thresholds give the so called safety margins.

Calculations are made with detailed, mechanistic codes that are run under conservative (i.e., pessimistic) hypotheses. Conservatism introduced in the calculations is aimed at overcoming uncertainties in the model representation of the actual plant behavior.

Lately, this traditional approach has been challenged by a more realistic, Best-Estimate (BE) analysis which sets forth the calculations of the safety margins under realistic assumptions. Results of such calculations are closer to the real behavior of the plant under investigation than those obtained from the conservative calculations.

On the other hand, the removal of conservatism leaves the results “unprotected” from uncertainties in the model representation of the plant real behavior. Hence, the feasibility of a more realistic approach to safety analysis depends on the possibility of properly quantifying and controlling the uncertainty associated to the estimated safety margins. This calls for repeated model runs within a probabilistic modeling of safety margins [Gavrilas et al., 2004; Martorell, 2007].

In general, uncertainty can be considered of two types: that due to inherent variability in the system behavior and that due to lack of knowledge and information on the system. The former type of uncertainty is often referred to as objective, aleatory, stochastic

whereas the latter is called subjective, epistemic, state-of-knowledge [Apostolakis, 1990; Helton, 2004].

The distinction between aleatory and epistemic uncertainty plays a particularly important role in the risk assessment framework applied to complex engineered systems. In the context of risk analysis, the aleatory uncertainty is related to the occurrence of the events which define the various possible accident scenarios whereas epistemic uncertainty arises from a lack of knowledge of fixed but poorly known parameter values entering the evaluation of the probabilities and consequences of the accident scenarios.

The present work addresses the epistemic uncertainty affecting the evaluation of the safety margins. Under the probabilistic viewpoint here undertaken to represent uncertainties, the BE code for safety margin evaluation needs to be repeatedly run with different values of the thermal-hydraulic parameters, sampled from predefined probability distributions; the outcomes of these runs are then statistically analyzed to estimate with a specified confidence a given percentile of the distribution of the safety parameter used to calculate the safety margin [Guba et al., 2003; Nutt et al., 2004]. Because of the large computing time required to run the BE code, the procedure can be computationally quite expensive.

To cope with the computational problem, in this work a single set of code input files and corresponding output data (i.e., maximum fuel cladding temperature) are used as input and output patterns for training and testing a multi-layered feedforward Artificial Neural Network [Mitchell et al., 1997, Zio 2006]. Once the network is trained, it can be used for estimating, in a negligible computation time, the safety parameters values needed for safety margin evaluation.

However, the use of ANN-based modeling (or any other empirical not physics-based modeling, for that matter) in safety critical applications for nuclear power plants raises concerns with regards to the model accuracy which must be not only verified but also quantified; in this paper, we resort to the bootstrap method for quantifying the uncertainty associated to the output of a multilayered feedforward neural network trained by the error-back propagation algorithm [Zio, 2006]. This allows the safety parameters to be estimated together with their estimation errors (see Appendix A).

The statistical analyses of the ANN evaluations for obtaining confidence intervals for safety parameters estimates relies on the use of Order Statistics (OS), along a non-parametric approach initially explored by [Wilks, 1941; Wilks, 1942]; this brings the advantage that the number of code calculations needed for safety margins evaluation is independent of the number of uncertain input parameters. Figure 1 shows a schematic sketch of the non-parametric procedure adopted; for ease of illustration, a single safety parameter y is considered.

By this procedure for safety margin calculation, the analyst can produce results with the level of confidence against uncertainty required for presenting a robust safety case to the Regulatory Authority.

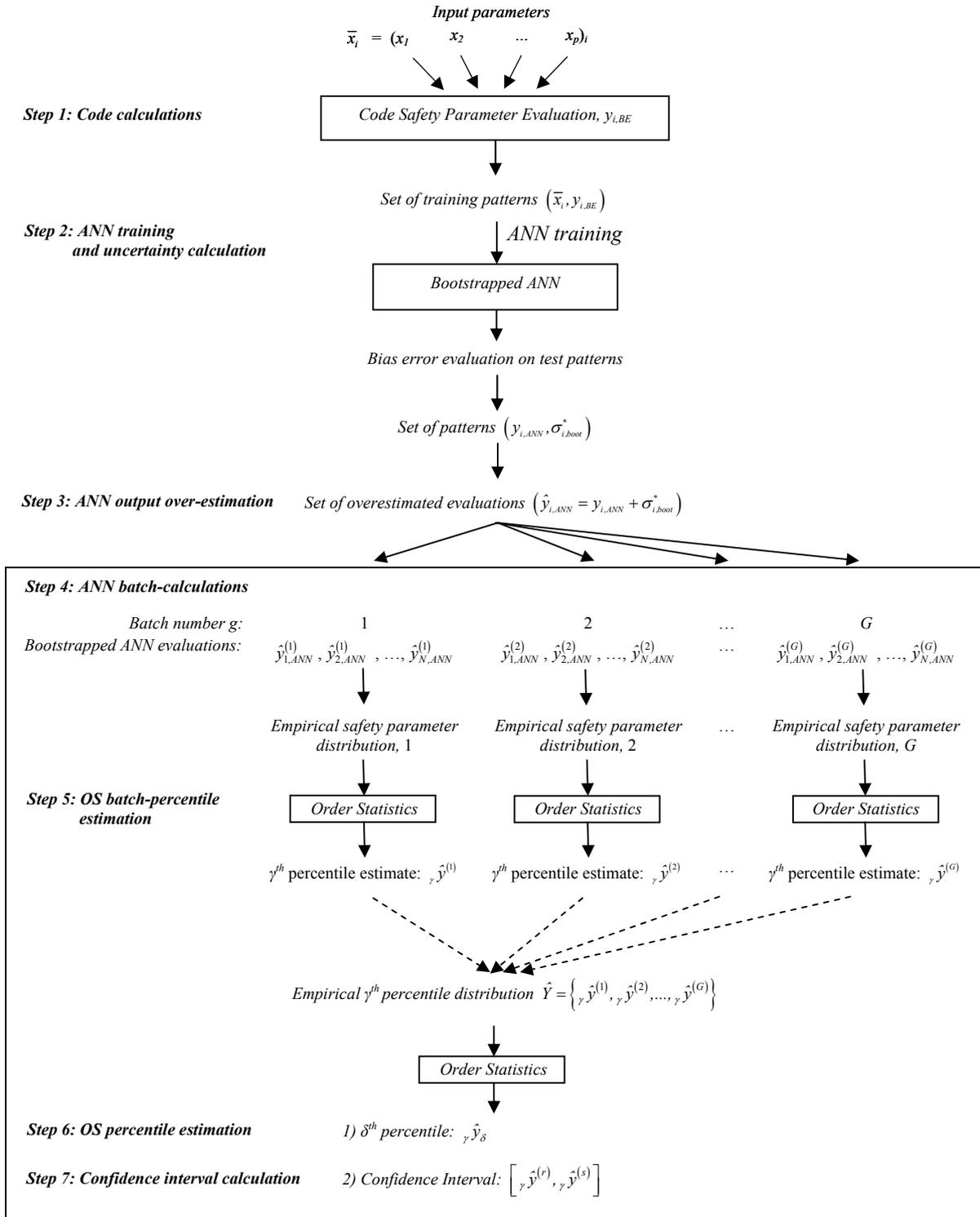


Figure 1 Flowchart of the non-parametric procedure for percentile and confidence interval estimation

The paper organization is as follows. In Section 2, the non parametric approach to the estimation of percentiles is briefly recalled. Section 3 is devoted to the presentation of the analytical case study used to illustrate the proposed approach: the specific artificial neural network used and the results of the application of the proposed approach to estimation of the uncertainty of its output are illustrated. Section 4 is devoted to the presentation of the realistic application: the main characteristics of the RBMK-1500 reactor are sketched, the GDH complete blockage accident scenario is described and the RELAP5/MOD3.2 simulations performed to analyze the system response to the accident scenario are presented; the specific neural model for the calculation of this accident scenario is introduced, the results of the application of the proposed approach to the estimation of the safety margin of the maximum fuel cladding temperature reached during the accident are provided and the results obtained by a parametric approach are reported for comparison. Conclusions are drawn in Section 5. Finally, in Appendix A, the basic principles underpinning the artificial neural network modeling paradigm are presented for completeness.

2 PROBABILISTIC APPROACH TO UNCERTAINTY QUANTIFICATION

The input vector \bar{x} of a BE code for NPP safety analysis is uncertain; the appropriate incorporation of this uncertainty onto the results and the presentation of its implication on their interpretation are fundamental components of the analysis.

Let the vector \bar{x}_0 define the vector of the nominal values of the input parameters of the BE code, typically assumed as the expected values $E[\bar{x}]$ of their distributions.

Corresponding to the nominal input values, the BE code output vector $\bar{y}_0 = f(\bar{x}_0)$ is the output of the model function $f(\cdot)$ implemented by the BE code and is expected to represent a largely safe state, well within the safety margins. In formal terms, this means that each one of the l output variables $\{y_{1_0}, y_{2_0}, \dots, y_{l_0}\}$, i.e. the components of \bar{y}_0 , fall within a predefined safety threshold interval, viz.:

$$y_{j_0} \in [L_j, U_j], j = 1, 2, \dots, l. \quad (1)$$

In presence of uncertainty in the input values \bar{x} , the plant is absolutely safe if its response \bar{y} falls in the safety envelope $\Psi = \{[L_j, U_j], j = 1, 2, \dots, l\}$ for every $\bar{x} \in X$, the set of all possible input vectors \bar{x} [Guba et al., 2003].

Given the impossibility of verifying the above safety conditions for all $\bar{x} \in X$, one is forced to address the problem probabilistically by generating a representative sample of independent input vectors $\bar{x}_k \in X, k=1, 2, \dots, N$ and then running the code for each of the input vectors to generate the corresponding output $\bar{y}_k, k=1, 2, \dots, N$: the sample of N independent output vectors realizations $\{\bar{y}_1, \bar{y}_2, \dots, \bar{y}_N\}$ carries information on the probability distribution of the safety output response \bar{y} ; from this information, one wants to draw conclusions on the safety conditions of the plant, with the required confidence.

2.1 *One-sided Order Statistics for percentile point estimates*

For ease of notation but without loss of generality, from now on we will discuss the case of a one-dimensional output y . The sample size N needed for obtaining the desired

confidence $\beta \in [0,1]$ when estimating the γ -percentile of the distribution of y is defined on the basis of the OS method, in its nonparametric formulation which applies independently from the type of probability distribution generating the data (in this case unknown) [Wilks, 1941; Wilks, 1942]. Denoting by ${}_{\gamma}y$ and ${}_{\gamma}\hat{y}$ the unknown true γ -percentile of the output distribution and its estimator, respectively, the probabilities γ and β are defined as $\gamma = P\{y < {}_{\gamma}y\}$ and $\beta = P\{{}_{\gamma}y < {}_{\gamma}\hat{y}\}$.

Once γ and β are fixed, the OS method for calculating the $(\beta|\gamma)$ -percentile estimate follows the lines of [Guba et al., 2003; Nutt et al., 2004] and amounts to:

- i) Determining the sample size N by fixing a positive integer m . The probability that at least m observations within a random sample of size N are greater than the γ -percentile of the distribution generating the sample is

$$p = \sum_{k=0}^{N-m} \binom{N}{k} \gamma^k (1-\gamma)^{N-k}$$

By Setting $p=\beta$, one can and compute the sample size N by solving the previous equation with respect to N .

- ii) Sorting the observations in the sample by increasing values, the element in the r^{th} position being the statistic of order r .
- iii) Estimating the γ -percentile by setting ${}_{\gamma}\hat{y}$ equal to the statistic of order $N-m+1$, i.e. the m^{th} largest observation in the sample; then $\beta = P\{{}_{\gamma}y < {}_{\gamma}\hat{y}\}$.

Note that higher values of m in step (i) imply higher values of the sample size N but generate less conservative estimates of the γ -percentile; in any case, the sample size N ,

i.e. the number of BE code runs, can be kept low because only intervals related to the γ^{th} percentile are estimated and not the full probability distribution generating the data.

2.2 *Artificial Neural Networks for empirical regression modeling*

The uncertainty relative to the estimator ${}_y\hat{y}$ would be captured by its distribution, if it were known; indeed this distribution would be estimated with arbitrary precision if one could draw a large (infinite) sample from it, i.e. if one could replicate the estimation procedure described in the previous Section for a large number of independent samples of size N drawn from the distribution of the output parameter y . However, in spite of the reduction in the number of runs allowed by the use of the OS method, the computational problem still remains because the complex models of plant dynamics used for NPP safety analysis are computationally very expensive and the collection of samples of size N may be extremely burdensome. One way to overcome this hurdle is to replace the slow-running BE code by a fast-running, empirical regression model. The response surface of the regression model is calibrated on the basis of a limited-size sample of input values drawn from the relative probability distribution and the corresponding outputs computed by the BE code.

In the present work, ANNs are proposed as regression models for their capability of modeling nonlinear input/output relationships. However, the ANNs empirical approximation of the system response introduces an additional source of uncertainty, which needs to be evaluated and represented in the safety margin estimation. This can be done by resorting to an ensemble of ANNs, each one trained on a different data set

bootstrapped from the original one [Zio, 2006]. Appendix A at the end of the paper contains some details on the bootstrapped ANN modeling technique.

2.3 The proposed approach for percentile point and confidence interval estimation

The proposed approach, sketched in Figure 1, addresses the problem of the evaluation of a point estimate of the γ -percentile and of a confidence interval associated to it, to be used for the safety margin evaluation. In what follows, the steps of the procedure are reported in detail (reference distributions and notations are shown in Figure 2):

- **Step 1: Code calculations.** Given a set of n_p independent input parameters values \bar{x}_i , $i=1,2,\dots,n_p$ sampled from the relative probability distribution, a set of n_p output values $y_{i,BE}$, $i=1,2,\dots,n_p$ are evaluated by the BE simulation code.
- **Step 2: ANN training and uncertainty calculation.** A bootstrapped ANN model, with bootstrap sample size B (see Appendix A.2), is trained to give the n_p patterns of estimates $(y_{i,ANN}, \sigma_{i,boot}^*)$, $i=1,2,\dots,n_p$ where $y_{i,ANN}$ is the neural fitted value corresponding to $y_{i,BE}$ and $\sigma_{i,boot}^*$ its regression error. The bias term of the neural network error is estimated by means of Eq. (8), Appendix A, on a data set D^* used for testing the ANN.
- **Step 3: ANN output over-estimation.** Conservatively, the regression error (e.g. one standard deviation) is added to each output of the ANN to give a conservative estimate $\hat{y}_{i,ANN} = y_{i,ANN} + \sigma_{i,boot}^*$. In Section 3.1, a motivation for this choice is provided.

- **Step 4: ANN batch-calculations.** G replicates of the trained bootstrapped ANN are independently fed each with a sample of N new input patterns. Thus, each of the G ANN generates a sample of size N of over-estimated output values: $\hat{y}_{n,ANN}^{(g)}$, $n=1,2,\dots,N, g=1,2,\dots,G$.
- **Step 5: OS batch-percentile estimation.** For $g=1,2,\dots,G$, the output sample of size N of the g^{th} batch is used to compute the $(\beta|\gamma)$ -percentile estimate ${}_{\gamma}\hat{y}^{(g)}$ by means of the OS method.
- **Step 6: OS percentile estimation.** The median of the distribution of ${}_{\gamma}\hat{y}$ is used as point estimator of the γ -percentile of the output distribution for safety margin evaluations (the median is a robust estimator for distribution-free statistics); the statistical median ${}_{\gamma}\hat{y}_{0.5}$ of the sample of the G $(\beta|\gamma)$ -percentile estimates $\hat{Y} = \{ {}_{\gamma}\hat{y}^{(1)}, {}_{\gamma}\hat{y}^{(2)}, \dots, {}_{\gamma}\hat{y}^{(G)} \}$ is used as estimate.
- **Step 7: Confidence interval calculation.** In alternative to the point estimate of Step 6, we generate a confidence interval estimate of the median of the distribution of the estimator ${}_{\gamma}\hat{y}$. Sort $\hat{Y} = \{ {}_{\gamma}\hat{y}^{(1)}, {}_{\gamma}\hat{y}^{(2)}, \dots, {}_{\gamma}\hat{y}^{(G)} \}$ by increasing values and let ${}_{\gamma}\hat{y}^{[1]}, {}_{\gamma}\hat{y}^{[2]}, \dots, {}_{\gamma}\hat{y}^{[G]}$ be the values of the order statistics. Set r and s to be positive integers satisfying the inequality $0 < r < (N+1)/2 < s \leq N$. Then the random interval $[{}_{\gamma}\hat{y}^{[r]}, {}_{\gamma}\hat{y}^{[s]}]$ covers the median of the distribution of the estimator ${}_{\gamma}\hat{y}$ with probability

$$\alpha = I(1/2, N-s+1, s) - I(1/2, N-r+1, r) \quad (2)$$

where $I(c, j, k)$ is the Regularized Incomplete Beta Function for non-singular cases [Kendall et al., 1979; Pál et al., 2002]. Hence, by fixing α we may find suitable r and s , for instance in a symmetric position with respect to $(N+1)/2$, such that $[\hat{y}^{[r]}, \hat{y}^{[s]}]$ is a level α confidence interval of the median of the distribution of \hat{y} .

Note that, given the conservative over-estimates computed in Step 3 and the fact that \hat{y} is the $(\beta\gamma)$ - estimator of the γ -percentile of the output distribution, we expect both the point estimate of Step 6 and the interval estimate of Step 7 to cover values larger than the true value of y ; see Figure 2 for an illustration of the analysis setting. The method is efficient if these estimates will not be too conservative while guaranteeing the required level of confidence.

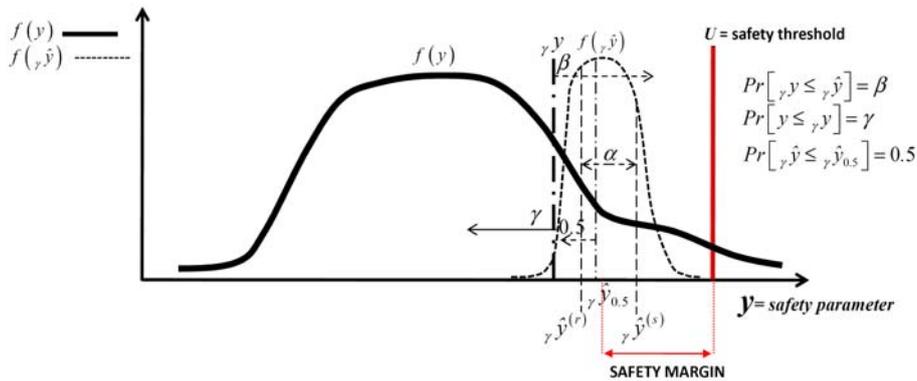


Figure 2 Sketch of the coverage value γ , the confidence β and the confidence interval level α ; representation of the (unknown) safety parameter probability distribution $f(y)$ and its γ^{th} percentile probability distribution $f(\hat{y})$

3 THE ANALYTICAL CASE STUDY

The approach for model output uncertainty quantification explained in Section 2.3 has been applied to a nonlinear two-dimensional analytical case study. The safety parameter y is deterministically defined as:

$$y = 10 \cdot (\cos(x_1) + \sin(x_2)) \quad (3)$$

where the input parameters x_1 and x_2 are uniformly and independently distributed in $[0, 360^\circ]$. The function (3) and the probability density function of y are shown in Figures 3 and 4, respectively.

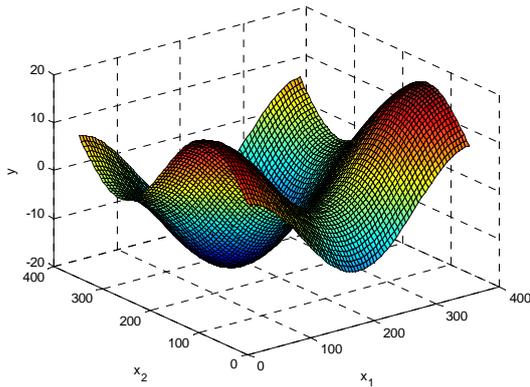


Figure 3 Surface of the analytical case study.

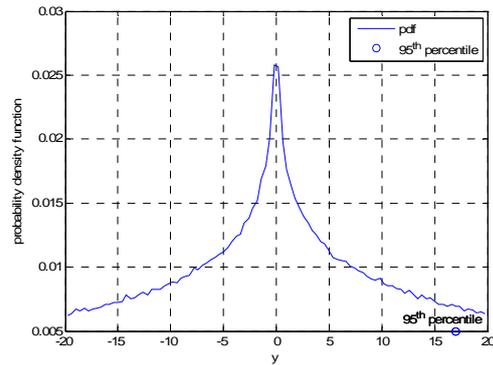


Figure 4 Probability density function constructed with 500,000 model output evaluations and its true 95th percentile.

As shown in Figure 4, the model output is strongly not normally distributed and its (true) 95th percentile is equal to 16.95.

3.1 The application of the non-parametric OS approach to percentile estimation

The results of the non-parametric procedure for percentile estimation are hereafter illustrated with reference to the procedural steps detailed in Section 2.3:

Step 1: Code calculations

$n_p=150$ patterns $\{(\bar{x}_i, y_{i, BE}), i=1, 2, \dots, 150\}$ have been generated for training the ANNs and $n_t=50$ for testing the trained ANNs.

Step 2: ANN training and uncertainty calculation.

The bootstrapped ANN regression model illustrated in Appendix A has been applied for predicting the output variable of Eq. (3). The number B of bootstrapped networks has been taken equal to 15.

All neural calculations have been performed with the software package NEural Simulation Tool (NEST) developed by the Laboratorio di Analisi di Segnale e di Analisi di Rischio (LASAR, Laboratory of Analysis of Signals and of Analysis of Risk, <http://lasar.cesnef.polimi.it>) of the Department of Energy of the Polytechnic of Milan, Italy.

In Figures 5 and 6 the bootstrapped neural network estimates $y_{i, ANN}$ (crosses) are plotted against the true values of the output variable $y_{i, BE}$ (circles). The bootstrapped ANN is very accurate.

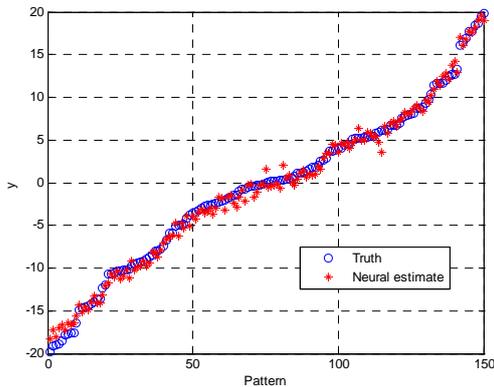


Figure 5 Bootstrapped ANN estimations for the 150 training patterns.

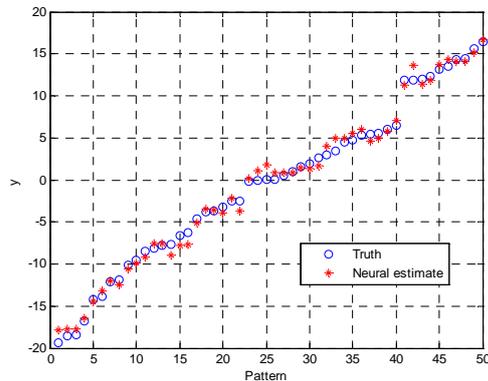


Figure 6 Bootstrapped ANN estimations for the 50 test patterns.

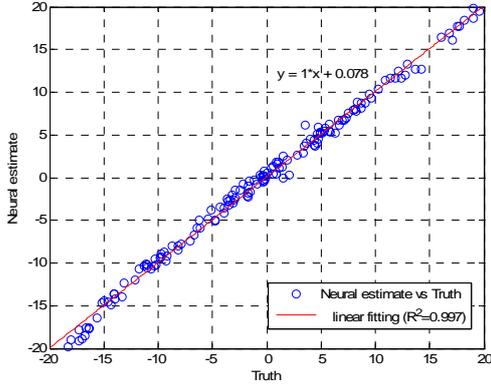


Figure 7 Linear fitting for 150 training Bootstrapped ANN estimations vs Truth.

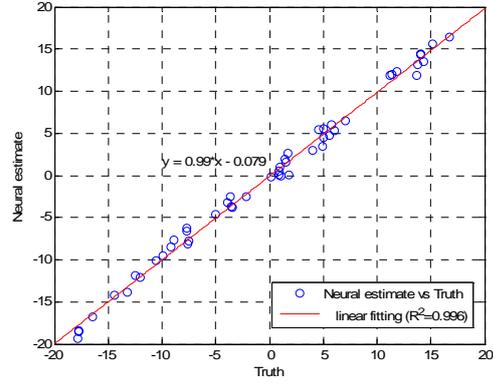


Figure 8 Linear fitting for 50 testing Bootstrapped ANN estimations vs Truth.

The values of the Pearson's coefficient R^2 reported in Figures 7 and 8 and the estimate of the absolute value of the bias equal to 0.66, evaluated resorting to Eq. (8), confirm the good accuracy of the trained neural network model.

Step 3: ANN output over-estimation.

The ANN output values $y_{i,ANN}$ are augmented as $\hat{y}_{i,ANN} = y_{i,ANN} + \sigma_{i,boot}^*$.

Step 4: ANN batch-calculations.

We take, $m=100$ and $\beta=\gamma=0.95$; this leads to a sample size $N=2,326$ for the OS $(\beta|\gamma)$ -percentile estimates. A number of $G=150$ batches of $N=2,326$ output values have been computed.

Step 5: OS batch-percentile estimation.

For each of the $G=150$ batches, the $(\beta|\gamma)$ -percentile estimate has been computed. The 150 independent estimates are collected in the sample $\hat{Y} = \{ {}_{0.95}\hat{y}^{(1)}, {}_{0.95}\hat{y}^{(2)}, \dots, {}_{0.95}\hat{y}^{(150)} \}$.

Step 6: OS percentile estimation.

The median ${}_{\gamma}\hat{y}_{0.5}$ of the sample \hat{Y} turns out to be equal to 18.59.

Step 7: Confidence interval calculation.

The confidence interval of level $\alpha=0.95$ for the median of the estimator ${}_{\gamma}\hat{y}$ turns out to be equal to [17.81, 19.56].

To evaluate the robustness of the proposed procedure, which combines ANN modeling and Order Statistics to estimate the 95th percentile of the safety parameter distribution, the evaluation procedure consisting of the previous Steps 1-7 has been repeated $k=50$ times: results are plotted in Figure 9, where the values of the point estimates obtained at Step 6 are represented by a square while the confidence intervals computed at Step 7 appear as vertical segments. It turns out that with frequency 0.98 the true value (16.95) for the 95th percentile of the distribution of y is smaller than the lowest extreme of the confidence interval for the median of the estimator ${}_{\gamma}\hat{y}$. Hence with confidence greater than the level 0.95 required by regulation for the safety margin quantification [Wallis, 2006] we are overestimating the true value of the 95th percentile of the distribution of y and yet these estimates are small enough to be used for safety margin evaluations.

To justify the over-estimation in Step 3 of the procedure illustrated in Section 2.3, the results obtained without ANN output over-estimation are shown in Figure 10: the confidence on the estimates in this case falls down to 0.68, which is not acceptable for safety margin quantification.

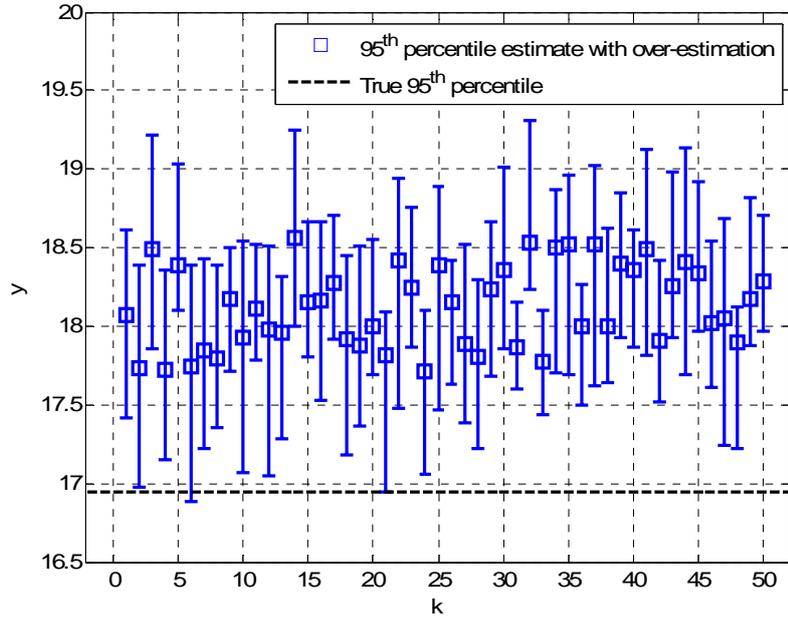


Figure 9 Representation of $k=50$ estimates of the 95th percentile of the safety parameter and corresponding confidence intervals

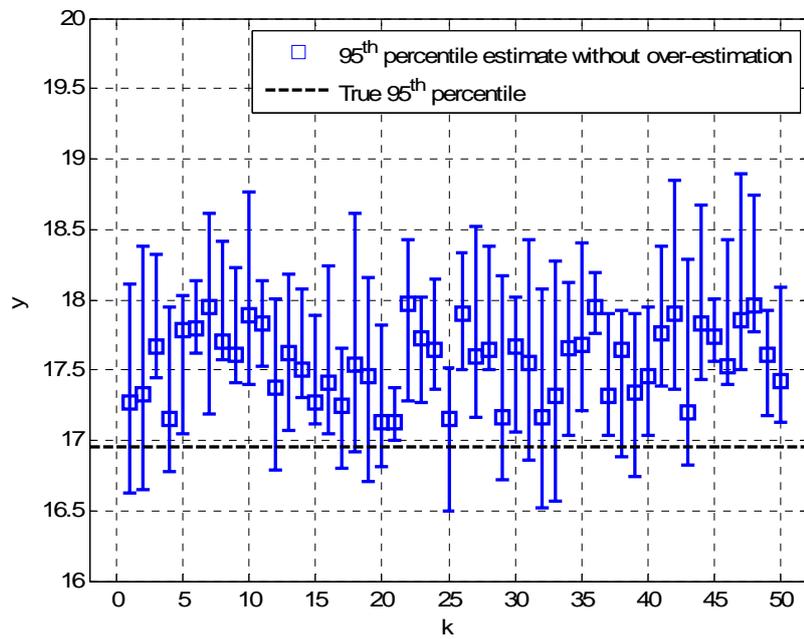


Figure 10 Representation of $k=50$ estimates of the 95th percentile of the safety parameter and corresponding confidence intervals without the ANN output over-estimation described in Step 3 of the procedure

4 THE GDH COMPLETE BLOCKAGE ACCIDENT SCENARIO IN THE RBMK-1500

The non-parametric procedure for percentile estimation introduced in Section 2.3 has been applied to the quantification of the safety margin relative to the maximum fuel cladding temperature reached during the accident scenario of complete blockage of a Group Distribution Header (GDH) of the RBMK-1500 nuclear reactor.

4.1 The RBMK-1500

The description of the RBMK-1500 refers to the Ignalina Nuclear Power Plant (NPP) in Lithuania [Ušpuras et al., 2006]. The RBMK-1500 is a graphite-moderated, boiling water, multi-channel reactor. The two units at Ignalina are designed to provide a saturated steam at 7.0 MPa. The maximum reactor rating is 4800 MW_{th}. Several design features of the RBMK-1500 are rather unique with respect to reactors of western design. The main distinguishing characteristic of the RBMK-type reactor is that each core fuel assembly is housed in an individual pressure tube.

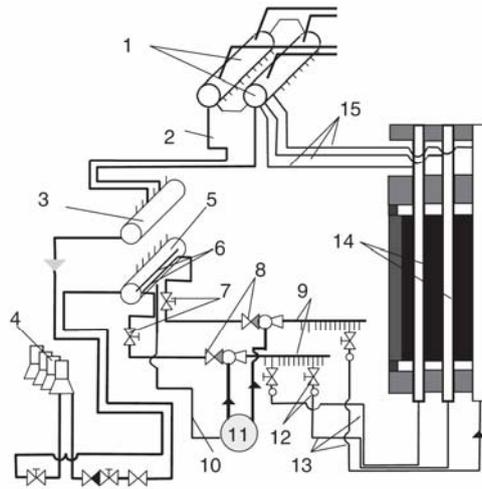


Figure 11 Ignalina NPP model nodalization scheme [Ušpuras et al., 2006]

The RBMK-1500 core contains 1661 pressurized fuel channels (FCs), inserted in a graphite block lattice. The Main Circulation Circuit (MCC) is divided into two loops. Figure 11 presents one such loop. The loop has two drum separators (1), which separate steam from the steam-water mixture coming from the core. Eight Main Circulation Pumps (MCPs) are used for the circulation of the cooling water. The MCPs (4), joined in groups of four pumps on each loop (three for normal operation and one in standby), feed the pressure headers (5) on each side of the reactor. Each pressure header provides coolant upwards through the reactor core block to 20 Group Distribution Headers (GDHs) (9). Each of them in turn feeds from 38 to 43 pressurized fuel channels (14). The flow in the channel is measured by a ball flow meter (12) and regulated by means of isolation and control valves. By flowing through the core, the coolant absorbs about 95% of the total energy released by the fuel elements. The steam-water mixture generated in the FCs flows through the steam-water pipes (15) to the Drum Separators (DSs) [Kaliatka et al., 2005].

4.2 The GDH complete blockage scenario

The accident scenario considered in the present study consists of a complete blockage of a GDH. This leads to a temporary decrease in the coolant flow rate in the FCs and to a corresponding increase in the cladding temperature which may reach values close to the maximum allowable limit of 700.00° C [Kopustinskas et al., 2005]. For this reason, this scenario is considered safety relevant and a careful analysis of it must be performed [Urbonas et al., 2003a].

4.3 RELAP5/MOD3.2 simulations of the accident scenario

Given the above mentioned safety concerns related to the GDH blockage scenario, a RELAP5/MOD3.2 model of the RBMK-1500 reactor has been implemented and used to simulate 480 accidental complete blockage transients, generated by sampling the involved input parameters from proper probability distributions suggested from previous experience and/or skilled operators [Kopustinskas, 2005]. As it will be explained in the next Section, these transients constitute the data base samples to be used for training the bootstrapped ANN embedded in the procedure for estimating a given percentile of the probability distribution of the maximum fuel cladding temperature reached during the accident and its safety margin. The interested reader may refer to the original works for further details on the RELAP5/MOD3.2 model implementation [Urbonas et al., 2003b].

In the accident transient simulations, it is assumed that the reactor operates at the stationary power of 2900 MWth. The coolant is supplied through the core by two MCPs in each MCC loop, up to the beginning of the accident (i.e. before the GDH blockage). This reactor state is chosen because in such conditions the reactor cooling of the core is the most complicated. Note that 2900 MWth is the maximum allowable power level when four MCPs are in operation, i.e. the worst power and coolant flow rate ratio is conservatively considered in the analysis. The calculations performed for such type of accident show a decrease in the coolant flow rate. Thus, the fuel cladding and pressure tube wall temperatures sharply increase and then start to decrease after reactor shutdown, which is initiated for protection against the decrease in coolant flow rate through the GDH.

Since the peak of the fuel cladding temperature in the maximum power channel may reach values close to the acceptance criteria temperature (700.00° C for fuel cladding), this is the chosen safety variable of interest y , and its safety margin must be estimated.

The relevant input parameters \bar{x} which may influence the fuel cladding temperature behavior may be divided in [Kopustinskas, 2005]:

- Initial conditions (coolant pressure, temperature and flow rate or power)
- RELAP5/MOD3.2 code model parameters, assumptions and correlations (e.g. different correlations for the calculation of friction loss and heat transfer).

A first preliminary investigation based on engineering judgment led to the identification of the following initial conditions as most important for the postulated accident analysis [Urbonas et al., 2003b; Ušpuras et al., 2006]:

- Pressure in the drum separator (x_1)
- Coolant flow rate through the MCPs (x_2)
- Feed water temperature (x_3)
- Amount of steam for in-house needs (x_4)
- Reactor thermal power (x_5)

As for the RELAP5/MOD3.2 code modeling parameters, the following are regarded relevant for the accidental transient:

- Water packing: it specifies whether the scheme of volume filling with water is to be used (x_6)
- Vertical stratification: it specifies whether the model of two-phase media vertical stratification is enabled or disabled (x_7)
- Modified PV term in the equations: it specifies whether the modified potential pressure energy model is applied or not (x_8)
- CCFL (counter current flow limit): on/off (x_9)
- Thermal front tracking: on/off (x_{10})
- Mixture level tracking: on/off (x_{11})

A last parameter considered to have an impact on the temperatures of the fuel cladding and fuel channel wall is the signal to start the reactor protection against the accident initiation, which determines the time when the reactor is shutdown in the fast mode (x_{12}). It is assumed that insertion of CPS rods is delayed by 1 second, with respect to such signal.

In conclusion, a total of twelve parameters are considered relevant. Of these, six are continuous (x_1 - x_5 and x_{12}) and six are binary (x_6 - x_{11}). The continuous parameter distributions have been obtained from error specifications in measure devices and from skilled-operator expertise, whereas the Boolean parameters are set as RELAP5/MOD3.2 inputs, with an arbitrary probability of 0.5 (Table 1).

Parameter	Range of parameter distribution		Mean	Standard deviations	Probability distribution
	Min	Max			
Initial conditions					
x_1 (Pressure in DS) [Pa]	6.79E+06	6.93E+06	6.86E+06	3.43E+04	Normal
x_2 (Coolant flow rate) [m ³ /h]	6860	7140	7000	70	Normal
x_3 (Feedwater temperature) [K]	458.52	467.78	463.15	2.32	Normal
x_4 (Steam for in-house needs) [m ³ /h]	227.7	232.3	230	1.15	Normal
x_5 (Reactor thermal power) [W]	2.81E+09	2.99E+09	2.90E+09	4.5E+07	Normal
Modelling parameters					
x_6 (Water packing)	0 (on)	1 (off)	1 (off)	-	Discrete
x_7 (Stratification)	0 (on)	1 (off)	0 (on)	-	Discrete
x_8 (PV term)	0 (on)	1 (off)	0 (off)	-	Discrete
x_9 (CCFL)	0 (on)	1 (off)	0 (off)	-	Discrete
x_{10} (Thermal front tracking)	0 (on)	1 (off)	0 (off)	-	Discrete
x_{11} (Mixture level tracking)	0 (on)	1 (off)	1 (on)	-	Discrete
x_{12} (Scram initiation time)	5.3	6.3	6.0	0.25	Normal

Table 1 Parameters which are regarded relevant with respect to the behaviour of the fuel cladding temperature [Ušpuras et al., 2006]

4.4 The application of the non-parametric OS approach to safety margin estimation

The application of the non-parametric procedure for percentile estimation introduced in Section 2.3 is hereafter illustrated with reference to the case study introduced in the previous paragraphs. Procedural steps are:

Step 1: BE code calculations

The $n_p=440$ patterns $\{(\bar{x}_i, y_{i,BE}), i = 1, 2, \dots, 440\}$ have been generated from the RELAP5/MOD3.2 simulations of the accidental scenario considered for training the ANNs and $n_t=40$ for testing the trained ANNs.

Step 2: ANN training and uncertainty calculation

The bootstrapped ANN regression model illustrated in Appendix A has been applied for prediction of the maximum fuel cladding temperature reached during the accidental scenario. The number B of bootstrapped networks has been taken equal to 15. In [Cadini et al., 2007], the improved accuracy of the bootstrapped neural network estimates with respect to those of the single best-trained ANN has been demonstrated for the study under analysis.

The distributions of the RELAP5/MOD3.2 simulations $\{y_{i,BE}, i = 1, 2, \dots, 480\}$ obtained in step 1 (Figures 12 and 13, solid line) is taken as reference for the comparison with the results obtained by the ANN estimations in the present step 2. In particular, its 95th percentile, which turns out to be 684.85° C, is taken as the (unknown) real 95th percentile $_{0.95}y$ of the maximum fuel cladding temperature distribution in the comparisons which follow.

Figures 12 and 13 show also the empirical cumulative distribution functions (cdfs) and the probability density functions (pdfs) constructed from 10,000 random bootstrapped-ANN estimations $\{\hat{y}_{i,ANN}, i = 1, 2, \dots, 10000\}$ (dashed-dotted lines). In Figure 13, the estimated regression error $\sigma_{i,boot}^*$ associated to each ANN estimation $\hat{y}_{i,ANN}$ is also reported (dashed line). The good match of the two pdfs in Figure 13 leads us to assert that

the accuracy in the estimates can be considered satisfactory for the needs of the safety margins estimation procedure, so that the bootstrapped ANN can be used as fast-running regression model in substitution of the complex slow-running RELAP5/MOD3.2 code.

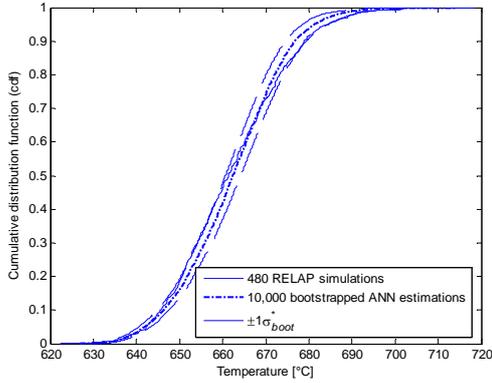


Figure 12 Maximum temperature empirical cdfs $\pm 1\sigma_{boot}^*$, constructed with 10,000 bootstrapped ANN simulations and with 480 RELAP5/MOD3.2 simulations

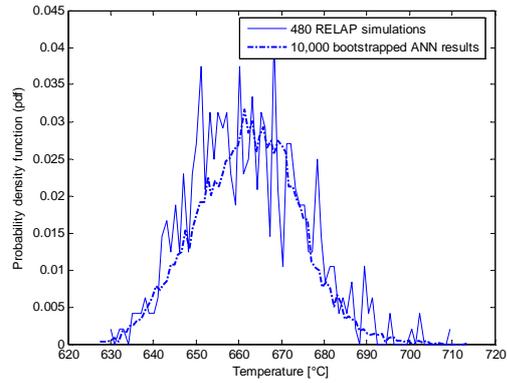


Figure 13 Maximum temperature empirical pdfs constructed with 10,000 Bootstrapped ANN simulations and with 480 RELAP5/MOD3.2 simulations

Moreover, by resorting to Eq. (8) of Appendix A one can compute the average of the absolute bias term in the bootstrapped ANN prediction error; this turns out to be equal to 8.22°C.

The safety margin is then computed as

$$M = \frac{U - \hat{y}}{\hat{y} - y_{ref}} \quad (4)$$

where \hat{y} is the temperature estimate considered (e.g., in the successive step 5 \hat{y} is equal to ${}_{\gamma}\hat{y}_{0.5}$, whereas in step 6 it is equal to ${}_{\gamma}\hat{y}_{0.5}^{(r)}$ or to ${}_{\gamma}\hat{y}_{0.5}^{(s)}$) and $y_{ref} = 297.00^{\circ}$ C is the reference pellet cladding temperature, taken equal to the sample mean of the 480 RELAP5/MOD3.2 values at the initial time of the accidental transients; the pellet cladding safety threshold limit U is set equal to 700.00° C by regulation [Urbonas et al., 2003a].

Step 3: ANN output over-estimation.

The ANN output values $y_{i,ANN}$ are augmented as $\hat{y}_{i,ANN} = y_{i,ANN} + \sigma_{i,boot}^*$.

Step 4: ANN batch-calculations.

We take, $m=100$ and $\beta=\gamma=0.95$; this leads to a sample size $N=2,326$ for the OS $(\beta|\gamma)$ -percentile estimates. A number of $G=150$ batches of $N=2,326$ output values have been computed. Running the RELAP5/MOD3.2 code these many times for different values of sampled inputs is impractical. On the contrary, $G=150$ batches of $N=2,326$ output values have been computed by exploiting the capability of the trained ANNs to compute in a short time a very large number of output estimates (in this case, the maximum fuel cladding temperature reached during the considered accidental scenario), in correspondence of different input parameter vectors sampled from the relative probability distributions.

Step 5: OS batch-percentile estimation.

For each of the $G=150$ batches, the $(\beta|\gamma)$ -percentile estimates have been computed and collected in the sample $\hat{Y} = \{ {}_{0.95}\hat{y}^{(1)}, {}_{0.95}\hat{y}^{(2)}, \dots, {}_{0.95}\hat{y}^{(150)} \}$.

Step 6: OS percentile estimation and uncertainty calculation.

The median of the sample \hat{Y} and its safety margin turn out to be equal to 688.37°C and $3.00\text{E-}02$, respectively.

Step 7: Confidence interval calculation with associated uncertainty.

The confidence interval of level $\alpha=0.95$ for the median of the estimator ${}_{\gamma}\hat{y}$ and for the safety margin turn out to be equal to $[685.56^\circ\text{C}, 691.35^\circ\text{C}]$ and $[2.19\text{E-}02, 3.72\text{E-}02]$, respectively (Figures 14 and 15).

analytical case study in Section 3), and the $\alpha=0.95$ confidence interval $[\hat{y}_{0.95}^{[4]}, \hat{y}_{0.95}^{[147]}] = [685.56, 691.35]$ meet the safety criterion of being less than $U=700.00^\circ\text{C}$, it can be concluded that the scenario is protected by a positive safety margin and can thus be considered safe.

4.5 Comparison with a parametric approach

For comparison, a statistical analysis relying on a parametric approach has been applied to $\hat{Y} = \{ \hat{y}_{0.95}^{(1)}, \hat{y}_{0.95}^{(2)}, \dots, \hat{y}_{0.95}^{(150)} \}$, the sample of $G=150$ ANN-based estimations of the 95th percentiles of the maximum fuel cladding temperature reached during the accident scenario of complete blockage of a Group Distribution Header (GDH) of the RBMK-1500 nuclear reactor.

The sample \hat{Y} has been first tested for Normality by means of the Lilliefors Test when mean and variance are unknown [Lilliefors, 1967]. The p-value = 0.094 supports the assumption of Normality for the distribution generating the data; hence the center of the distribution is taken to be its mean and is estimated with the mean of the sample \hat{Y} , which turns out to be 688.89°C . The safety margin is $2.83\text{E-}02$.

Moreover, the standard symmetric 95% confidence interval for the mean of the Normal distribution when the variance is unknown, based on the t-distribution with 149 degrees of freedom, turns out to be $[685.60^\circ\text{C}, 691.33^\circ\text{C}]$ while the corresponding interval for the safety margin is $[2.19\text{E-}02, 3.70\text{E-}02]$. (Figures 16 and 17).

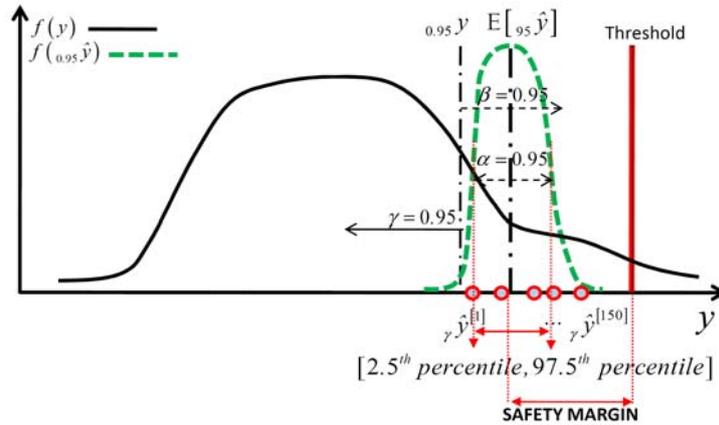


Figure 16 Sketch of the results provided with the parametric approach

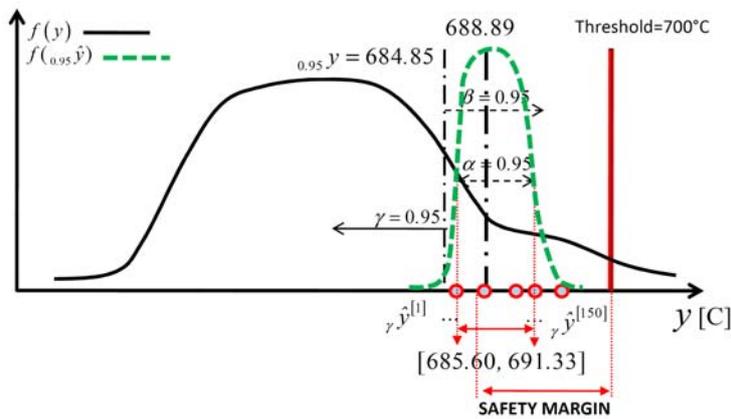


Figure 17 Representation of the γ^{th} percentile estimate and its confidence interval obtained with the approach-distribution with 149 degrees of freedom.

Notice the good agreement of the results obtained with the non-parametric and parametric approaches, Sections 4.4 and 4.5, respectively. However, it is to be noted that the hypothesis of Normality of the distribution underlying the data is not general and the parametric approach is thus not applicable to all cases; on the contrary, the non-parametric approach here proposed for safety margin quantification is general and independent of the distribution.

5 CONCLUSIONS

A framework for estimating safety margins has been proposed within a probabilistic approach for accounting the uncertainties associated to the relevant parameters of a safety analysis of a nuclear power plant. The procedure has been verified on an analytical case study and applied to the maximum fuel cladding temperature reached during a complete group distribution blockage scenario in a RBMK-1500 nuclear reactor.

Simulated accident transients have been used for training and testing a bootstrapped ANN model for predicting the maximum fuel cladding temperature for different sets of values of 12 input and model parameters relevant for the simulation.

Non-parametric Order Statistics has been exploited to support a limited number of calculations and utilized to provide confidence intervals on the percentiles. The trained ANNs have been exploited to provide in a fast and accurate way, in comparison to computationally burdensome BE code estimations, the needed number of calculations. For comparison, confidence intervals and percentile estimates have been computed also resorting to a parametric approach.

The procedure gives a reliable (the estimate is very near to the true 95th percentile), robust (confidence intervals are very narrow) and conservative (high probability that the lower bound of the confidence interval lies above the true 95th percentile) estimate of the 95th percentile of the safety parameter distribution.

The possibility of running a high number of simulations by the bootstrapped ANN model is fundamental for building the required confidence in the safety of the system to make a robust case to the Regulatory Authority, while properly accounting for the uncertainties in the input and model parameters and in the estimates themselves.

The procedure may be recommended to add robustness and reliability to the conclusions drawn from safety analyses of nuclear power plants.

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APPENDIX A “BOOTSTRAPPED” NEURAL NETWORKS

Artificial neural networks are information processing systems composed of simple processing elements (*nodes*) linked by weighted *synaptic* connections [Rumelhart et al., 1986; Muller et al., 1991; Mitchell 1997]. The resulting empirical models are capable of reconstructing the complex nonlinear input/output relations underpinning real systems and processes by combining multiple simple functions.

A.1 Regression by neural networks

In all generality, let us consider an ANN for performing a task of nonlinear regression, i.e. estimating the underlying nonlinear relationship existing between a vector of input variables \bar{x} and an output target y , assumed one-dimensional for simplicity of illustration. The ANN is trained with a finite set of n_p input/output data examples (patterns):

$$D \equiv \{(\bar{x}_i, y_i), i = 1, 2, \dots, n_p\}.$$

A similar finite set of n_t input/output data examples (patterns) is used for testing the ANN:

$$D^* \equiv \{(\bar{x}_i, y_i), i = 1, 2, \dots, n_t\}$$

It can be assumed that the target y is related to the input vector \bar{x} by an unknown nonlinear deterministic function $\mu_y(\bar{x})$ corrupted by a noise $\varepsilon(\bar{x})$, viz.

$$y(\bar{x}) = \mu_y(\bar{x}) + \varepsilon(\bar{x}) \quad \varepsilon(\bar{x}) : N(0, \sigma_\varepsilon^2(\bar{x})) \quad (5)$$

The objective of the regression task is to estimate $\mu_y(\bar{x})$ by means of a regression function $f(\bar{x}; \bar{w}^*)$ dependent on the set of synaptic weights \bar{w}^* to be properly determined on the basis of the available set D . The ANN parameters \bar{w}^* are usually obtained by a training procedure which aims at minimizing the quadratic error function:

$$E = \frac{1}{2n_p} \sum_{i=1}^{n_p} (\hat{y}_i^* - y_i)^2 \quad (6)$$

where $\hat{y}_i^* = f(\bar{x}_i; \bar{w}^*)$ is the network output corresponding to input \bar{x}_i . If the network architecture and training parameters are suitably chosen and the minimization done to determine the weights values is successful, the obtained function $f(\bar{x}; \bar{w}^*)$ gives a good estimate of the unknown, true function $\mu_y(\bar{x})$. Indeed, it is possible to show that in the ideal case of an infinite training data set and perfect minimization algorithm, a neural network trained to minimize the error function in (6) provides a function $f(\cdot)$ which performs a mapping from the input \bar{x} into the expected value of the target y , i.e. the true deterministic function $E[y|\bar{x}] = \mu_y(\bar{x})$ [Bishop, 1995]. In other words, the network averages over the noise on the data and discovers the underlying deterministic generator. Unfortunately, in practice, any training set is finite and there is no guarantee that the selected minimization algorithm achieves the global minimum in finite computation time.

A.2 Bootstrapped neural networks for increasing and quantifying accuracy

In practical regression problems and in the case of ANN estimation, it is crucial to properly account for the various sources of uncertainty affecting the determination of the weights \bar{w}^* [Tibshirani, 1996; Twomey et al., 1998; Dybowski et al., 2000].

If we assume (5), we can derive an expression for the expected prediction error of a regression fit $f(\bar{x}, \bar{w}^*)$ at an input vector \bar{x} :

$$\begin{aligned} Err(\bar{x}) &= \sigma_\varepsilon^2 + \left\{ f(\bar{x}; \bar{w}^*) - \mu_y(\bar{x}) \right\}^2 + E \left\{ \left[f(\bar{x}; \bar{w}^*) - E \left[f(\bar{x}; \bar{w}^*) \right] \right]^2 \right\} \\ &= \sigma_\varepsilon^2 + Bias^2 \left(f(\bar{x}; \bar{w}^*) \right) + Var \left(f(\bar{x}; \bar{w}^*) \right) \end{aligned} \quad (7)$$

The first term is the variance of the target around its true mean $\mu_y(\bar{x})$ and cannot be avoided no matter how well we estimate $\mu_y(\bar{x})$, unless $\sigma_\varepsilon^2 = 0$ (which happens to be the model assumption in our case studies). The second term is the squared bias, the amount by which the average of our estimate differs from the true mean; the last term is the variance, i.e the expected squared deviation of $f(\bar{x}, \bar{w}^*)$ around its mean. Typically the more complex we make the model, the lower the (squared) bias but the higher the variance [Hastie et al., 2001]. However, in many applications the variance term indeed dominates the bias term [Stuart, 1992] and, furthermore, if it were possible to compute the bias component its value should be used as an index of the accuracy of the regression function $f(\bar{x}; \bar{w}^*)$.

For the estimation of the average of the absolute *bias term* one can compute:

$$\varepsilon_{bias} = \frac{1}{n_t} \sum_{i=1}^{n_t} \left| f(\bar{x}_i; \bar{w}^*) - \mu_y(\bar{x}_i) \right| \quad (8)$$

where n_t is the number of input patterns in the set D^* used for testing the bootstrapped neural network capabilities.

For the estimation of $Var\left(f\left(\bar{x};\bar{w}^*\right)\right)$, the *expected squared deviation of the neural networks outputs around its mean*, the bootstrap method can be used. This entails that a number B of bootstrap samples be drawn at random with replacement from the original training set of n_p input/output patterns $D \equiv \{(\bar{x}, y)\}$. The generic b^{th} sample D_b is constituted by the same number n_p of input/output patterns, drawn among those in D , although, due to sampling with replacement, some of the patterns in D will appear more than once in D_b whereas some will not appear at all [Efron, 1979; Efron et al., 1993]. Each bootstrap set D_b is then used as data set for training a different neural network to give a regression function $\hat{y}_b^*(\bar{x}) = f\left(\bar{x};\bar{w}_b^*\right)$, where \bar{w}_b^* is the thereby obtained vector of network weight values (Figure 18). Then, in correspondence of a new input \bar{x} , the bootstrapped neural network estimate $y_{ANN}(\bar{x})$ is given by the average of the B regression functions $\hat{y}_b^*(\bar{x}) = f\left(\bar{x};\bar{w}_b^*\right)$, i.e.:

$$y_{ANN}(\bar{x}) = f\left(\bar{x};\{\bar{w}_b^*, b = 1, 2, \dots, B\}\right) = \frac{\sum_{b=1}^B f\left(\bar{x};\bar{w}_b^*\right)}{B} = \frac{\sum_{b=1}^B \hat{y}_b^*(\bar{x})}{B} = f\left(\bar{x}, \bar{w}^*\right) \quad (9)$$

and the estimate of the standard deviation of $y_{ANN}(\bar{x})$ is given by:

$$\sigma_{boot}^*(\bar{x}) = \sqrt{\frac{1}{B-1} \sum_{b=1}^B \left[\hat{y}_b^*(\bar{x}) - y_{ANN}(\bar{x}) \right]^2} \quad (10)$$

From the theory and practice of ensemble empirical models, it can be shown that the estimate $y_{ANN}(\bar{x})$ in (9) is in general more accurate than the estimate of the best-trained network in the bootstrap ensemble of B neural networks trained for the estimation task

[Krogh et al., 1995; Franke and Neumann, 2000; Cadini et al., 2007]. Further details on the method and an application in the nuclear field may be found in [Zio, 2006].

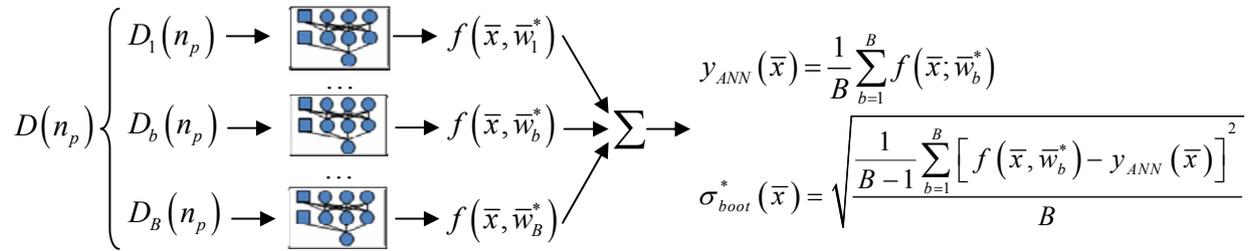


Figure 18 Scheme of bootstrapped ANN estimations

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Dipartimento di Matematica “F. Brioschi”,
Politecnico di Milano, Via Bonardi 9 - 20133 Milano (Italy)

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