# Surrogate modelling for solving optimization problems with polymorphic uncertain data

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**Abstract**

The solution of optimization problems with polymorphic uncertain data requires to combine stochastic and non-stochastic approaches. In this paper, a concept is presented, which allows one to consider uncertain a priori parameters and uncertain design parameters quantified by stochastic numbers and intervals. To solve optimization problems in structural mechanics by means of iterative optimization algorithms (e.g. particle swarm optimization), often multiple runs of nonlinear finite element models with varying a priori and design parameters have to be performed. For each design to be optimized, an interval analysis in combination with Monte Carlo simulations is necessary. This can only be realized by substituting the nonlinear finite element model by numerically efficient surrogate models. In this paper, a strategy for neural network based surrogate modelling is presented. Instead of just replacing the deterministic finite element simulation, it is focused on surrogate models to replace the stochastic simulation. The approach is verified by an analytical solution and applied to optimize the concrete cover of a reinforced concrete bridge structure taking the variability of material parameters and construction imprecision into account.

Keywords: Surrogate Model, Artificial Neural Network, Optimization, Polymorphic Uncertainty

## 1 Introduction

Uncertain parameters can be quantified by stochastic distributions within the structural design process. In [1], an overview on reliability-based design optimization approaches is presented. In general, a surrogate optimization problem has to be defined, because the solution of an optimization problem requires deterministic measures. Such measures are mean values, variances or quantile values of the original objective function, which allows one to consider the robustness by optimizing the mean value and minimizing the variability, see e.g. [2], and [3].

In addition to stochastic models, uncertain parameters can be described by intervals or fuzzy numbers. Surrogate objectives can be formulated by means of worst case scenarios, e.g. minimizing the upper bound of an interval objective function, in case of interval parameters or by means of defuzzified measures (e.g. fuzzy mean, fuzzy centroid) in case of fuzzy parameters. Stochastic and non-stochastic models can be combined to polymorphic uncertainty models within structural optimization approaches, see e.g. [4] and [5].

In this paper, optimization approaches are presented, which allow to combine stochastic and interval design and a priori parameters. A particle swarm optimization algorithm [6] is applied to solve surrogate optimization problems, e.g. to minimize the worst case mean value of an objective function. This requires to perform Monte Carlo simulations and optimization-based interval analyses of deterministic structural simulations for each optimization run. In order to reduce the computational effort of the deterministic simulation and the Monte Carlo simulation, artificial neural network (ANN) surrogate models are applied. Whereas ANN surrogate models have already been developed to replace deterministic simulations within stochastic analyses, see e.g. [7–10], or to replace interval simulations within interval stochastic analyses, see e.g. [11], an approach for replacing the stochastic simulation with ANN surrogate models is introduced in this paper.

After a verification test, the presented surrogate modelling strategy is applied to minimize the crack widths of a reinforced concrete bridge structure. A nonlinear finite element model is utilized to compute the load bearing capacity and the crack patterns of the structure. Based on the finite element simulation results, an ANN surrogate model is trained to approximate the objective function. Within the optimization, the Young's modulus of concrete is modelled as a stochastic a priori parameter and the position of the reinforcement layers are defined as interval design parameters, with a fixed radius and midpoints to be optimized. Based on Monte Carlo simulation results of the ANN surrogate model, another ANN is trained to replace the Monte Carlo simulation within the optimization runs.

## 2 Optimization with polymorphic uncertain data

Optimization with polymorphic uncertain data means, that stochastic and non-stochastic uncertain parameters are combined to solve an optimization problem. It is classified into uncertain a priori parameters, which cannot be optimized, and design parameters, which are to be optimized. Here, optimization approaches combining stochastic numbers and intervals are presented, which results in the following possible parameter representations:

- uncertain a priori parameters
  - stochastic numbers $A$
  - intervals $\overline{a}$
- design parameters
  - deterministic numbers $d$
  - stochastic numbers $D$
  - intervals $\overline{d}$

Whereas a stochastic number $X$ is defined by its probability density function $f(x)$, an interval $\overline{x} = [{}_{l}x,\ {}_{u}x]$ is quantified by its lower and upper interval bounds ${}_{l}x$ and ${}_{u}x$, respectively, or by its midpoint

$$ {}_{m}x = \frac{1}{2} \cdot ({}_{l}x + {}_{u}x) \ , \tag{1} $$

and radius

$$ {}_{r}x = \frac{1}{2} \cdot ({}_{u}x - {}_{l}x) \ . \tag{2} $$

To solve optimization problems with uncertain a priori or design parameters, surrogate objectives have to be defined, because the minimization or maximization of an objective function $Z$ requires a deterministic representation. In case of stochastic uncertainty, typical surrogate objectives to be optimized are the mean value $\mu(Z)$, the standard deviation $\sigma(Z)$ or quantiles of $Z$. The surrogate objectives can also be combined resulting in a multiple objective optimization, e.g. minimizing the mean value and the standard deviation of an objective function to obtain a robust optimal design. In case of interval uncertainty, the midpoint ${}_{m}z$, the radius ${}_{r}z$, the lower bound ${}_{l}z$ or the upper bound ${}_{u}z$ of the objective function can be defined as surrogate objectives, e.g. resulting in a worst case optimization, if the upper bound of the interval objective function is minimized.

If both, intervals and stochastic numbers are considered within an optimization problem, the surrogate objectives for stochastic uncertainty and interval uncertainty can be combined, e.g. worst case mean value $\min\{\max\{\mu(Z)\}\}$, which means that the upper bound of the mean value of the objective function is minimized. This is visualized in Figure 1, for the combination of an interval design parameter $\overline{d}$ (with fixed radius ${}_{r}d$ and midpoint ${}_{m}d$ to be optimized) and stochastic a priori parameters. It can be seen, that for each deterministic design $d$, the value of the objective function $Z$ is a stochastic distribution with a mean value $\mu(Z(d))$ and for an interval design $\overline{d}$, an interval of mean values is obtained. The optimal design is marked by the optimal interval midpoint ${}_{m}d$.

Optimization problems with stochastic and interval parameters can be solved by two possible approaches, see Figure 2. In both approaches, four computational loops are required and in the first loop,

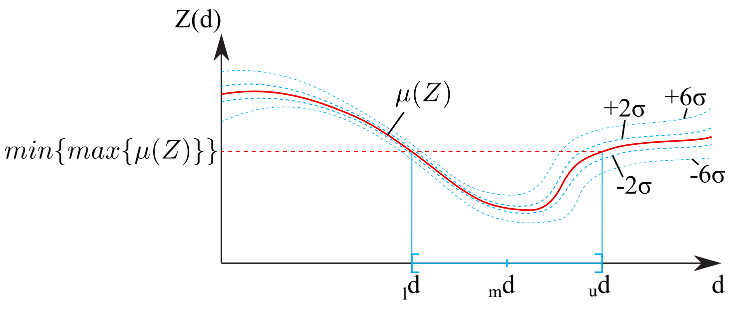
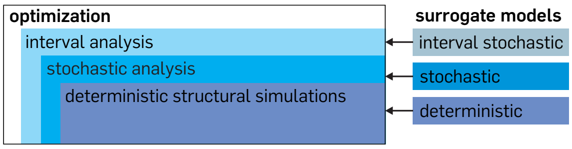
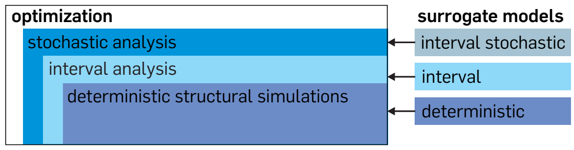



Figure 1: Objective function $Z$ of an optimization task with stochastic a priori parameters and an interval design parameter $\overline{d}$.

an optimization algorithm, e.g. a particle swarm optimization algorithm [6], is applied to solve the optimization problem with a surrogate objective, where also constraints can be considered. The fourth loop contains the deterministic structural simulation. The interval dominated approach requires an interval analysis (e.g. by using an optimization-based approach according to [12]) with stochastic realizations in the second loop and a stochastic analysis (e.g. by using Monte Carlo simulation) in the third loop, see Figure 2a. Within the stochastics dominated approach, a stochastic analysis with interval samples (e.g. Interval Monte Carlo simulation [13]) is performed in the second loop and an interval analysis (e.g. by using an optimization-based approach according to [12]) in the third loop, see Figure 2b.




(a) Interval analysis with stochastic realizations (interval dominated approach).




(b) Stochastic analysis with interval samples (stochastics dominated approach).

Figure 2: Computational schemes for optimization tasks with interval and stochastic parameters.

If numerical simulation techniques are applied for the second and third loops, such as the Monte Carlo simulation for the stochastic analysis and an optimization-based interval analysis, a high number of deterministic structural simulations (samples) are required. In case of detailed numerical models, e.g. based on the finite element method, numerically efficient surrogate models can help to solve optimization problems with polymorphic uncertain parameters.

## 3 Neural network based surrogate modelling

Several artificial neural network (ANN) approaches have been developed to approximate time consuming FE simulations in structural mechanics, see e.g. [14]. In [15] and [16], different network architectures are presented. Here, it is focused on feedforward neural networks. They are used to map the inputs (realizations of the uncertain a priori and design parameters) onto the outputs (corresponding value of the objective function). A feedforward neural network consists of an input layer, a number of hidden layers and an output layer. The neurons of each layer have synaptic connections to the neurons in the previous and following layers. Whereas the number of input and output neurons are given by the approximation problem (i.e. number of design and uncertain a priori parameters and number of objective functions), the number of hidden layers and hidden neurons have to be defined according to the complexity of the objective functions to be approximated.

Starting from the input layer to the output layer, the signals of a neuron in a feedforward ANN are computed by

$$x_i^{(m)} = \varphi_i^{(m)} \left( \nu_i^{(m)} \right) = \varphi_i^{(m)} \left( \sum_{h=1}^{H} \left[ x_h^{(m-1)} \cdot w_{ih}^{(m)} \right] + b_i^{(m)} \right) , \tag{3}$$

where $\varphi_i^{(m)}(.)$ is the activation function of neuron $i$ in layer $(m)$. The argument $\nu_i^{(m)}$ of the activation function contains the sum of all output signals $x_h^{(m-1)}$ of the previous layer $(m-1)$ multiplied by the corresponding synaptic weights $w_{ih}^{(m)}$ and adding a bias value $b_i^{(m)}$. Different activation functions $\varphi_i^{(m)}(.)$ can be used, e.g. linear function, logistic function (sigmoid function), hyperbolic tangent function or area hyperbolic sine function.

The weights and bias values of the ANN are determined within the network training. For the ANN approximation of an objective function, a sufficient number of supporting points are defined (e.g. by regular grids, random sampling or Latin hypercube sampling) to create patterns of input and output data. The whole data set is divided into training, testing and verification data to guarantee a good approximation performance and to avoid overfitting. Backpropagation algorithms, see e.g. [15], are the most commonly used approaches to train an ANN by minimizing the error between the network outputs and the desired responses at the supporting points.

In general, ANN surrogate models are used to approximate the deterministic simulation model. However, in case of simulations with polymorphic uncertain parameters, also the interval analysis or the stochastic analysis can be replaced by surrogate models. To solve optimization problems, it would be beneficial, if all a priori uncertain parameters are part of the neural network approximation, because they are fixed and cannot be changed during the optimization, and just the design parameters are defined as

ANN inputs. In Figure 2, four possible surrogate modelling strategies are shown for optimization tasks with interval and stochastic parameters:

- surrogate model for deterministic simulation
- surrogate model for interval analysis
- surrogate model for stochastic analysis
- surrogate model for interval stochastic analysis

To replace the interval analysis, see Figure 2b, either the surrogate objective (e.g. midpoint, lower or upper bound of the objective function) is defined as ANN output and a ANN is trained with deterministic data or the whole interval analysis is replaced by an ANN with interval signal processing, see e.g. [17]. The second approach has been applied in [11] to replace the interval analyses within an Interval Monte Carlo simulation.

In this paper, a concept to replace the stochastic analysis according to Figure 2a is presented. The ANN is trained to approximate the surrogate objective (e.g. the mean value) to be minimized or maximized. This allows one to avoid time consuming Monte Carlo simulations during the optimization. In case of FE simulations, it may be necessary to work with two levels of surrogates. At the first level, the deterministic FE simulation is replaced by an ANN, which is then used to train another ANN replacing the stochastic simulation at the second level. This means that at each supporting point of the second level ANN, a Monte Carlo simulation is performed with the first level ANN to get the desired responses (e.g. mean values).

Both concepts, i.e. to replace the interval analysis and to replace the stochastic analysis, can be combined within interval stochastic surrogate models. In [18], a similar concept has been introduced to map fuzzy bunch parameters with ANNs for fuzzy stochastic analyses.

# 4 Examples

## 4.1 Verification with analytical solution

The proposed neural network surrogate modelling approach for the stochastic simulation is verified by an analytical solution of an optimization problem

$$\min\left\{\max\left\{\mu\left(Z(d_1,\overline{d}_2,D_3)\right)\right\}\right\}, \text{ with } Z(d_1,\overline{d}_2,D_3) = {d_1}^2 + {\overline{d}_2}^2 + D_3 + {\overline{a}_1}^2 + A_2 + 1\,, \tag{4}$$

considering three design parameters (deterministic number $d_1$, interval $\overline{d}_2$ and stochastic number $D_3$, see Table 1) and two additional uncertain a priori parameters (interval $\overline{a}_1$ and stochastic number $A_2$, see Table 2).

Table 1: Design parameters of the optimization problem according to (4).

| parameter | type | search space |
|---|---|---|
| $d_1$ | deterministic | $[-5,\ 5]$ |
| $\overline{d}_2$ | interval, midpoint ${}_m d_2$ to be optimized, fixed radius ${}_r d_2 = 1$ | $[-9,\ 9]$ |
| $D_3$ | Gaussian, mean value $\mu(D_3)$ to be optimized, fixed standard deviation $\sigma(D_3) = 0.5$ | $[-4,\ 4]$ |

Table 2: Uncertain a priori parameters of the optimization problem according to (4).

| parameter | type |
|---|---|
| $\overline{a}_1$ | interval, midpoint ${}_m a_1 = 1.2$, radius ${}_r a_1 = 1.8$ |
| $A_2$ | Gaussian, mean value $\mu(A_2) = 0$, standard deviation $\sigma(A_2) = 0.75$ |

The analytical solution of the optimization problem (4) with polymorphic uncertain parameters is $\mu(Z(d_1,\overline{d}_2,D_3)) = 7$ with the optimal design parameters $d_1 = 0$, ${}_m d_2 = 0$, $\mu(D_3) = -4$.

In [19], the optimization problem (4) has been solved by a particle swarm optimization algorithm [6] for the interval dominated and the stochastics dominated approaches according to Figure 2. It has been investigated, that the interval dominated approach was about 10 times faster than the stochastics dominated approach and that for both approaches the relative deviation $Z_{rel} = \frac{Z_{num} - Z_{an}}{Z_{an}}$ of the numerically computed optimum $Z_{num}$ with respect to the analytically computed optimum $Z_{an}$ converges to zero with an increasing number of samples of the Monte Carlo simulation. But for the interval dominated approach, the optimum $Z_{num} > Z_{an}$, whereas for the stochastics dominated approach $Z_{num} < Z_{an}$, i.e. the interval dominated approach is more reliable than the stochastics dominated approach, see [19].

In order to verify the presented ANN surrogate modelling approach, a feedforward neural network with one hidden layer (4-5-1 architecture) is trained to approximate the objective function $\mu\left(Z(d_1, \overline{d}_2, D_3)\right)$, see Figure 3. This means that the Monte Carlo simulation loop within the optimization is replaced by the ANN. Inputs of the neural network are realizations $d_1$, ${}_m d_2$ and $\mu(D_3)$ of the three design parameters and realizations $a_1$ of the interval a priori parameter $\overline{a}_1$, see Figure 3. Here, 1296 supporting points (a regular grid $6 \times 6 \times 6 \times 6$ of the four dimensional input space) are used to train, test and verify the ANN with 60%, 20% and 20% of the data, respectively. For each of the 1296 supporting points, a Monte Carlo simulation with varying stochastic design parameter $D_3$ and varying stochastic a priori parameter $A_2$ is performed to obtain the corresponding target output value. In order to investigate the sensitivity of the sample size within the Monte Carlo simulation, four ANNs are created with 1,000, 3,000, 5,000 and 10,000 samples, respectively. The prediction performance of all ANNs is of high quality with a coefficient of determination close to 1.0.

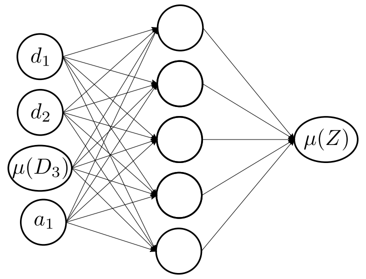



Figure 3: Feedforward neural network for the approximation of the objective function $\mu(Z)$ according to the optimization problem (4).

In Table 3, the relative deviation $Z_{rel}$ of the numerically computed optimum $Z_{num}$ with respect to the analytically computed optimum $Z_{an}$ is presented for the four ANNs created with different sample sizes. It can be seen, that the optimization problem can be solved with the ANN surrogate model with similar accuracy compared to the original solution without ANN. The ANN solution could further be improved, if more supporting points are used to generate the ANN.

Table 3: Relative deviation $Z_{rel}$ of the numerically computed optimum $Z_{num}$ with respect to the analytically computed optimum $Z_{an}$; comparison of the interval dominated approach without and with ANN surrogate model.

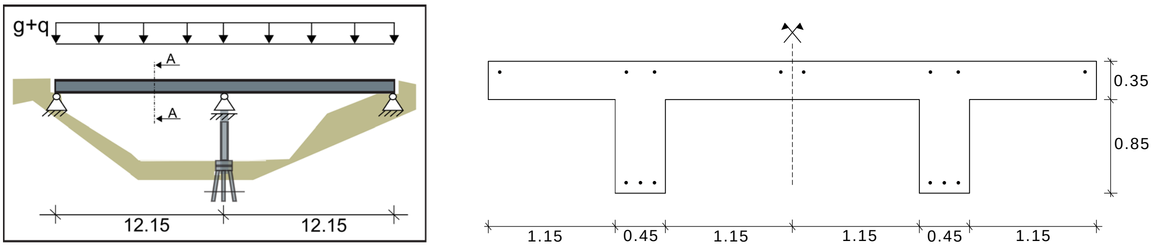
| number of samples | $Z_{rel}$ without ANN $\left[\cdot 10^{-3}\right]$ | $Z_{rel}$ with ANN $\left[\cdot 10^{-3}\right]$ |
|---|---|---|
| 1,000 | 7.86 | 3.49 |
| 3,000 | 3.00 | 3.03 |
| 5,000 | 2.69 | −2.37 |
| 10,000 | 0.80 | −2.43 |

### 4.2 Optimization of the reinforcement layout of a reinforced concrete bridge structure

The proposed ANN surrogate modelling approach is applied to optimize the reinforcement layout of a reinforced concrete bridge structure. The structural system and the cross section of the two-span bridge is shown in Figure 4. To investigate the cracking behaviour under long-term loading, the bridge is subjected to its self weight $g = 67.25$ kN/m and a constant traffic loading $q = 22.2$ kN/m$^2$ over the whole bridge deck.

The load bearing capacity and the crack patterns of the structure are analysed by a finite element model. In this model, the reinforcement bars are considered by a smeared formulation taking the bond slip mechanism into account. The concrete material model is based on [20] and for the steel reinforcement, an elasto-plastic model is adopted. Due to the double symmetric system and loading conditions only $\frac{1}{4}$ of the structure has to be computed.

In Figure 5, the distribution of the internal crack variable $\alpha_R$ is shown. In a post-processing, the crack width $w_i$ for each finite element is calculated using the internal crack variable $\alpha_R$, see [21]. This




(a) Structural system and loading. (b) Cross section (A–A).

Figure 4: Two-span bridge structure (dimensions in [m]).

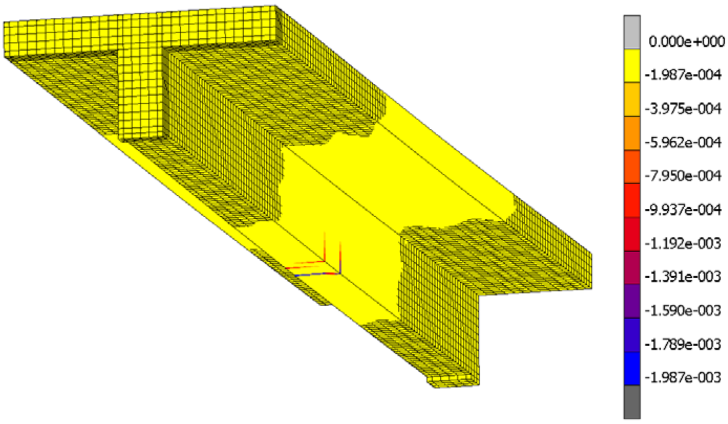



Figure 5: Finite element model of the bridge structure and computed crack pattern (represented by values of the internal crack variable $\alpha_R$).

allows one to evaluate the exposed lateral surface of reinforcement $M$ [mm$^2$] based on the crack widths at the reinforcement layers, see [19], which is defined as a durability measure in this work.

In order to minimize the exposed lateral surface of reinforcement, an optimization task has to be solved. Within this optimization, the Young's modulus $E_c$ of concrete is considered as a stochastic a priori parameter (Gaussian distribution with mean value $\mu = 33,300$ N/mm$^2$ and standard deviation $\sigma = 400$ N/mm$^2$). The design parameters $\overline{h}_{bottom}$ and $\overline{h}_{top}$ (position of the reinforcement rebars with respect to the upper and lower edge of the cross section, respectively) are defined as intervals with fixed radii and midpoints to be optimized. To consider both, stochastic and interval uncertainty within the optimization, the minimization of the worst-case mean value of the exposed lateral surface of reinforcement is defined as objective

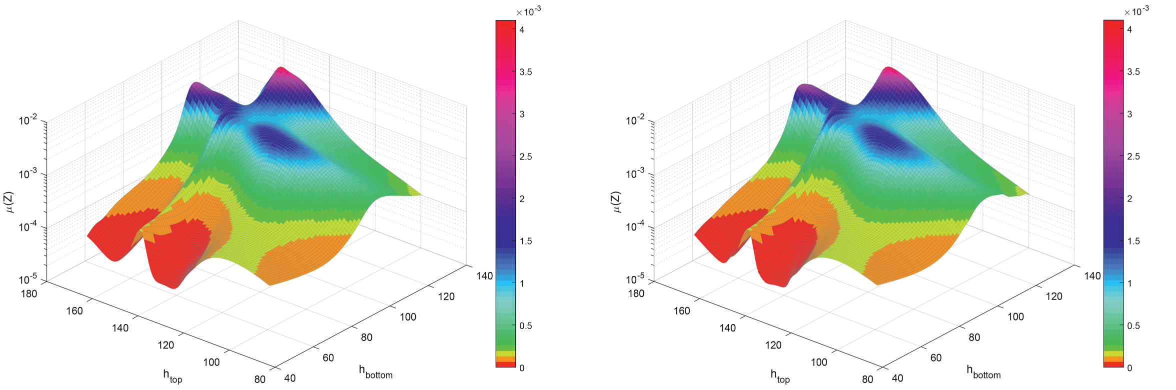
$$\min\left\{\max\left\{\mu\left(M\left(\overline{h}_{bottom},\overline{h}_{top}\right)\right)\right\}\right\} \ . \tag{5}$$

As a constraint of the optimization problem, the accepted failure probability with respect to the load bearing capacity of the bridge structure is defined as $P_{f,tol} \leq 10^{-4}$.

In [19], optimization runs for different reinforcement layouts (number and diameter of rebars) of the described bridge structure have already been performed for deterministic, interval and the described polymorphic uncertain conditions, i.e. stochastic a priori parameter and interval design parameters. The influence of the radius of the interval design parameters has been investigated in [22]. Here, it is focused on the proposed multilevel ANN surrogate modelling approach.

Based on the results of 90 FE simulations with varying realizations of the interval design parameters $\overline{h}_{bottom}$ and $\overline{h}_{top}$ and the stochastic a priori parameter $E_c$, two neural networks are trained to predict the exposed lateral surface of the reinforcement $M$ (objective function) and the load bearing capacity $lbc$ (to evaluate the failure probability constraint), respectively. After training and testing, the first neural network with a 3-10-5-1 architecture is applied to compute the mean values $\mu\,(M)$ of the exposed lateral surface of the reinforcement in the design space, see Figure 6a. The sensitivity of the sample size to the objective function has been investigated. Here, 100,000 samples of the Gaussian distributed Young's modulus $E_c$ are used to approximate the objective function.

To solve the optimization problem, a particle swarm optimization algorithm is applied. Here, a swarm with six particles is used and the search for the global optimum is repeated three times. In each search




(a) Mean values of 100,000 samples with ANN approximation of the deterministic simulation.

(b) Additional ANN approximation of the stochastic simulation.

Figure 6: Objective function $\mu\left(M\right)$ in the design space (logarithmic scale).

step, for each particle an optimization-based interval analysis is required and a Monte Carlo simulation has to be performed for each run of this additional internal optimization. In order to replace the Monte Carlo simulation within the optimization, another neural network with 2-10-4-1 architecture is trained to approximate the dependency of realizations of the interval design parameters $\overline{h}_{bottom}$ and $\overline{h}_{top}$ (inputs) to the objective function $\mu\left(M\right)$ (output). Based on the first neural network, 6,561 supporting points (regular $81 \times 81$ grid) are used to train (60%), test (20%) and verify (20%) this additional ANN with 100,000 samples of the stochastic a priori parameter $E_c$. The resulting ANN approximation of the objective function in the design space is shown in Figure 6b, which shows a very good agreement with the reference solution to be approximated, see Figure 6a. This ANN is then applied to compute the optimal design $\min\left\{\max\left\{\mu\left(M\left(\overline{h}_{bottom}, \overline{h}_{top}\right)\right)\right\}\right\}$ just by solving an optimization-based interval analysis for each optimization run. This reduces the computation time approximately by a factor of three to four.

The results of both approaches, i.e. the ANN approximation of the deterministic simulation and the additional ANN approximation of the stochastic simulation, are presented in Table 4 and Table 5, respectively. The additional ANN approximation of the stochastic simulation leads to almost the same results compared to the pure ANN approximation of the deterministic simulation. Here, the constraints have only be checked at the end of the optimization, because the evaluation of the failure probability in each iteration step of the optimization is too time consuming. It should be noted that for both approaches the constraint $P_{f,tol} \leq 10^{-4}$ (accepted failure probability with respect to the load bearing capacity of the bridge structure) is slightly exceeded for ${}_{r}h_{bottom/top} = 10$mm.

Table 4: Results of the optimization with ANN approximation of the deterministic simulation for varying interval radii ${}_{r}h_{bottom}$ / ${}_{r}h_{top}$ of the design parameters; value of the objective function $\max\left\{\mu\left(M\right)\right\}$, midpoints of the best designs, computation time for three optimization runs and failure probability $P_f$.

| ${}_{r}h_{bottom/top}$ [mm] | $\max\left\{\mu\left(M\right)\right\}$ [mm$^2$] | ${}_{m}h_{bottom}$ [mm] | ${}_{m}h_{top}$ [mm] | time [s] | $P_f$ |
|---|---|---|---|---|---|
| 0 | 7.88E-05 | 55.0000 | 142.8696 | 20.5 | 2.29E-05 |
| 5 | 1.59E-04 | 60.0000 | 142.9992 | 4273.5 | 7.10E-05 |
| 10 | 4.86E-04 | 65.0000 | 140.2368 | 3708 | 1.39E-04 |

Table 5: Results of the optimization with additional ANN approximation of the stochastic simulation for varying interval radii ${}_{r}h_{bottom}$ / ${}_{r}h_{top}$ of the design parameters; value of the objective function $\max\left\{\mu\left(M\right)\right\}$, midpoints of the best designs, computation time for three optimization runs and failure probability $P_f$.

| ${}_{r}h_{bottom/top}$ [mm] | $\max\left\{\mu\left(M\right)\right\}$ [mm$^2$] | ${}_{m}h_{bottom}$ [mm] | ${}_{m}h_{top}$ [mm] | time [s] | $P_f$ |
|---|---|---|---|---|---|
| 0 | 7.68E-05 | 55.0000 | 138.1468 | 7.5 | 1.27E-05 |
| 5 | 1.47E-04 | 60.0000 | 142.6607 | 1076.5 | 7.27E-05 |
| 10 | 4.82E-04 | 65.0000 | 140.4340 | 1175.5 | 1.39E-04 |

## 5 Conclusions

In this paper, a neural network based surrogate modelling strategy has been presented to solve optimization problems in structural mechanics considering stochastic and interval parameters. A first artificial neural network is trained to approximate the deterministic finite element analysis. Based on this neural network, a second neural network is created to replace the stochastic analysis (Monte Carlo simulation) within the optimization runs. This surrogate modelling strategy has been verified by an analytical solution, and it has been applied to optimize the cracking behaviour of a reinforced concrete bridge structure. The results show good approximation and prediction capabilities and a reduction of the computation time by a factor of three to four.

In future works, the approximation quality of the surrogate models can further be improved by generating additional training and test points close to the optimal designs and close to the limit state functions adaptively during the optimization. It would also be beneficial, if the time consuming constraints check can be incorporated into the surrogate model for the stochastic analysis. Moreover, the whole interval stochastic simulation could be replaced by another surrogate model, where only the design parameters are inputs and the influence of all a priori uncertain parameters are captured by the neural network parameters.

## Acknowledgments

This research is supported by the German Research Foundation within Subproject 6 of the Priority Programme SPP 1886 "Polymorphic uncertainty modelling for the numerical design of structures", which is gratefully acknowledged by the authors.

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