Neural network simulation of deterministic and stochastic processes

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1. Introduction

The methods of computer simulation have been proved as very powerful tools for the exploration of different complex processes [1]. They gain a considerable attention in recent years, when being used for adequate forecasting of the behaviour of explored systems under different external or internal conditions. Classical approximation methods are generally used for the analysis of well-known analytical expressions, which are far too simple to describe the real physical processes. For the correct interpretation of the experimental data computer simulation must be included in the process of data analysis. One of the forms of such application is a simulation-based fitting (SBF) [1]. The idea of SBF is the approximation of experimental data by synthetic data obtained *via* simulation modeling. In comparison to standard analytical data fitting techniques, SBF has the advantage that it fits natural physical parameters of the system itself and gives a direct insight in how they affect the experimental characteristics of the system.

However, in some cases it is not necessary to operate with a simulation model (or a "white box" model), which gives precise results but is far more computationally expensive than analytical approximation. For example, in SBF only parameters of the model are modified, when its structure holds constant. In such a case, it may be useful to perform a "black box" modeling, which still operates with real physical parameters but can be performed much faster. In the current work, it is proposed to use artificial neural networks (ANNs) [2] as "black box" simulators of physical processes.

Two completely distinct cases are considered below: the neural simulation of deterministic physical processes, and ANN simulation of stochastic ones.

2. Approximation of a deterministic process

The global scheme of ANN utilization is shown in fig. 1. Here ANN is applied exactly in the same way as a simulation model: it transforms input parameters (7) into output values (8). The training procedure is rather obvious: the representative training set (2, 3) is generated by a special algorithm (1) and the network can be trained on it by a standard "back-propagation error" method [2].
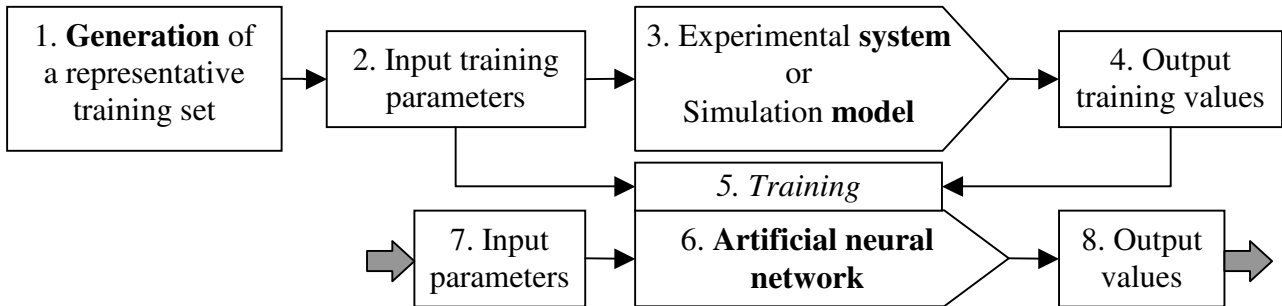

Fig. 1. Standard scheme of ANN approximation of deterministic process.

To generate a representative set of input parameters a kind of grid algorithm can be used. However, in this case the size of a training set should be known well before the training, because grid methods hamper the increase of parameter point (knots) density. Another algorithm was proposed in [3] and presented in fig. 2.
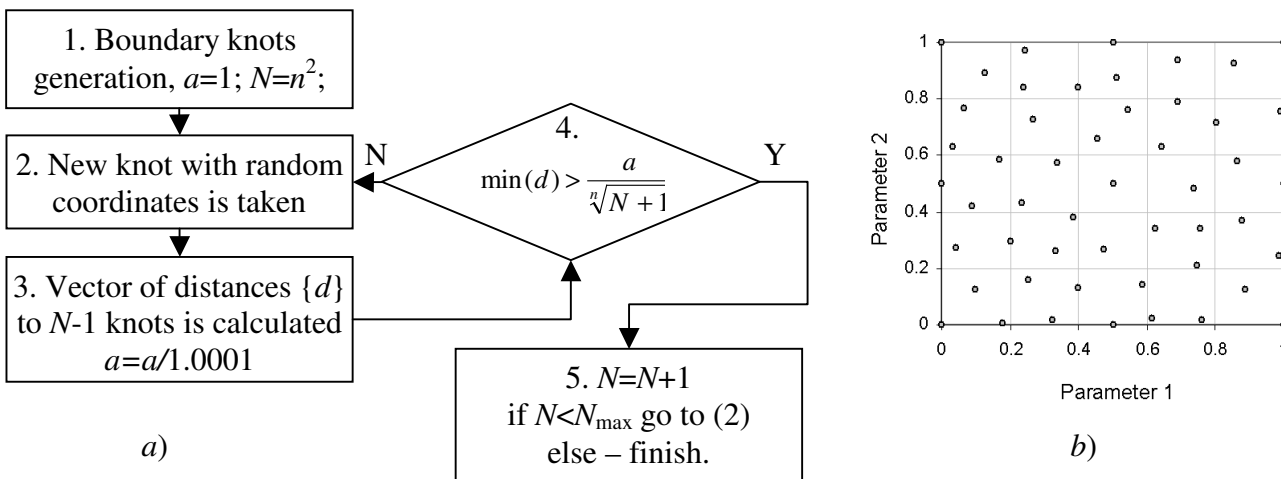

Fig. 2. Proposed algorithm of knot generation (a) and the result for n=2 (b).

Where n – dimensionality of the parametric space; N – the number of found knots.

The application of the scheme gives a uniform infill of the two-dimensional parameter space. Furthermore, the infill itself remains random and can easily be continued.

The ANN approximation of a deterministic process was applied to study the resonance energy transfer [4] in complex membrane-protein systems and gave the increase of the SBF speed by the factor of 10^4 [3].

3. Approximation of a stochastic process

To simulate a stochastic processes two approach can be proposed. The first one – is to use a stochastic ANN (for example, Boltzmann machine). However, this area of ANN is not completely studied yet and there are unsolved problems in network structure determination and training. Another approach is application of standard feed-forward networks with slight modifications. To utilize a deterministic network for generation of a random signal one should put into it a source of randomness. Fortunately, it is possible to do without significant structural changes – the random signal can be given into ANN inputs. In fact, such a network operates as an abstract function which transfers the set of uniform random values $\{x_i\} \subset \mathbf{R}$ to arbitrary distributed $\{y_j\} \subset \mathbf{Y}$.
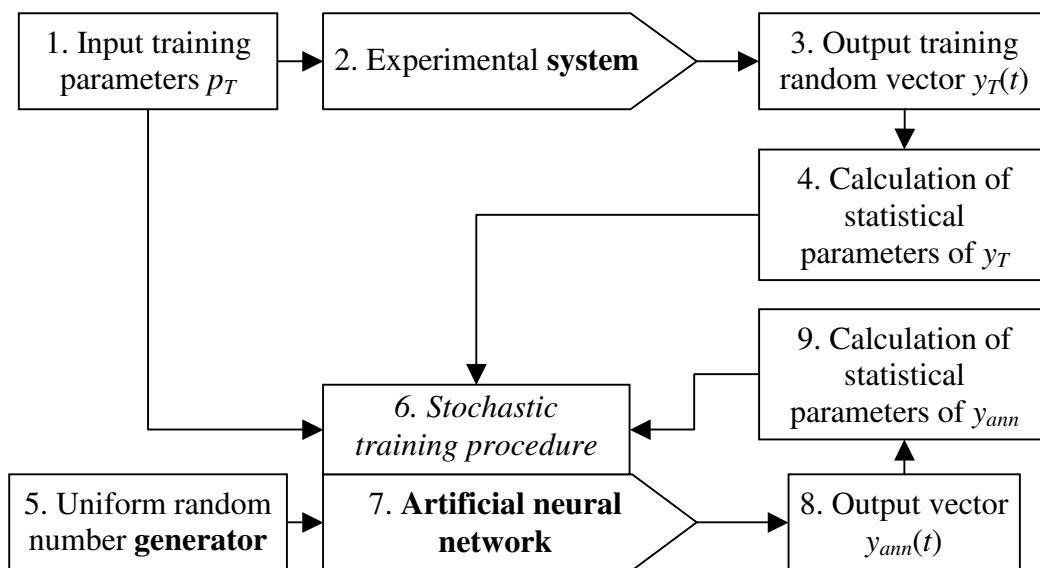

Fig. 3. Training of ANN for the approximation of stochastic signal.

It should be noted, that standard "back-propagation error" methods are not applicable to train ANN in this case. We propose the scheme shown in fig. 3. Each training pair is presented by a vector of input parameters p_T (1) and a sufficiently long output random signal $y_T(t)$ (3). From $y_T(t)$ several statistical parameters are calculated: mean, standard deviation, estimation of probability density, minimal and maximal values. During training, parameters p_T (1) together with a set of random vectors $x(t) \subset \mathbf{R}$ (5) are given to ANN which produce a sufficiently long random vector $y_{ann}(t)$. For it the same statistical parameters are calculated (9). The weighted comparison of (4) and (9) gives the error of ANN. The ANN weight coefficients can be modified iteratively using one of standard stochastic training algorithm [2].

To test this methodology the random signal given by eq. 1 was successfully generated by a 3 layer perceptron with 4x4x1 neurons.

$$y(t) = p_1 \cdot n^2(t) + p_2, \quad (1)$$

where p_1, p_2 – constant parameters, $n(t)$ – Gaussian stochastic signal with $m=0$, $\sigma=1$. Two uniformly distributed random signals were taken as $\{x_i\}$.

The proposed approach is applicable only for δ-correlated stochastic signals. Special transformations (convolution, sum) or ANN with feedback should be used.

References

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