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Development of the Algorithm for Selection of Appropriate Numerical Modeling Approach

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Abstract: This paper is dealing with review of different modeling approaches, available in contemporary literature, and analyses of their applicability on real technological processes. During the theoretical discussion the scope of potential options of techniques available for complex systems modeling are presented. Both analytical and statistical modeling approaches are described. The most important part of the paper is dealing with development of the algorithm for selection of appropriate numerical modeling approach – ASANMA, based on the structure of the system and the scope of input variables of the investigated process. Presented assumptions are based on real-life examples of the numerical models of the real systems. Developed algorithm can be used by decision makers for selection of the appropriate numerical modeling approach, in the practice.

Keywords: Optimization, komplex systems, numerical modeling

1 Introduction

Most of management processes are presenting very complex systems defined with large number of constituting elements and their interrelations. If placed on the level of general system theory (GST), each of such process could be defined as a complex system with one or more output variables and large number of input variables. Still on the level of GST, optimization of such systems is actually consisting in obtaining desired value of output variable (variables) which should be inside the defined outlying levels. This could be achieved in two ways. First way is based on control and regulation of input variables (both controlled and disturbances), which is based on defined controller unit of the system. The second way is based on possibility to perform controlled and designed changes on the structure of the system in question.

However, considering the complexity of the systems, both methods require adequate model of the investigated system which would be the basis of its further optimization. This is because the controller unit is actually defined as inversion of mathematical model equation of the object of control and, on the other hand, the change of the structure inside the real system can be too expensive if it is not based on prior model based experiments. Also, it could lead to wrong reorganization of the system structure.

Considering that in operations management, there is a belief that absolute optimization of any system cannot be achieved, each system should be the object of further optimization in the future. If defining an adequately accurate model of the system, it could be used as a tool for another iteration of optimization, considering that it can result with prediction of output values based on different scenarios and combinations of input variables [1].

Accordingly, development of accurate model of the process is of essential importance in contemporary operations management, considering that this is enabling much easier way of the process parameters acquisition, which is of crucial importance for complex systems optimization. At the bottom line, the most important aims of the system (process) modeling can be listed as follows: Using the model instead of real system to achieve system parameters; Avoiding the risk of experiments on real system; Obtaining the results of prediction whose analysis should enable effective operational management and optimization of the real system; Lower expenses resulting from model, instead of system, optimization.

Accordingly, selection of the most appropriate modeling approach, of the real complex process, is of crucial importance in achieving these aims. This paper is dealing with the development of the algorithm that can be of use to decision makers when selecting the most appropriate modeling approach for complex processes optimization. The algorithm is developed based on previous experience in modeling of real complex systems.

2 Development of the Algorithm for Selection of Appropriate Numerical Modeling Approach - ASANMA

2.1 Background

In spite of the fact of intensive development of the modeling methods in different fields of science and technology, it can be stated that unique classification of all types of models isn't developed yet. Having this in mind, general classification is placing all models in one of two groups: the class of symbolic (in most cases numerical) and the class of real (physical, material) models. Based on such general classification, the object of research presented in this paper is actually the symbolic models, e.g. numerical models. Symbolic models are describing the object, process or appearance on some of languages (symbols) characteristically for the objects nature. To further explain the symbolic language, it should be started from the fact that each scientific field developed its own symbolism during its historical evaluation. The first language used to describe each scientific discipline was, of course, verbal language. Next scientific language was the language of mathematics pronounced by its symbolic abbreviations, relations and logical dependences. Starting with James Watt and his centrifugal "fly ball" governor, which was the first system of automotive regulation, the development of contemporary mathematical modeling started [2]. However, since Watt was practitioner, inventor and engineer, he was not the one who developed the first mathematical model of this first dynamic system controller unit. Actually, the first theoretic who described this system using numerical model was James Clerk Maxwell [3]. He wrote a famous paper "On governors" that is widely considered a classic in feedback control theory and is used as inspiration for researchers, even today [4]. Subsequently, further research was conducted on the field of dynamic system optimization and control, starting with Routh [5] and Hurwitz [6] who investigated the stability of linear systems, in parallel with Lyapunov [7] who introduced modeling of nonlinear systems for the first time, over Lorentz [8] and his famous butterfly effect up to contemporary investigations present in recent research [9-12].

For a while in history of mathematical modeling, each scientific and technical field developed its own language of the symbols. However, resulting from the intensive development of informational technology during 80ties and 90ties, the possibilities for modeling different appearances are strongly increasing. This again led to certain standardization of symbolic models and their broad application which leads to generality of computer simulation and modeling implementation. Accordingly, mathematical language once again becomes major modeling tool. Each scientific field is subsequently adjusting its symbolism to standard mathematical expressions [13].

2.2 Clasification of modeling approaches

Aware of the fact that mathematical model has to mirror the real technological process as better as possible, as well as the cognition of the limits to which contemporary mathematical apparatus can reach; the question of level of real process idealization arises. Accordingly, primarily characteristics of the process should not be neglected, on one hand, while mathematical model should not be too complex, on the other. Too complex mathematical model is lingering the subsequent mathematical analysis. Also, complexity narrows the applicability of the model on a small surrounding of an equilibrium point of the system. Accordingly, the first modeling technique, that will be denoted as (M1) in following text, is based on the assumption that the mathematical model of an object is presented in the form of differential equations assemble. With systems, presented by differential equations assemble, the structure of the model is emerging directly from the known theoretical background and scientific validity of the system. This modeling aproach is widely recogniyed as the “First principle modeling”. For M1 modeling approach, as a precognition, it is necessary to know the structure of the investigated system and nature of the system reflected in some physical law that describes its behavior. Subsequently, the solutions of the differential equations assemble can be obtained using the computer simulation after introducing standard input signals. Then, the real system (the object of control) is induced with the same input signals while the output (response) of the system is measured. Comparing the results of the differential equations solution with the outputs of the real system, the conclusions on validity of constructed model can be brought. On the other hand, since there is no real linear system existing in the nature, success of this modeling approach is based on differential equations linearization, in the surrounding of an equilibrium point. This is resulting with difficulties of complex systems modeling, which can have more than one stabile state and this way many equilibrium points [1, 14-16]. The real system’s dynamical behavior is additionally aggravating this modeling approach. Subsequently, this modeling approach is mostly applicable for simple real (physical) systems and, of course, for abstract systems before their construction.

The second modeling approach, that will be denoted as (M2) in following text, is based on experimentally obtained, or measured, functional dependences of the real object under the non stationary regime. Using the measured output of the system, obtained after introducing predefined input signals, mathematical model of the object can be defined. In this case it is not necessary to know the structure of the system (relations among the elements, number of elements and their characteristics), neither the physical law of its behavior. In this approach, it is sufficient to collect the outputs, after introducing predefined inputs to the system and this way to form a data base which can be used for further modeling procedure. This is why, this type of modeling, is called a “black box modeling” [13, 17, 18]. This type of real process modeling is attaining more and more application in the operations management, because of the practical reasons based on its applicability.

Before further development of the mathematical model, based on the M2 modeling approach, the decision maker must assess is the system liable to predefined design of experiments or not. If the answer is “yes” than, further modeling should be based on design of experiments which can be performed using the factorial experimental design or the Taguchi method [19]. This modeling approach will be further indexed as M2.1.

On the other hand, if the investigated system is not liable to the predefined design of experiments, in the M2 approach, there are two potential possibilities to define numerical model of the system.

The first one (analytical) is based on choosing the most adequate model equation from the variety of existing potential numerical model equations, available in literature (M2.2.).

In the cases where alredy existing mathematical model equations do not present adequate accuracy of obtained model, modeling approach M2.3 (statistical modeling) can be of use. As already indicated, both linear and nonlinear statistics could be applied in obtaining the final model. However, there are some strong indicators, which can be of use when deciding which approach (liner or nonlinear) are more appropriate for modeling the data obtained from the specific process measurements. The first step in the decision making about applicability of linear or nonlinear statistical tools, for modeling, should be the analysis of correlation between the variables of the system. For definition of the correlation dependence in the form: output of the process (Y) = *f* input of the process (X_i; i = 1÷ n), bivariate correlation analysis should be performed. As the result of this analysis Pearson Correlation (PC) coefficients with responding statistical significance should be calculated.

To finally define the dependence of the output parameter as the function of the input parameters, using the linear statistics tool, for example multiple linear regression analysis (MLRA), with acceptable level of fitting (strong correlation), it is necessary that the values of PCs are above 0.5 with statistical significance ($p \leq 0.05$) for most of dependences between Y and X_i [20, 21].

However, even then, obtained MLRA model should be further tested for accuracy. The most appropriate test for defining the accuracy of a MLRA model is ANOVA. Significant *F statistics* is indicating that using the model is better than guessing the mean. Also, if the significance value of the F statistic is less than 0.05, this means that the variations explained by the model are not due the chance. *Regression* displays information about the variation accounted for by the model, while *residual* displays information about the variation that is not accounted for by the model. The ratio of regression to residual is advocating the level on which the dependent variable (Y) values are explained by the model. This ratio is also equal to the value of coefficient of determination between measured and model calculated Y values. Finally, the *collinearity* analysis of obtained MLRA models coefficients should be performed. If for most predictors (X_i), the values of the *partial* and *part* correlations drop sharply from the *zero-order* correlation this means that much of the variance in Y that is explained by X_i is also explained by other variables. The *tolerance* is the percentage of the variance in a given predictor that cannot be explained by the other predictors. Thus, relatively small tolerances in case of some of predictors show that large percentage of the variance in a given dependent variable (Y) can be explained by the other predictors. Also a *variance inflation factor* (VIF) greater than 2 is usually considered problematic for the model predictors. Also, important factor of the collinearity analysis is *condition index*. Values of condition index greater than 15 indicate a possible problem with collinearity, greater than 30 a serious problem.

Accordingly, if the PCs are large enough, with statistical significance below 0.05 and also ANOVA indicators and collinearity analysis are at acceptable level, than obtained MLRA model can be regarded as adequate for accurately prediction of output variable of the process. This modeling approach will be indexed as M2.3.1.

The models equations obtained using MLRA approach are in the form: $Y = a \cdot X_1 + b \cdot X_2 + \ldots + n \cdot X_n$, (with a,b, ..,n presenting the coefficient of model equation). If such equation can be used as adequate description of interdependence between input (X_i) and output variable (Y) of the process, this is a benefit because it is possible to calculate the values of Y for any combination of X_i values. However, there aren't that many cases of complex business or management processes in which the linear modeling approach would yield high accuracy of prediction (above 70%).

In cases where the linear statistics tools wouldn't result with high enough accuracy, nonlinear statistics should be used. Meaning, low value of correlation between two variables doesn't automatically mean that interdependence of their behavior does not exist. This is only an indicator that linear modeling approach cannot describe their inter correlation. This is usually good indicator that further modeling should be based on dynamic behavior of the variables [16]. This modeling approach, based on nonlinear statistics, will be indexed as M2.3.2. In such cases, modeling is usually facilitated using nonlinear statistic approaches such are, for example, Artificial Neural Networks (ANNs) - in case that input variables do not have wide range during whole time interval of observation [22-24] or Adaptive-Network-Based Fuzzy Inference System for variables with wide range of change [25,26].

ANNs modeling approach will be indexed as M2.3.2.1 in following text. Artificial neural networks can be viewed as nonlinear approaches to multivariate statistical methods, not bound by assumptions of normality or linearity. Although neural networks originated outside the field of statistics and have even been seen as an alternative to statistical methods in some circles, there are signs that this viewpoint is initiating an appreciation of the manners in which neural networks complement classical statistics [27,28]. The general example of ANN used in the development of the model is in the form of a network which consists of three layers of nodes (Figure 1).

The layers, described as input, hidden and output layers, comprise *i, j* and *k* numbers of processing nodes, respectively. Each node in the input (hidden) layer is linked to all the nodes in the hidden (output) layer using weighted connections. In addition to the *i* and *j* numbers of input and hidden nodes, the ANN architecture also houses a bias node (with a fixed output +1) in its input and hidden layers and they provide additional adjustable parameters (weights) for model fitting. The number of the nodes (i) in the ANN network input layer is equal to the number of inputs in the process, whereas the number of output nodes (k) equals the number of process outputs. However, the number of hidden nodes (j) is an adjustable parameter the magnitude of which is determined by issues, such as the desired approximation and generalization capabilities of the network model [29]. The employment of an ANN usually comprises three phases. First is the training phase, which is achieved using 70–80 % of randomly selected data from the starting data set. During this phase, the correction of the weighted parameters of the connections is achieved through the necessary number of iterations, until the mean squared error between the calculated and measured outputs of the network is minimal. During the second phase, the remaining 20–30 % of the data is used for testing the "trained" network. In this phase, the network uses the weighted parameters determined during the first phase. These new data, excluded during the network learning stage, are now incorporated as the new input values (Xi) that are then transformed into the new outputs (Yi). The third phase is a validation of the network on a new data set. This data set usually consists of the data from the new experimental measurements of the same process. The validation phase presents the final level of a successful or unsuccessful prediction obtained by using the network developed in the two previous stages on a new data set [28].

However, in some cases when almost all input variables of the system have wide range of relative change (ratio of variance compared to range), modeling approach based on one rule describing the dynamic changes of input variables, belonging to group of nonlinear statistic analysis methods (such are ANNs), probably wouldn't result with accurate enough prediction. In such cases, further modeling approach should be based on Adaptive-Network-Based Fuzzy Inference System (ANFIS). This modeling approach will be indexed as M2.3.2.2 in following text.

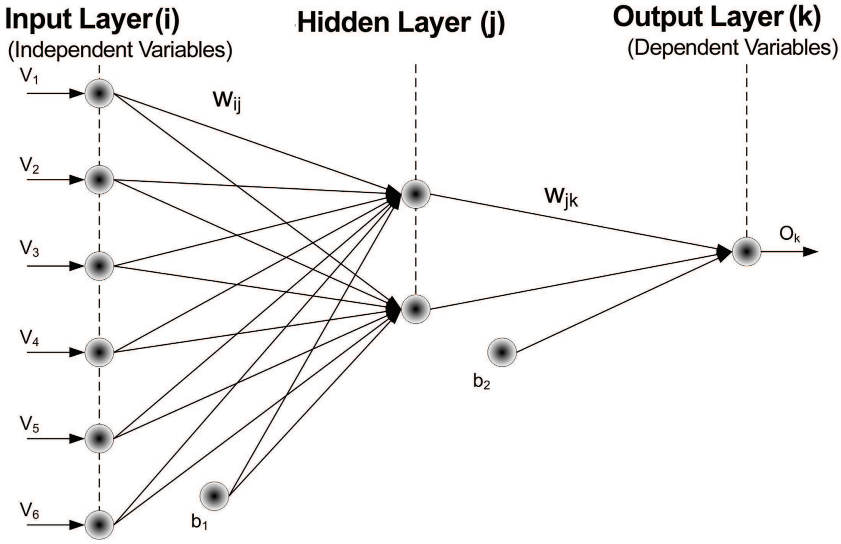

Figure 1

General example of ANN structure (prevedi)

As a basis for construction of a set of fuzzy if-then rules the ANFIS system, based on selected membership functions, can be used. The ANFIS structure is obtained by embedding the fuzzy interference system into the framework of adaptive networks [30]. Similar as ANN, an adaptive network is a network structure consisting of a number of nodes connected through directional links. The outputs of these adaptive nodes depend on modifiable parameters pertaining to these nodes [31]. The pattern in which these parameters should be iteratively varied, aiming to minimize the final error, is specified by the learning rule. Also, according to [32], the fuzzy inference system (FIS) is a framework based on fuzzy set theory and fuzzy if – then rules. Three main components of a FIS structure are: a rule base, a database, and a reasoning mechanism. The appropriate number of if – then rules, for levels of ranges of input variables, is located in the rule base. The example of a rule is "if Brent Oil price is high, than Dow Jones Global index is also high," where items such are low or high are representing the linguistic variables. The database defines the membership functions applied in fuzzy rules and the reasoning mechanism performs the inference procedure [30]. This way, for example that there are two input variables (X_1 and X_2), and assuming that their ranges can be divided in two levels, there would be the rule base with two rules for modeling the value of output variable Y:

Rule 1: If X_1 is in the range A_1 and X_2 is in the range B_1, then $f_1 = p_1x_1 + q_1x_2 + r_1$ … (1)

Rule 2: If X_1 is in the range A_2 and X_2 is in the range B_2, then $f_2 = p_2x_1 + q_2x_2 + r_2$ … (2)

In the case $f(x_1, x_2)$ is a first-order polynomial, and then the model is called a first-order Sugeno fuzzy model. Compared to classical three layers ANN network, ANFIS architecture can be presented with five layers (Figure 2). Where X_1 and X_2 are inputs to nodes in layer 1, A_i and B_i are the linguistic label of the ranges of input variables (small, large, etc), associated with the node function. Membership functions of nodes located in layer 1 ($O_i^1 = \mu A_i(X_i)$ or $O_i^2 = \mu B_i(X_i)$) specifies the degree to which the given X_i satisfies the quantifier A_i, B_i, etc.

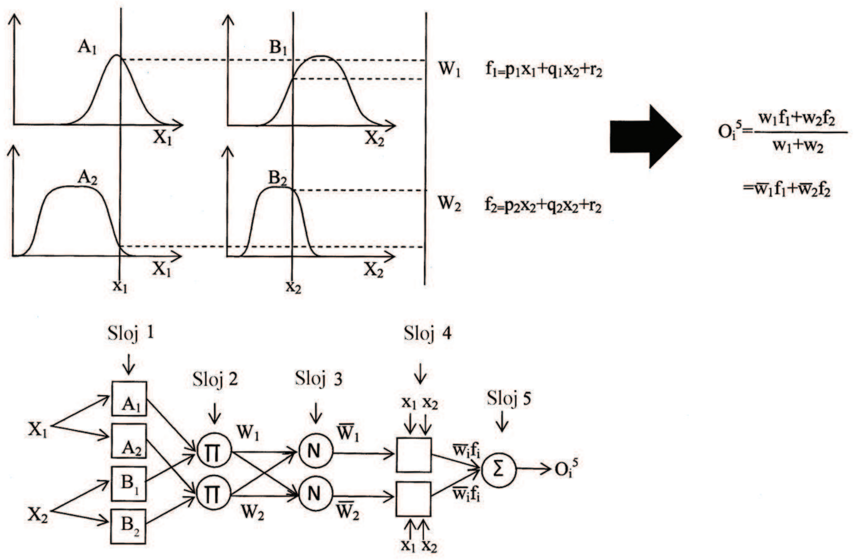

Figure 2

General example of ANFIS architecture

Usually, membership functions are either bell- shaped with maximum equal to 1 and minimum equal to 0, or Gaussian function. Nodes located in the layer 2 are multipliers, which are multiplying the signals exiting the layer 1 nodes. For example $O_i^2 = W_i = \mu A_i(X_i) \times \mu B_i(X_i)$, $i = 1, 2$, etc. Output of each node is representing the firing strength of a rule. The *i*-th node of layer 3 calculates the ratio of *i*-th rules firing strength to sum of all rules firing strengths. This way $O_i^3 = \overline{W_i} = W_i / (W_1 + W_2 + \ldots)$, $i = 1, 2, \ldots$ Every node *i* in the layer 4 has a node function of following type: $O_i^4 = \overline{W_i} \cdot f_1 = \overline{W_i} \cdot (p_i x_1 + q_i x_2 + r_i)$, where p_i, q_i and r_i will be referred to as consequent parameters. The single node of layer 5 is the node that computes the overall output as the summation of all incoming signals i.e.,

$$O_i^5 = \sum_i \overline{W_i f_i} = \frac{\sum_i W_i f_i}{\sum_i W_i} \tag{3}$$

Training of the parameters in the ANFIS structure is accommodated according to the hybrid learning rule algorithm which is the integration of the gradient descent method and the least square methods. In the forward pass of the algorithm, functional signals go forward until layer 4 and the consequent parameters are identified by the least squares method to minimize the measured error. In the back propagation pass, the premise parameters are updated by the gradient descent method [30].

2.3 The ASANMA algorithm

Based on above clasification and justification of modeling approaches, following algorithm for appropriate selection of the adequate numerical modeling approach – ASANMA can be presented (Appendix 1). This algorithm can be of use of decision makers when selecting the most appropriate modelin texchniquest for the systems which are the objest of their interest, in accordance to above defined criterions.

3 Conclusions

This paper is presenting the development of the decision making tool applicable for selection of the appropriate modeling approcah in atempt to define numerical model of complex business or management system. The obtained decision making tool is in the form of algorithm. The acronim of abtained algorithm is ASANMA (Algorithm for Selection of Appropriate Numerical Modeling Approach). All theoretical beckground presented in this manuscript is based on knowledge obtained during modeling of real complex systems in practice. However, due to the page limitaition exampleas of real life systems modeling are not presented in the text of the paper.

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Appendix 1 Algorithm for selection of appropriate numerical modeling approach – ASANMA