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A New Method for Building Proxy Models Using Simulated Annealing

Mohammad Reza Mahdiani and Ehsan Khamehchi

Faculty of Petroleum Engineering, Amirkabir University of Technology
(Tehran Polytechnic), Hafez Avenue, Tehran, Iran

Abstract: There are various types of proxy models in literatures. But most of them are not accurate enough. Among them artificial neutral network (ANN) can be accurate but it's aggressively dependent to its internal parameters and thus different run of that leads to different models with different accuracy, hence a created model of that necessarily in not the best one. In this paper, an attempt has been made to find a new artificial intelligence method which will be called simulated annealing programming (SAP) to create proxy models. It's highly accurate but roughly independent of its internal parameters. In this method, simulated annealing is applied on a tree structure to change its shape to a form in which its corresponding equation has minimum errors in predicting the outputs. Afterwards, using a test function, this model has been compared with the artificial neural network and its applicability has been discussed. It is observed that the in new introduced model different runs lead to similar models, which all are high accurate.

Key words: Artificial Intelligence · Simulated Annealing · Modeling · Proxy Model · Artificial Neural Network · Optimization

INTRODUCTION

There are various cases in experimental science in which a parameter needs to be calculated and usually it is a function of some other parameters. The most accurate method for finding its value is experiment or at least simulation, but both are expensive and time consuming. So finding a model that can predict the concerned parameter using some other parameters is necessary. This relation which is called the proxy model calculates the result rapidly and cheaply but a little less accurately than an experimental one [1, 2]. There are a lot of methods for creating proxy models. In 1951, G. E.P. Box and K.B. Wilson [3, 4] introduced response surface methodology in which a n-degree polynomial (usually second-degree) is fitted on the experimental points. This method's applicability is not good when the number of input parameters increases. Another one is splines which was introduced by Jerome Fridman in 1991 [5] and are some kind of polynomials, work well in low degrees, but become very complex at high degrees. Polynomial regression is not an accurate method [6]. Afterwards, the Kriging method was introduced by Matron [7] in 1965. This method is less complex and more accurate than the previous ones, but its problem is having limited applicability and not being used easily in different problems. In 1995, the artificial neural network was introduced by Anderson [8]. This method just needs to be trained and after that it can estimate the results and be used easily in different problems [9; 10]. However, it has its own problems that will be discussed in validation of the new model. This model is the most common method that is used in different fields of science. In 2011 Liu [11] used multi-proxies in digital signs for security purposes. In 2014 Mitrut [12] studied the ways of tuning proxy models. He studied the problem in economic problems. But in this study we try to find a model that satisfies the problem of neutral network.

Building the Model: As previously mentioned, the most common method for creating proxy models is the artificial neural network, but this method has its own weaknesses, for example it leads to different models in different runs and thus the user is not sure about its model. In this paper, an attempt is made to find a better model using the simulated annealing optimization method.

Corresponding Author: Ehsan Khamehchi, Faculty of Petroleum Engineering, Amirkabir University of Technology (Tehran Polytechnic), Hafez Avenue, Tehran, Iran.

For this means, the tree representation has been used. This representation is so flexible and can be used in different fields of science such as computer programming, mathematic equations, circuit design, creating models and identification of steady state [13], kinetic orders [14] and differential equations [15, 16]. A tree representation can be seen in Figure 1. A tree stands for an equation. Here we want to find an equation which have the least error.

Simulated annealing is based on the slow cooling and creation of crystals. In this method, we have two functions of temperature and free thermodynamic energy. Temperature determines the chance of acceptance of bad solutions and free thermodynamic energy is in fact our objective function [17, 18, 19, 20].

In the usual algorithm, the s is a series of numbers, but here we suppose that as a tree. By this definition, the algorithm can be continued normally, while the only problem is the neighbor. We need a new definition for neighbor which can be applied in tree structure.

Neighbor: We suppose a tree as a crystal. For increasing the size of the crystal in a non-deficient way some new molecule should be added in suitable places and the molecules on a bad position should be removed. Using this three methods are defined to optimize the size of the tree structure.

- Adding a sub tree: a sub tree is created randomly and it is added to a random node in a tree. In this method, the node that is common between the tree and sub tree takes the values of the sub tree (Figure 2).
- Removing a sub tree: a node and its entire connected branch are removed and a random acceptable value is put in the place of the removed node (Figure 3).
- Exchanging nodes: Two nodes are selected randomly and their place with all their connected branches will be exchanged (Figure 4).

In this study, the chance of occurrence of all the above methods was equal. So with this definition and considering the trees as the state and energy as the average error of the estimated value that the equation of the tree causes, the SAP algorithm is similar to the normal simulated annealing.

Validation of the New Model and Discussion: As previously stated, the most common method that is used for creating a proxy model is the artificial neural network. Now, The new model's applicability will be compared with ANN.

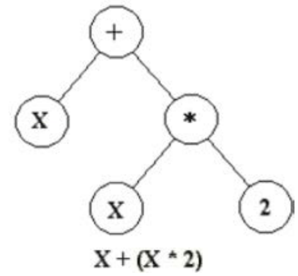

Fig. 1: Tree structure

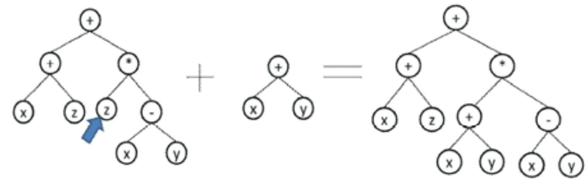

Fig. 2: Addition of sub trees

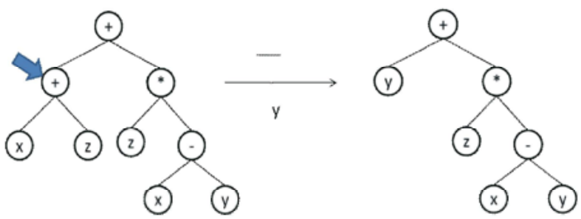

Fig. 3: Removal of sub tree

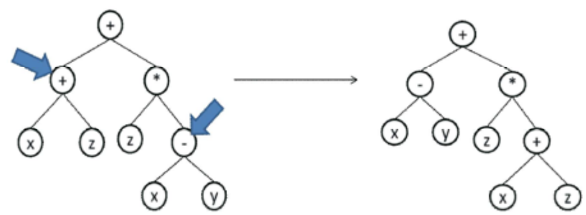

Fig. 4: Exchanging nodes

Hence, a test function is proposed, as follows:

$$u = 1.2131323\, x^3 y + 2.3123/t - 0.1241322/y \times \sin(0.004343\, x) + 0.123123 \times z \times y \times 0.1142 + 1.3 \times y + 0.0023 \times \exp(0.012 \times x \times (t \times 0.121/z)) \quad (1)$$

This equation contains different kinds of polynomial, exponential, rational and trigonometric terms. For testing the model, a dataset containing 200 real values was generated randomly in a space filling manner for x, y, z and t. Then u was calculated using equation (1), this value being considered as the exact value. 40 data were put aside as test data and the remaining data were used for training the model. The range of train and test data can be seen in Table 1 and Table 2. Using this data, two proxy models were built by SAP and ANN. The values of nodes

Table 1: Range of parameter of train data

Train	x	y	z	t
Max	9.994873	9.999702	9.972108	9.988733
Min	0.028674	0.006838	0.024819	0.017996

Table 2: Range of parameter of test data

Test	x	y	z	t
Max	9.493251	9.850664	9.972485	9.987296
Min	0.732238	0.035938	0.372502	0.692979

Table 3: Simulated Annealing Parameters

Annealing Function	Fast annealing
Re annealing interval	100
Temperature Update Function	Exponential
Temperature Update Coefficient	0.96
Initial temperature	100
Stop Tolerance	1.00E-5
maximum tree depth	10

Table 4: Artificial Neural Network Properties

Data division	Random
Training	Levenberg-Marquart
Performance	Mean Square Error
Stop tolerance	1.00E-05

Table 5: Statistical Properties of Artificial Neural Network and Simulated Annealing Programming on Test Model

	ANN	SAP
Mean	10.43658	0.51561
Median	0.595413	0.04615
Max	210.5117	7.765074

Table 6: The Result of Different Runs of the Artificial Neural Network on test Data

Run no.	Mean	Median	Max
1	46.77233	19.12397	577.7813
2	10.43658	0.595413	210.5117
3	44.30893	2.111942	1097.308
4	22.76321	2.289386	527.5528
5	323.3914	20.97607	5300.766

of the SAP model were {"+", "-', "/","*"}. The parameter of the SAP model and the ANN model can be seen in Table 3, as well as, the statistical properties of the SAP and ANN model can be seen in Table 5. As can be seen in the ANN model, some estimated values are very far from the exact values, but in the SAP model this cannot be seen, because the max relative error and the average error of the ANN is much greater than the SAP model. Even if we ignore the points with large error, the SAP model is again better than ANN, so we consider the value of median, in which the ANN has a median 12 times greater than SAP. With all this in mind, in this example, both models estimates are acceptable (Figure 5).

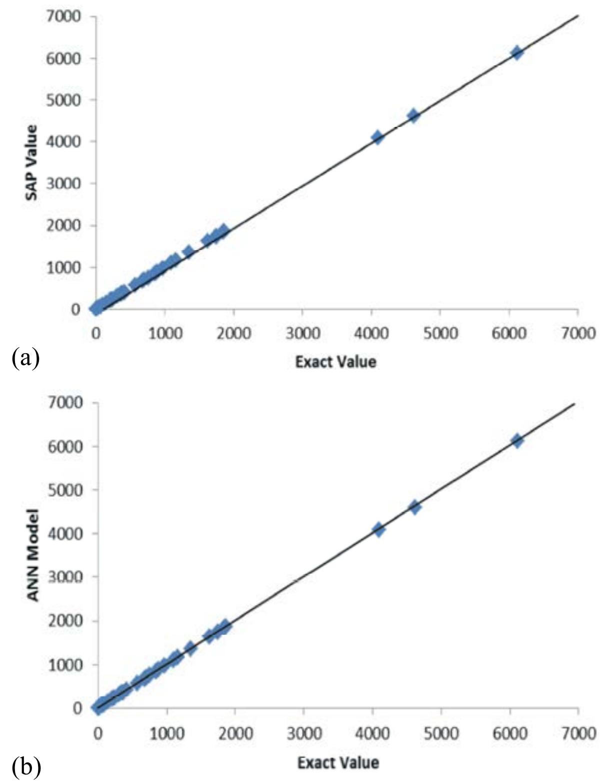

Fig. 5: (a) crossplot of SAP model versus exact data (b) crossplot of ANN model versus exact data

The error distribution of the ANN model can be seen in Figure 6 (a). As it can be seen in this figure, despite the fact that the most error distribution is near zero, some underestimation and overestimation of about 200% and -100% can be seen. It is clear that the data was accurate and this underestimation and overestimation is due to the deficiency of the model. The error distribution of the SAP model can be seen in Figure 6 (b). In this figure, most of the errors are near zero once more, but despite the ANN model there is no huge overestimation and underestimation (just about 8% and -3%). Another issue is the different model that different runs of ANN create. Of course it is one of the advantages of the ANN that it is quicker than the SAP, but the problem is that different runs lead to different solutions with different accuracy, so the user cannot be sure that his run has the best solutions or a new run can lead to a better one. For example, for the model of this paper, the program was repeatedly run and the best one was selected. The statistical properties of 5 runs can be seen in Table 6. However, if enough time was given to SAP it would lead to the best solution in each run.

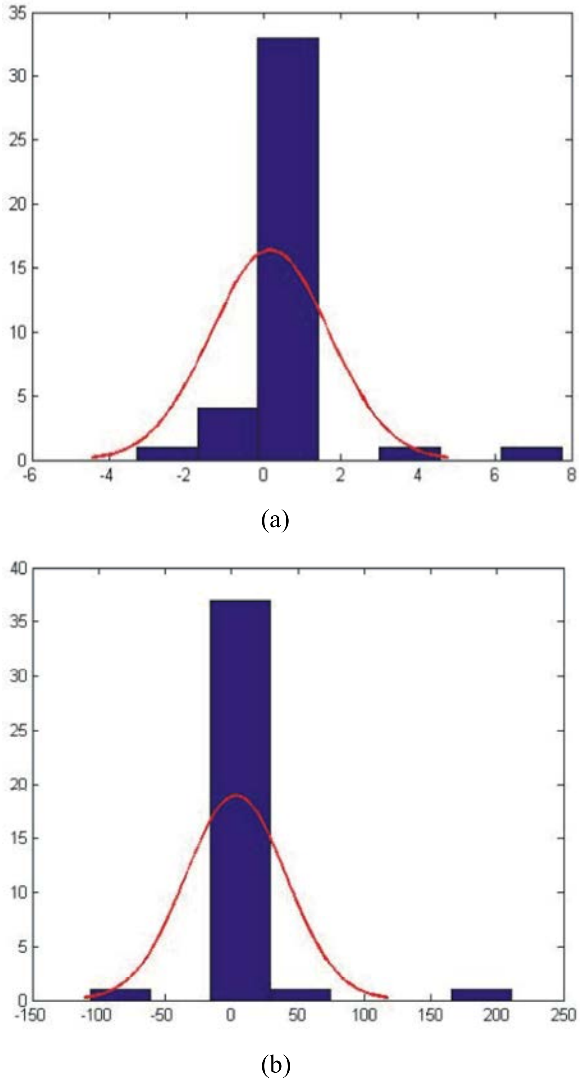

Fig. 6: (a) Error distribution of SAP Model on Test data (b) Error distribution of ANN Model on Test data

CONCLUSION

- The new SAP model can build the models with acceptable accuracy.
- The estimation of the SAP model is near the exact value and usually does not have the huge underestimation and over estimations.
- Different runs of the neural network can lead to different solutions but the results of different runs of SAP are close to each other and to the best solution. Thus just with one run it can be ensured that the best models is found.

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