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Volume II: Applications

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Systems Research Institute
Polish Academy of Sciences
Newelska 6, 01-447 Warsaw, Poland
www.ibspan.waw.pl

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Generalized net model of the process of the prognosis biomass accumulation using TEMPO-amine metal complexes with neural network

Galina Grigorova[1] Krassimir Vassilev[2], Sotir Sotirov[3]
University "Prof . d-r Asen Zlatarov" – Burgas, Bulgaria,
e-mails: [1]galinakirova@abv.bg; [2]kvasilev@btu.bg, [3]ssotirov@btu.bg

Abstract:

The proposed generalized net will give us a possibility for using a feed-forward neural network based on backpropagation algorithm used for prognosis biomass accumulation. The prognosis of the data is very important for many real processes.

Key words: Neural networks, biomass accumulation, prognosis

1. Introduction

Like all live creatures, microorganisms exist in unity and coherence with the environment. From there, they obtain the substances necessary for growth. In the same environment, they excrete the unnecessary substances generated throughout their life. Therefore, the life activities of the microorganisms are in close relationship with the environmental conditions. Every change in these conditions has certain favorable or unfavorable effect on the microbial cell. These effects depend on the biological resistance of the microorganism and the duration and nature of the effects of the changed conditions. In some cases, the changed environmental conditions favor the growth of the microorganisms while in others they slow it down or stop it. In some cases, changes take place in the microorganisms which allow them adapting to the new environment. That is why the study and knowledge on the effects environment exerts on the microorganisms are quite important both for the industrial use of microorganisms and the fight to overcome their negative influences. By deliberate change of conditions, one could accelerate or stop the development of microorganisms, thus eliminating the unwanted and enhancing the growth of the wanted bacterial species.

The chemical composition of the medium has certain effect on the life activity of the microorganisms. Many chemical elements change the medium reaction, stimulate, quell or stop microorganism growth. On the other hand, a great number of chemical substances kill microbial cells at higher or slower rate.

1.1. Influence of medium reaction

Medium reaction, i.e. the degree of acidity or alkalescency, depends on the concentrations of hydrogen (H+) and hydroxyl (HO^-) ions.

Microorganisms require certain medium reaction for their life activity. The optimal medium reaction is different for the different microbial species. Most often it is pH 7,0 but sometimes it varies between 5,0 and 9.0. Some microorganisms grow better in acidic medium (at pH below 7,0): lactic acid and acetic acid bacteria grow best in medium of pH 5.0 while fungi and yeast in media with pH from 3,5 to 6,0.

The change of hydrogen ion concentration (pH) in the medium to values lower or higher than the optimal for certain kind of microorganisms suppresses their life activity and kills them later. The highest resistances to changes in pH have the spores. The change of medium pH changes the electric charge on cell surface, disturbs the colloid equilibrium of the protoplasm and decrease the activity of the microbial enzymes. Thus, cell metabolism is disturbed which results in slower or stopped life activity of the microorganisms.

Some microorganisms change the reaction of the medium during their growth, thus limiting their own growth. For instance, the lactic acid bacteria accumulate such quantities of lactic acid in the medium where they reside which further quells their growth. Other microorganisms regulate the reaction of the medium they live in by themselves. They excrete substances which acidify or alkalify the medium thus inhibiting pH changes to ranges unfavorable for bacteria growth.

1.2.Influence of chemical substances

Chemical substances have varying effects on the microorganisms depending on substance nature, its concentration, duration of presence, etc.

Many chemical compounds have toxic effect on microorganisms. Their influence depends of the nature of the chemical substance and its concentration. At low concentrations, lots of toxic chemical substances facilitate the growth and life activity of the microorganisms. At higher concentrations, some toxic compounds curb life activity without killing the microorganisms. At high concentrations, the toxic substances destroy both vegetative microbial forms and spores, i.e. they act as bactericides.

1.3.Mechanism of action.

The bactericide substances act upon microbial cells by several ways:

After penetrating the microbial cell, the bactericide substance causes protoplasm coagulation. This is the effect of salts of heavy metals, alcohols, phenol, aldehydes, etc.

After penetration the microbial cell, the bactericide substance stems the operation of some enzyme systems. Sulfonamides and antibiotics are examples of this group.

Other substances induce changes in the hereditary factor (DNA). Such effect exert some dyes like acridine orange, etc.

Many bactericide substances accumulate on cell surface, thus disturbing the cell metabolisms.

5.Some substances destroy cell walls and microorganism structure. Such effect exert the quaternary ammonium salts and other surfactants.

2. Experimental

2.1. Preparation of molybdenum complex

To 20 ml bidistilled water, 0.24 g (1.45x10-3 M) TEMPO-amine(4-amino-2,2,6,6-tetramethylpiperidine-1-oxyl) were added and the solution was acidified with diluted nitric acid to pH 2.0 – 2.2. To 20 ml bidistilled water, 0.23 g (6.9x10-3 M) sodium molybdate were added and the solution was acidified with diluted nitric acid to pH 2.0 – 2.2. The two solutions were mixed at room temperature under vigorous agitation. The precipitation obtained was washed with distilled water until neutral reaction. The complex obtained was dried under vacuum at 40°C until constant weight. The complex of sodium tungstenate with TEMPO-amine was obtained by similar procedure.

2.2. Preparation of vanadium complex

To 20 ml bidistilled water, 0,24 g (1.45x10-3 M) TEMPO-amine and 1.83 g (7.25x10-3 M) vanadyl sulphate were added. The solution obtained was stirred intensely at room temperature for 12 h and then kept in refrigerator for 24 h. The precipitate obtained was washed with distilled water until neutral reaction. The complex obtained was dried in vacuum at 40°C until constant weight. The nickel complex with TEMPO-amine was prepared by the same technique

2.3. Antimicrobial activities

The antimicrobial activities of the complexes obtained were determined by comparing the growth cultures in pure nutrient and one containing some of the complexes studied. The optical density was measured at wavelength of λmax 420 nm. All the experiments were carried out on a rotating shaker at 37oC for 12 h, at concentration of antibacterial compounds of 120 mg/L.

The aim of the present work is to study the antibacterial activity of complexes of Tempo-amine with heavy metals on the growth of Escherichia coli bacteria, also here we can use neural networks as a tool for one-dimensional prognosis of the biomass accumulation.

3. Prognosis with multilayer neural network of the Escherichia coli

In a series of papers the process of functioning and the results of the work of different types of neural networks (NN) [4] are described by Generalized Nets [1,2]. Here, we shall discuss the process for prognosis with trained of feed-forward Neural Networks.

The different types of NNs can be implemented in different ways [6] and can be learned by different algorithms [3, 9, 10, 11, 12].

Prognosis with NN allows prognosis for one-dimensional and n-dimensional function and as a base for the base we use neural network learned with BackPropagarion algorithm [3].

During the process of the prognosis with NN we can train it with data that has been once saved. This type of learning data is used as a part of the data provided in the input of the NN and other data – to the output.

The process of learning can be represented in the following order:

- from the series of the data $x_1, x_2, x_3, \ldots\ldots, x_N$, to the input we put m values, where N – number measuring, m – number of inputs of the NN. Let the values be: $P = x_{i+1,} x_{i+2,} x_{i+3,} \ldots, x_{i+m}$, and the output has next value from the series of measurement $T = x_{i+m+1}$ (for i = 0, 1, 2, 3, 4, 5…, N-m-1);
- series from the measurements from the inputs P and the next value from the series T constructed learning couples (P, T), where T is a target. We use the BackPropagation algorithm;
- i begin from zero and increase with 1 to N-m-1.

Process of the prognosis use follow algorithm:

- in the input of the NN we put next m values from the series. The result value come from the output;
- this result value is added to the learning series P with number x_{N+1};
- the next prognosis is based on the series with $N+1$ elements.

Table 1

1	2	3	4	5	6
Time, h	Standard	TEMPO+ VO^{2+}	TEMPO+ Ni^{2+}	TEMPO+ MoO_2^{2+}	TEMPO+ WO_2^{2+}
0	0,155	0.157	0.152	0.154	0.155
1	0.167	0.175	0.174	0.178	0.165
2	0.215	0.188	0.229	0.230	0.210
3	0.407	0.203	0.246	0.250	0.241
4	0.792	0.240	0.269	0.298	0.280
5	1.020	0.288	0.350	0.360	0.350
6	1.271	0.501	0.388	0.401	0.385
7	1.430	0.740	0.510	0.580	0.480
8	1.500	1.011	0.685	0.695	0.650
9	1.565	1.284	0.910	0.920	0.810
10	1.698	1.350	0.950	1.155	0.908
11	1.765	1.400	0.971	1.311	0.975
12	1.780	1.420	1.042	1.488	1.155
13*	1.778	1.394	0.961	1.298	0.984
14*	1.869	1.497	1.189	1.470	1.212
Error.1 %	0.7%	0.4%	1.04%	1.01%	1.02%
Error.2 %	5%	5.6%	6.9%	1.2%	4.9%

In a Table1 we present data for biomass accumulation. Different column present different complexes_added to solution. In first 12 rows are data for real values. The next 2 rows (number 13* and 14*) are prognosis data each type of solution, based on all first eleven values.

As can see the error are small percent. In column 2, 3, 4, and 5 we collect data and after that we made prognosis and calculate error. Only in column 6 we used prognosis.

Based on this data we can see that:

1. The results indicate that the predicted values are identical with the values obtained experimentally for concentration of biomass.
2. Using a mathematical model one can predict the next values from the kinetic curve.
3. Using the “Artificial neural networks” method one can predict the

bacteriostatic effect of complexes of heavy metals on bacteria *E.coli.*

4. A gn-model

The model describing the work and learning of the multilayer perceptron is proposed in Fig. 1.

Initially the following tokens enter in the GN:

- in place S_{data} - β-token with characteristic "biomass data for training of the neural network";
- in place S_{ez} - γ-token with characteristic "least square error for learning";
- in place S_{wb} - δ-token with characteristic "initial value of the weight coefficients and biases".

Initially the following token stays in the GN:

- in place S_{Str} stays α-token with characteristic "available architectures of the feedforward neural networks and transfer functions".

The GN is presented by a set of transitions [1, 2]:

$$A = \{ Z_1, Z_2, Z_3, Z_4, Z_5\},$$

where transitions describe the following processes:
Z_1- Defining of the learning couples $\{p_1, t_1\}$, $\{p_2, t_2\}$, ..., $\{p_Q, t_Q\}$;
Z_2- Calculating the outputs of the neural network (feed forward);
Z_3- Determination $e^2 < E_{max}$;
Z_4- Learning the neural network (backward)
Z_5- Determination learning for the all learning couples.

Transitions of the GN-model have the following forms.

$$Z_1 = < \{S_{Str}, S_{data}, S_{52}, S_{A1}\}, \{S_{11}, S_{12}\}, R_1, M_1, \wedge (S_{Str}, S_{data}, S_{52}, S_{A1}) >$$

$$R_1 = \begin{array}{c|cc} & S_{21} & S_{A2} \\ \hline S_{Str} & True & False \\ S_{data} & False & True \\ S_{52} & True & False \\ S_{A1} & True & True \end{array}$$

In position S_{21} enter token with characteristic "the next learning couples (p,t)".

In position S_{A2} enter token with characteristic ”learning couples $\{p_1, t_1\}$, $\{p_2, t_2\}$, ..., $\{p_Q, t_Q\}$,”.

$$Z_2 = < \{S_{51}, S_{wb}, S_{11}, S_{41}, S_{A2}\}, \{S_{pr}, S_{21}, S_{22}, S_{A2}\}, R_2, M_2, \wedge (S_{a2}, \vee (S_{41}, S_{51}), \vee (S_{11}, S_{wb})) >$$

$$R_2 = \begin{array}{c|cccc} & S_{pr} & S_{21} & S_{22} & S_{A2} \\ \hline S_{51} & True & False & False & False \\ S_{wb} & False & False & False & True \\ S_{11} & False & False & False & True \\ S_{41} & False & False & False & True \\ S_{A2} & False & True & True & False \end{array}$$

In positions S_{21} and S_{22} enter tokens with characteristics ” least square error on the output of the neural network”.

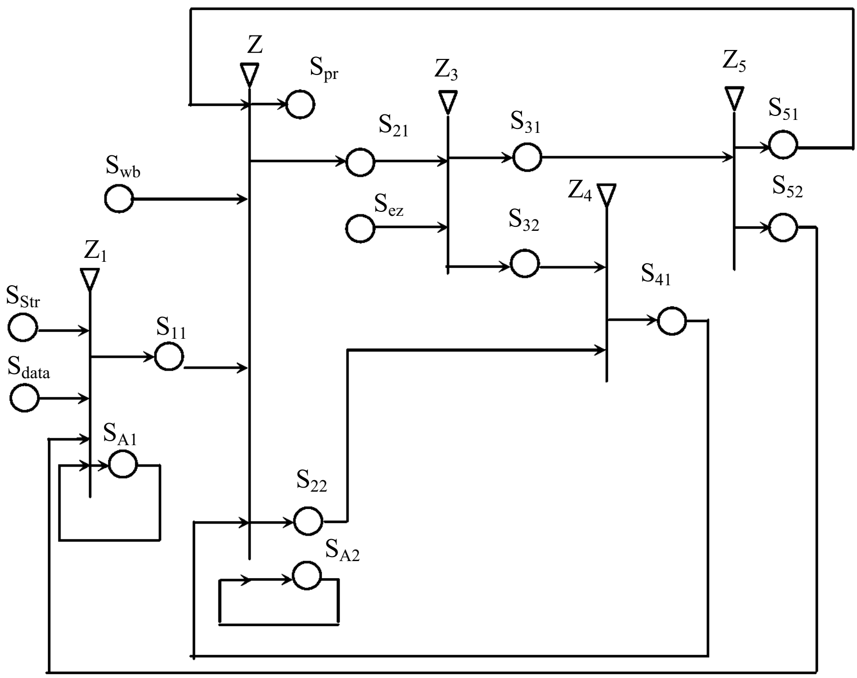

Fig. 1 GN model of the process of the prognosis biomass accumulation with neural network

In position S_{pr} enter token with characteristic "prognosis value from the neural network based on the experimental data".

In position S_{A2} enter token with characteristic "(w,b)".

$$Z_3 = < \{S_{21}, S_{ez}\}, \{S_{31}, S_{32}\}, R_3, M_3, \wedge (S_{31}, S_{ez}) >$$

$$R_3 = \begin{array}{c|cc} & S_{31} & S_{32} \\ \hline S_{21} & W_{21,21} & W_{21,32} \\ S_{ez} & W_{ez,31} & W_{ez,32} \end{array}$$

where:

$W_{21,31}$ = "$e^2 < E_{max}$";

$W_{ez,31}$ = "$e^2 < E_{max}$";

$W_{21,32}$ = "$e^2 > E_{max}$";

$W_{ez,32}$ = "$e^2 > E_{max}$".

The neural network is full learned where $e^2 > E_{max}$

In position S_{31} enter token with characteristic "learned neural network".

In position S_{32} enter token with characteristic " least square error on the output of the neural network".

$$Z_4 = < \{S_{32}, S_{22}\}, \{S_{41}\}, R_4, M_4, \wedge (S_{32}, S_{22}) >$$

$$R_4 = \begin{array}{c|c} & S_{41} \\ \hline S_{22} & True \\ S_{22} & True \end{array}$$

In position S_{41} enter token with characteristic "$W(k+1);b(k+1)$".

$$Z_5 = < \{S_{31}\}, \{S_{51}, S_{52}\}, R_5, M_5, \wedge (S_{31}) >$$

$$R_5 = \begin{array}{c|cc} & S_{51} & S_{52} \\ \hline S_{31} & W_{31,51} & W_{31,52} \end{array}$$

Where

$W_{31,51}$=" $i = N\text{-}m\text{-}1$";

$W_{31,52}$=" $i \neq N\text{-}m\text{-}1$";

In positions S_{51} and S_{52} enters token with characteristics "New weight coefficients and biases ($W(k+1);b(k+1)$) for all learning couples".

5. Conclusions

Prognosis process with neural network allows prognosis of the one and multиfunction based on the feedforward neural network. In this case usually

uses algorithm with backward propagation of the error – BackPropagation. For constructing a model of Feedforward Neural Network are used generalized nets because they allow their simulation and tracing their behavior in future, their management and respectively a selection of proper structure for solving the set problem.
Also we proof that using a mathematical model one can predict the next values from the kinetic curve. Using the "Artificial neural networks" method one can predict the bacteriostatic effect of complexes of heavy metals on bacteria E.Coli.

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The papers presented in this Volume 2 constitute a collection of contributions, both of a foundational and applied type, by both well-known experts and young researchers in various fields of broadly perceived intelligent systems.
It may be viewed as a result of fruitful discussions held during the Eleventh International Workshop on Intuitionistic Fuzzy Sets and Generalized Nets (IWIFSGN-2012) organized in Warsaw on October 12, 2012 by the Systems Research Institute, Polish Academy of Sciences, in Warsaw, Poland, Institute of Biophysics and Biomedical Engineering, Bulgarian Academy of Sciences in Sofia, Bulgaria, and WIT - Warsaw School of Information Technology in Warsaw, Poland, and co-organized by: the Matej Bel University, Banska Bystrica, Slovakia, Universidad Publica de Navarra, Pamplona, Spain, Universidade de Tras-Os-Montes e Alto Douro, Vila Real, Portugal, Prof. Asen Zlatarov University, Burgas, Bulgaria, and the University of Westminster, Harrow, UK:

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The consecutive International Workshops on Intuitionistic Fuzzy Sets and Generalized Nets (IWIFSGNs) have been meant to provide a forum for the presentation of new results and for scientific discussion on new developments in foundations and applications of intuitionistic fuzzy sets and generalized nets pioneered by Professor Krassimir T. Atanassov. Other topics related to broadly perceived representation and processing of uncertain and imprecise information and intelligent systems have also been included. The Eleventh International Workshop on Intuitionistic Fuzzy Sets and Generalized Nets (IWIFSGN-2012) is a continuation of this undertaking, and provides many new ideas and results in the areas concerned.

We hope that a collection of main contributions presented at the Workshop, completed with many papers by leading experts who have not been able to participate, will provide a source of much needed information on recent trends in the topics considered.

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