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Journal of Chromatography A, 722 (1996) 233–243

JOURNAL OF
CHROMATOGRAPHY A

Determining the characteristics of water pollutants by neural sensors and pattern recognition methods

Vitaly Yatsenko

Department of Control Systems, Institute of Cybernetics, Kiev, Ukraine

Abstract

In this paper we have researched the influence of pollutants on such biological objects as photosynthesizing systems in order to reveal the capabilities and features of their application as the controlling sensor in integral ecological monitoring microsystems. It is proposed to elaborate upon the intelligent sensor on the basis of: (1) neural network technologies; (2) the possibility to separate the characteristics of the substances dissolved in water by means of the methods which recognize patterns in a functional space of the fluorescence curves; (3) the results of the chromatographic analysis of standard water samples. This sensor allows to predict water state and to make the optimal decisions for correcting an ecosystem's condition. The efficiency of such a system for water analysis can be improved using the dual measurement principle. This principle suggests identification of a biosensor model according to experimental data.

1. Introduction

Ecological monitoring of the environment is one of the most important tasks of the natural sciences. As a rule, the existing systems used for the analysis and control of an ecological system, function according to the principles of discovery of signs characterizing the actions of certain types of pollutants (direct measurements). At the same time, some pollutants may remain unidentified if the actions of them upon an ecological system are insufficiently explored (i.e., either a physical or a mathematical model may be absent) or if these pollutants cannot be detected with the help of existing monitoring methods. Such imperfections, observed when the ecological monitoring systems are designed, may be overcome if systems oriented to integral pollution sensors are created. In particular, bio-objects in which life processes depend upon the state of the environment can play this role.

Any pollutant exhibits a tendency to be stored in air, water, silt, plants and animals, and disturbs their life. As for severeness, the pollutants may be classified as lethal, dangerous, harmful, latent, indifferent or comfortable. The first three classifications are caused by harmful matters in a bio-object at concentrations of levels about one hundred to one thousand times higher than the limit of possible concentration (LPC). Such concentrations are obtainable in a sufficiently simple way by direct measurements. The LPC-level concentrations, especially when many factors are active, cause hidden, latent reactions. The direct measurement of such pollutants is difficult and is associated with use of very expensive equipment.

SSDI 0021-9673(95)00571-4

Moreover, during the direct measurements, the influence of such pollutants may remain nearly undetected or undetected for a long period of time.

Living objects are sensitive to the influence of low concentrations of pollutants and react upon them when normal physiological processes are disturbed. This feature of bio-objects is proposed as a sensor able to record data about the integral state of an environment.

The author offers a method by means of which the substances dissolved in water can be analyzed under dynamic conditions when separate components interact with the sensitive element containing photosynthetic objects. Since these components influence the objects in a different way, there appears the possibility to separate the characteristics of the components by means of the methods recognizing patterns in a functional space of the fluorescence curves. Contrary to the classic chromatography, this method may find more applications and, moreover, it is adaptable to measurement conditions. Also, it is possible to use the chromatographic data at the sensor training stage, to perform parallel data processing and scientific analysis. The requirements for sample preparation are low.

2. Experimental

2.1. Materials

Plants, algae, photosynthesizing bacteria, extracted reaction centers (RCs), Langmuir–Blodgett–Shefer films taken from reaction centers of *Rh. Sphaeroides* purple bacteria were used to examine the photosynthetic objects. The pure films and the films affected by atrazine solution were investigated experimentally. Also, we examined samples of water taken from different artificial ponds, and such pollutants as heavy metals, chemical toxicants and herbicides of different concentrations were detected there. The samples were characterized by numbers in the range [0,1] and this interval shows the degree of ecological purity of water.

2.2. Methods

The influence exerted by different pollutants on the functional characteristics of the photosynthetic objects in a sensitive element was assessed. The curves of delayed fluorescence and of fluorescence induction were examined for this purpose. The distinctive features of these curves were used to analyze the polluted water. The pattern recognition methods were implemented on a neural chip with probabilistic neurons, and the experimental results obtained for the examined water samples were used to train this chip (the water component composition was known here in advance). The sensitive element characteristics "degradation" was corrected by the method of bilinear identification of the sensor model and the correcting potential on the membrane was changed. All the mentioned methods permit to provide the sensor with the robust features, to implement the principle of dual measurement and to foresee qualitative non-parametric assessments of low concentrations of pollutants in water ponds. The assessments can be further improved if the chromatographic analysis results are delivered to the chip input.

2.3. Apparatus

Fig. 1 depicts the experimental system, which includes: a film-type biosensor; a neural chip based on probabilistic neurons and located at the sensor output (Section 4); and a bilinear model identifier located in the feedback circuit (Section 3). The signals coming from converter 8 and photodetector 6 are the input signals for this identifier. The latter generates the required control signal value at the feedback circuit output. The proposed scheme provides dual control principle realization, and here the biosensor operation mode as well as the mode in which the whole monitoring system functions are thus optimized. When the reverse bilinear system is used as signal converter 8, the neural chip may not be applied.

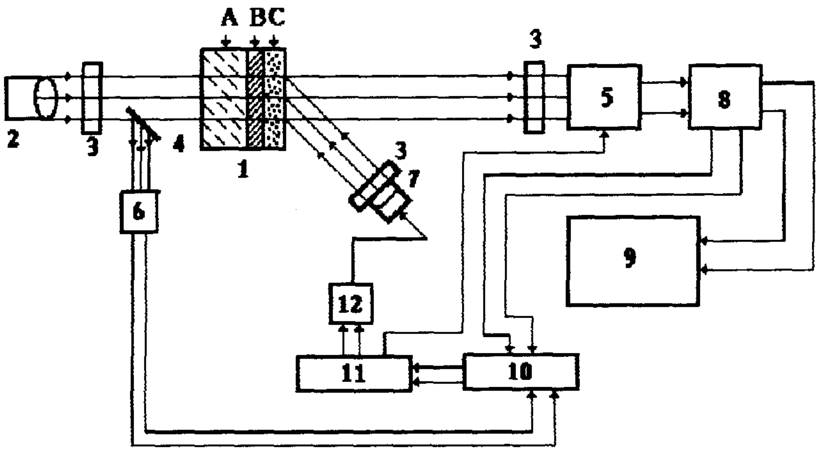

Fig. 1. Experimental eco-object state estimation setup based on a film-type biodetector. 1 = Biodetector (A = crystal plate, B = lipid layer, C = monolayers of purple bacteria RC); 2 = the source of continuous light; 3 = interferometric filters; 4 = semitransparent glass plate; 5 = photodetector with preamplifier, 6 = photodetector with preamplifier and converter; 7 = flash lamp; 8 = signal converter; 9 = neural chip; 10 = bilinear model identifier; 11 = feedback unit; 12 = control signal generator.

2.4. Measurements

At present, many papers are known (or have been published) in which the influence of pollutants on object functioning has been studied.

These investigations were aimed at revealing the influence on both the spectral characteristics of such objects [1–5] and the dynamics of charges in photosynthesizing materials. The results of numerical simulation of photosynthesizing-system dynamics are described in detail in [6–9].

In particular, the essential influence of pollutants on spectral characteristics of radiation of the chlorophyll-bearing materials was discovered. We should also note the papers where influence of pollutants on the kinetics of a charge moving along an electron-transport circuit of photosynthesizing systems is explored. Thus, the existence of different pollutants in a system blocks, at one stage or another, the movement of a photoexcited electron along an electron-transport circuit of photosystems of plants or bacteria and causes, therefore, the disturbance of the kinetics of relaxation of a biological system under its photoexcitation.

Such disturbances are revealed in optical characteristics of photosynthesizing objects in the following ways:

- relaxation times for a system change under pulsed optical excitation in absorption bands of chlorophyll-bearing pigments;
- the slow fluorescence and the form of the induction fluorescence curve are changed when an object is acted upon by continuous optical excitation.

We have analyzed the optical features of some green plants and photosynthesizing bacteria [6,7,10] and the extracting RCs and the Langmuir–Blodgett–Shefer films on their base in order to reveal the possibility to use them in computer-aided ecological monitoring systems. The kinetics of photomobilized electron recombination in photosynthetic bacteria RCs was considered. Analytic solution of equations which describe the electron-conformation transitions in both the limiting cases with "fast" and "slow" diffusion in conformational coordinate space were found. According to the experimental data the conformational potentials of a system with electrons on the pigment and on the primary acceptor were considered. The possibility of electron-transfer efficiency control due to light-induced intensity was shown. Let us dwell on some characteristics which are the most evident ones for application of the bio-objects, namely, green plants and algae, for the above-mentioned purposes.

Fig. 2 depicts the curves of fluorescence induction of green plant leaves that are in a healthy environment and ones that were acted upon for 2 min by an atrazine–water solution (under the LPC-level concentration: about 10^{-5} M). These curves are recorded in no more than 2 min and easily define the features associated with the presence of herbicides in an environment. Such facts make it possible to construct an integral ecological monitoring system on the basis of such a type of a biosensor. Note that the curves of induction of fluorescence of plants are also disturbed when actions of heavy metals and of a wide range of toxicants of chemical nature occur.

Another object of our particular interest is the RC of purple bacteria *Rb. Sphaeroides*. The analysis of their absorption spectra shows essential changes at the wavelength region 750–900 nm under the action of saturating optical pumping. These changes are due to photooxidation of the RC and they manifest also in the recovery kinetics of the RC under pulsed optical excitation. As well established now the herbicides substitute the secondary quinone acceptors from their localization sites in the RC, causing the sufficient changes of RC recovery kinetics. Fig. 3 shows the recovery kinetics of isolated *Rb. Sphaeroides* RC suspensions with (Fig. 3c) and

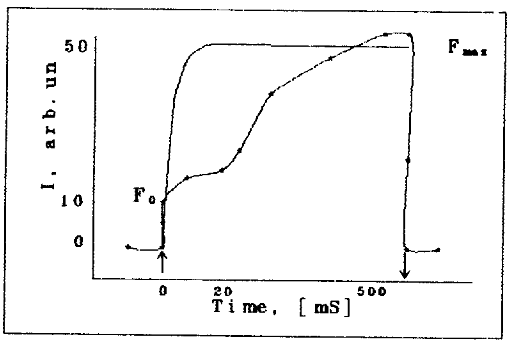

Fig. 2. Curves of fluorescence induction for green plants leaf. Solid line for plants in unpolluted water; (*) for plants in water solution of atrazine. Arrows indicate: ↑ the moment of turning on the acting light; ↓ the moment of turning off the light.

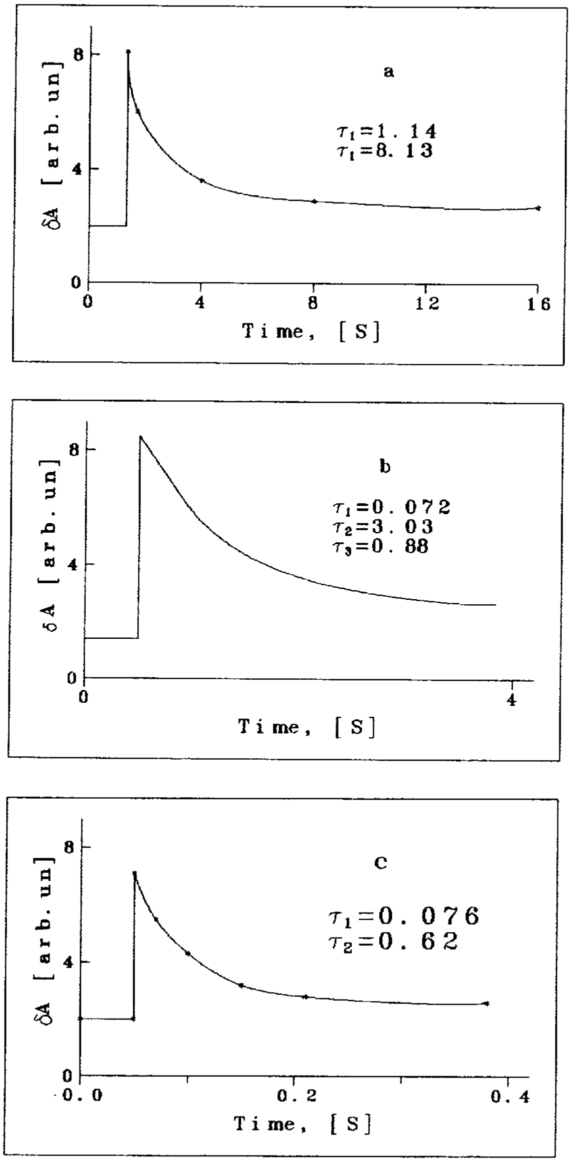

Fig. 3. Electron donor recovery kinetics of *Rb. Spheroids* RCs without addition of inhibitors under pulsed optical excitation: (a) by He–Ne laser ($\lambda = 633$ nm, $\tau = 1$ s); (b) by Xe-lamp ($\lambda = 450$–650 nm, $\tau = 10$ μs). (c) The curve shows the corresponding dependence for a RC suspension with atrazine (10^{-7} M) under Xe-lamp excitation. The times (in s) of the best exponential approximation of the experimental curves by the calculated ones are given in the figures.

without (Fig. 3a, b) addition of herbicides. One can see the presence of only the short-time component in the curves on Fig. 3c. Thus, the herbicides are well detected optically in the experiments on the recovery kinetics of purple bacteria RC suspensions. The main result is that the characteristic time of recovery is much shorter for the samples with herbicides than for those without herbicides.

It is evident that film-type sensors (see this section below) may be essentially more suitable for computer-aided controlled ecological monitoring systems to be designed. We have studied the recovery kinetics of Langmuir films of RC *Rb. Sphaeroides*. Fig. 4a presents the curve for the samples in the natural unpolluted ecological system (water). This curve is almost the same as for suspensions of RC with unblocked electron transition from the primary to secondary quinone acceptor (see Fig. 3a). After immersion of the films into the water solution of atrazine (10^{-5}–10^{-7} M) the electron transfer onto the secondary acceptor was blocked. This was revealed experimentally by increasing of the short-living component weight (Fig. 4b).

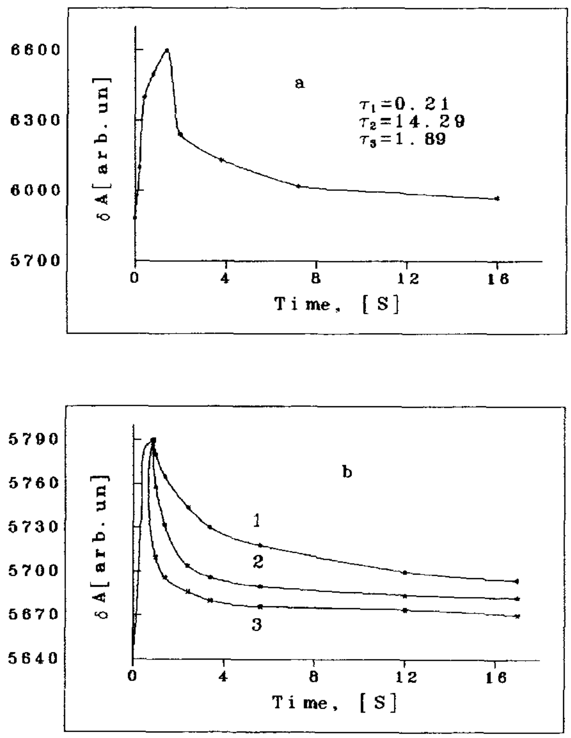

Fig. 4. Electron donor recovery kinetics of Langmuir-film RCs (20 monolayers) following He–Ne laser pulsed (1 s) excitation before (a) and after (b) 5 min processing with an atrazine water solution. The times and the weights of the best exponential approximation of the experimental curve by the calculated one are given in (a). For (b): curve 1 corresponds to the sample processed with atrazine solution of 10^{-7} M [the best approximations with $\tau_1 = 0.21$ (50%), $\tau_2 = 13.0$ (20%), $\tau_3 = 1.89$ (30%)]; curve 2 corresponds to 10^{-6} M atrazine solution [$\tau_1 = 0.21$ (70%), $\tau_2 = 12.0$ (20%), $\tau_3 = 1.89$ (10%)]; curve 3 is for 10^{-5} M atrazine solution [$\tau_1 = 0.21$ (88%), $\tau_2 = 11.11$ (12%)].

One should point out that the studied Langmuir films were of rather good quality, but improvement of their optical characteristics is necessary for further practical application. These films can serve as the basis of the sensors used in ecological monitoring systems, but the task for the nearest future consists in making our sensors more perfect.

In conclusion, it may be noted that right now it is possible to model ecological monitoring systems using (as the biosensors) green plants fixing the useful data, in particular, in the form of a disturbed fluorescence induction curve. On the basis of such sensors, integral ecological monitoring systems can be designed both for separate ecological objects and for more extended systems.

3. Identification of a bilinear approximation to a sensitive biosensor element

The identification of a sensitive biosensor element (SBE) based on approximation of the input–output map with certain simple models has appeared recently.

In the continuous-time case these simple models are bilinear systems (BS), given by:

$$\dot{x}(t) = \left[A_0 + \sum_{i=1}^{p} u_i(t) A_i \right] x(t),$$

$$y(t) = \lambda x(t), \tag{1}$$

where the state is $x \in R^n$ and the (scalar) output is $y(t)$; $u_1(t)$ is measured signal; $u_2(t), \ldots, u_p(t)$ are the control inputs of the biosensor. The approximation result is as follows:

Let $J \subset [0,\infty)$ and $C \subset [C^*(J)]^P$ be compact sets, where $C^*(J)$ denotes the space of continuous functions $J \to R$, with the supreme norm. A functional $J \times C \to R$ is said to be causal if and only if its value in $t \in J$, for $(u_1, \ldots, u_p) \in C$, does not depend on $u_1(r), \ldots, u_p(r)$ for all $t < \tau$; then

Theorem 1. Any causal and continuous functional $J \times C \to R$ can be arbitrarily closely approximated by BSs.
This result has been independently obtained by Susmann [11]. In the discrete-time case, the former result is not valid, as can be seen with the classic counter example $y(t) = u^2(t-1)$. However, a similar result can be shown replacing BSs by state-affiance systems:

$$x(t+1) = \left[A_0 + \sum_{i=1}^{p} f_i(u_1(t), \ldots, u_m(t)) A_i \right] x(t),$$

$$y(t) = \lambda x(t), \tag{2}$$

where $x \in R^n$, $y(t)$ is scalar and $f_i(u_1(t), \ldots, u_m(t))$ are monomials in the inputs $u_1(t), \ldots, u_m(t)$. An input–output map is continuous if and only if for every t the output depends continuously on the inputs $u_1(j), \ldots, u_m(j)$, with $0 < j < t-1$.

Theorem 2. Any continuous SBE map input–output can be arbitrarily closely approximated on a finite time interval and with bounded inputs by state-affine systems.

At the identification stage it seems convenient, for computational reasons, to use discrete models, as presented by Hang Van Mien and Normand-Cyrot [12]. They used a least-squares method on a single-input–single-output SBE, verifying the following conditions: i) the input–output map can be linearized at several operating points, ii) an operating point is described by certain measurable parameters $\theta \in R^{m-k}$ which, in the state-affine approximation, play the same role as control inputs where $u_{k+1}, \ldots, u_m$ are the parameters θ. In applications, the difficulty lies in the determination of the number of parameters, their physical meaning and their relation with the dynamic behaviour of the system. However, we want to present the excellent results obtained when these inconveniences can be overcome, as in the cases presented in the paper referred to.

In spite of what has been previously said, continuous-time analysis should not be discarded, since it is common in practice when processes and systems described by differential equations are found. This is the motivation for our work on the proposed identification method based on an approximating model given by Eq. 1. The technique used is of the Ritz–Galerkin kind [13]. The hypotheses i) and ii) mentioned above are not needed, although it is required that the states of the SBE must be observable.

3.1. Identification procedure

Let $z(t) \in R^n$ be the output variables of an SBE when the inputs are $u_1(t), \ldots, u_p(t)$. Both $z(t)$ and $u(t)$ are assumed to be measured. We shall determine coefficients A_i, $i = 1, \ldots, p$, in such a way that the system in Eq. 1 will produce states $x(t)$ close, in some sense, to $z(t)$, when the inputs are $u_i(t)$ in the time interval $[0,T]$. In order to achieve this, we shall follow the ideas presented in [6]. Let $\{\mu_k(t)\}_{k=0}^{\infty}$ be a basis of $L^2[0,T]$ and define $u_0(t) \equiv 1$. The system in Eq. 1 can be written as:

$$\dot{x}(t) = \left[\sum_{j=0}^{p} u_j(t) A_j \right] x(t). \tag{3}$$

Observe that the apparently more general

$$\dot{y}(t) = \left[\sum_{j=0}^{p} u_j(t) M_j \right] y(t) + \sum_{j=1}^{p} u_j(t) B_j \tag{4}$$

can be written in the form of Eq. 2 by defining

$$x = \begin{bmatrix} y \\ 1 \end{bmatrix}, \quad A_j = [M_j \vdots B_j] \tag{5}$$

with $B_0 = 0$. Integrating Eq. 3, multiplying by γ_k and integrating from 0 to T, results in

$$b_k^t \triangleq \int_0^T \gamma_k [x(t) - x(0)] \, dt$$

$$= \int_0^T \gamma_k(t) \, dt \int_0^t \sum_{j=0}^{p} u_j(s) A_j x(s) \, ds. \tag{6}$$

Calling Γ_k the primitive of γ_k,

$$b_k^t = \sum_{j=0}^{p} A_j \int_0^T u_j(s)x(s)[\Gamma_k(T) - \Gamma_k(s)]\, ds. \qquad (7)$$

The integral on the right-hand side is defined as $(g^{jk})^t$. Eq. 7 can be repeated in k, until the same number of equations as unknowns is obtained. It can be seen that the number of functions γ_k required is $L = (p+1)n - 1$. Proceeding in this manner we obtain the system of equations

$$Qa = b, \qquad (8)$$

where

$$Q = \begin{bmatrix} q^{00} & q^{10} & \cdots & q^{L0} \\ q^{01} & q^{11} & \cdots & Q^{L1} \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ q^{0L} & q^{1L} & \cdots & q^{LL} \end{bmatrix},$$

$$b = \begin{bmatrix} b_0 \\ b_1 \\ \cdot \\ \cdot \\ \cdot \\ b_L \end{bmatrix} (L+1) \times n, \quad a = \begin{bmatrix} A_0^t \\ A_1^t \\ \cdot \\ \cdot \\ \cdot \\ A_p^t \end{bmatrix} (L+1) \times n.$$

Solving the linear system of Eqs. 8, calculate the coefficients of the system in Eq. 3. This solution is always possible because of the linear independence of the γ_k's. Furthermore, it must be noticed that we require $u_i(t) \neq u_j(t)$, $0 \leq i$, $j \leq p$. It is possible to built a rectangular system of the form of Eq. 8 adding equations corresponding to γ_k's with $k > L$; and then solving by least squares. We considered the following equation of the SBE

$$\ddot{y} - ay - by - cy^3 = u(y),$$

or its equivalent

$$\dot{q}_1 = q_2,$$

$$\dot{q}_2 = aq_2 + bq_1 + cq_1^3 + u(t). \qquad (9)$$

The order n of the approximation BS is not known, hence different approximations are made by incorporating additional states. The observed states are (q_1,q_2) and powers and products of q_1 and q_2 are incorporated to augment the dimension of the approximation. This is justified since the functionals of the SBE are analytic, and then we can naturally introduce power series involving those terms. A formal proof and the relationship with Volterra series was given by Brockett [14]. The pollutant characteristics assessment method is presented in [15]. The bilinear models are given by

$$\dot{x} = A_0 x + A_1 xu,$$

where $x \in R^n$ and u contains scalar functions. The identification procedure is used to obtain the matrices A_0 and A_1. The independent functions γ_k used in this example were the Laguerre polynomials.

4. Separation of pollutant characteristics by neural chips

4.1. Requirements for standard samples of polluted water

The present point suggests that it is necessary to make use of a neural chip based on probabilistic neurons and used to recognize the characteristics of water pollutants. It is supposed that the results of chromatographic analysis can be delivered to the chip input. However, when the neural processing method is applied, it can also compete with the chromatographic methods.

In all the cases, when derivation of a mathematical model adequate for an object is not successful at some investigation stage, but there are only experimental data characterizing the behaviour of this object under various disturbing actions, pattern recognition training methods can be used [10].

The main requirements for the pattern recognition training methods are: guarantee of quality and reliability of object state recognition performed by the solution rules yielded by the training process; these solution rules must be easily interpretable and, from the technical point of view, they also must be easily implementable when it is necessary to create a special pattern recognition system; possibility to operate with object properties of different types.

Let us represent some types of pollutant concentration prognostication problems which can be formulated and solved within the framework of the pattern recognition training problem and let us take the water environment state assessment problems as the example when the assessment is made pursuant to indirect measurements.

Assume that the investigation object is the water assay and there exists some measuring facility based on biosensors and an electrical or optical signal is recorded at the facility output. The parameters characterizing such a signal (frequency, phase, amplitude characteristics, etc.) are hereafter referred to as the indirect measurements. Here follow the series of experiments. A water assay is taken and the direct measurements are performed (chemical analysis, etc.) and according to these results an expert (an expert group) yields the integral water quality assessment made according to the proper assessment scale. For instance: "Water" = ("distilled", "spring", "drinking", "industrial", "domestic"), or: " Water" = ("very pure", "pure", "more likely pure", "more likely polluted", "polluted", "polluted very much"). As the result of all such experiments, we have an L-length observation sample V on which the object subsets $V_1, V_2, \ldots, V_m$ ($V = \cup_{j=1}^{m} V_j$; $V_j \cap Vy_k = \emptyset$ when $j \neq k$) are determined and they correspond to the water quality classes (patterns) $V_1^*, V_2^*, \ldots, V_m^*$ identified with respect to the assessment scale. Every object $v \in V$ is described by the vector of values $x = (x_1, x_2, \ldots, x_s)$ of the indirect measurements.

The observation sample V is the data required for the training algorithm to operate. Pursuant to the above-mentioned requirements made with respect to recognition systems, state the pattern recognition training problem as follows.

Let V_j be a subset of training sample objects which corresponds to a pattern V_j^* and let V_j^- be an object subset corresponding to the rest of patterns V_j^*.

It is said that when using the training sample V it is required to find sets of signs in the space where every object set V_j can be separated from the set V_j^- by the solution rule $F(x)$ that belongs to a solution rule set Φ. And here, the quality of recognition of new objects done by the rule $F(x)$ must be guaranteed with reliability $1 - \eta$ and this quality is not lower than the value [8]

$$\epsilon = \frac{\ln N - \ln \eta}{L},$$

as specified in advance. Here N is the extension function of a solution rule set Φ.

To solve the problem in such a statement, recognition training algorithms may be used.

During the training process, the most informative indirect measurements and the ones meeting the pattern sign definition are selected from the indirect measurement set. The final result of the training procedure is the set of solution rules which permit to prognosticate a water state pursuant to the indirect measurements. And the quality and reliability of the work under the new data are guaranteed for the obtained solution rules.

4.2. Separating pollutant characteristics by a stochastic neural chip

The intelligent sensor is the device with the neural chip. We use a neural chip with symmetric recurrent connections where each neural element is stochastic and the firing depends on the weighted sum of inputs.

Let us consider a neural chip consisting of n neurons, and let $w_{ij} = w_{ji}$ be the symmetric connection weight between the ith neuron and the jth neuron. The self-recurrent connection ω_{ii} is assumed to be zero. Let h_i be the threshold of the ith neuron. The potential of the ith neuron is defined by

$$U_i = \sum_{j=0}^{n} w_{ij} x_j. \tag{11}$$

Each neuron changes its state asynchronously depending on U_i, where the new state, x_i, of the ith neuron is equal to 1 with probability $p(U_i)$ and is equal to 0 with probability $1 - p(U_i)$.

The vector $x = (x_1, \ldots, x_n)$ is called the state of the neural chip. A state transition is mathematically described by a Markov chain with 2^n states x. When all the neurons are connected, they form an ergodic Marcov chain, having a unique stationary distribution $\mu(x)$. Every initial state x converges to $f(x)$, and state x appears with relative frequency $f(x)$ over a long course of time.

Let $\nu(x)$ be the probability distribution over x with which an ecological information source emits a signal x. Signals are generated independently subject to $\nu(x)$ and are presented to a neural chip. This chip is required to modify its connection weights and thresholds so that it will simulate the ecological information source. It is required that the stationary distribution $f(x)$ of the neural chip becomes as close to $\nu(x)$ as possible. The learning rule is given by

$$\Delta w_{ij} = \Delta w_{ji} = \epsilon(\nu_{ij} - f_{ij}), \tag{12}$$

where ϵ is small constant, ν_{ij} is the relative frequency that both x_i and x_j are jointly excited under probability distribution $\nu(x)$, and f_{ij} is the relative frequency that both x_i and x_j are jointly excited under $f(x)$, that is, when the neural chip is running freely.

The learning rule is realized by the Hebbian synaptic modification method in two phases [16]. In the first phase, the input learning phase, the connection weight w_{ij} is increased by a small amount whenever both x_i and x_j are exited by an input x; hence, on average the increment of w_{ij} is proportional to v_{ij}. In the second phase, the free or antilearning phase, w_{ij} is decreased by the same small amount whenever both x_i and x_j are excited by the free state transition; hence, the decrement of w_{ij} is proportional to p_{ij} on average.

We consider a situation where the neurons are divided into two parts, namely visible neurons and hidden neurons. Visible neurons are divided further into input and output neurons. In the learning phase, inputs are applied directly to visible neurons. Inputs are represented by a vector $x_{\rm V} = (x_{\rm I}, x_{\rm O})$ for visible neurons, where $x_{\rm I}$ and $x_{\rm O}$ correspond to the states on the input and output neurons, respectively, and components on hidden neurons have meaning in this phase. A visible input $x_{\rm V}$ is generated from the ecological information source. Its joint probability distribution is denoted by $\nu(x_{\rm I}, x_{\rm O})$.

In the working or recalling phase, only the input part $x_{\rm I}$ of the $x_{\rm V}$ is applied. The stochastic state transitions take place under this condition of fixed $x_{\rm I}$, so that the conditional stationary distribution $f(x_{\rm H}, x_{\rm O}/x_{\rm I})$ is realized, where $x_{\rm H}$ denotes the states on the hidden neurons. The distribution can be calculated from the connection weights, thresholds and the fixed $x_{\rm I}$.

In the more general case a Boltzmann machine is required to realize the conditional probability distribution $\nu(x_{\rm O}/x_{\rm I})$ of the ecological state of water as faithfully as possible by learning. The distribution of the state of the hidden neurons is of no concern, but $f(x_{\rm O}, x_{\rm I})$ should be as close to $\nu(x_{\rm O}, x_{\rm I})$ as possible.

It can also be shown [17], that the learning rule gives a stochastic gradient descent of the conditional Kullback information

$$I[\nu;f] = \sum \nu(x_{\rm I})\nu(x_{\rm O}/x_{\rm I}) \log \frac{\nu(x_{\rm I}, x_{\rm O})}{f(x_{\rm I}, x_{\rm O})}, \tag{13}$$

where ν_{ij} denotes the relative frequency of $x_i = x_j = 1$ under the condition that $x_{\rm I}$ and $x_{\rm O}$ are fixed and f_{ij} is the relative frequency in the restricted free run when only $x_{\rm I}$ is fixed.

Another solution of this problem is also possible. Introduce, for instance, the notions "pure water" and "polluted water". According to the direct measurement results, an expert determines the degree of belonging of a given observation object to the "pure water" and "polluted water" notion. The degree of belonging is specified by a number taken from the closed interval [0,1]. For example, if some given observation object is the "pure water" notion standard, then the degree of belonging for it is equal to 1 and, by contrast, its degree of belonging to the "polluted water" notion is equal to 0.

The training is over, and the pattern recognition system yields the prognosis with respect to water quality as the degree of belonging of this observation object to the "pure water" or "polluted water" notion.

Within the framework of the pattern recognition training problem, not only the problem associated with prognostication made with respect to indirect measurements of water quality can be solved, but also the problem of prognostication of concentration of different chemical agents and elements (e.g., herbicides) in this water. In this case, it is guaranteed with reliability $1-\eta$ that the probability of deviation of a prognosticated value from a real value by more than $2g$ does not exceed the value e specified in advance.

5. Results and discussion

1. The theoretical and experimental investigations as well as the sensor signal processing methods and the environment state assessment methods based on neural network technologies are considered here. These investigations can be the basis for improvement of the sensitive sensor elements. The results of studying the neural sensor are based on the novel principles of information processing performed in physical and biological systems. It is proposed here that the intelligent sensor be elaborated on the basis of: 1) neural network technologies; 2) the possibility to use the chromatographic characteristics of different pollution components in water.

2. Experimental investigations were performed using photosynthetic bacteria to study the influence of herbicides on optical properties of the RC. In the presence of herbicides at the LPC-level, essential changes of the RC's recovery kinetics were observed.

3. Langmuir films of *Rh. Sphaeroides* purple bacteria RCs were determined to be a good detector of water pollution.

4. The influence of herbicides, heavy metals and some other pollutants (toxicants) on the operation of the green-plant photosynthesis apparatus was analyzed experimentally. The analysis was performed pursuant to the results concerning the influence on kinetic-fluorescent characteristics of plants. The fluorescence induction curves of green plants adequately reflect their response to unfavourable conditions present in the environment.

5. The choice of a non-linear identification method for biosensor dynamics was substantiated. Algorithms were proposed for identification of the non-linear model with respect to the experimental input and output data and on the basis of the Ritz–Galerkin method. The possibility of performing the system analysis of biosensor dynamics and construction of an inverse model to classify the pollutants was determined [15]. Information was also obtained about the character of the processes running in polluted water.

6. Training algorithms which guarantee the quality and reliability of recognizing the water state are proposed and theoretically substantiated. This quality is not lower than the value specified in advance. In this case, it becomes possible to operate with biosensors of different types.

7. Intelligent sensors provide a new microsystem for treating the wide variety of ecological pollutants. Information geometry that originates from the intrinsic properties of a smooth family of probability distributions is also appropriate to the study of the manifold of sensors. The manifold of simple intelligent sensor with no hidden units is proved to be l-flat and m-flat, so that it possesses nice properties. The present paper, together with [16], is the first step in constructing a mathematical theory of sensors.

Acknowledgements

The author is indebted to the members of the Scientific Foundation of Scientists and Researchers on Molecular Cybernetics and Informatics for the fruitful collaboration during which a number of problems were discussed and for the materials dedicated to the R&D activities which were represented by them. Also, I would like to express my gratitude to Prof. Hiroyuki Hatano and to Dr. Toshichiko Hanai for the great attention paid by them to my research work.

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