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THE CONSTRUCTIVE IMPLEMENTATION OF LIEBIG'S LAW OF THE MINIMUM IN THE PARADIGM OF SYNTHESIS OF A NEURAL NETWORK SUBJECT STATE CLASSIFIER

Abstract. Liebig's law of the minimum is one of the fundamental laws in ecology, which states that the most significant factor for the organism is the factor that deviates most from its optimal value and at the same time most significantly limits the successful life of the organism, being the weakest link in the chain of its ecologic needs. Therefore it is very important to identify the weak link in the life of organisms while classifying and predicting ecologic conditions. However, taking into account ambiguity of the factor influence, compensation of the influence of some factors by others, as well as the synergistic effect of influencing the result, Liebig's law should be considered as a law operating under conditions of a high degree of uncertainty, which makes it difficult to apply it effectively in some cases. **The purpose of the article** is to find a deterministic relationship of input factors with an objective function (a set of indicators of the study subject state), which involves the synthesis of an ensemble of neural network models with forced learning on retrospective data examples, to ensure their adequacy, performance and accuracy, to create an algorithm for modifying the value of input factors for a given class the state of the study subject for a pragmatic, highly effective use of Liebig's law in practice. In the paper it is considered a technology for quantitative evaluation of the determining force of influencing factors on the organism state based on the synthesis of an ensemble of adequate models of the relationship between the space of input factors and the state of the study subject. A quantitative differential evaluation of the influence of input factors on the state of the subject was carried out; the adaptation of input factors to the objective state of the study subject was algorithmized. It expands the possibilities of practical application of the Liebig's law of the minimum, both in the quantitative evaluation of problematic ecologic factors, and in their variations to achieve the required state of the subject. The invariance of the developed technology for the quantitative evaluation of the determining force of the input factors to the features of the subject area has been established, which makes it possible to extend the obtained results to the animal and plant world and emphasizes the universality of the provisions of Liebig's law.

Keywords: Liebig's law of the minimum, neural network, ensemble of neural network models with forced learning.

Introduction

Liebig's law of the minimum, formulated by J. Liebig in 1840, is one of the fundamental laws in ecology. It states that the most significant factor for the organism is the factor that deviates most from its optimal value and at the same time most significantly limits the successful life of the organism being the weakest link in the chain of its ecological needs [1, 2]. Therefore, it is very important to identify the weak link in the life of organisms while classifying and predicting of the ecologic conditions. However, it should be noted that the effect of a certain factor on various body functions is ambiguous: optimum for some processes is not the optimum for others, and vice versa. In addition, the absence or deficiency of some ecologic factors can be compensated by another factor with similar influence. Sometimes there is a synergistic effect of influencing the result and not always in the direction of increasing the positive effect. This allows us to state that Liebig's law should be considered as a law operating in conditions of a high degree of uncertainty, which makes it difficult to apply it effectively in practice in some cases [2-4]. Thus, for its pragmatic, highly effective use in practice, it's necessary to develop a technology for finding the deterministic dependence of the influencing factors on the body state, convert this dependence into a strict analytical and publicly available form and develop an algorithm for fast and reliable modification of the set of input factors to bring the body to the objective (optimal) state.

Purpose of the study is to develop a technology for evaluation of the influence of factors on the body state based on the synthesis of an ensemble of adequate models of the relationship between the space of input factors and the state of the study subject, to provide a quantitative evaluation of this influence and to make algorithm of the adaptation of the input factors to the objective state of the study subject. This expands the possibilities of applying Liebig's law of the minimum, both in quantitative evaluation of problematic ecologic factors and in their variations to achieve the required state of the subject.

Task is to find a deterministic relationship between input factors and an objective function (set of indicators of the state of the study subject), which involves the synthesis of an ensemble of neural network models with forced learning on examples of retrospective data, to ensure their adequacy, performance and accuracy, to create an algorithm for modifying the value of input factors for a given class of state of study subject [3-7].

Results of research

Let's establish the deterministic relationship of input ecologic factors with the state of the subject in the

classical way, using the Kolmogorov-Arnold theorem about the representation of a function of several arguments through the sum of the compositions of functions of one variable [3], taking into account its analytical transformation to the Hecht-Nielsen neural network format [3-4]:

$$y(x) = \alpha \sum_{i=1}^{H} v_i \left(w_{i1}x_1 + w_{i2}x_2 + ... + w_{in}x_n + u_i \right), \quad (1)$$

where H is training sample dimension; α, v are internal parameters of the neural network; n is number of neurons; $w_{i1}, w_{i2}, ..., w_{in}$ are neuron weights. Then the adequacy of this statement (1) is achieved by forced training of the neural network on a representative sample of examples.

Next, it is necessary to calculate the determining force of the input ecologic factors.

It is appropriate to solve this problem using a practical evaluation of the Kharkevich information measure [3,4], with the justification that any purposeful activity is based on information that can be used for differential factor analysis (of biological systems in our case). According to A.A. Kharkevich, there is a deterministic relationship of information with the state and purposeful behavior of the study object. And the measure of the conditionality of the information value is determined by the probability of achieving the objective from the received information at multifactorial influence on the study object [3,4]:

$$I_i^j = \log_2 (P_i^j / P^j), \quad (2)$$

where P^j and P_i^j are the probabilities of objective achieving, respectively, before and after receiving information from the i-th factor; I_i^j is a quantitative measure of the determining force of the i-th factor to bring the study object into the j-th state.

The choice of this measure is due to the meaning of the variables P_i^j and P^j, fixing, respectively, the probability of the object's transition to the j-th state under the influence of the i-th factor and the probability of an arbitrary transition of the object to the same state. Expression (2) directly determines quantity of information I_i^j that affects the object at presence of i-th factor. When quantity of information $I_i^j > 0$, the i-th factor contributes to the transition of the object into the j- th state; when $I_i^j < 0$, it prevents this transition; when $I_i^j = 0$, it does not affect the transition in any way, the object is indifferent to the control action.

In the context of Liebig's law, this property implies the ability to evaluate quantitatively the strength and direction of ecologic factors through the magnitude and sign of the information conditioning them. At the same time, there are no fundamental restrictions on the nature of the study object, the determining force and the number of influencing factors, which is essential when justi-

fying the application of this approach to modeling the scheme for implementing Liebig's law of the minimum. In this case, the decision-maker has information about the determining force of all input factors without exception.

With this approach, the practical solution of this problem is reduced to minimizing the error function of an artificial neural network during its forced training on the examples of the set of initial historical data in a given subject area [3-7]. In practice, the problem of synthesizing of an adequate neural network is solved expertly on the platform of a standard package of technical data analysis [8].

Thus, the algorithm for implementing Liebig's law of minimum can be represented as follows: the states of the study subject, as images, are described in the language of their informative features, transformed into a representative sample of historical precedents, fed to the input of a neural network with a variable structure, teaching methods, initial conditions, etc. [4]. After training the ensemble of models, the best one by performance, accuracy and speed is selected from it. If necessary, a separate application is created, for example, in the "macro" option implementation mode.

Expanding the capabilities of Liebig's law, it is appropriate to implement the option of modifying the values of input factors for a given state of the study subject. This is achieved by forming a residual (error) function between the current and target state of the study subject of the form:

$$E(X) = \frac{1}{2} \sum_{i=1}^{M} (y_i(x) - y_{iz})^2, \quad (3)$$

where $y_i(x)$ and y_{iz} are, respectively, the current and objective vectors of the state indicators of the study subject. Next, the gradient of this error is calculated by the vector of input ecologic factors and the modification of the space of input factors is based on the following computational procedures [3]:

$$X^{t+1} = X^t - \eta_1 \cdot grad\ E(X^t), \quad (4)$$

where

$$grad\ E(x_1, x_2, ..., x_n) = \begin{Vmatrix} \dfrac{\partial f}{\partial x_1}(x_1, x_2, ..., x_n) \\ \dfrac{\partial f}{\partial x_2}(x_1, x_2, ..., x_n) \\ .... \\ \dfrac{\partial f}{\partial x_n}(x_1, x_2, ..., x_n) \end{Vmatrix} \quad (5)$$

are components of residual function gradient.

Instrumental implementation of these computational procedures is carried out by one of the known methods, for example, by the method of synthesis of a dual neural network [3, 4]. In the process of neural network model training two types of gradient of a complex function are implemented: first one is formed from the partial derivatives of the network error function by its

weight coefficients; the second one is formed from the partial derivatives of the mismatch function of the current and objective states according to the set of input control factors [7]. The functional diagram of the process is shown in Fig. 1.
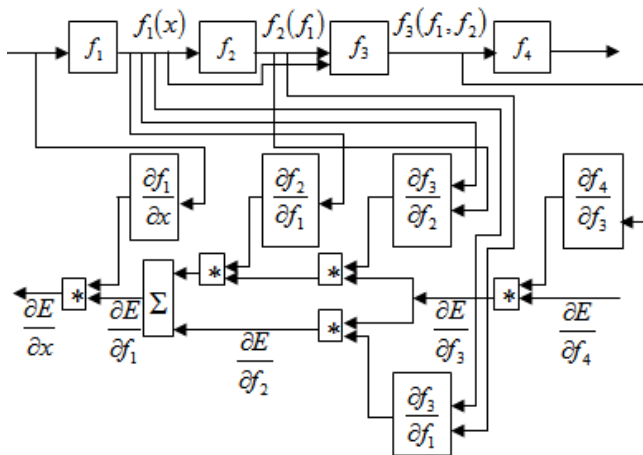

Fig. 1. The functional diagram of the synthesis of a dual neural network

The current state $y_i(x)$ is instrumentally estimated in the process of solving of $y_i(x)$ classification problem arising from a more general formal problem of pattern recognition according to the following rule:

$$G\left[H\left(\omega,\left\{\omega_g\right\}\right)\right], \Rightarrow Sup, \qquad (6)$$

where $\left[H(\omega,\left\{\omega_g\right\})\right]$ is the rule for assigning a subject to the appropriate class (k), $\omega_g \in \Omega_k$, $\left\{\omega\right\}$ is set of objects in the class. Solution of (6) is achieved by optimizing of rule (6) using one of the well-known methods [3, 4].

In order to form a training sample from the database, it was used real information about the number of sick patients, depending on the ecologic load in the region (Fig. 2). Based on this set, a training sample was formed with the allocation of three classes based on their description in the space of 10 features (ecologic factors) (Fig. 3).

The neural network training procedure is implemented on the platform of a standard package of technical data analysis by a neural network module in the "Decision Wizard" and "Network Designer" modes with a variety of training methods, types of models, sample power, dimension of input factors, activation functions, architecture and network complexity [3, 8].

In our example, the performance acceptable for practice (97%) in the classification mode was achieved within (50-70) learning epochs, which is clearly illustrated by the table of characteristics of synthesized neural networks and training graphs for the best models from the entire saved ensemble (Fig. 4, 5)/

The stable convergence of the iterative process and the performance acceptable for practice on the training and test sets, as well as the test control of the user's observations by the values of the user corresponding to the true classes [3,4] allow us to assert that the synthesized models adequately implement the analytical deterministic dependence (1) of the subject's states on the set of input ecological factors. Thus it is possible to convert efficiently the results of the approximation of the sought functional dependence (1) into an evaluation of the determining strength of each factor on class of the subject's state. This task was instrumentally solved by activating the sensitivity evaluation option of the neural network module of the technical analysis package [8], and the result is presented in (Fig. 6) for the network with the best performance from the final ensemble of models (Fig. 4).

Код места	Числ. Насел. Тыс.чел овек	Число обращ.	%	NO	SO2	CO	Cn(H2 O)n	MnO2	NH3	SiO2	C6H5C H3	CH3(CH2) 3OOCH	CH3C OCH3
1	1317.2			4841,78	11348	7253,4	589,29	2,05	1111	480,97	79,14	19,81	33,27
2	296.2	13277	4,48	2836,73	4748	2504,7	31,31	0,36	1006	20,09	37,44	10,04	26,66
3	21.0	11971	57.1	30,31	567,7	189,59	4,65	0,01	17	3,47	0,09	0,02	0,03
4	69.7	8959	12,85	172,81	290	628,68	15,23	0,11	2,68	107,87	12,29	1,61	1,06
5	88.7	11996	13.52	120,1	420	361,32	8,97	0,17	7,3	11,02	1,38	0,36	0,66
6	49.3	14877	30.18	30,59	208,9	309,83	15,13	0,03	2,6	8,37	1,95	0,4	0,7
7	42.6	15502	36.39	19,74	171,9	85,9	2,89	0,01	3,08	4,65	0,5	0,19	0,07
8	45.6	12423	27.24	45,89	66,99	95,42	6,25	0,01	4,1	1,37	0,07	0,04	0,01

Fig. 2. Fragment from the data set of the ecological load of the regions

1 Пер1	2 Пер2	3 Пер3	4 Пер4	5 Пер5	6 Пер6	7 Пер7	8 Пер8	9 Пер9	10 Пер10	11 НовПер
2836,73	4748,08	2504,72	31,31	0,36	1005,71	20,09	37,44	10,04	26,66	1
30,31	567,72	189,59	4,65	0,01	17	3,47	0,09	0,02	0,03	3
172,81	289,97	628,68	15,23	0,11	2,68	107,87	12,29	1,61	1,06	1
120,1	419,96	361,32	8,97	0,17	7,3	11,02	1,38	0,36	0,66	1
30,59	208,9	309,83	15,13	0,03	2,6	8,37	1,95	0,4	0,7	2
19,74	171,92	85,9	2,89	0,01	3,08	4,65	0,5	0,19	0,07	3
45,89	66,99	95,42	6,25	0,01	4,1	1,37	0,07	0,04	0,01	2
45,06	569,2	218,76	2,63	0,01	5,96	30,35	1,34	0,12	0,06	2

Fig. 3. Fragment of a training sample with 10 variables and 3 classes

N	Архитектура	Производительность обуч.	Контр. производительн ость.	Тест. производительн ость.	Алгоритм обучения	Функция ошибки	Ф-я актив. скрытых нейр.	Ф-я актив. выходных нейр.
2	MLP 10-8-3	99,00498	100,0000	97,61905	BFGS 75	Энтропия	Гиперболическая	Софтмакс
3	MLP 10-8-3	84,07960	92,8571	76,19048	BFGS 16	Энтропия	Гиперболическая	Софтмакс
4	MLP 10-8-3	97,51244	92,8571	90,47619	BFGS 66	Энтропия	Гиперболическая	Софтмакс
5	MLP 10-8-3	97,01493	97,6190	95,23810	BFGS 58	Энтропия	Гиперболическая	Софтмакс
6	MLP 10-8-3	96,51741	92,8571	88,09524	BFGS 76	Энтропия	Гиперболическая	Софтмакс

Итоги моделей (Таблица)

Fig. 4. The characteristics of the ensemble of synthesized models
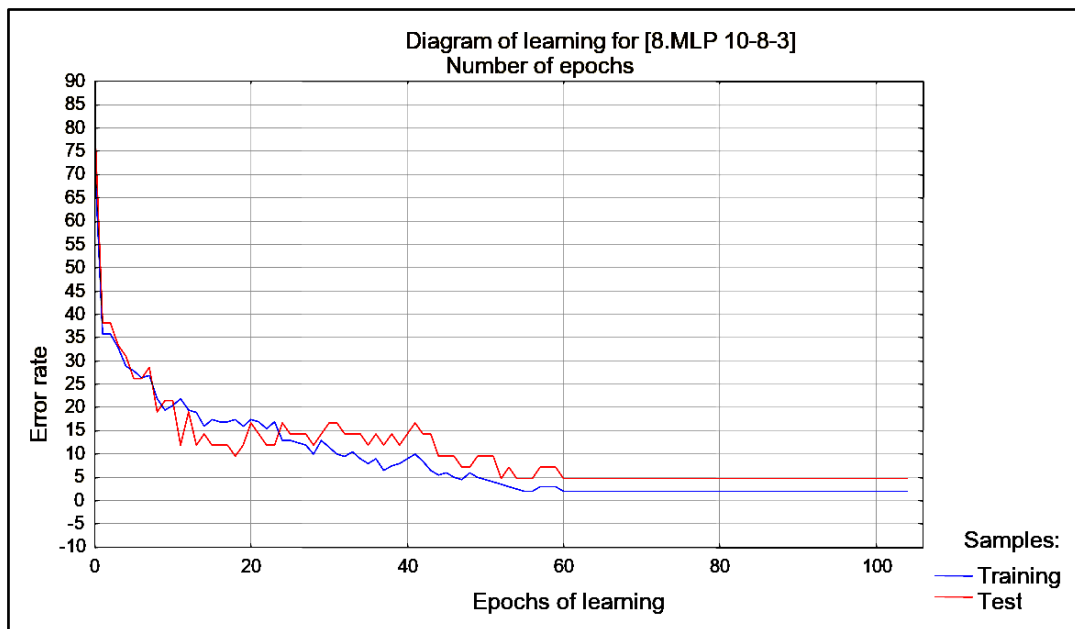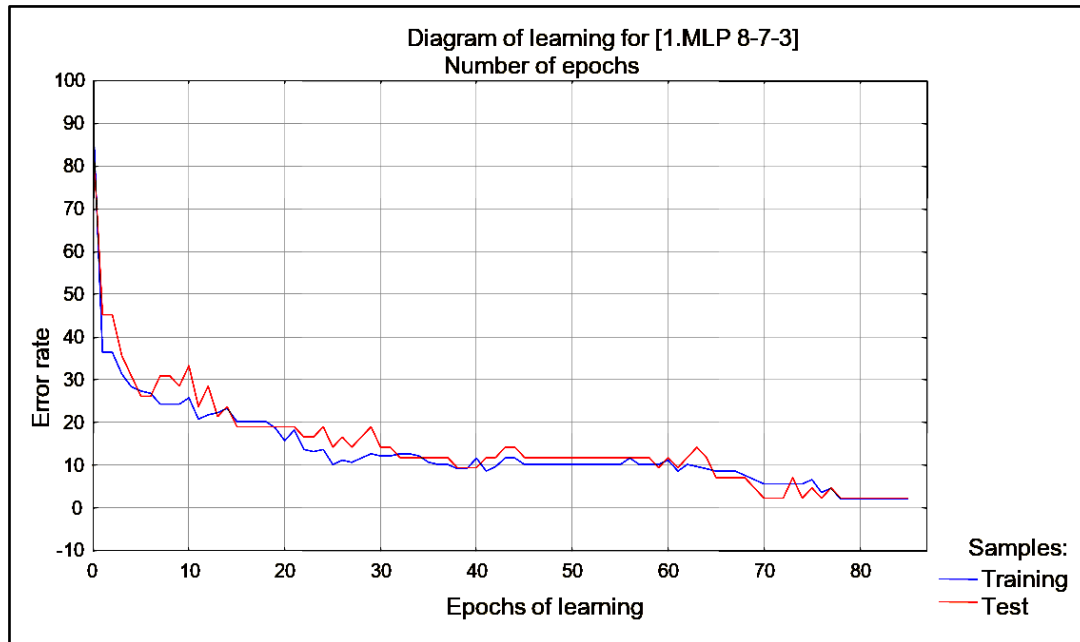
Fig. 5. Diagrams of convergence of the learning process under different initial conditions

Сети	Пер10	Пер1	Пер3	Пер5	Пер6	Пер7	Пер8	Пер4	Пер9	Пер2
6.MLP 10-8-3	79,07091	38,29908	32,07745	28,77438	28,66677	18,06126	16,18869	14,53044	7,581324	6,227305

Чувствительность (Таблица данных1)
Выборки: Обучающая

Fig. 6. Results of evaluation of the relative sensitivity of input factors

The higher the sensitivity of the factor, the more I_i^j – quantitative measure of the determining force of the *i*-th factor to transfer the study object into the *j*-th state according to expression (2).

This is the solution of the problem of constructive implementation of the Liebig's law of minimum, when a differential quantitative evaluation of the determinative force of each factor on the state of the study object is obtained.

After that, it is not difficult to select expertly the user values for a given state of the subject or automatically activate an algorithm for search of the required ratio of factors to ensure the objective state, implementing a functional scheme for the synthesis of a dual neural network (Fig. 1).

In this case, Liebig's law acquires an additional property: not only to fix the degree of influence of each factor on the study object, but also to purposefully change the state of this object by expert or program modification of the values of the input set of factors.

Conclusion

It was developed a technology for quantitative evaluation of the determining force of influencing factors on the organism state based on the synthesis of an ensemble of adequate models of the relationship between the space of input factors and the state of the study subject. A quantitative differential evaluation of the influence of input factors on the state of the subject was carried out; the adaptation of input factors to the objective state of the study subject was algorithmized. It expands the possibilities of practical application of the Liebig's law of the minimum, both in the quantitative evaluation of problematic ecologic factors, and in their variations to achieve the required state of the subject. The invariance of the developed technology for the quantitative evaluation of the determining force of the input factors to the features of the subject area has been established, which makes it possible to extend the obtained results to the animal and plant world and emphasizes the universality of the provisions of Liebig's law.

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Конструктивна реалізація закону мінімуму Лібіха в парадигмі синтезу нейромережного класифікатора станів суб'єкта

С. П. Альошин, О. М. Гайтан, О. Є. Зима

Анотація. Закон мінімуму Лібіха – один з фундаментальних законів в екології, який гласить, що найбільш значущий для організму той фактор, який найбільше відхиляється від його оптимального значення і при цьому найбільш істотно обмежує успішну життєдіяльність організму, будучи найслабшою ланкою в ланцюзі його екологічних потреб. Тому під час класифікації та прогнозуванні екологічних умов дуже важливо визначити слабку ланку в житті організмів. Однак з огляду на неоднозначність впливу факторів, компенсацію впливу одних факторів іншими, а також наявність синергетичного ефекту впливу на результат, можна констатувати, що закон Лібіха слід розглядати як закон, що діє в умовах високого ступеня невизначеності, що в ряді випадків ускладнює ефективність його застосування на практиці. Мета статті – знайти детермінований зв'язок вхідних факторів з цільовою функцією (набором показників стану суб'єкта аналізу), що передбачає синтез ансамблю нейромережевих моделей з примусовим навчанням на прикладах ретроспективних даних, забезпечити їх адекватність, продуктивність і точність, створити алгоритм модифікації значення вхідних факторів під заданий клас стану суб'єкта дослідження для прагматичного, високоефективного використання закону Лібіха на практиці. В роботі розроблена технологія кількісної оцінки детермінуючої сили факторів, що впливають на стан організму, на основі синтезу ансамблю адекватних моделей зв'язку простору вхідних факторів зі станом суб'єкта аналізу. Проведена кількісна диференціальна оцінка впливу вхідних факторів на стан суб'єкта, алгоритмізована адаптація вхідних факторів до цільового стану суб'єкта дослідження. Це розширює можливості практичного застосування закону мінімуму Лібіха, як у кількісній оцінці проблемних екологічних факторів, так і в варіаціях ними для досягнення необхідного стану суб'єкта. Встановлено інваріантність розробленої технології кількісної оцінки детермінуючої сили вхідних факторів до особливостей предметної області, що дозволяє поширити отримані результати на тваринний і рослинний світ та підкреслює універсальність положень закону Лібіха.

Ключові слова: закон Лібіха про мінімум, нейронна мережа, ансамбль нейронних мережевих моделей з примусовим навчанням.