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THE METHODOLOGY OF MATHEMATICAL MODELING IN INFORMATION-ANALYTICAL SYSTEMS OF THE SCIENTIFIC SPHERE

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ABSTRACT

Currently, the information-analytical systems are widely applied to solve problems of information support and to justify decision-making in the management of complex systems for various purposes, including in the scientific sphere. Since the mathematical models for the analysis of the science development, when making management decisions, are of the utmost importance, the authors focus on the need to include the mathematical modeling subsystem in the information-analytical systems of the scientific sphere. The article presents the methodological issues of development of a complex of mathematical models of different levels. It is concluded, that the estimate of the state of the scientific sphere, forecasting its development and analysis of consequences of possible management decisions according to the results of modeling on the offered set of mathematical models will improve the effectiveness of the made decisions.

Keywords: *Scientific Sphere, Information-Analytical System, Scientometrics, Mathematical Modeling.*

1. INTRODUCTION

The question of mathematical modeling of the scientific sphere was prepared by extensive researches in this sphere, from the philosophical understanding of science as a phenomenon [7] to constructing qualitative models of the science development [6], [13]. The application of methods for the science research by measuring publishing activity parameters has led to the emergence of scientometrics, which helped to identify many empirical regularities in the scientific sphere [2], [11], [9], [10]. The achievements in studies of thermodynamics of nonequilibrium systems and discovery of self-organizing complex systems contributed to the emergence of science synergetics [23], [12], [15], the mathematical apparatus of which is extensively used in the modeling of social and economic systems and can be applied to research of science itself, as a social system [21], [22], [8], [17].

In recent years, the information-analytical systems (IAS), developed to provide information-analytical support of the tasks of managing complex systems of various levels from business concerns to large industrial regions, have been widely spread [1], [19]. IAS for collecting, analysis and processing of data are widely used in the scientific sphere (ISTINA – Intelligent System Case Studies of Scientific and Technical Information. MSU // (Electronic resource); Information-analytical system “Nauka”. Samara State Technical University // (Electronic resource)).

A remarkable feature of IAS is an opportunity of collecting primary data from diverse data sources. Data may have different presentation formats and be located in different storage systems, from simple text tables and drawings to databases, including in the sub-level IAS.

In the current IAS extraction, transformation and loading of data is carried out using specially created ETL-tools (extraction, transformation, loading).

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They contain functions and protocols of data extraction from various transaction low-level sources, their transformation and consolidation, as well as loading into target analytic databases – data warehouses and data marts. At the transformation stage the necessary calculations are carried out and data redundancy is eliminated.

Data warehouses, being one of the main parts of the IAS architecture, are primary data sources for comprehensive analysis of all information, available at the given level of the IAS architecture. Data marts are built, as a rule, on the information from the data warehouse and are more specialized data sources for analytical processing. The analytical IAS block accumulates modern software tools allowing to conduct comprehensive analysis of information. They help you successfully to navigate through large amounts of data, to analyze information, to make objective conclusions on the analysis and to make reasonable decisions, to make forecasts, reducing the risks of making wrong decisions to the allowable minimum.

Data mining tools are used by analysts for access to information, its visualization, multidimensional analysis and formation of reports, both predetermined in a form and structure and arbitrary ones. As input information for business analysis are pre-processed data from the data warehouse or presented in data marts.

In IAS of the scientific sphere due to their specific nature tools for data analysis should contain a rather powerful block of mathematical modeling and forecasting the science development in addition to the universal methods: statistical data analysis, OLAP (online analytical processing), etc.

2. METHODS

It is impossible to manage a complex dynamic system, which science is, without knowing its internal characteristics. The application of mathematics in the science research is complicated, first of all, by lack of clear quantitative characteristics reflecting such concepts as scientific knowledge, scientific productivity, value of a scientific result, etc. However, some parameters, describing the scientific process, are still subject to exact measurement, in particular, the number of scientific publications. Besides, the methods of qualitative research of dynamics of the development of science, as a complex system, can say a lot of things about its state and prospects.

To solve the problems of statistical forecasting, as well as to make simulation modeling of the scientific process knowledge of the laws of distribution of the scientific productivity to an array of publications and an array of researchers is of paramount importance.

Today, the Zipf-Pareto distribution law, which seems to reflect the underlying structural characteristics of complex systems, which contribute to the integrity and sustainability, agrees with the experimental data [21].

$$p(x) \sim \frac{\alpha}{x^{\alpha+1}}, \quad (1)$$

where $\alpha=\mu/\lambda$ – characteristic distribution exponent, λ – intensity of the process, μ – distribution parameter.

The offered method of constructing the mathematical model of dynamics of the scientific activities and its verification consists in the following: we describe a model of the scientific activities, forming an array of information (for example, an array of scientific publications), on the basis of enough plausible hypotheses. If the structural regularities of the obtained array coincide with the Zipf-Pareto law, the plausibility of the model will be rather high.

The external regulation of parameters of the complex system, which is especially connected with the structural changes, requires qualitative research of the system behavior. It is important to clarify the states of the system stability in this case.

For the qualitative description of dynamics of the system by mathematical methods the most promising is using the conclusions of nonlinear thermodynamics [23], which are applied to modeling of complex systems of various nature. As first approximation we can consider formalization of the known qualitative model of the science development of T. Kuhn [6] by methods of nonlinear thermodynamics.

According to T. Kuhn development of science has a stick-slip nature and occurs by “scientific revolutions” which divide the long periods of “normal science”. During these periods, the scientists obtain research results within the dominant paradigm. Thus “anomalous” discoveries, which can not be explained from the standpoint of the current paradigm, are accumulated. When the number of “anomalous” discoveries and facts exceeds some critical volume, there is a crisis of the accepted system of scientific concepts. During the crisis, the standard limitations are weakened, and there is a plenty of competing hypotheses. From a

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plenty of hypotheses one, which serves as a new paradigm, is selected. There is a stick-slip transition of science to the new qualitative state and the new period of "normal science" starts.

The offered method consists in presenting science as an open non-linear thermodynamic system, the development of which can be considered as the consecutive transition from the current state to the number of states with decreasing entropy (increase in the system organization), and the initial state must be quite far from the equilibrium one. It is known, that next to the stationary state (thermodynamic equilibrium) Prigozhin's theorem of minimum entropy production in such states is valid [15], the system is stable and not able to develop.

For systems, far from equilibrium, as a result of nonlinear effects a situation, in which the system becomes unstable when changing the corresponding parameters, emerges. These systems acquire an ability to the evolutionary development, because, becoming unstable, they acquire a property to pass to the new stationary state with lower entropy (greater structural complexity) as a result of fluctuations or other processes. An important question arises: whether an artificial transition of the system to the required structural state is possible, and what are the conditions of stability of its functioning?

Regulating the scientific activities is really used not in all science as a whole but in the particular, rather narrow spheres of scientific research. They are characterized by rather serious limitations. These limitations include: knowledge intensity of the research area, amount of financing, etc.

According to the offered method the research activities of the limited scientific community in the limited subject area in the simplified form can be presented as the development of biological population. This will allow to use a rather well developed mathematical apparatus of modeling dynamics of similar systems.

3. RESULTS

3.1. Mathematical Model Of Dynamics Of The Scientific Activities

Let us present the mathematical model of the scientific activities as a randomized branching multiplication process with increasing productivity and limited work of time in the subject area. We introduce a notion of the scientist's state, which is characterized by the number of articles, published by him, x, and the transition from one state to another one means publishing a new scientific article. The probability of such transition is equal to the probability of writing and publishing a new article. A flow of the published scientific articles can be considered as sequence of rare events. The probability of writing of an article at the moment must depend on the number of articles, which have been already written by a scientist, i. e. the probability of transition to the new state at interval t, t+Δt must be a function of the state, in which a scientist is at the moment t. These assumptions allow us to consider our process as the Poisson process of pure multiplication [3]. It means, that the process of formation of an array of publications can be considered as the stochastic process of Markov type which is defined by the following postulates:

- probability of transition $x \to x + 1$ at interval t, $t+\Delta t$ is $\lambda(x)\Delta t + o(\Delta t)$, i.e. it is proportional to interval Δt;
- probability of two and more transitions for Δt is $o(\Delta t)$, i.e. it is negligible;
- probability of lack of transitions at interval Δt is $1 - (\lambda(x)\Delta t + o(\Delta t))$ respectively.

Now we can find the probability of scientist's being in the state x at the moment $t+\Delta t$:

$$p_x(t + \Delta t) = (1 - \lambda(x)\Delta t)\, p_x(t) + \lambda(x - 1)\,\Delta t\, p_{x-1}(t) + o(\Delta t). \qquad (2)$$

In the limit at $\Delta t \to 0$ we obtain a system of differential equations for the probability of scientist's being in the state x at the moment t.

$$\frac{dp_0}{dt} = -\lambda_0 p_0(t),$$
$$\frac{dp_x(t)}{dt} = -\lambda(x)p_x(t) + \lambda(x-1)p_{x-1}(t), x = 1,2,. \qquad (3)$$

We believe, that $p_x(0) = \begin{cases} 1, x = 1, \\ 0, x \neq 1, \end{cases}$

i.e. at the initial time a scientist has only one published article.

We assume, that $\lambda(x) = \lambda x$, i.e. density function of the transition to the new state is linear dependence on the previous state with proportionality coefficient λ.

Solving the system of differential equations (3) for the probability of scientist's being in the state x at the moment t.

$$p_x(t) = \begin{cases} e^{-\lambda t}(1 - e^{-\lambda t})^{x-1}, x = 1,2,\ldots, \\ 0, x = 0, \end{cases} \qquad (4)$$

Then the mathematical expectation of the process (an average number of articles which have been written by a scientist for time t) can be expressed by the formula

$$x_t = e^{\lambda t}, \qquad (5)$$

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which coincides with the law of exponential growth of number of publications, well-known in the science of science, and is experimental confirmation of our model.

In the scientific sense parameter λ can be interpreted as a relative increase in the number of articles per time unit. This can be seen by differentiating mathematical expectation:

$$\frac{dx}{dt} \equiv \dot{x}_t = \lambda \dot{e}^{\lambda t} = \lambda x_t, \quad (6)$$

from which we obtain $\lambda = \frac{\dot{x}_t}{x_t}$.

To obtain the distribution of the scientific productivity of scientists to the information array of scientific publications, this value should be averaged over a plenty of scientists with different time of work on the given subject. Let us make an elementary assumption, that the probability of termination of work on the given subject is constant at each moment of time and is defined by two factors: the increasing productivity in solving new tasks due to experience acquisition in the given field (number of articles which have been already published) and the increasing difficulty of finding new tasks due to exhaustion of the subject. We come to the exponential distribution of time of work in the given scientific sphere:

$$p(t) = \mu e^{-t\mu}, \quad (7)$$

where $\mu = 1/t_{av}$, t_{av} – average time of work of scientists in the given subject area.

Thus, taking into account that $p_x(t) \equiv p(x/t)$, we write:

$$p(x) = \int_0^\infty p(t)p(x/t)dt = \int_0^\infty \mu e^{-t\mu} e^{-\lambda t}(1-e^{-\lambda t})^{x-1} \quad (8)$$

Having integrated this expression, we obtain the distribution proportional to the beta function:

$$p(x) = \frac{\mu}{\lambda} B\left(x, \frac{\mu}{\lambda}+1\right) = \alpha B(x, \alpha+1), x = 1, 2, \quad (9)$$

where

$B(x, \alpha+1) = G(x)G(\alpha+1)/G(x+\alpha+1)$ - beta function;

$G(x)=(x-1)!$ – gamma function; $\alpha=\mu/\lambda$ – characteristic exponent.

We can show, that at $x \to \infty$

$$G(x)/G(x+\alpha+1) \to \frac{1}{x^{\alpha+1}}. \quad (10)$$

Substituting this expression into the formula for the probability distribution, we obtain:

$$p(x) \sim \alpha G(\alpha+1)\frac{1}{x^{\alpha+1}}. \quad (11)$$

Assuming, that for small α

$$G(\alpha+1) \approx 1, \quad (12)$$

we obtain a normalized form of the Zipf-Pareto law:

$$p(x) \sim \frac{\alpha}{x^{\alpha+1}}. \quad (13)$$

Thus, we can state with enough certainty, that the mathematical model, presenting the scientific activities, as a randomized branching multiplication process with increasing productivity and limited work of time in the subject area is to a certain extent adequate to the nature of the process, being modelled.

3.2. Qualitative Mathematical Models Of The Science Development

Very promising for qualitative predictive estimates of dynamics of various aspects of the scientific sphere is a mathematical apparatus of the catastrophe theory [14]. The base of this theory is a notion of the structural stability of the system in terms of the stability of the phase portrait of the dynamical system in relation to the change of its parameters. At the boundaries among these stable structures the critical modes appear, upon the transition through which the phase portrait changes in the process of changing the control parameters, and the system jumps to the new state.

In spite of the fact, that the catastrophe theory is the tool of the qualitative analysis, this does not in any way diminish its importance, because the qualitative methods of dynamics research are often the most informative in the analysis of complex systems.

The catastrophe theory is a theory of structural stability of a special class of differential equations with an arbitrary number of variables. The feature of these equations is that their right-hand sides must be presented as a gradient system, which is the mathematical description of the movement in the field of force with potential $F(\bar{x}, \bar{\lambda})$:

$$\dot{x}_i = -\frac{\partial F(\bar{x}, \bar{\lambda})}{\partial x_i}, \; i = 1, \ldots, n, \quad (14)$$

where $\bar{x}$ - vector of variables, $\bar{\lambda}$ – vector of parameters.

It is interesting, that at the number of parameters, not exceeding four, Thom's theorem [18] is valid; it states that there is no more than seven elementary catastrophes in the system irrespective of the number of phase variables.

For the elementary and the most carefully studied case with one phase variable the number of elementary catastrophes is equal to four. In this case any system can be considered as gradient. In this case any system can be considered as the gradient

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one. According to Thom's theorem [18], any smooth function can have only two types of features (catastrophes), called "fold" and "cusp". If there is one parameter, the "fold" catastrophe has potential F(x, a)= $\frac{x^3}{3} - ax$. If there are two parameters a and b, the "cusp" catastrophe has potential F(x,a,b) = $\frac{x^4}{4} - b\frac{x^2}{2} - ax$.

Substituting the "cusp" potential into the equation (14), into the right-hand side, we obtain the cubic equation, the stability of which can be investigated by algebraic methods.

$$\dot{x}_i = -\frac{\partial F}{\partial x} = -x^3 + bx + a, \text{ i=1, 2, …} \quad (15)$$

We find the stationary points of this equation as the roots of the cubic equation:

$$x^3 - bx - a = 0. \quad (16)$$

The analysis of the solutions of this equation, when changing values of the parameters, shows that the "cusp" catastrophe has five qualitative features: bimodality, inaccessible region, sudden jump (catastrophe), hysteresis and divergence.

Interpreting the substantial sense of parameters a, b and the phase variable x differently, the qualitative forecast of dynamics of the scientific sphere in various terms can be made. For example, if parameter a is a number of publications, describing the new results, obtained in the framework of the current paradigm, and b is a number of publications describing the new results, contradicting the current paradigm, there is a catastrophe leading to the change of the paradigm.

3.3. Mathematical Models Of Science Taking Into Account Resource Limitations

We can obtain the mathematical expressions separately for the model of dynamics of the scientific publications and dynamics of the scientific community of scientists working in the limited subject area.

We will consider the development of the scientific sphere as the process of obtaining scientific results being implemented in the form of a sequence of publications y(t), representing the units of scientific information. As the limited resource we will choose a number of unresolved problems I (t). We will call it knowledge intensity of the subject area. Thus, we believe, that in the process of development of the scientific sphere the number of unresolved problems I (t) decreases, and the speed of their resolving, as a rule, increases due to already accumulated knowledge.

Let us obtain equations for dynamics of scientific publications. For this purpose we will assume, that the increase in the number of publications (the speed of development of the scientific sphere) Δy for time Δt is proportional to some function V (I), reflecting a chance to resolve one of the available I problems, with proportionality coefficient k: Δy=kV(I)Δt. Similarly, to decrease the number of unresolved problems, we obtain expression: ΔI =-V(I)yΔt.

In the limit case we obtain the following system of differential equations:

$$\frac{dI}{dt} = -V(I)\,y, \frac{dy}{dt} = kV(I)\,y. \quad (17)$$

Let us assume, that function $V(I)$ is linear, i.e. we believe, that an opportunity to resolve new unresolved problem is proportional to their number. Then

$$V(I) = \lambda I, \quad (18)$$

where λ – proportionality coefficient.
After substitution we obtain a system of equations:

$$\begin{cases} \frac{dI}{dt} = -\lambda I y, \\ \frac{dy}{dt} = k\lambda I y. \end{cases} \quad (19)$$

Substituting the right-hand side of the first equation: $\lambda I y = -\frac{dI}{dt}$ into the second one, we obtain:

$$\frac{dy}{dt} = -k\,\frac{dI}{dt}. \quad (20)$$

Integrating this equation with respect to time t, we obtain, that y+kI≡const≡L

The solution to this system of equations can be written in the following form:

$$y(t) = \frac{L}{1 + ae^{-\lambda L(t-t_c)}}, \quad (21)$$

where a – coefficient determined by the initial conditions, t_c – curve parameter.

Expression (21) in the graphic form represents a logistic curve. Beginning from the moment of time t=0, (beginning of the subject area research), dependence of publishing activity on time y(t) has exponential nature. It corresponds to the period of rapid development of a new subject area, when the number of unresolved scientific problems I is rather great. Such nature of dynamics of the subject area continues to take place to the moment of time tc, after which decrease in knowledge intensity of the subject area (resource exhaustion) starts affecting, and the system gradually comes to the saturation state.

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Dynamics of the community of scientists, working in some subject area, is defined by two opposite processes: coming of new researchers, involved by scientific prospects, and leaving of researchers because of completion of researches, exhaustion of the subject area and other reasons. The scientific community can be presented as a dissipative structure which can stably operate subject to its continuous feeding with the constant flow of information, which can be identified with the flow of scientific literature on the subject, i.e. array of publications I(t).

The amount of array I(t) characterizes a cash stock of scientific knowledge. In dynamics it can be increased due to receipt of new publications and be decreased due to works, which have been already used by the scientific community to gain new knowledge, which has lost its scientific value or has not been understood. We can write:

$$\dot{I} = \nu - \lambda I x - \alpha I, \qquad (22)$$

where x – current size of the scientific community,

ν – speed of coming of new researchers to the scientific community,

λ – the proportionality coefficient determined by the probability of scientist's finding useful publications,

α – the proportionality coefficient characterizing the speed of flow decreasing I(t) due to unused information.

For the scientific community dynamics of its number can be expressed by the following equation:

$$\dot{x} = k\lambda I x - \beta x, \qquad (23)$$

where x – current size of the scientific community,

k – coefficient of increase in the number of researchers,

λ – coefficient of using information,

β – intensity of the dissipative process of decrease in the number of researchers.

We obtain a system of differential equations:

$$\begin{cases} \dfrac{dI}{dt} = \nu - \lambda I x - \alpha I, \\ \dfrac{dx}{dt} = k\lambda I x - \beta x. \end{cases} \qquad (24)$$

Without loss of generality, we can make the following simplifications: we assume, that the speed of information input flow is proportional to its maximum value ν≡ αImax , intensity α=β≡Q. Then the system (24) can be rewritten as:

$$\begin{cases} \dfrac{dI}{dt} = Q(Imax - I) - \lambda I x, \\ \dfrac{dx}{dt} = k\lambda I x - Qx, \end{cases} \qquad (24)$$

The obtained equations are similar to the equations describing the processes of development of biological populations [20], [16]. Some results, obtained in the analysis of the specified processes in biology, can be used in the analysis of dynamics of the scientific community. For example, the solution in quadratures of the system (24) results in the logistic function:

$$y(t) = \frac{L}{1 + \alpha e^{-\lambda L t)}}, \qquad (25)$$

where $\alpha = L/x(0)$ – coefficient determined by the initial parameters of the scientific community,

$L = kI_{max} - Q/\lambda$ – "size of environment",

λ – coefficient of using information,

k – coefficient of increase in the number of researchers.

The qualitative analysis of the system (24) to obtain the conditions of its stability shows, that the system is stable at $\frac{dx}{dt} = k\lambda I x - Qx \geq 0$. Thus, in the saturation state, when $I = Imax$, we obtain

$$y(t)\; k\lambda I_{max} \geq Q. \qquad (26)$$

In practice, this is confirmed, when we observe the phenomena of disintegration or decay of the subject area as a result of decrease in the information flow.

On the whole, it should be noted, that there is a rather extensive range of formalizations, describing processes, similar to the considered ones, which can be used for constructing mathematical models of development of the subject area, in mathematical language.

4. DISCUSSION

The authors have described the methodology of mathematical modeling of the processes, characterizing dynamics of the scientific activities, based on the system of rather simplified assumptions. Despite its simplicity, this methodology allows us to estimate a number of very essential factors in regulating of the scientific sphere.

One of the most essential aspects of the intelligent analysis of information in IAS of the scientific sphere is ensuring forecasting the science development and calculating possible consequences

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of the made management decisions. It is especially important in modern conditions of significant cost of scientific research.

Regulation of the processes of the science development due to the limited resources, especially material ones, is substantially connected with an ability to distinguish a new promising direction of research in due time, to count the amount of the necessary financial support, to carry out the required structural changes, to organize training of specialists.

Studying distribution (13) of the number of publications in various areas of research, it is possible to find out signs of the exponential growth of publishing activity early enough, that can testify to emergence of breakthrough scientific results. Involving experts from the given subject area will help to analyze the found regularity in more detail and qualitatively. If the result is confirmed, there is a reason to increase funding for research in the subject area.

However, it is impossible to solve scientific problems only by bringing the material resources in the development of the scientific sphere. Costs and results in science are connected in the complex non-linear way, that's why extensive methods do not always lead to the result. Hopes are laid on the science intensification by its structural organization and optimal management, as well as by creation of interdisciplinary groups. The fact is, that as a result of extensive growth the science approaches saturation and then, like any evolving system, enters a new phase of its development by the complexity of its structure. The external management of such a process is associated with certain risks. The need for qualitative research of the stability of functioning of the created organizational structures and forecasting their scientific productivity comes to the forefront. The study of phase trajectories of the system behaviour, constructed on the model (16), is helpful in this case. Besides, satisfying condition (26) can serve as an exponent of stable dynamics of the research subject area.

Forecasting the science development is possible on the basis of mathematical modeling, especially as the Zipf-Pareto distribution law (13), to which distribution of the scientific productivity submits, indicates the need for the critical attitude to forecasting by statistical methods, as dispersion is theoretically infinite [21]. Therefore, the modeling of the processes of the science dynamics, taking into account limitations of the subject area on the basis of expressions (21, 25), will allow to make predictive estimates of its development taking into account the accuracy of parameter settings of models.

5. CONCLUSIONS

Since the mathematical models for the analysis of the science development, when making management decisions, are of great importance, it is necessary to take into account results of mathematical modeling of the science dynamics.

The article presents the methodological issues of development of mathematical modeling of the scientific sphere. The authors assume, that the estimate of the scientific sphere state, forecasting its development and analysis of consequences of possible management decisions according to the results of modeling on the offered set of mathematical models will improve the effectiveness of the made decisions. The paper considers the models constructed on very simplified presentation. At this stage, issues of complex interaction of science, equipment, technologies and industrial production, as well as social aspects of science are disregarded. The authors see further research in the development of indicators which are necessary to form computational algorithms of information-analytical system of the scientific sphere and to conduct scientometric calculations, using an array of publications in the field of social sciences and humanities.

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