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DEVELOPMENT OF A MODEL OF OPTIMAL PRODUCTION OF PHARMACEUTICAL PRODUCTS

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ABSTRACT

The article discusses the development of methods and models for the optimal production of pharmaceutical products, taking into account the specifics of the production of drugs and aimed at improving the efficiency of enterprise management and increasing profits, as well as the creation of mathematical tools that implement this model and methods.

KEYWORDS: *Model, Optimization, Fuzzy Set Theory, Membership Function, Objective Function, Pharmaceutical Products*

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INTRODUCTION

In the early process of drug discovery, machine learning has many potential applications, from the initial screening of drug compounds to predicting drug success. More specifically, AI can play a role in the task of drug identification and verification; goals based on phenotypic and multitarget drug discoveries; reuse of the drug; and identification of biomarkers. The introduction of AI for drug trials can shorten the time it takes for a drug to obtain approval and market, thus lowering the overall cost. Ideally, this will also lead to lower drug costs for patients, offering them more treatment options.

In well-known works, the solution of problems of modeling and making semi-structured decisions is carried out, in most cases, on the basis of the theory of fuzzy sets. An alternative concept of multi-agent distributed intelligent systems with interaction and competition among agents differs from the classical approach in the following: each intelligent agent acts completely autonomously; each intelligent agent offers a solution to a common problem (not only his own), each agent has full access to all available information; a general solution to a problem is defined as a proposal of one of the concurrently functioning agents on the basis of competition (not by coordinating and integrating private decisions of agents, which are often performed in an iterative mode); the cooperation of agents forms the necessary behavior of the entire system; actions related to cooperation and competition in the system are carried out simultaneously (not sequentially). At the same time, promising issues of the synthesis of integrated soft models, including fuzzy-neural ones using evolutionary algorithms for creating artificial intelligence systems for the production of drugs, are currently insufficiently studied.

In fact, the entire field of application of AI solutions can be conditionally divided into several large groups. Artificial intelligence (AI) is defined as computer systems capable of performing tasks that would normally require human intelligence. It consists of three different types: human-made algorithms, machine learning, and deep learning. The group of analytical solutions and systems includes all types of "intellectual", "cognitive" analysis, predictive, or predictive, analytics (predicting the probability of occurrence of events) and building scenario models. Now artificial intelligence helps to analyze data as deeply as it was impossible with simple analysis: to look for hidden patterns, identify cause-effect relationships and make predictions based on the analysis of thousands of similar events.

The pharmaceutical industry is one of the most dynamic industries, and is the first to respond to all changes in the market, including technological ones. Therefore, innovations that can optimize costly processes of production, promotion and sale of goods almost instantly appear on the pharmaceutical market. The analytical report "Artificial Intelligence: next frontier for connected pharma" [1] shows that in the pharmaceutical industry, artificial intelligence technologies are already in demand at three stages of the production and business process: in drug formula development (R & D), pharmacovigilance and marketing.

In the near future, artificial intelligence will help companies also manage relationships with customers and partners, as well as coordinate the work of production, purchasing and sales services.

The development of a single drug takes up to $ 2.6 billion on average and up to 14 years, according to estimates by Tufts University and the US Food and Drug Administration [2]. At the same time, not all drugs successfully enter the market.

The complexity of R&D is that researchers have to study tens of thousands of molecules in order to find "candidates" for inclusion in a drug by trial and error, then thoroughly test them and find the ratio of components that is effective in treating a specific disease. Analyzing all chemical compositions is a complex and costly process, even for large companies. Currently, most computing solutions emerging in healthcare do not rely on independent computer intelligence as such.Instead; they are based on man-made algorithms. These are evidence-based approaches programmed by researchers or clinicians. Once the known data is embedded in algorithms, computers can subsequently extract the information and apply it to a given problem. For example, in oncology, using consensus algorithms combined with the clinical, demographic and medical history of each individual patient, a computer can review available treatment alternatives and recommend the most appropriate drug combination. Unlike human-created algorithms, "machine learning" relies on so-called neural networks. It is a computer system modeled on the human brain. Machine learning uses multilevel probabilistic analysis that allows computers to simulate the processing of data in the human mind. Thus, even programmers cannot tell how the computer gets its final solution. Until now, the use of machine learning for drug production has been limited. However, its potential applications are numerous and potentially game-changing.

Among Other Uses, Machine Learning Can Be Used To

- Detection and diagnosis of diseases.
- Drug discovery.

Under the following assumptions, the proposed method determines the demand with high accuracy.

- The distributor does not get rid of the purchased products, ie production is spent only on the needs of the population.
- The needs of the population are always met. When the population comes to purchase products, the products are always in stock, because distributors always replenish the manufacturer's stocks on time.

- The distributor does not replenish the stock of products until it runs out (or the quantity drops below the stock).

MODEL OF OPTIMAL MANUFACTURING OF PHARMACEUTICAL PRODUCTS

The principle of the method is as follows:

As it was said, it is necessary to use information on the date and volume of sales of products for each distributor separately. If there are n distributors, we have $y_{j,i}$ data from each, which denote the volume of the i-th purchase of the j-th distributor, perfect at a moment in time $t_{j,i}$.

At the first stage, we compose a step function from the data:

$$f(t) = \begin{cases} \sum_{j=1}^{n} \frac{y_{j,i}}{t_{j,i+1} - t_{j,i}} \\ i : t_{j,i} \le t < t_{j,i+1} \end{cases} \tag{1}$$

A model has been developed for optimal planning of sales and production of pharmaceutical products using a multistep discrete controlled process. The planning period is divided into intervals (steps) with numbers from O to T. In the study, the optimal planning problem is formulated as finding the sizes of series *j* for all types of products *i* at all steps *j*, at which the objective function$Q$, denoting the profit of the enterprise, will be maximum:

$$Q = \sum_{i=1}^{N} \sum_{j=0}^{T} \left[\min(S_{i,j-1}, F_{i,j}) * C_i - x_{i,j} * p_i - S_{i,j-1} * p_{H\, i-1}(x_{i,j}) * A_i \right] \tag{2}$$

$$Q \to \max$$

with restrictions:

$$S_i - 1 = Const_i \qquad (i : 0 \ldots N) \tag{3}$$

$$S_{i,j} = S_{i,j-1} + x_{i,j} - \max(S_{i,j-1}, F_{i,j}) \qquad (i : 0 \ldots N;\ j : 0 \ldots T) \tag{4}$$

$$\sum_{i=1}^{N} S_{i,j} * V_i \le \text{warehouse volume} \qquad (j : 0 \ldots T) \tag{5}$$

$$x_{i,j} \le \sum_{i=0}^{T} F_{i,j+1} \qquad (i : 0 \ldots N;\ j : 0 \ldots T) \tag{6}$$

$$\sum_{i \in \bar{\ }_a} x_{a,j} \le \max_a \qquad (a : 1 \ldots ¶;\ j : 0 \ldots T) \tag{7}$$

$$K_{start} + Q_j \ge P(J) \qquad (J : 0 \ldots T) \tag{8}$$

where:

N – number of different types of products;

T – the period for which planning takes place;

$S_{i,j}$ –the number of products of the i-th product at the end of step j (in the warehouse);

$F_{i,j}$– demand for products of the i-th type in step j;

c_i– the selling price of a unit of production of the i-th type;

$x_{i,j}$ – number of products of the i-th type;

p_i – the cost of producing a unit of product of the i-type;

A_i – expenses for certification of products of the i-type;

$P_{н\ i}$ – storage costs of one unit of the i-type product;

$Const_i$ – quantity of products available before planning starts;

V_i– volume occupied by one unit of i-type product;

$T_{yearH\ \ i}$ – shelf life of products of the i-th type (number of steps to end);

$\bar{}_{a}$ - a group (set) of products that require the production of the work of the same workshop, equipment;

¶ - the number of product groups that are subject to restrictions on production capacity;

K_{start} -start-up capital available at the beginning of planning;

$P(J)$ - the limit below which the finances of the enterprise should not fall (for example, salary costs, loan payments, etc.);

Q_j - total profit from J steps, similar to the expression of the objective function.

The resulting optimization problem is very difficult to solve by the method of Lagrange multipliers or gradient methods.The solution to this problem is possible by the method of fuzzy programming, which allows finding the optimal solution to multistep problems.

FUZZY PROGRAMMING METHOD

The general model of the Fuzzy inequalities and linear programming problem with a precise target function is as follows[3]:

subject for $Max\ \ c^T x$,

$$\begin{aligned} A_i x \le b_i, \quad (i = 1, 2, ..., m), \\ x \ge 0 \end{aligned} \tag{9}$$

here≤ is called “Fuzzy less or equal to it” and should be understood as a function of properly selected affiliation.

Parametric programming methods can be used to solve such ambiguous linear programming problems. Here, the indefinite constraints are converted to explicit constraints by selecting the relevance function for each constraint. The content of the relevance function, agar $A_i x \le b_i$, means, *I*-this means that the restriction is absolutely satisfied, here $A_i x \le b_i + p_i$.

$$\text{«}_i(A_i x) = \begin{cases} 1, & A_i x < b_i, \\ 1 - \dfrac{A_i x - b_i}{p_i}, & b_i \le A_i x < b_i + p_i, \\ 0, & A_i x > b_i + p_i, \end{cases} \tag{10}$$

here $A_i\,(i = 1, 2, ..., m)$ means the *i*-th row of *A*.

The objective function must be uncertain to solve type problems (9)and to create a relevance function, it is necessary to solve the following two linear programming problems:

$$\begin{array}{ll} (LB(b)) & (LB(b+p)) \\ Max\ c^T x & Max\ c^T x \\ Ax \le b, & Ax \le +bp \\ x \ge 0 & x \ge 0 \end{array}$$

Here $p = (p_1, p_2, ..., p_m)^T -$ (9) is the tolerance vector for the m constraints.

Let Z_0 and Z_1 be the values of $(LB(b))$ and $(LB(b+p))$, respectively.

Now, using Z_0 and Z_1, the linear relation function for the objective function is constructed as follows:

$$\text{«}_0(c^T x) = \begin{cases} 1, & c^T x < Z_1, \\ 1 - \dfrac{Z_1 - c^T x}{Z_1 - Z_0}, & Z_0 \le c^T x \le Z_1, \\ 0, & c^T x > Z_1, \end{cases}$$

The constraints are the same as the corresponding functions (10).

Now using the above belonging functions, $\text{«}_i\,(i = 0, 1, 2, ..., m)$ and following the principles of Bellman and Zadeh,(9) problem

subject for Max *α*,

$$\text{«}_0(x) \ge a,$$

$$\text{«}_0 \ge a,\ (I, 1, 2, ...m),$$

$$a \in [0,1],\ x \ge 0.$$

the following is a solution to the exact linear programming problem.

subject for Max α,

$$
\begin{aligned}
& c^T x \geq Z_1 - (1-a)(Z_1 - Z_0), \\
& A_i x \leq b_i + (1-a)\, p_i, \\
& a \in [0,1], x \geq 0.
\end{aligned}
$$

CONCLUSIONS

The main advantage of Fuzzy target programming is that it can be converted to a traditional linear programming model.Another advantage is that goal setting is symmetrical with setting limits.Finally, the concept of permissible degradation aspiration level is consistent with real decision making.

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