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# MATHEMATICAL MODELING IN ECONOMICS OF EFFICIENCY OF INVESTMENT PORTFOLIOS BY THE CLUSTER ANALYSIS METHOD FOR SMALL CHEMICAL PROJECTS IN THE INNOVATION INFRASTRUCTURE OF THE REPUBLIC OF TATARSTAN

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# **Igor Leonidovich Beilin**

Kazan Federal University, Institute of Management, Economics and Finance, Kazan 420008, Russian Federation

Abstract. The most important component of the innovation policy in the Republic of Tatarstan is building and further development of an effective innovation infrastructure. It is necessary for ensuring the transfer of innovative inventions in production and reinforcement of its place in the market. The Republic of Tatarstan has the most highly developed and the most competitive petrochemical cluster compared to other sectors of the economy at both the federal and international levels. It includes not only high-performance science-intensive inventions in the extraction and processing of oil, but also chemistry of high-molecular compounds, plastics and synthetic rubbers. Small innovative projects in the field of polymers due to good scientific elaboration, high production flexibility, availability of raw materials in their own region and large demand for the product, and relatively low capital investments unlike large-scale oil production, can significantly improve the economic efficiency of the entire petrochemical cluster of the Republic of Tatarstan. Over the past decade, the amount of domestic expenditures on research in the region has increased by more than 10 times, amounting to 68.2 billion rubles in 2016. In terms of total costs for technological, marketing and organizational innovations, Tatarstan ranks third among the regions of Russia. The first and second places are occupied by Samara (94.1 billion rubles) and Nizhny Novgorod (89 billion rubles) regions, respectively.

**Keywords:** mathematical modeling in economics, innovation infrastructure, profitability index (PI), internal rate of return (IRR), cluster analysis, nearest-neighbor principle, farthest neighbor principle, innovative chemical project.

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## **1. INTRODUCTION**

Mathematical modeling in economics of investment portfolios efficiency for small chemical projects in the innovation infrastructure of the Republic of Tatarstan can significantly increase the opportunities for attracting investments in this sphere. Cluster analysis is one of the most modern and universal tools of hierarchical organization of economic indicators for a large number of small innovative projects. As discussed in this paper, such indicators include, among others, the profitability index (PI) and the internal rate of return on investment (IRR). Work in new conditions requires adjusting the mechanisms of support and protection of domestic producers, and in a number of areas it is necessary to improve the regulatory framework at the federal level.

### 2. LITERATURE REVIEW

The active enterprises shipping most products nanotechnological OJSC are Nizhnekamskneftekhim, OJSC Kazanorgsintez, OJSC Karpov Khimzavod, Fuzo KAMAZ Trake Rus LLC, KVART CJSC, Danaflex-Nano LLC, Ledel LLC, Research and Development Center Inkomsistem. The Republic not only actively works with nanotechnology, but also prepares specialists in this field.

The key problems in the development of design and research activities in the field of the nanoindustry are the lack of a mechanism for stimulating the project activity in the field of nanotechnology, the ineffective interaction of scientific teams and industrial enterprises of the republic, and the lack of innovative projects in the field of nanotechnology for own resources required at the initial stage of the projects for commercialization of intellectual property in the field of nanoindustry. In order to develop innovative production in the republic, it was decided to create special infrastructure projects in Tatarstan, such as the economical zone of the technology-innovative type "Innopolis".

After a slight decline in investment amounts in fixed assets in 2014, in 2016 there was an increase in investment, reaching the level of 2013. As a result, investments in fixed assets in 2016 amounted to 6,324 million rubles.

Currently, the leading role among the multifarious development institutions in the republic is played by

the special economic zone of the industrialproduction type "Alabuga" (JSC SEZ IPT "Alabuga"). The special economic zone is a center of gravity for investors implementing prospective high-tech projects in basic clusters of economy: petrochemical complex, automotive industry and construction industry. At the end of 2016, 34 companies became residents of JSC "SEZ IPT "Alabuga". In 2015, 9 companies were granted the status of the site's resident, including 6 companies with the participation of foreign capital. The new residents were LLC Armstrong Building Products (USA) (production of counter ceiling systems), LLC Khabi Logistica Elabuga (Germany) (creation of a manufacturing and distributing center for product suppliers of McDonald's restaurants), LLC RMA Rus (Germany) (production of ball valves for gas pipelines), LLC EkoTechnologies-Alabuga (Russia) (recycling of worn-out tires into a rubber powder), East Balt Yelabuga LLC (USA) (production of bakery products), LLC NTC MSP (Russia) (production of exhaust gas aftertreatment systems for cars), LLC "ZM Volga (USA) (production of protection anticorrosion products, abrasive materials, hollow glass beads, industrial adhesive materials and adhesives), LLC Tatplastic (Russia) (production of plastic household products) and LLC Joshkunoz-Alabuga (Turkey) (manufacture of stamped parts for car bodies).

According to the planned timetables for the implementation of the projects, the total commissioning of 9 new enterprises is scheduled for the end of 2016. The volume of declared investments of these enterprises is 13.3 billion rubles. These companies expect to employ about 2488 people at their facilities. The enterprises existing for today in IPT" JSC "SEZ Alabuga" are high-tech manufactures producing world-class products oriented to substite imported goods.

Cluster analysis is a convenient method for identifying homogeneous groups of objects called clusters (Pourrajabi ,Moulavi, Campello, Zimek, Sander & Goebel, 2014). Cluster objects for many characteristics differ from objects that do not belong to this cluster. Small innovative chemical projects in the process of innovation transfer are interested in segmenting their client bases in order to better orient them, for example, to price strategies (Beilin, 2016). An important problem in the application of cluster analysis is the decision on how many clusters should be obtained from the data. Sometimes we ourselves specify the number of elements that must be obtained from the data. For example, if you need to find out what characteristics distinguish frequent customers from occasional customers, then you need to find two different clusters. However, we usually do not know the exact number of clusters, and then we come up with a compromise. On the one hand, we want to make clusters understandable and effective, what means a small number of them. On the other hand, a large number of clusters makes it possible to identify more segments and more subtle differences between segments (Roman

Resnick, Susan, Davatzikos & Christos, 2011) In an extreme case, you can call each consumer separately (micromarketing) to determine the best set of characteristics for specific purposes.

# 3. METHODS AND STAGES OF THE STUDY

Hierarchical procedures for clustering are characterized by a tree-like structure formed during the analysis. Most hierarchical methods fall into a category called agglomeration clustering. Initially, this type of procedure begins with each object representing a separate cluster (Huth, 2008). Then these clusters are consistently combined with regard to their similarities. First, the two most similar clusters are combined into a new cluster at the bottom of the hierarchy. In the next step, another pair of clusters is combined and linked by a higher level of hierarchy, and so on. This allows the hierarchy of clusters to set from the bottom up.

The hierarchy of clusters can also be created from the top down. In such a partitioning clustering, all objects are first combined into one cluster, which is then gradually split up. In both types of clustering (agglomeration and separatory clusterization, also called the "nearest neighbor" method and the "farthest neighbor" method), the cluster at a higher level of the hierarchy always covers all clusters of a lower level. (Roman, Resnick, Susan, Davatzikos, Christos, 2011) This means that an object assigned to a particular cluster cannot be reassigned to another cluster.

There are various measures to express the similarity between pairs of objects (Dolnicar & Lazarevski, 2009). A simple way to evaluate the proximity of two objects is a direct line between them. For example, when we look at a scatter plot, we can easily see that the length of a line connecting one pair of observations will be shorter than the line connecting the other pair of observations. This type of distance is also called Euclidean distance (or rectilinear distance) and is the most commonly used. To use the hierarchical clustering procedure, it is necessary to express these distances mathematically.

$$d_{a,b} = \left(\sum_{j=1}^{n} (x_{aj} - x_{bj})^2\right)^{\frac{1}{2}}$$

There are also alternative distance measures: a distance between urban quarters, which uses the sum of absolute differences of variables. This distance measure is often called the Manhattan metric, since it recalls the distance traveled between two points in the city.

$$\boldsymbol{d}_{\boldsymbol{a},\boldsymbol{b}} = \sum_{j=1}^{n} \left| \boldsymbol{X}_{\boldsymbol{a}j} - \boldsymbol{X}_{\boldsymbol{b}j} \right|$$

Having determined the measure of distance or similarity, it becomes necessary to decide which one clustering algorithm to choose (Larson, Bradlow, & Fader, 2005). There are four types of effective agglomerate clustering procedures.

Single connection (nearest neighbor): the distance between two clusters corresponds to the shortest distance between any two members in two clusters.

Complete connection (farthest neighbor): an opposition approach to a single connection. It is suggested that the distance between two clusters corresponds to the largest distance between any two members in two clusters.

Average connection: the distance between two clusters is defined as the average distance between all pairs of members of two clusters.

Central connection: with this approach, the geometric center (centroid) of each cluster is first calculated. This is done by calculating the average values of variables of all objects in a particular cluster. The distance between two clusters is equal to the distance between two centroids.

# 4. THE RESULTS OF THE STUDY AND THEIR PRACTICAL IMPORTANCE

Considering the progressiveness and range of the innovative activity in the chemical industry of the Republic of Tatarstan, it seemed to us urgent to conduct a cluster analysis of two investment portfolios of the innovative projects "Copolymer +" (Beilin & Arkhireev, 2011), (Beilin & Arkhireev, 2006) and "Polycarbonate Analogs" (Beilin & Arkhireev, 2005), (), each of which is characterized by two

features (Table 1, 2): the profitability index (PI) and the internal rate of return on investment (IRR):

$$PI = \sum_{k=1}^{n} \frac{P_{k}}{(1+r)^{k}} / \sum_{j=1}^{m} \frac{IC_{j}}{(1+i)^{j}}$$

$$IRR = r_1 + \frac{NPV_1}{NPV_1 - NPV_2} \cdot (r_2 - r_1)$$

Innovation	Innovative project number								
project	1	2	3	4	5	6th	7th		
efficiency									
indicator									
PI	2	3	6	1	8	2	4		
IRR,%	10	15	22	9	14	11	17		

Table 1.Efficiency Indicators of the Investment Portfolio consisted of seven innovative projects "Copolymer +".



Fig. 1.The results of the hierarchical classification of objects in the form of a dendrogram of cluster analysis based on the "nearest neighbor" principle for the investment portfolio of seven innovative projects "Copolymer +".



Fig. 2. The results of the hierarchical classification of objects in the form of a dendrogram for cluster analysis

based on the "farthest neighbor" principle for the investment portfolio of seven innovative projects "Copolymer +".

Innovation	Innovative project number								
project	1	2	3	4	5	6th			
efficiency									
indicator									
PI	5	7th	4	3	1	5			
IRR,%	15	18	12	19	16	14			

Table 2.Performance Indicators of the Investment Portfolio consisted from six innovative projects "Polycarbonate Analogs"



Fig. 3.The results of the hierarchical classification of objects in the form of a dendrogram for cluster analysis based on the "nearest neighbor" principle for the investment portfolio of six innovative projects "Polycarbonate analogs".



Fig. 4. The results of the hierarchical classification of objects in the form of a dendrogram for cluster analysis

based on the "farthest neighbor" principle for the investment portfolio of six innovative projects "Polycarbonate analogs."

### 5. SUMMARY

Thus, for the investment portfolio of the seven innovative projects "Copolymer +", a more distinct result was obtained in the cluster analysis (Figure 1.2) based on the "farthest neighbor" principle: two clusters [No. 1, No. 6, No. 4] and [No. 2, No.7, No.5, No.3], the distance between which was equal to P = 13.93. For the investment portfolio of six innovative projects "Polycarbonate analogs", both the "nearest neighbor" method and the "farthest neighbor" method provide the same result (Fig. 3, 4): clusters [No. 1, No. 6, No. 3] and [No. 4, No. 5, No. 2], the distance between which is P = 4.12 and P = 7.07, respectively.

# 6. CONCLUSION

The key link in the chain of innovative infrastructure of Tatarstan is the Technopolis "Khimgrad". By the end of 2015, there were about two hundred enterprises on its territory, what is 11% more than in 2014. The volume of their output was 11,348 million rubles (almost 30% higher than the level of 2014). Since 2011, 7.4 billion rubles of private investments have been attracted by residents.

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