Intelligent Geopolymer Characterisation System Using Multicriteria Analysis and Markov Chains

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Abstract

The advantages of hybrid intelligent systems are the common objective of the exploited model, the possibility of extension, and adaptation to loads through scaling. A smart system and algorithm for hybrid implementation of criterion evaluation and probabilistic dynamics of slobostructured geopolymer basic characteristics in real time are proposed based on the coupling of Markov chains and multicriteria optimization methods. The advantages of hybrid intelligent systems lie in the overall objective of the proposed model, scalability, and adaptability to workloads through scaling. The computational basis of calculations was the digitalization of technology study and analysis of physical-mechanical properties of geopolymers. The optimal composition of geopolymer structure elements for the given technology of their production was determined. The results of modeling the parameters of target functions have shown the advantages of the digitalization of technologies in the analysis of the physical and mechanical properties of geopolymers. The use of the analytical apparatus of Markov chains allowed us to rank the coefficients of multicriteria optimization and to increase the accuracy of calculations.

Keywords

Multi-criteria optimization, Markov chains, Target function parameters, Coefficient ranking, Hybrid models

1. Introduction

Geopolymers are a new class of building material designed to replace Portland cement. High carbon dioxide emissions accompany the production process of Portland cement. Modern cement plants worldwide emit about 1.5 billion tons of CO_2 annually. Geopolymers are becoming an environmentally friendly alternative to Portland cement. The properties and applications of geopolymers depend on their chemical structure and the ratio of components.

The search for the optimum composition of geopolymers with high strength and performance properties is becoming an urgent problem in construction, architecture, and noise protection structures. The practical application of the results of studies on estimating geopolymer mixtures with given physical and mechanical properties is limited to the empirical selection of the composition of geopolymer components and the establishment of their variation ranges [1-4]. Reaching an extremum of one of the properties is accompanied by a decrease in the other properties by a particular value.

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However, even in this case, the point of optimum formulation is determined with a large margin of error.

Information processing based on mathematical modeling of the composition of geopolymer compositions is related to the selection of solutions in weakly structured problems with quantitative and qualitative parameters used as input variables and unstructured with qualitative description only. Considering their significance, collective decision-making based on quantitative and qualitative criteria is the main direction of research on creating an intelligent system of geopolymer characteristics to determine the ranking of criteria using Markov chains and subsequent multicriteria optimization. Such a hybrid model begins as a system using one autonomous method and ends up as a system using another way. The coupling of experimental results on geopolymer mixture formulation with their processing by methods of multicriteria optimization and Markov chains form the basis of the present work.

The authors' main contributions are the following:

- the methodology of complex use of Markov chains for determination of weight coefficients of multicriteria optimization was proposed;
- modeling of target function parameters was performed, the results of which revealed the advantages of digitalization of technologies in the analysis of geopolymers properties;
- based on the results of modeling, a scheme of hybrid implementation of criterion evaluation and probabilistic dynamics of weakly structured data was proposed.

The aim of the work is not only to investigate the physical and technological parameters of different geopolymer compositions but also to simulate these properties using multicriteria Optimisation and Markov chains.

2. Literary review

The scientific field of intelligent material characterization systems using a hybrid implementation of Markov chains and criteria methods includes a synergistic combination of semantically integrated technologies defining the architecture and information exchange process and developing communication between the components.

In [5-7], discrete Markov chains have been used for strategy development in various industries, in [8] medical research, [9] coronavirus control, [10] navigation systems, [11] international relations, [12] student performance evaluation, in [13] in structural transformations.

Criterion methods are ways of describing alternative solutions in quantitative terms. Each decision leads to a particular outcome and therefore expresses the effectiveness of the process and its overall value. In [14] an evaluation of the composition of the main power chains of an asphalt concrete mixture based on discrete element methods is presented. In [15], a model for quantitative risk assessment of a structural hierarchical system used in the petrochemical industry is described. The use of fuzzy sets theory and genetic algorithms for the composition of communication services is presented in [16]. An optimality criterion-based algorithm for efficient optimization of laminated composite design using simultaneous resizing and scaling is presented in [17]. An assessment of the weighted effectiveness of lattice criterion methods is presented in [18]. A hybrid firefly-inspired approach for optimal web composition is described in [19]. Modeling the use of Markov chains covers a wide class of probabilistic dynamics, allowing one to trace trends and causes of changes in the properties of one's subject domain. However, it should be noted that the presented arsenal of Markov chain implementation tools lacks methodological unity and represents only some aspects that are treated separately and used for different purposes. Markov chains represent an integrated element of forecasting mechanics based on an integrated approach with criteria methods.

The influence of material structure on the mechanical properties of geopolymers obtained using additive technologies is presented in [20]. Comparative studies using atomic force microscopy, X-ray spectroscopy, and Fourier transform infrared spectroscopy in [21], the influence of structure on the strength properties of geopolymer characteristics in [22]. Optimization of matrix compositions affecting the mechanical properties of geopolymer composites with short carbon fibers in [23], development of hybrid geopolymers for structural materials in [24]. The problem of optimizing the composition of geopolymer mixtures with the help of an intelligent system of multicriteria optimization and Markov chains is relevant and timely.

The main multicriteria optimization techniques used in the cited sources are criterion convolution, main criterion optimization, and sequential concession method. The practical applications of criterion methods are wide and varied. The main disadvantage of global optimization for all geopolymer parameters is the high computational complexity of target functions. For most practical optimization problems, analytical expressions of limiting functions are unknown. Their general patterns, trends, and possibilities are considered and used in developing the hybrid implementation method.

The unsolved part of the general problem of building intelligent systems of multicriteria multiobjective optimization is their equivalence when replacing the original criteria with general aggregated criteria, i.e., the exclusion of ranking of private criteria by their importance. This significantly reduces the accuracy of multicriteria optimization evaluation.

3. Material and Method

Geopolymers' physical-mechanical and technological properties were used as research materials: their quantitative values and priority probabilities of the main characteristics that ultimately determine the weight composition of the mixture components. The technology of geopolymers production, their formulation properties, chemical composition, and structure are presented, which are the basis of input information for the study of investigated properties.

The main constituents of geopolymer are calcined clay, aluminosilicate materials, bentonite, and kaolin. The local concrete industry in the Czech Republic uses aggregates in the form of fine and coarse sand. The aggregates smaller than 4.75 mm are considered fine sand, and coarse sand larger than 4.75 mm. The totals in the present work were obtained in crushed form. Most of the particles were gravel-type with particle sizes ranging from 4.0 to 8.0 mm and fine sand with particle diameters of 0.063 mm to 2.0 mm [3]. Binder is provided České lupkové závody, a.s by commercial name L_k. In preparing the binder mixture based on the inorganic polymer, five parts by weight of cement and four pieces of activator are usually used.

The mixtures were prepared by two following steps: (1) To begin with starting materials, a geopolymer mortar was prepared by mixing metakaolin-based geopolymer materials with an alkaline solution in a predetermined ratio (liquid to solid) by mechanical stirring for five minutes; (2) afterward, the aggregates were added to the geopolymer mortar mixture and the mixture was homogenized by the mechanical stirring with five minutes. Directly after mixing, the fresh mortar and concrete were poured into the plastic molds and vibrated for 2 minutes on the vibration table to remove air voids. Specimens were covered with a plastic bag for 24 hrs after casting. There are two ways to cure these samples:

(i) These samples were cured at room temperature for 3 days after casting. Next, the pieces were removed from the molds and left in laboratory ambient conditions until the day of the test. The sample ages for the latter tests were 7, 14, and 28 days.

(ii) All the mixtures were cured in an oven without delay at the specific curing temperature for 24 hr and 48 hr ranging from 60 ^{o}C ÷ 90 ^{o}C. Samples were molded in the oven after the curing process and continued at ambient conditions for 2 days.

The samples prepared with different mixing ratio aggregate content are presented in Table 1.

4. Methodology

The algorithm of implementation of multicriteria evaluation and probabilistic dynamics of weakly structured data developed according to the described methodology is presented in Fig.1.

The algorithm has a cross-sectional structure and consists of a transient probability matrix algorithm using Markov chains and a criterion approach for determining the optimal geopolymer composition. Two aspects determine the dynamics of the process: the initial probability distribution and the transition probability matrix. Markov chains allow prioritizing each physical and mechanical parameter analyzed. Based on the calculations performed in the first part of the algorithm, we obtain the values of weight coefficients for each physical-mechanical parameter of the geopolymer. The use of Markov chains reveals the essence and interrelation of the main physical and mechanical parameters of geopolymers with the probability of their manifestation under various manifestations of the external environment. The novelty of Markov chains application is the replacement of equal-step time intervals by a discrete sequence of states. Markov chains are a powerful tool that provides fundamental reasoning of a decision on the basis of processing a large number of experimental data, some of which constitute a database of data obtained with one or another probability. Criterion evaluations are carried out based on Laplace, Wald, and Hurwitz criteria and additive, multiplicative and complementary multiplicative convolution. The general cross-validation algorithm takes into account the necessary operations and building blocks for constructing a hybrid model for determining the optimal geopolymer composition. Hybrid implementation of Markov chains combined with quantitative multicriteria optimization evaluations were used as research methods.

Table 1
Composition of fresh geopolymer concrete mixes

Starting Materials (g)			Aggregates(g)			
Fly ash	Cement	Alkaline solution	Fine sand	Coarse aggregate	Water	Samples names
200	100	85	190	380	45	No. 1
150	130	110	190	380	40	No. 2
150	130	150	190	380	-	No. 3
100	150	180	190	380	-	No. 4
100	150	180	90	480	-	No. 5
100	90	140	90	580	-	No. 6

The conceptual model of multicriteria decision-making with fuzzy input data provides equality of weight coefficients of used criteria. The range of mechanical, thermal, and technological properties variation is determined by setting the extremum of the boundaries of the target values of the requirements. In this case, the existing methods have not considered the additional values found through empirical observation of the characteristics, which significantly reduces the effectiveness of optimization methods for multiple criteria since decision-making occurs under conditions of uncertainty and risk. Therefore, it is necessary to modernize the multicriteria optimization methods, which consist of the transition from vector to scalar optimization. This operation manifests convolution functions of qualitative criteria into a single generalizing one.

The need to rank the weight coefficients of criteria requires the creation of an intelligent system in which the weight coefficients of criteria will be determined through the apparatus of Markov chains. The technology of intelligent systems is considered as an information-computing system with intelligent support. From these positions, the intelligent system of geopolymer characteristics is presented as a technical system capable of solving creative problems belonging to this subject area, which are stored in the knowledge base in the form of a functional semantic network.

When building an intelligent system of geopolymers characteristics, the ability to solve problems by a declarative description of the condition, control the processes of computation in the dialogue mode, and synthesize computational algorithms capable of solving poorly formalized problems were taken into account. The main stages of building an intelligent system of geopolymer characteristics were: work with quantitative information, mathematical calculations, storage and exchange of information, and interpretation of results. The sequence of models underlying the intelligent system of geopolymers characteristics included Markov chains for determining the ranking of criteria, multicriteria optimization models, and cross-algorithms of their hybrid implementation. When ranking criteria using Markov chains each state of the parameters characterising the information situation of determining the mechanical properties of geopolymers for a given recipe for their preparation is assigned a certain probability, which is written as a line of the state matrix. The matrix of intensities or transitions of the system describes the wandering of the system over its states. The matrix is compiled so that the sum of the probabilities in the rows of the matrix is always equal to 1. In analysing the state matrix, all possible states of the parameters are enumerated with their probabilities, i.e. we are dealing with a stochastic transition matrix, the set of vectors inside which reflects the values of probabilities between gradations. These iterations are made for various combinations of parameters. Since the processes of obtaining the mechanical properties of geopolymers by changing their formulations do not have a constant time reference, we will use the stages that characterise the successive approximation of the states' approach to achieving the intended goal as time. In this case, we will replace the time with the step number.

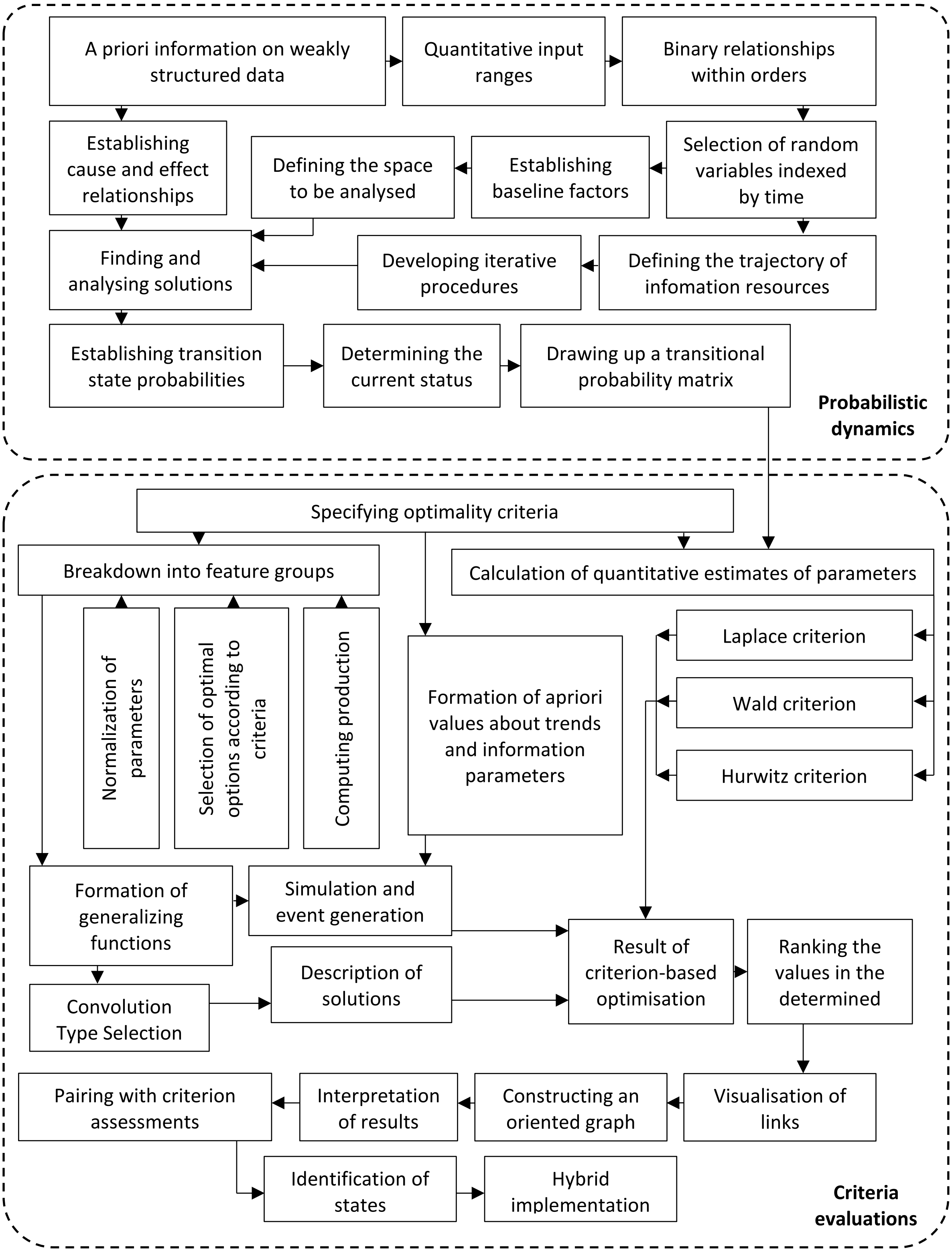

Figure 1: Hybrid implementation of criterion-based estimation and probabilistic dynamics of weakly structured data

Making decisions under uncertain and risky conditions begins with constructing a payoff matrix. The payoff matrix is a simplified formal model of an actual conflict situation. Mathematically, formalisation means that certain rules for the interaction of parties, choices of actions, and specific outcomes for the selected actions have been developed, and the necessary information is available. The term "payoff matrix" is synonymous with the term "performance matrix" [25].

$$R = \begin{pmatrix} & \Pi_1 & \Pi_2 & \cdots & \Pi_n \\ \hline q_1 & \delta y_{11} & \delta y_{12} & \cdots & \delta y_{1n} \\ q_2 & \delta y_{21} & \delta y_{22} & \cdots & \delta y_{2n} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ q_m & \delta y_{m1} & \delta y_{m2} & \cdots & \delta y_{mn} \end{pmatrix} \quad (1)$$

where $q_1,\ldots,q_i,\ldots,q_m$ – weight composition of sample components, $\Pi_1,\ldots,\Pi_i,\ldots,\Pi_n$ – analysed parameters (physical and mechanical, thermophysical, chemical, operational and technological, economic), δy_{ij} – relative deviation of the j-th parameter from the target.

To determine the element of the matrix, one of the methods used is the estimation of a scalar vector – the method of selection by arranging objects according to the model. In this case, converting from estimating a vector to a scalar of the objects is necessary. The functions used in solving the multicriteria problem as convolution functions of the vector arguments $y_i = (y_{i1},\ldots,y_{ij},\ldots, y_{in})$ into scalars $\delta y_{ij} = f(y_i)$. Vector argument convolution serves to reduce the number of criteria. Its purpose is to replace the original criteria with common criteria. The convolution operation is also called aggregation of partial criteria. The method is applied if private criteria can be ranked in descending order of their importance so that the importance of each pair of neighboring criteria does not differ significantly. Their normalization is applied to compensate for the small values of some criteria with large values in other criteria. The most straightforward scalar function that provides a linear order of objects is the penalty function, which is formed to the extreme importance of features.

$$f_{ш}(y_i) = \sum_{j=1}^{n} \Delta y_{ij} \quad (2)$$

where: Under the deviation Δy_{ij} from the ideal target by the j-th feature, we understand the absolute value of the difference $\Delta y_{ij} = |y_j - c_{j,extr}|$, where the ideal target when maximizing the j-th feature is denoted as $c_{j,extr} = y_{j,\max}$, and when minimizing the j-th feature, as $c_{j,extr} = y_{j,\min}$. The condition to correctly use function (9) is to employ a general absolute scale to measure all features.

As for the sample, we want to refer to a class of objects characterized by a general target $h = (c_1,\ldots, c_j,\ldots, c_n)$. Let us introduce a measure of the overall deviation from the target, which allows finding the object closest to the sample and ranking the objects based on their distance to the target. Consider a sample with attributes formed by equality constraints ($y_j = c_j$). The deviation of the j-th feature in any direction from the specified point $c_j(c_j \pm \Delta y_j)$ indicates the extent to which an object deviates from the target concerning this attribute. Then, the relative deviation of the j-th feature from the target is determined as,

$$\delta y_{ij} = \begin{cases} \dfrac{|y_{ij} - c_j|}{y_{j,\max} - c_j}; \; y_{ij} > c_j; \\ \dfrac{|y_{ij} - c_j|}{c_j - y_{j,\max}}; \; y_{ij} < c_j. \end{cases} \quad (3)$$

where i – line number; j – matrix column number.

As parameters, the best values of the analyzed parameters need to be chosen according to the perspective of the problem being addressed - these can be maximum, minimum, or average values from the experimental sample. With this approach, the formula will shift the integer quantities about the scale (0.1). However, with such parameter selection, the corresponding elements of the matrix coincide with the necessarily observed values, leading to. Using the convolution sum results in the corresponding feature being lost from the overall evaluation of the object, and using the convolution product will lead to a reduction to 0. A clear way to avoid such situations is to extend each feature's upper (maximum) or lower (minimum) limits by the same percentage. Below, each analyzed parameter's maximum (minimum) values have been increased (decreased) by 1%.

Scalar optimization requires additional knowledge about the properties of the generalized objective functions, characteristics scale, and weighting coefficients. Since this knowledge is domain-specific, the order of objects in an n-dimensional space cannot be explicitly determined. Therefore, it is crucial to study the influence of the properties of the generalized objective functions, characteristic scales, and weighting coefficients on the optimization results.

The following generalizing multicriteria utility functions have been used in theoretical analysis.

Additive Convolution

$$\delta y_i = \sum_{j=1}^{n} \omega_j \delta y_{ij} \tag{4}$$

where ω_j – importance (weighting factor) j-th sign, $\sum_{j=1}^{n} \omega_j = 1$.

Power multiplicative convolution

$$\delta y_i = \prod_{j=1}^{n} \left(\delta y_{ij}\right)^{\omega_j} \tag{5}$$

Additional multiplicative convolution

$$\delta y_i = 1 - \prod_{j=1}^{n} \left(1 - \omega_j \delta y_{ij}\right) \tag{6}$$

The best object is considered to have the minimum values of functions.

Savage (Wald) criterion (minimum-maximum)

$$Z_v = \min_i \max_j \delta y_{ij} \tag{7}$$

Laplace criterion (minimum-minimum)

$$Z_L = \min_i \min_j \delta y_{ij} \tag{8}$$

Hurwitz criterion

$$Z_{hw} = \min_i \left\{ \rho \min_j \delta y_{ij} + (1-\rho) \max_j \delta y_{ij} \right\} \tag{9}$$

where $0 \le \rho \le 1$ – the indicator of pessimism, in the calculations, was taken equal to 0.5.

The generalized additive function synthesizes the mass index of an object. It reflects the total value of individual characteristics, taking into account their importance. The direct product function prioritizes objects with consistent estimates for all indices, reflecting individual indices' homogeneity. The complementary product function has the opposite property. The advantage of a complementary product function over other product functions is its ability to accept zero feature values. With direct product functions, special care is needed to avoid scalar estimates of vectors with a component value of zero.

The Savage criterion is a safety criterion, used to achieve maximally guaranteed results under the worst conditions. It accepts the maximum negative development of the situation, where a selected strategy avoids both excessive wins and losses. The worst-case option (the strategy of destiny) is taken into account. It can use when strategy selection errors could lead to catastrophic consequences when decisions are made only once and cannot be changed in the future.

The Laplace criterion determines the strategy that maximizes gains in an uncertain state of the environment. The one with the lowest score according to the Laplace criterion is the best option. This criterion represents extreme optimism, not taking into account any negative outcomes except for the best one. This risk level from the negative impact of changes in the external environment is not considered. It should be noted that situations requiring the application of such a criterion are not limited only to optimists, who cannot be corrected but also to those who are trapped and must adhere to the principle of "do or break". The main drawback of this criterion relates to the fact that when finding the average payoff level, the offsetting effect of small payoffs can occur.

The Hurwitz criterion guides the selection of recommended solutions based on a range of characteristic average outcomes between extreme pessimism and unrestrained optimism. The Hurwitz criterion is related to introducing a weight parameter $0 \leq \rho \leq 1$, called the pessimism index. The assumption about the environment's behavior is that for any alternative choice, the worst choice is made with probability ρ, and the best choice is made with probability $(1 - \rho)$. When $\rho = 0$ the Hurwitz criterion coincides with the Laplace criterion at maximum, and when $\rho = 1$ – with the Wald criterion at maximum. By using the Hurwitz criterion, we apply more significant information under the conditions of Wald, Savage, and Laplace. The main drawback of this criterion is that it only considers two outcomes – the worst and the best.

Additionally, there is difficulty in specifying a pessimism index, ρ. The assumption is that every rational decision-maker must select appropriate maximum or minimum strategies. Caution is required.

The hybrid intelligent system is a set of statistical simulation models in which the qualitative side of loosely structured problems and performance evaluation of processes for determining the mechanical properties of geopolymers are solved using Markov chains, while criterion methods are used for quantitative inference, and the final result best adapts the results of both applications. The quantitative side of loosely structured tasks and process performance evaluation is solved using Markov chains, while criterion methods are used for quantitative conclusions, and the final result best adapts the results of both applications.

5. Experiment

Compressive strength testing of mortar was performed as per AS 1012.9 using (Ø46 x 92) mm diameter cylindrical molds. ASTM C39 was conducted for compressive strength tests of hardened concrete, using (Ø100 × 200) mm cylinder molds. Three sample cylinders were tested, with the experimental values averaged.

The density of geopolymer composite materials was measured according to standard CSN EN 1936 and was estimated by dividing the mass of the sample by its volume. The testing samples with (Ø100 x 200) mm dimensions were used to measure the density after 28 days.

The compressive strength is measured on a VEB Werktoff Prufmaschinen Leipzig, 500 kN, ambient condition temperature 23 ± 2 °C, and relative humidity 65 %. The samples are cured and tested by the standard ASTM C 31/C 31M. Values are the averages of four separate tests. Data that deviated by more than 10 % were eliminated. The loading was displacement-controlled at a constant rate of 2.4 mm/min for all the tests. At least two cylinders are tested at the same age and the average strength is reported as the test result to the nearest 0.1 MPa.

The modulus of elasticity by the equation:

$$E_c = 2707\sqrt{f_{cm}} + 5300, \tag{10}$$

where f_{cm} is compressive strength, MPa.

In order to obtain different mechanical properties of geopolymers, necessary for multicriteria optimization of their composition, the conditions of their curing were changed from the beginning of the process of formation of the geopolymer mixture structure after 7, 14, 28, 90 days. The obtained results of mechanical properties of geopolymers are presented in Table 2.

6. Result and Discussion

The presented methods and results of determining the mechanical properties of geopolymers through their relationship with the mechanism of structure formation were used as a basis for the construction of the transition probability matrix in Table 3, in which the current initial value of the probabilities of mechanical properties is represented as the first row of the matrix, and the subsequent ones - as rows denoting transitions to subsequent states. The sum of probabilities in each row is equal to 1. Processing of this matrix by the method of Markov chain calculation allows determining values of weighting coefficients ω_j.

Table 2

Mechanical properties of geopolymer concrete

Samples	Density, ρ, kg/m^3	Compressive strength, σ_c, MPa	Modulus of Elasticity in compression, GPa	Splitting tensile strength, MPa
7M1	2112	6.58	12.24	1.03
14M1	2073	7.13	12.53	1.07
28M1	2057	8.94	13.39	1.20
90M1	1999	9.09	13.46	1.21
7M2	2135	7.25	9.76	0.68
14M2	2104	9.12	11.52	0.85
28M2	2093	9.75	12.03	0.90
90M2	2033	10.05	12.27	0.92
7M3	2195	20.85	17.89	1.46
14M3	2168	24.76	19.21	1.59
28M3	2146	29.76	20.63	1.73
90M3	2003	29.96	20.68	1.73
7M4	2222	19.23	17.27	1.40
14M4	2230	26.44	19.72	1.64
28M4	2167	28.11	20.19	1.69
90M4	1984	28.41	20.27	1.69
7M5	2250	26.61	19.77	1.64
14M5	2153	28.03	20.17	1.68
28M5	2164	31.49	21.06	1.77
90M5	2035	31.97	21.18	1.78
7M6	2250	22.18	18.36	1.51
14M6	2233	27.76	20.09	1.68
28M6	2176	28.61	20.32	1.70
90M6	2104	29.88	20.66	1.73

Note: 7M1 means 7 is day curing, and M1 is mixture number 1.

Table 3

Transition probability matrix

Current state / Subsequent state	Compressive strength	Density	Young's modulus	Splitting tensile strength
Compressive strength	0,4000	0,3000	0,2000	0,1000
Density	0,5000	0,2500	0,1600	0,0900
Young's modulus	0,5500	0,1500	0,1100	0,1900
Splitting tensile strength	0,3500	0,1000	0,2000	0,3000

The initial state vector in accordance with Table 3 can be written in the form:

$$P(0) = [0.4000, 0.3000, 0.2000, 0.1000] \quad (11)$$

The transition probability matrix has the following form:

$$T = \begin{bmatrix} 0.4000 & 0.3000 & 0.2000 & 0.1000 \\ 0.5000 & 0.2500 & 0.1600 & 0.0900 \\ 0.5500 & 0.1500 & 0.1100 & 0.1900 \\ 0.3500 & 0.1000 & 0.2500 & 0.3000 \end{bmatrix} \quad (12)$$

Multiplying the initial state vector *P*(0) by the matrix of transition probabilities *T*, we obtain the probability distribution at the first stage of decision-making *P*(1). In accordance with the methodology for calculating Markov chains, this probability will be equal to:

$$P(1) = P(0) \times T = [0.4550, 0.2350, 0.1750, 0.1350] \quad (13)$$

Multiplying the state vector P(1) by the matrix of transition probabilities T, we obtain the probability distribution at the next decision-making stage P(2):

$$P(2) = P(1) \times T = [0.4430, 0.2350, 0.1816, 0.1404] \quad (14)$$

Multiplying the state vector P(2) by the matrix of transition probabilities T, we obtain the probability distribution at the next decision-making stage P(3):

$$P(3) = P(2) \times T = [0.4437, 0.2329, 0.1813, 0.1421] \quad (15)$$

We repeat similar calculations until constant stationary values of the state vector are reached:

$$P(4) = P(3) \times T = [0.4434, 0.2327, 0.1815, 0.1424] \quad (16)$$

$$P(5) = P(4) \times T = [0.4434, 0.2327, 0.1814, 0.1425] \quad (17)$$

$$P(6) = P(5) \times T = [0.4434, 0.2327, 0.1814, 0.1425] \quad (18)$$

Starting from the fifth step, the values of the state vector stop changing. Thus, we have the following set of weight coefficients for the mechanical parameters of geopolymers:

- compressive strength $\omega = 0.4434$
- density $\omega = 0.2327$
- Young's modulus $\omega = 0.1814$
- Splitting tensile strength $\omega = 0.1425$

The method of criteria convolution consists in transformation of vector criterion into scalar one and manifests itself in assigning coefficients of initial criteria of its subsequent ectremization on the set of admissible variants. In its sense, the convolution is a weighted average of the initial criteria. The condition for using convolution of criteria is their reduction to a single scale, i.e. normalisation. In single-criteria or scalar optimisation, a single objective function is defined over a set of decision options. In multicriteria optimisation there are several such functions at once, forming a vector criterion.

The solution to a scalar optimisation problem is considered to be the element that maximises or minimises the target function. In the case of multicriteria vector optimisation, there is maximisation for one criterion and minimisation for the rest. The set of solutions is represented as a set of selectable vectors.

Table 4.
Matrix of dimensionless values of deviations of mechanical parameters from optimal values

Samples	Density, ω =0.2327	Compressive strength, ω =0.4434	Young's modulus, ω =0.1814	Splitting tensile strength, ω =0.1425
7M1	0.5171	1.0000	0.7868	0.6868
14M1	0.3806	0.9786	0.7618	0.6511
28M1	0.3247	0.9082	0.6879	0.5348
90M1	0.1217	0.9023	0.6819	0.5258
7M2	0.5976	0.9739	1.0000	1.0000
14M2	0.4891	0.9012	0.8486	0.8479
28M2	0.4506	0.8767	0.8048	0.8031
90M2	0.2407	0.8650	0.7842	0.7852
7M3	0.8075	0.4449	0.3010	0.3022
14M3	0.7130	0.2928	0.1875	0.1859
28M3	0.6361	0.0984	0.0655	0.0606
90M3	0.1357	0.0906	0.0612	0.0606
7M4	0.9020	0.5079	0.3543	0.3558
14M4	0.9300	0.2275	0.1437	0.1411
28M4	0.7095	0.1625	0.1033	0.0964
90M4	0.0692	0.1509	0.0964	0.0964
7M5	1.0000	0.2209	0.1394	0.1411
14M5	0.6606	0.1656	0.1050	0.1053
28M5	0.6990	0.0311	0.0285	0.0248
90M5	0.2477	0.0124	0.0182	0.0159
7M6	1.0000	0.3932	0.2606	0.2574
14M6	0.9405	0.1762	0.1119	0.1053
28M6	0.7410	0.1431	0.0921	0.0874
90M6	0.4891	0.0937	0.0629	0.0606

The methodology of calculations of parameters of target functions based on multi-criteria analysis using Laplace, Hurwitz, and Wald criteria requires consistent use and finding experimental values of deviations from the priority location of targets. The results of calculations and values of convolutions and criteria for determining the optimality of mechanical parameters of geopolymers are presented in Table 5

The calculations were carried out in the Maple computer mathematics system. Table 4,5 presents the results of calculations by formulas (3–9) for each group of mechanical parameters. Based on expert assessments, the optimal values of the parameters were established (maximum or minimum values from Table 2): density - minimum; compressive strength, splitting tensile strength, Young's modulus - maximum;

Table 5 uses the following designations: ya — additive convolution (4); yms - multiplicative convolution (5); ymd - additional multiplicative convolution (6); Vald - Wald criterion (7); Laplace - Laplace criterion (8); Hurwitz - Hurwitz criterion (9). The optimal values of the criteria and convolutions are highlighted in bold and in color.

Table 5.
Values of convolutions and criteria for determining the optimality of mechanical parameters of geopolymers

Samples	min	max	(max+min)/2	y_a	y_{ms}	y_{md}
7M1	0.5171	1.0000	0.7585	0.8043	0.7784	0.6213
14M1	0.3806	0.9786	0.6796	0.7534	0.7083	0.5966
28M1	0.3247	0.9082	0.6164	0.6792	0.6303	0.5535
90M1	0.1217	0.9023	0.5120	0.6270	0.4982	0.5274
7M2	0.5976	1.0000	0.7988	0.8948	0.8767	0.6566
14M2	0.4891	0.9012	0.6951	0.7882	0.7666	0.6042
28M2	0.4506	0.8767	0.6636	0.7540	0.7302	0.5862
90M2	0.2407	0.8650	0.5528	0.6937	0.6223	0.5567
7M3	0.3010	0.8075	0.5543	0.4828	0.4506	0.4102
14M3	0.1859	0.7130	0.4494	0.3563	0.3114	0.3175
28M3	0.0606	0.6361	0.3483	0.2121	0.1317	0.2018
90M3	0.0606	0.1357	0.0982	0.0915	0.0875	0.0887
7M4	0.3543	0.9020	0.6282	0.5501	0.5169	0.4562
14M4	0.1411	0.9300	0.5356	0.3635	0.2714	0.3276
28M4	0.0964	0.7095	0.4030	0.2697	0.1958	0.2502
90M4	0.0692	0.1509	0.1101	0.1142	0.1089	0.1104
7M5	0.1394	1.0000	0.5697	0.3760	0.2709	0.3389
14M5	0.1050	0.6606	0.3828	0.2612	0.1973	0.2423
28M5	0.0248	0.6990	0.3619	0.1852	0.0612	0.1814
90M5	0.0124	0.2477	0.1300	**0.0687**	**0.0277**	**0.0680**
7M6	0.2574	1.0000	0.6287	0.4910	0.4269	0.4185
14M6	0.1053	0.9405	0.5229	0.3323	0.2227	0.3051
28M6	0.0874	0.7410	0.4142	0.2651	0.1806	0.2474
90M6	0.0606	0.4891	0.2749	0.1754	0.1203	0.1676
	Vald	Laplas	Hurwitz			
	0.1357	0.0124	0.5062			

An analysis of the results obtained allows us to state that the depreciation of convolutions (additive, multiplicative, and additional multiplicative) gives an unambiguous conclusion - the optimal composition of 90M5. The Laplace criterion also indicates the composition of 90M5. The optimum composition of geopolymer mixtures was determined: 100 g of fly ash, 150 g of cement, 180 g of activator solution, 90 g of fine sand, 480 g of coarse aggregate.

The Wald criterion gives the optimal composition 90M3, while it should be noted that the values of the convolutions and the Laplace criterion (minimum) for this composition are also close to the minimum values. Therefore, the 90M3 composition can be put in second place in terms of optimal mechanical properties.

The Hurwitz criterion significantly depends on the pessimism coefficient ρ (see formula (9)), the choice of which is subjective and greatly changes the result. Therefore, the Hurwitz criterion should be considered an auxiliary one and its discrepancy with the general trend should not be considered.

7. Conclusions

The proposed intellectual system of multi-criteria evaluation using Markov chains has been developed in the hybrid implementation of structured and unstructured problems of obtaining optimal characteristics of geopolymers. Combining subjective and objective elements of decision selection this approach represents a new way of information processing based on mathematical modelling and probabilistic dynamics.

The simulation of target function parameters has shown the advantage of evaluating the digitalization of technologies in the analysis of geopolymer properties, where the qualitative side of loosely structured problems is solved with the help of Markov chains, while for quantitative conclusions criterion methods are used, and the final result best combines the results of both applications.

The methodology of the complex use of Markov chains in combination with optimization criteria is the basis for the application of the target functions to increase the reliability of the parameter estimation for determining the optimal composition and structure of geopolymers when changing their manufacturing technologies.

Prospects for further research of the authors consist in the creation of hybrid models of quantitative and qualitative methods of experimental data processing in combination with prediction methods, where the method presented in the article can be used at the stage of data preprocessing

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