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Development and Multi-Objective Optimization of Cosmetic Cream Formulations Using Artificial Neural Networks and Genetic Algorithms

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ABSTRACT

In recent years, demand for herbal cosmetics has grown due to their safety, efficacy, and eco-friendliness. Yet, herbal skincare formulations often lack standardization, leading to variable quality. This study focuses on developing and optimizing a herbal moisturizing cream using artificial intelligence (AI) in formulation design. Fourteen natural ingredients, including aloe vera, shea butter, almond oil, hyaluronic acid, and essential oils, were combined into 30 experimental formulations through a Simplex Lattice mixture design. Key properties—pH, viscosity, permeation, and moisturizing ability—were measured and modeled using a fuzzy logic neural network integrated with a genetic algorithm. The optimal formula was then evaluated for texture, absorption, spreadability, and stability. Integrating I(14)-HL(2)-O(4) with genetic algorithms highlights an effective approach for standardizing and optimizing herbal cosmetic formulations, offering a scientific basis for creating high-quality, consistent skincare products.

Introduction

Optimizing cosmetic formulations, particularly skin creams, is challenging due to nonlinear interactions among actives, excipients, emulsifiers, and preservatives, affecting viscosity, pH, permeability, stability, and moisturizing performance. Traditional Design of Experiments (DoE) methods—such as OFAT, Box–Behnken, and Response Surface Methodology—are limited by linear or quadratic assumptions and sensitivity to experimental noise, often requiring extensive trials and high costs [1]. In contrast, artificial intelligence (AI) offers robust solutions by learning from data, capturing complex nonlinear relationships, and enabling multi-objective optimization. Hybrid approaches combining artificial neural networks (ANN), fuzzy logic, and genetic algorithms (GA) [2] are particularly effective: ANNs model nonlinear input–output relationships directly from training data, fuzzy logic handles uncertainty and qualitative sensory attributes, and GAs perform global optimization to identify ingredient combinations that achieve target

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properties such as viscosity, pH, and moisturizing efficacy [3]. This AI-assisted strategy enhances predictive accuracy, reduces trial-and-error experimentation, and supports rational, data-driven design of high-performance cosmetic formulations [4]. The integration of ANN, fuzzy logic, and GA establishes an intelligent optimization system: ANN captures input–output relationships, fuzzy logic manages uncertainty, and GA identifies the optimal formulation [5]. This strategy accelerates development, reduces experimental trials, and enhances product quality. In moisturizing cream design, it enables precise balancing of oil–water phases, emulsifiers, emollients, and active ingredients to achieve key attributes such as appropriate viscosity, physiological pH, effective skin absorption, and sustained hydration [6]. However, traditional formulation optimization approaches often rely on empirical experience and classical experimental designs such as Response Surface Methodology (RSM) or Box–Behnken design, which are time- and resource-consuming and struggle to address nonlinear and multi-objective relationships between formulation components and product characteristics [7].

Artificial intelligence (AI) is emerging as a powerful tool in formulation design and decision-making. This study employs a hybrid AI framework—ANN to capture ingredient-attribute relationships, fuzzy logic to handle uncertainty, and GA to optimize component ratios—for skin cream development [5]. Target parameters include viscosity, pH, permeability, and moisturizing efficacy. The integrated approach reduces experimental trials, shortens development time, and ensures consistent, high-quality formulations compared with traditional methods [1].

This study aims to develop and optimize a fast-absorbing turmeric ointment by predicting product performance from the physicochemical properties of raw materials. An integrated AI framework combining Simplex Lattice mixture design, Genetic Algorithm (GA), and Adaptive Neuro-Fuzzy Inference System (ANFIS) is proposed to model nonlinear ingredient–attribute relationships and identify optimal formulations. This approach minimizes experimental workload, reduces cost and time, and enables the design of skin creams with high moisturizing efficacy, rapid transdermal absorption, and stable performance, thereby providing a scientific foundation for advanced cosmetic development.

Materials and Methods

Materials and Equipment

Pharmaceutical-grade ingredients used included aloe vera extract, coconut oil, shea butter, almond oil, hyaluronic acid, glycerin, beeswax, xanthan gum, lecithin, olive oil, vitamin B5, vitamin E, and various natural essential oils. Key instruments comprised a high-speed homogenizer (IKA EUROSTAR 60), pH meter (HANNA Edge), magnetic stirrer (DAIHAN Scientific), analytical balance (JA203P), and standard laboratory tools for formulation and evaluation of cream absorption and stability. Computational tools included Design-Expert for Simplex Lattice mixture design and INForm software for AI-based optimization modeling.

Formulation Methods

Experimental Procedure

The herbal moisturizing ointment was formulated in three main stages after accurately preparing all ingredients according to the predetermined composition. Raw materials included aloe vera extract, coconut oil, shea butter, almond oil, hyaluronic acid (HA), glycerin, beeswax, xanthan gum, lecithin, olive oil, vitamin B5, vitamin E, and natural essential oils. In Stage 1, the aqueous phase (Phase A) was prepared with water-soluble components to hydrate xanthan gum and form the cream base. Specifically, 52.91 g distilled water, 0.59 g xanthan gum, 0.58 g HA, 6.63 g glycerin, 1.12 g vitamin B5, and 13.43 g aloe vera extract were stirred in a 250 mL beaker at 70 °C until homogeneous. In Stage 2, the oil phase (Phase B) was prepared by mixing 10.57 g almond oil, 6.84 g shea butter, 3.51 g beeswax, 2.36 g lecithin, 6.82 g olive oil, and 1.11 g vitamin E in a 100 mL beaker, stirring at 70 °C until a uniform transparent oil phase was obtained. In the final emulsification stage, Phase A was gradually added to Phase B under high-speed homogenization (10,000 rpm) to ensure even dispersion of components and formation of a stable emulsion system. The mixture was homogenized for 15–30 minutes until complete homogeneity was achieved. The final product was a 100 g batch of herbal moisturizing cream characterized by high stability, good skin permeability, and compliance with quality requirements for cosmetic skincare products [8,9].

Designing An Intelligent Model

To systematically design a moisturizing cream, the Simplex Lattice mixture design in Design-Expert software was employed. An experimental matrix of 30 formulations with varying ingredient ratios was generated to explore the formulation space. Each formulation combined core components in different proportions and was evaluated for four critical properties: pH (y_1, skin compatibility), absorption rate (y_2, permeation efficiency), moisture retention (y_3, hydration duration), and viscosity (y_4, rheological behavior). The dataset (x_1–x_{14} inputs, y_1–y_4 outputs) provided the basis for building a predictive model using Artificial Neural Network (ANN) integrated with Genetic Algorithm (GA). The ANN captured complex nonlinear input–output relationships, while GA enabled multi-objective optimization of formulation parameters. For preliminary approximation or when ANN training remained incomplete, a second-order polynomial regression model was also applied to describe correlations between formulation variables and product responses. This hybrid modeling framework offered both robustness and flexibility in guiding the rational development of optimized moisturizing cream formulations [1]:

$$y_k = b_0 + \sum_{i=1}^{14} b_i x_i + \sum_{i=1}^{14} \sum_{j}^{14} b_{ij} x_i x_j \quad (k = 1,2,3,4) \qquad (1)$$

Where: y_k: is the predicted property (pH, absorption time, moisture retention, or viscosity); β_0, β_i, β_{ij}: are regression coefficients of ingredients from Design-Expert.

Based on the experimental matrix, an artificial neural network (ANN) with architecture I(14)–HL(2)–O(4) was constructed, where 14 inputs represented formulation variables, 2 hidden neurons captured nonlinear interactions, and 4 outputs predicted pH, absorption rate, moisture retention, and viscosity. The ANN was trained using supervised backpropagation for 1000 iterations with a convergence error of 0.001. After training, it was integrated with a genetic algorithm (GA) via INForm to determine optimal ingredient ratios. This hybrid ANN–GA system combined predictive modeling with multi-objective optimization, effectively capturing complex input–output relationships. The optimal formulation predicted by the model was prepared and experimentally validated, confirming its accuracy and consistency with product quality requirements.

Quality Evaluation of The Cream

All cream samples were evaluated for physicochemical and sensory attributes, including pH, absorption time (s), moisture retention (h), viscosity (mPa·s, equivalent to cP), spreadability, phase stability, color, and fragrance. Skin penetration and sensory feel were additionally examined to ensure consumer acceptability and product performance [10]. pH measurement: Triethanolamine was gradually added under continuous stirring to adjust the formulation, and pH was determined using a calibrated pH meter [11]. Triethanolamine is a strongly alkaline agent (1% solution ≈ pH 10) commonly used in cosmetics to achieve skin-compatible pH. Viscosity: Samples were analyzed with an IKA ROTAVISC me-vi rotational viscometer (spindle SP-3, 5 min). Each experiment was performed in triplicate, and measurements deviating more than 2.5% from the mean were excluded.

Spreadability: A 1.0 g sample was placed between two identical glass plates (diameter 8 cm, weight 25.37 g). After 1 min, the spreading area was measured; acceptable formulations met general topical standards [11,12]. Sensory evaluation: Creams were visually inspected for texture, homogeneity, color, and fragrance. Acceptable samples exhibited a soft, smooth, uniform appearance, light brown color, and characteristic coconut oil scent. Stability was confirmed by the absence of phase separation, solidification, discoloration, or liquefaction at 37 °C. Adhesion and spread on skin were also assessed under well-lit conditions [12].The spreadability of the cream is determined using the formula:

$$S = \frac{d^2 p}{4} \qquad (2)$$

In this study, the spreadability (S) was expressed in g·cm/s, with an acceptable range of 30–40 cm². In this context, d represents the average diameter obtained from two repeated measurements. The cream samples were considered to meet the quality standards if they satisfied all criteria, including organoleptic properties, pH, emulsion type, stability, and spreadability.

Results and discussion

Formulation Matrix Development

An experimental matrix of 30 moisturizing cream formulations was constructed using the Simplex Lattice mixture design. Fourteen ingredients served as independent variables with proportions varied within predefined limits: distilled water (x_1), aloe vera extract (x_2), glycerin (x_3), hyaluronic acid (x_4), almond oil (x_5), shea butter (x_6), beeswax (x_7), soy lecithin (x_8), olive oil (x_9), xanthan gum (x_{10}), panthenol (x_{11}), vitamin E (x_{12}), grapefruit essential oil (x_{13}), and rose essential oil (x_{14}). Ingredient ranges were adapted from commercial formulations and cosmetic formulation standards (Table S1, Table S2). The dependent variables included pH (y_1), absorption time (y_2, s), moisture retention (y_3, h), and viscosity (y_4, mPa·s). These parameters were selected as critical quality indicators, reflecting skin compatibility, permeation efficiency, hydration duration, and rheological performance. Their inclusion

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was guided by standard references and cosmetic evaluation guidelines (Table 1), ensuring both scientific validity and practical relevance for assessing product performance.

Table 1: Standard Variation Ranges of Skin Cream Properties

Cream Properties	notation	Min	Max
pH	y_1	5.97	6.24
Absorption time (seconds)	y_2	27.37	28.23
Moisture retention (hours)	y_3	9.37	9.61
Viscosity (mPa·s)	y_4	118704	118954

The cream preparation process, detailed in the Methods section, consisted of three main stages, combining hydrophobic and hydrophilic phases to form a stable emulsion and homogeneous cream base. The experimental matrix was then used to construct a neuro-fuzzy neural network with architecture I(14)–HL(2)–O(4). Each output property was modeled separately using backpropagation. Training was performed over 1000 epochs with momentum 0.7, learning rate 0.7, error tolerance 0.001, and random seed 10000. A sigmoid transfer function was applied to neurons in both hidden and output layers. After training, the neural network exhibited strong statistical performance, as presented in Table 2.

Table 2: Optimal cream formulation from the I(14)–HL(2)–O(4) neural network, with predictive performance validated experimentally

Cream Properties	notation	Model quality			Predictibility of model		
		R^2	values F	MSE	Predicted properties	Empirical Evaluation	Relative Error, %
pH	y_1	0.9985	75.395	0.000097	6.10	6.01	1.5
Absorption time (seconds)	y_2	0.9995	263.618	0.000098	27.80	27.30	1.8
Moisture retention (hours)	y_3	0.9995	243.710	0.000100	9.49	9.5	0.84
Viscosity (mPa·s)	y_4	0.9994	204.807	0.000111	118829.06	119200.0	0.31

Optimal ingredients of herb cream formulation from I(14)–HL(2)–O(4) neural network

Ingredients	notation	Percentage ratio (% w/w)	Ingredients	notation	Percentage ratio (% w/w)
Distilled Water	x_1	52.91	Soy Lecithin	x_8	2.36
Aloe Vera Extract	x_2	13.43	Olive	x_9	6.82
Glycerin	x_3	6.63	Xanthan Gum	x_{10}	0.59
Hyaluronic acid (HA)	x_4	0.58	Panthenol (B5)	x_{11}	1.12
Almond Oil	x_5	10.57	Vitamin E	x_{12}	1.11
Shea Butter	x_6	6.84	Grapefruit Essential Oil	x_{13}	0.87
Beeswax	x_7	3.51	Rose Essential Oil	x_{14}	1.16

The experimental results and constructed artificial neural network (ANN) confirmed consistent causal relationships in the herbal cream formulations. Across 30 trials, predicted and experimental values of four key properties showed strong agreement, demonstrating high model reliability and predictive accuracy. The optimal ANN architecture, I(14)–HL(2)–O(4), developed using INForm, was integrated with a genetic algorithm (GA) to optimize formulation design. The GA explored the formulation space through multi-objective optimization functions, each tailored to specific product attributes. Four desirability functions—UpHill, DownHill, Tent, and Flat—were employed. pH was optimized with an UpHill function, targeting ~6.10, the physiological level ideal for skin compatibility. Moisture retention was also optimized with an UpHill function, as prolonged hydration is desirable in skincare. Absorption time was optimized using a Tent function, ensuring the cream penetrates effectively without being too rapid (poor film formation) or too slow (greasy sensation). Viscosity was optimized with a Flat function, maintaining values within an acceptable range for stable texture, spreadability, and user satisfaction. This integrated ANN–GA approach effectively balanced multiple objectives, providing an intelligent and efficient method for developing optimized moisturizing cream formulations.

By applying tailored objective functions within the GA framework, the model identified the optimal combination of 14 ingredients to achieve desirable pH, absorption rate, moisturizing efficacy, and rheological properties simultaneously. The resulting formulation, summarized in Table 2, demonstrates a robust intelligent design strategy that reduces trial-and-error experiments while improving product quality [12].

To evaluate the predictive performance of the neuro-fuzzy model [I(14)–HL(2)–O(4)], the optimized cream formulation was prepared and experimentally validated. Measured values of pH (y_1), absorption time (y_2), moisture retention (y_3), and viscosity (y_4) were compared with predicted values, with relative errors consistently below 2% (Table 2). The skin absorption ability was determined by observing the rate and extent of product penetration on an artificial skin surface, using parameters such as absorption time. Meanwhile, the moisturizing ability was evaluated over time by measuring skin hydration levels before and after product application. These assessments provide essential information on the product's performance in terms of skin compatibility and hydration efficacy. This strong agreement confirmed the accuracy and robustness of the model for topical cream optimization. The optimized-experimental formulation exhibited nearly neutral pH (~6.01), ensuring skin compatibility and low irritation risk; rapid absorption (~27 s), indicating efficient permeation without greasy residue; long-lasting hydration (~9.5 h), confirming sustained moisturizing efficacy; and stable viscosity (~119,000 mPa·s), supporting favorable rheology and user comfort. Collectively, these results demonstrate that the integrated approach—combining mixture design, ANN modeling, and genetic algorithms—provides a powerful and reliable framework for multi-objective optimization of cosmetic formulations. The 3D response surface plots (Fig. 1) illustrate relationships between key formulation components and product attributes of the moisturizing cream—pH (y_1), absorption time (y_2), moisture retention (y_3), and viscosity (y_4). These plots were generated from the ANN model I(14)–HL(2)–O(4) integrated with an optimization algorithm. For pH (y_1), almond oil (x_5), aloe vera extract (x_2), and grapefruit essential oil (x_{13}) showed the strongest influence. Increasing x_5 or x_2 slightly elevated pH, enabling the formulation to reach a near-neutral value (~6.2), consistent with the objective of ensuring skin physiological compatibility.

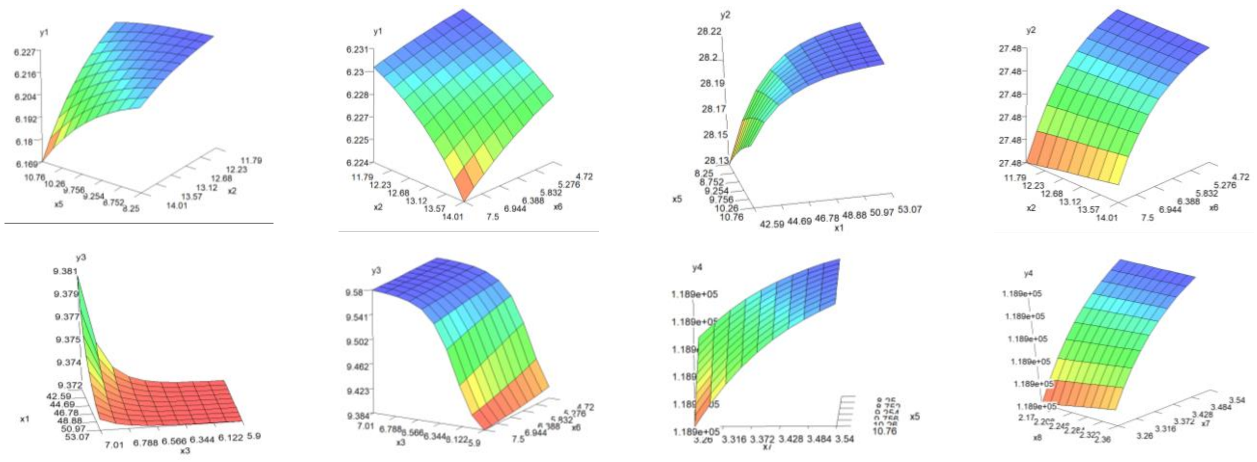

Fig. 1. Optimal response surface targets corresponding to each cream property

Absorption time (y_2): The response plots emphasized the influence of distilled water (x_1), aloe vera extract (x_2), and shea butter (x_6). An increase in x_1 combined with a reduction in x_6 improved absorption efficiency, while higher levels of x_1 and x_2 yielded faster absorption times (~27.4–28.2 s), indicating effective permeation without greasy residue. Moisture retention (y_3): Glycerin (x_3) and shea butter (x_6) were identified as major contributors. Increasing x_3 and reducing x_6 extended hydration, with retention times ranging from 9.38 to 9.58 h. These findings confirm glycerin's established role as a potent humectant and highlight the modulatory effect of x_6 on viscosity and skin adhesion. Viscosity (y_4): Beeswax (x_7), almond oil (x_5),

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and olive oil (x_9) were primary determinants of viscosity. Elevated concentrations of x_7 and x_9 increased viscosity, stabilizing near 119,000 mPa·s, thereby ensuring optimal rheological behavior for smooth, uniform spreading without excessive thickness.

Collectively, the response surface plots revealed nonlinear interactions between formulation components and product attributes. These bivariate effects were effectively captured by the ANN–GA framework, which successfully guided the development of a moisturizing cream that fulfills functional, sensory, and performance requirements. The optimal formulation obtained from the I(14)–HL(2)–O(4) ANN–GA model represents a globally optimized emollient cream, demonstrating the practical potential of integrating artificial neural networks, genetic algorithms, and Simplex Lattice mixture design for herbal-based cosmetic development.

A 30-run experimental matrix provided a comprehensive dataset for AI training, enabling reliable prediction of key cream attributes—pH, absorption rate, moisture retention, and viscosity—prior to experimental validation. Predicted outcomes closely matched experimental values, with relative errors within acceptable limits, confirming the robustness and accuracy of the model. The optimized formulation not only satisfied technical criteria but also met aesthetic and sensory requirements, including uniform texture, natural color and scent, rapid absorption, long-lasting hydration, and storage stability. The incorporation of natural ingredients such as aloe vera, hyaluronic acid, almond oil, shea butter, and essential oils further improved skin compatibility, safety, and consumer appeal. Overall, the study demonstrates that AI-assisted optimization can effectively reduce trial-and-error experimentation while achieving a stable, high-quality, and market-relevant moisturizing cream [12]. Furthermore, the formulation process was standardized through a rationally designed three-stage procedure: (i) aqueous phase preparation, (ii) oil phase blending, and (iii) emulsification. This systematic approach not only ensures batch-to-batch reproducibility and consistent product quality but also facilitates scalability, thereby supporting potential transition from laboratory development to industrial-scale manufacturing.

Conclusion

This study developed an optimized herbal moisturizing cream using an artificial neural network [I(14)–HL(2)–O(4)] integrated with a genetic algorithm. The hybrid model accurately predicted key quality attributes—pH, absorption time, moisture retention, and viscosity—with relative errors below 2%. The optimized formulation exhibited favorable characteristics for topical application, fulfilled aesthetic and functional requirements, and maintained excellent physical stability. These results highlight the effectiveness of combining ANN, GA, and experimental design as a robust strategy for optimizing natural cosmetic formulations, reducing trial-and-error experimentation, and supporting the development of safe, high-performance, and market-relevant products.

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