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Review Article

Artificial Neural Network In Pharmaceutical And Cosmeceutical Research

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ABSTRACT

The presented collection of studies highlights the diverse applications of Artificial Neural Networks (ANNs) in pharmaceuticals and cosmeceuticals. Various researchers employ ANNs to optimize pharmaceutical formulations, predict drug release, and explore drug-target interactions. The studies demonstrate ANNs' superiority in handling complex relationships and learning from data patterns, offering enhanced accuracy in optimization and prediction tasks. Applications range from predicting skin permeability and toxicity to formulating stable oil-in-water emulsions and optimizing liposome size. ANNs prove valuable in drug discovery, providing insights into chemogenomic space and identifying potential new targets. The review emphasizes the growing significance of ANNs in revolutionizing approaches to pharmaceutical and cosmetic research. In this there is a discussion on the integration of computer science with theoretical bases, specifically nonlinear dynamics and chaos theory, to create intelligent agents such as artificial neural networks (ANNs). The goal is to address problems of high complexity by allowing these networks to adapt dynamically. The integration of computer science with theoretical bases enables the development of intelligent agents, with ANNs being highlighted as an example. ANNs are described as capable of adapting dynamically to complex problems. ANNs are noted for their ability to reproduce the dynamic interaction of multiple factors simultaneously. This characteristic is beneficial for

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studying complexity in various contexts. Integrating computer science principles, nonlinear dynamics, and chaos theory with artificial neural networks provides a powerful toolset for studying complex systems, inside the body. The adaptability and capacity for dynamic interaction modeling make ANNs particularly well-suited for addressing challenges associated with high complexity and individualized healthcare. Artificial neural networks can also be used as computational tools with significant potential for analyzing cosmological data. It emphasizes their applications in modelling data, saving computational time, and classifying objects, highlighting the qualities that make ANNs a promising alternative for data analysis in cosmology.

INTRODUCTION

ANNs are computational models inspired by the structure and function of the human brain. They consist of interconnected nodes (neurons) organized into layers. Neural networks can be trained on large datasets to learn complex patterns and relationships, making them effective in tasks such as classification, regression, and pattern recognition. ANNs are described as a branch of machine learning models. They are computational systems inspired by the principles of neuronal organization found in biological neural networks. ANNs are based on principles discovered by connectionism in biological neural networks. This implies that the structure and functioning of ANNs are inspired by how neurons are organized and connected in animal brains.

- **Artificial Neurons:**
  ANNs consist of connected units or nodes called artificial neurons. These artificial counterparts loosely model the neurons found in biological brains.
- **Connections (Edges):**
  The connections between neurons in ANNs are referred to as edges. Similar to synapses in biological brains, these connections allow the transmission of signals between neurons.
- **Signal Transmission:**
  Each connection can transmit a signal, which is represented as a real number. The artificial neurons receive signals, process them, and can then transmit signals to connected neurons.

Structure of artificial neural network

1. **Input Layer:**

Receiving External Data: The input layer is the initial layer of the neural network that receives data from the external world. This data could be anything that the neural network needs to analyse, process, or learn about.

2. **Hidden Layers:**

Transformation of Input Data:

The input data then passes through one or more hidden layers. The hidden layers perform transformations on the input data using weighted connections and activation functions. These transformations are crucial for the network to extract relevant features and patterns from the input.

Feature Extraction:

The hidden layers are responsible for extracting valuable features and representations from the input data, making the network capable of learning complex relationships and patterns.

3. **Output Layer:**

Providing Final Output:

The processed data from the hidden layers is then sent to the output layer. The output layer produces the final result or response of the neural network based on the patterns and features learned during the training process.

Response to Input Data:

The output layer's response could take various forms depending on the nature of the task the neural network is designed for. It could be a classification label, a numerical value, or any other relevant output.

4. **Data Transformation Pipeline:**

Value Addition:

The overall process involves a transformation pipeline where input data is successively processed by the hidden layers to extract valuable information before reaching the output layer.

Learning and Adaptation:

During the learning phase (training), the weights of the connections in the network are adjusted to minimize the difference between the predicted output and the actual output, enabling the network to adapt and improve its performance over time.

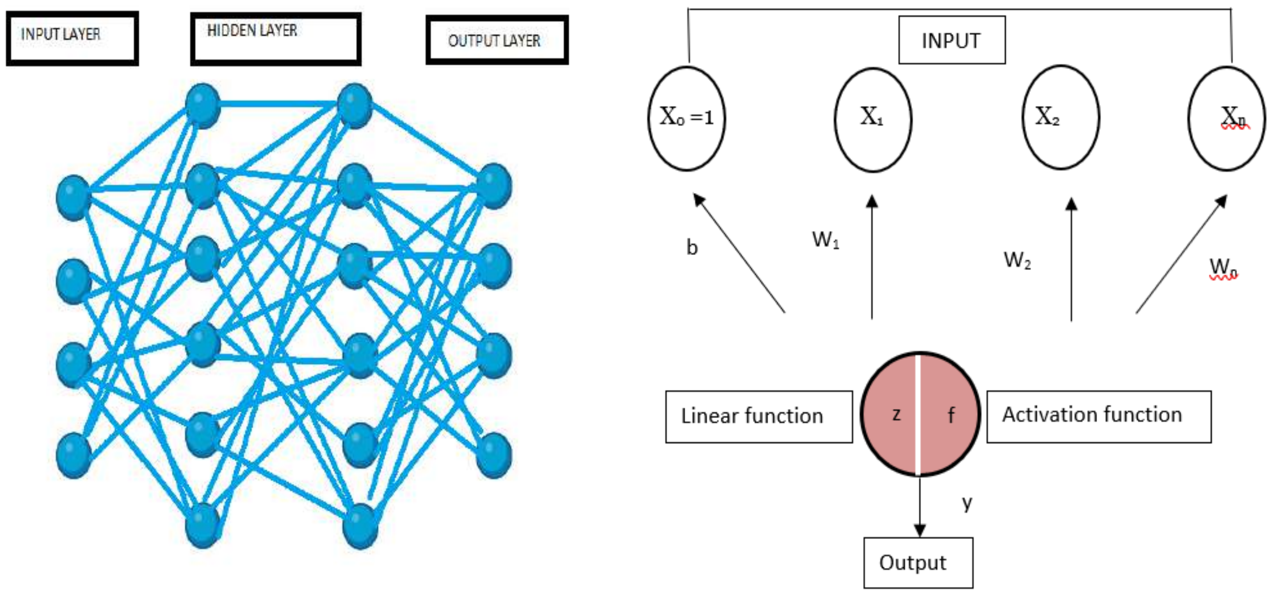

Figure No: 1 Structure of artificial neural network

The structure and operations of artificial neural networks closely mimic the workings of human neurons. The input layer receives external input, the hidden layer computes weighted sums, and the connections between neurons are adjusted during training to optimize the network's performance. This parallelism with biological neural networks is a key factor in the effectiveness of artificial neural networks in learning and making predictions from complex data. The structure of artificial neural networks is inspired by the organization of biological neurons found in the human brain.

Components of artificial neurons:

Single Neuron (Perceptron):

a. The left panel illustrates a single neuron, often referred to as a perceptron.
b. Numerical inputs (x) from a dataset are multiplied by individual weights (w).
c. The products of these multiplications are summed together along with a numerical bias term.
d. A mathematical "activation" function converts this sum into a value between 0 and 1, representing the output of the neuron.

Feed Forward Neural Network:

a. The right panel illustrates a simple "feed forward" neural network.
b. In a feed-forward network, neurons are organized into layers (input layer, hidden layers, and output layer).
c. Information is propagated from the input layer to the output layer based on weights and bias factors, as described in the left panel.

Training Process:

a. During the training of the network, numerical values arriving at the output layer are compared against the correct or desired solution.

b. The prediction error is computed based on the disparity between the predicted and desired outcomes.
c. Individual weights of the network are then adjusted in a process known as backpropagation to minimize the error.
d. The network iteratively refines its weights to generate outputs that progressively align more closely with the desired solutions.

Fundamentals of Neural Networks:

a. Architecture:

Neural networks consist of input, hidden, and output layers. Connections between nodes have associated weights that are adjusted during training.

b. Training:

ANNs learn from data through a process of forward and backward propagation. During training, the network adjusts its parameters to minimize the difference between predicted and actual outputs.

c. Activation Functions:

Neurons use activation functions to introduce non-linearity into the network, enabling it to learn complex relationships.

Forward and Backward Propagation:

a. The training process involves both forward and backward propagation of information.
b. Forward propagation refers to the flow of input data through the network, producing an output.
c. Backward propagation involves adjusting the weights based on the computed error, moving backward through the network to refine the model.

Components of Biological Neurons:

The key components of biological neurons, including the cell body (soma), dendrites, and axon, serve as a blueprint for the architecture of artificial neural networks.

Biological Neuron Components:

Soma (Cell Body):

Processes impulses.

Dendrites:

Receive impulses.

Axon: Transfers impulses to other neurons.

Corresponding Elements in ANNs:

Input Nodes:

Analogous to dendrites, these nodes receive input signals in artificial neural networks.

Hidden Layer Nodes:

Correspond to the soma in biological neurons. They compute and process the input signals received from the input nodes.

Output Layer Nodes:

Analogous to the axon, these nodes compute the final output by processing the results from the hidden layer nodes, using activation functions.

Biological Neuron	**Artificial Neuron**
Dendrite	Inputs
Cell nucleus or Soma	Nodes
Synapses	Weights
Axon	Output
Biological Neuron	Artificial Neuron

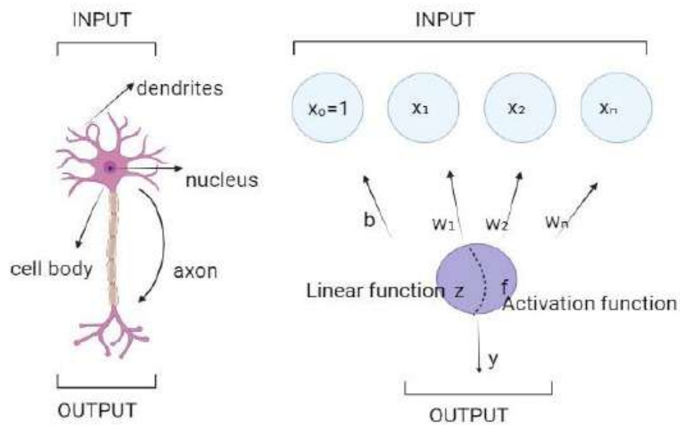

Table 2 difference between artificial and biological neuron

How do artificial neural network works?

Training Set:

Purpose:

ANNs are trained using a set of data known as a training set.

Example:

In the example given, the goal is to teach an ANN to recognize a cat, so the training set consists of thousands of different images of cats.

Learning Process:

Exposure to Data: The ANN is exposed to a diverse set of examples to learn and identify patterns related to the target concept (e.g., a cat).

Training Iterations: The learning process involves multiple iterations to fine-tune the network's ability to recognize specific features or characteristics.

Testing and Evaluation:

Verification:

After training, the performance of the ANN needs to be verified to ensure it can correctly classify images.

Classification Task:

The ANN is tasked with classifying new images as either containing a cat or not.

Backpropagation:

Adjusting Weights:

If the ANN makes incorrect classifications during testing, backpropagation is employed to adjust the weights of the connections within the network.

Error Correction:

Backpropagation involves fine-tuning the weights based on the error rate obtained during the testing phase.

Iteration and Improvement:

Iterative Process: The training and testing process, along with backpropagation, is repeated iteratively.

Continuous Learning:

The ANN continues to learn and improve its performance with each iteration.

Convergence:

Minimizing Error Rates:

The goal is to continue the process until the ANN can correctly recognize a cat in an image with minimal possible error rates.

Optimizing Performance:

a. Convergence is achieved when the network's performance is optimized for accurate and reliable recognition.
b. ANNs offer a virtual method for predicting how drugs will affect the body. This prediction capability contributes to improving patient care by providing insights into drug behaviour and efficacy

Advantages of artificial neural networks in healthcare and cosmetics.

Nonlinear Statistical Modelling:

ANNs are effective in handling nonlinear relationships between variables. This is particularly useful in situations where traditional methods like logistic regression may struggle to capture complex interactions.

Alternative to Logistic Regression:

Logistic regression is a commonly used method for predictive modelling in medicine. The passage suggests that ANNs can offer an alternative or complementary approach, providing more flexibility in capturing intricate relationships.

Reduced Need for Formal Statistical Training:

Users may require less formal statistical training to use ANNs effectively. This suggests that ANNs offer a user-friendly interface, making them accessible to a broader audience within the medical field.

Detection of Complex Non-linear Relationships:

efficiency can be advantageous in real-time applications or situations where quick decision-making is essential.

Handling Noisy or Missing Information:

ANNs can operate effectively even when dealing with noisy or incomplete data. This adaptability is crucial in real-world scenarios where data may not always be perfect or complete.

Generalization to Unseen Data:

ANNs are capable of detecting and representing complex non-linear relationships and interactions between dependent and independent variables. This is a significant advantage in scenarios where relationships are intricate and not easily characterized by linear models.

Incorporation of Literature-Based and Experimental Data:

ANNs can integrate information from various sources, including literature-based and experimental data. This ability to combine different types of data can enhance the robustness and comprehensiveness of the models.

Fast and Simple Operation:

ANNs offer fast and simple operations due to a compact representation of knowledge through weight and threshold value matrices. This

ANNs can generalize well to unseen data. This is important for creating models that can perform reliably on new and previously unseen cases.

Inductive Learning from Training Data:

ANNs can learn inductively from training data, meaning they can recognize patterns and trends that may not be explicitly programmed into the model. This is valuable for capturing the complexity of real-world data.

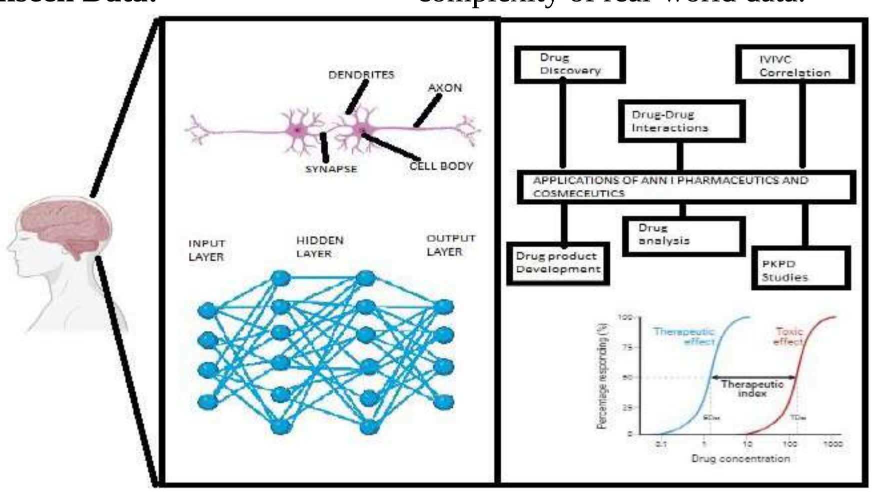

Figure 2 application of ANN in healthcare

ANN is the analytical technique used in pharmaceutical manufacturing.

Industry 4.0 Transformation:

a. Industry 4.0 is transforming manufacturing industries through digitalization, automation, and big data.

b. The goal is to achieve interconnected systems, autonomous decision-making, and the establishment of smart factories.

Role of Machine Learning, Specifically ANNs:

Machine learning techniques, particularly artificial neural networks (ANN), are identified as powerful tools to address computational tasks in the context of Industry 4.0.

Application in the Pharmaceutical Industry:

a. The advancements in Industry 4.0 have extended to the pharmaceutical industry.
b. The Process Analytical Technology (PAT) initiative is mentioned, which focuses on real-time analysis, science-based, and risk-based flexible production.

Systematic Review of ANNs:

The current state of artificial neural networks is systematically reviewed for the most common manufacturing steps of solid pharmaceutical products.

Contribution to Intelligent Manufacturing:

The ultimate goal is to contribute to the implementation of intelligent manufacturing lines with automated quality assurance in the pharmaceutical industry

Advantages of artificial neural networks in Cosmeceutics.

- The computer-aided model used for predicting the stability of various enzymes in the skin.

  For eg: ANN is used for predicting the stability of collagen.

Importance of Collagen:

Collagen is the most abundant protein in the human body.

The instability of collagen is associated with various important diseases, such as Osteogenesis imperfecta, Ehlers-Danlos syndrome, skin aging, fine lines, wrinkles, and collagenopathy.

Collagen Triple Helix Stability:

The stability of the collagen triple helix is closely related to its amino acid sequence, particularly the Gly-X-Y motif.

Computational Methods:

Many research groups have employed computational methods to investigate collagen's structure and its relationship with stability.

Markov Chain Model:

a. Data on a large number of collagen-like peptides were assembled.
b. The first Markov chain model was built to predict collagen stability at different temperatures by analyzing the amino acid sequence.
c. A set of 102 peptides with experimentally determined melting temperatures was used for model training.

Dataset Split and ANN Models:

a. The dataset was split into two classes, stable and unstable, based on melting temperatures.
b. Artificial neural network (ANN) models were built to predict collagen stability at various temperatures (38°C, 35°C, 30°C, and 25°C).
c. Models exhibited high accuracy, ranging between 82% and 92% for stability predictions.
d. Validation:
e. Several cross-validation procedures were performed to validate the developed model.
f. Outcome:
g. The method allows for fast and accurate predictions of collagen stability at different temperatures.

Benefits for Cosmological Research:

Versatility:

ANNs are versatile and can adapt to various types of data and research questions in cosmology.

Efficiency:

The ability of ANNs to handle large datasets and complex relationships can lead to more efficient analysis and modeling of cosmological phenomena.

ARTIFICIAL NEURAL NETWORK in analysis

The method adopted for determining the comparative study of collagen in the body using ANN is explained below.

Software and Normalization:

- Statistical 6.0 was used for constructing the ANN models.
- All variables used in the models were normalized to the same scale.

Model Validation:

- The classical method of leave-one-out was employed for model validation.
- Various statistical parameters, including the Mathews correlation coefficient (MCC) and the ROC curve, were calculated and reported for each model.

Detection of Outliers:

- The study investigated the presence of outlier cases.
- Outliers were considered if there was confusion between the training and validation series.

ANN Algorithms:

Different algorithms were used to construct the ANN models, including:

a. Probabilistic neural networks (PNN)
b. Multi-layer perceptrons (MLP)
c. Radial basis functions (RBF)
d. Linear neural networks (LNN)

Training Periods and Algorithms:

a. ANNs went through one-step testing (one training period) and later two-step testing (two training periods) of the training algorithms.
b. In the two-step training, various algorithms were combined, such as back-propagation, Levenberg-Marquardt, quick propagation, quasi-Newton, and conjugated gradient descent.
c. Combinations of two different methods were tested using a different number of epochs to train the ANN, ranging from 10 to 100,000 epochs.

ROC Curve and Model Selection:

- To obtain the ROC curve using the ANN models, linear neural networks (LNN) were built.
- The selected LNN model was the one most similar to the Linear Discriminant Analysis (LDA) final model.

BENEFITS OF ANN IN COSMECEUTICALS-

Popularity of ANN Algorithms in Bioinformatics: ANN algorithms are well-established tools in bioinformatics and are widely used by various research groups for constructing classification models.

Previous Success with ANN Models:

The author's group has employed ANN models on multiple occasions with favourable results in previous studies.

Analysis of Collagen Peptides:

In one of study, the focus is on analysing the structure of 102 collagen peptides and predicting their stability using ANN models.

Energy Variation and Backbone Analysis:

- The approach involves describing energy variation throughout the protein backbone, particularly in the case of collagen.
- The calculation proceeds through the backbone, analyzing three residues at a time.
- Cycles are calculated for three possible combinations: Gly-X-Y, X-Gly-Y, and X-Y-Gly, relative to the amino acids at positions X and Y.

Molecular Descriptors for Discrimination:

- The π_k, Θ_k, and ϑ_k values are used as molecular descriptors to discriminate between stable and unstable peptide collagen structures.
- These descriptors are utilized as invariants in a Markov chain (MC) model to identify electron delocalization in protein backbones.

- There is another type of neural network CNN [convolutional neural network] which specializes in image tasks.
- Convolutional Neural Networks (CNN), to assist in choosing the best skincare product based on different skin types.

Complexity in Choosing Skincare Products:

The complexity of choosing skincare products is acknowledged, leading to the development of a predictive approach.

Utilization of AI Algorithm (CNN):

- An AI algorithm is employed to address the complexity, leveraging its capability to handle vast amounts of unstructured data and produce promising results.
- Convolutional Neural Networks (CNN) are specifically chosen for the system.

Dataset and Skin Types:

The model is trained on a dataset scraped from the internet, comprising four classes of skin types: normal, dry, oily, and combination.

Python Packages and Tools:

The CNN model is implemented using Python 3 with various packages, including Numpy, OpenCV, Matplotlib, TensorFlow, Keras, and Sklearn.

Training and Testing:

- The model undergoes training and testing phases to establish accuracy.
- The goal is to achieve high accuracy in detecting different skin types using the trained model.

Product Recommendations:

- Suitable skincare products for each class of skin types are compiled in a file.
- After detecting the skin type, the system fetches the appropriate products from the file.

Outcome:

The result is a system that suggests the best composition of cosmetic products tailored to specific skin types.

High Accuracy as a Goal:

The primary objective is to achieve high accuracy in detecting skin types, ensuring the reliability of the suggested skincare product recommendations. This approach combines AI, particularly CNN, with a dataset of different skin types to create a system that accurately recommends skincare products. The use of Python packages facilitates the implementation of the CNN model, and the end goal is to provide users with reliable suggestions for skincare based on their skin type.

Application of ANN

Applications in Cosmology:

Data Modeling:

ANNs can be used to model and analyze cosmological data. This involves training the network on observed data to learn the underlying patterns and structures, enabling predictions or reconstructions of cosmological phenomena.

Computational Efficiency:

Neural networks can significantly reduce computational time in numerical simulations and tasks. They can approximate complex functions, offering a faster alternative to traditional methods in certain scenarios.

Classification of Objects:

ANNs can classify celestial objects based on their observed properties. For example, they can classify stars, galaxies, or other astronomical entities in large datasets more efficiently than traditional methods.

HALAL COSMETICS:

Halal cosmetics refer to beauty and personal care products that comply with Islamic principles and are considered permissible (halal) for use by Muslims. The concept of halal in cosmetics is rooted in Islamic dietary laws and ethical considerations. Here are some key aspects of halal cosmetics:

Ingredients:

Halal cosmetics are formulated with ingredients that are considered permissible in Islam. This includes avoiding ingredients derived from pork or its by-products, alcohol, and any other substances prohibited by Islamic dietary laws.

Animal Testing:

Many halal cosmetics are cruelty-free, meaning they do not involve animal testing. This aligns with Islamic principles that emphasize compassion and ethical treatment of animals.

Cross-Contamination:

Manufacturers of halal cosmetics take precautions to prevent cross-contamination with non-halal ingredients during the production process. This ensures the purity and adherence to halal standards.

Fragrances:

The use of alcohol-based fragrances is a common concern in halal cosmetics. Some halal cosmetic brands opt for alcohol-free fragrances to comply with Islamic principles.

Certification:

Some halal cosmetic products may carry certification from recognized halal certifying bodies. These certifications provide assurance to consumers that the products meet specific halal standards.

Ethical and Sustainable Practices:

Beyond halal considerations, some consumers also look for cosmetic brands that adhere to ethical and sustainable practices. This may include environmentally friendly packaging, fair labor practices, and social responsibility.

Consumer Awareness:

The demand for halal cosmetics has grown globally, driven by an increasing awareness among consumers about the ingredients in their beauty products and a desire for products that align with their religious or ethical beliefs.

ANN in halal cosmetics:

Cosmetic Technology Advancement:

The advancement in cosmetic technologies involves the application of multivariate statistical techniques, specifically artificial neural networks (ANN). ANN is used to optimize cosmetic formulations, providing a more efficient and effective method compared to traditional laborious and cumbersome formulation approaches.

Okara as a Promising Halal Cosmetic Ingredient:

Okara, a by-product of soy-based product production, has been identified as a promising ingredient for halal cosmetics. The use of okara in cosmetics aligns with the principles of halal, provided essential aspects of production adhere to Shariah requirements.

Plant-Derived Ingredient Considerations:

Okara being a plant-derived ingredient adds to its appeal, especially for consumers who prefer natural and sustainable cosmetic options. Incorporating okara as a cosmetic ingredient requires careful attention to the use of permissible substances, manufacturing processes, storage, packaging, and delivery, ensuring compliance with Shariah requirements. The aim is to develop an optimized halal cosmetic soap formulation that includes okara. The specific goal is to use artificial neural networks to achieve the desired hardness of the soap, demonstrating the versatility of ANN in cosmetic product development.

Optimization through Artificial Neural Networks (ANN):

ANN is employed to optimize the formulation of the halal cosmetic soap. The use of ANN allows for a data-driven approach, enabling the identification of the most effective combination of ingredients to achieve the desired soap hardness.

ANN in healthcare sector

the increasing use of machine-learning techniques, particularly artificial neural networks (ANN), in the healthcare sector, focusing on improving organizational decision-making.

Integration of Machine Learning in Healthcare:

- Healthcare organizations are leveraging machine-learning techniques, specifically artificial neural networks (ANN), to enhance care delivery while aiming for cost reduction.

- The application of ANN in healthcare is not only limited to diagnosis but is increasingly being used to inform decisions related to healthcare management.

Seminal Review of ANN Applications:

- It mentions a seminal review conducted on the applications of ANN to health care organizational decision-making.
- The review involved screening 3,397 articles from six databases with coverage of Health Administration, Computer Science, and Business Administration.

Study Characteristics:

- The review extracted various characteristics from the selected 80 articles, including the aim of the studies, methodology employed, and the context in which ANN was applied.
- Articles included in the review were published between 1997 and 2018 and originated from 24 countries, with a substantial portion from the United States.

Types of ANN Used:

The study identifies different types of ANN used in healthcare applications, including general ANN, feed-forward networks, and hybrid models.

The reported accuracy of these ANN models varied across studies, ranging from 50% to 100%.

Levels of Decision-Making:

The text notes that the majority of ANN applications in healthcare informed decision-making at the micro-level, occurring between patients and healthcare providers.

Fewer applications were found at the meso-level (intra-organizational decision-making) and macro-level (system, policy, or inter-organizational decision-making).

Global Perspectives and Drivers:

- The review highlights the global nature of the research, with contributions from authors in various countries.
- The identification of key characteristics and drivers for the market uptake of ANN in health care organizational decision-making is emphasized. This suggests an interest in understanding factors influencing the adoption of these technologies.

Accuracy Variation and Adoption Guidance:

- Mention is made of the reported accuracy of ANN models varying between studies.
- The purpose of the review is to identify key characteristics and drivers to guide further adoption of ANN for health care organizational decision-making.
- This scoping review addresses the perceived lack of coherence in understanding the applications of ANN in health care organizational decision-making. It seeks to overcome limitations in existing reviews by offering a comprehensive overview of the diverse applications of ANN at various decision-making levels within the healthcare context.

Lack of Coherence and Motivation for the Review:

- Despite the prominence of ANN in various applications, there is a perceived lack of coherence regarding its applications and potential to inform decision-making at different levels in health care organizations.
- The motivation for the review arises from a need for a broad understanding of the various applications of ANN in health care, addressing the interdisciplinary gap between organizational behavior and computer science.

Challenges in Keeping Abreast of Advancements:

- The sheer abundance and complexity of reported uses of ANN in health care make it challenging for practitioners and researchers to stay updated on new advancements and trends.

- Adopters of ANN or those new to the field of AI may find the scope and terminology of neural computing challenging.

Limitations of Current Reviews:

- The literature review highlights limitations in existing reviews on the applications of ANN in health care.
- Some reviews are deemed too specific, focusing on a particular disease or type of neural network, while others are considered too broad, encompassing data mining or AI techniques without providing insights specific to ANN.

Scope of the Scoping Review:

- The overarching goal of the scoping review is to provide a comprehensive overview of the various applications of ANN in health care organizational decision-making at different levels: micro, meso, and macro.
- These levels refer to decisions made on the micro-level involving individual patients, the meso-level concerning group decisions at departmental or organizational levels, and the macro-level involving larger groups or public organizations making decisions based on public interest.
- Identification of Literature and Methodologies:
- The review aims to identify the nature and extent of relevant literature on the applications of ANN in health care.
- The methodologies and contexts used in the identified literature will be described to provide a comprehensive understanding of how ANN is applied in different healthcare decision-making scenarios.
- the fundamental concepts of pharmacokinetic (PK) and pharmacodynamic (PD) models, which play crucial roles in drug development and evaluation.

Pharmacokinetic Models (PK):

- PK models involve a set of linked differential equations.
- These models enable the relationship between the administered dose, patient characteristics, and the timing of drug administration with changes in drug concentrations over time in the body.
- The equations in PK models incorporate biological information, such as anatomy, physiology, and biochemistry.
- Parameters in the equations, representing factors like rates of dissolution, metabolism, and transport, are adjusted during model development to ensure the model's predictions closely match empirical data.

Pharmacodynamic Models (PD):

- PD models focus on capturing the temporal effects of a drug on the body.
- Examples include the inhibition of an enzyme or changes in the expression of a specific protein in response to drug administration.
- Similar to PK models, PD models use mathematical approaches to represent and predict the dynamic interactions between a drug and its target within the body.

Combined PK/PD Models:

- A combined PK/PD model integrates both pharmacokinetic and pharmacodynamic components.
- This comprehensive model provides predictions not only for changes in drug concentrations in specific bodily compartments over time (PK aspect) but also for the time course of one or more biological effects resulting from these concentration changes (PD aspect).
- The combined model allows for a more holistic understanding of how a drug behaves in the body and how its effects manifest over time.

Model Development and Adjustment:

- During the development of these models, parameters and equations are adjusted.
- The goal is to ensure that the model accurately predicts the observed empirical data, aligning the theoretical predictions with the actual behavior of the drug in the body.
- The challenges in developing models for time-dependent changes in drug concentrations and their biological effects, and it highlights the application of artificial neural networks (ANNs) by CDER researchers.

Challenges in Model Development:

Model development is challenging due to the complex nature of physiological mechanisms governing time-dependent changes in drug concentrations and their effects in individual patients.

Application of Artificial Neural Networks (ANNs):

- CDER researchers have explored the use of artificial neural networks to address modeling problems in this context.
- ANN methods offer a flexible and powerful approach to capturing complex relationships and patterns in data.

Recurrent Neural Network (RNN) for PD Response:

CDER scientists have specifically developed a model based on a type of recurrent neural network (RNN).

This RNN is designed to simulate the time course of a pharmacodynamic (PD) response that is not directly related to drug concentration but develops latently through complex biological intermediate steps.1

Testing Machine Learning Capability in PD Modeling:

- To evaluate the capability of machine learning in modeling PD in this scenario, researchers first constructed a mechanistic Pharmacokinetic/Pharmacodynamic (PK/PD) model.
- The focus was on a hypothetical drug with a delayed biological response (a change in the concentration of a biomarker) to changes in drug concentration.

Generation of Simulated Data:

Using the PK/PD model, researchers generated simulated data, including both PK and PD profiles. Simulated data was generated for patients with varying demographics and weights who received the drug daily over a seven-day period. the researchers aimed to assess how well machine learning, specifically using an RNN-based model, could capture the complexities of a delayed pharmacodynamic response to changes in drug concentration. The use of simulated data allows for controlled testing and validation of the model's performance under different conditions and patient characteristics. This approach represents an innovative application of artificial neural networks in addressing challenges in pharmacodynamic modeling within the drug development context.

Choice of LSTM RNN:

- The researchers opted for a long short-term memory recurrent neural network (LSTM RNN) due to its demonstrated success in predicting sequential data, such as sentences.
- LSTMs are known for their ability to capture long-term dependencies in sequential data, making them suitable for modeling scenarios with intricate temporal relationships.

Model Construction and Variation:

- Several LSTM RNN models were constructed with variations in the number of hidden layers and perceptrons.
- The variability in model architecture allows researchers to explore the impact of different network complexities on predictive performance.

Training Data and Predictive Variables:

- The LSTM RNN models were trained using time sequences of plasma concentrations simulated by a mechanistic model.
- Patient baseline pharmacodynamic (PD) values and demographics were also included as input variables for training.

Specific Dosing Schedule:

The models were trained to predict the PD response under a specific dosing schedule.

This focused approach allowed researchers to assess how well the LSTM RNN models could capture the complex dynamics of PD responses in relation to the simulated drug concentrations.

Selection of the Best Performing Model:

- After constructing several LSTM RNN models, the researchers identified the simplest model that predicted the PD response with an acceptable level of error.
- This model was considered the most efficient and accurate in capturing the desired predictions.
- Application to Different Dosing Schedules:
- The selected LSTM RNN model, which demonstrated acceptable error in predicting the PD response under the specific dosing schedule, was then applied to predict PD responses for patients given the drug according to different schedules.
- This step extends the model's utility to assess its generalization capability across various dosing scenarios.
- The performance of the LSTM RNN machine learning model in predicting pharmacodynamic (PD) responses, particularly under different dosing regimens.
- Prediction of PD Response Under Different

Dosing Regimens:

- The machine learning model, specifically the LSTM RNN, demonstrated accuracy in predicting the pharmacodynamic (PD) response of individuals treated with dosing regimens that differed from the once-daily regimen used during model construction.
- This finding is crucial as it indicates the model's ability to generalize and accurately predict responses even when the dosing schedules vary, which is common in the drug development process.

Significance for Drug Development:

- The ability of the model to predict responses under different dosing regimens is particularly significant for drug development.
- Dosing regimens often undergo changes during the development process based on various factors, including safety, efficacy, and patient tolerability. The model's adaptability to different regimens enhances its utility in real-world scenarios.

Testing with Sparse Data:

- The authors also tested the LSTM RNN model when trained with sparse data.
- The model could accurately predict the PD response when the dosing regimen was the same as that used for training (once daily).
- However, the model faced challenges in accurately predicting responses for patients on twice- or thrice-daily regimens.

Limitations in Predicting Different Dosing Frequencies:

- The limitation in accurately predicting responses for patients on more frequent dosing regimens (twice or thrice daily) suggests potential challenges for the model when faced with variations in dosing frequency.
- The collaboration between scientists from the machine learning and mechanistic modeling disciplines holds great promise for advancing drug development and personalized medicine.

Overlapping Concepts:

By bringing together experts from both fields, researchers can identify commonalities in concepts. Machine learning models, which are data-driven, and mechanistic models, which are based on a deep understanding of biological processes, may share underlying principles and ideas.

Equations and Model Structures

There may be similarities in the equations used in mechanistic models and those employed in machine learning algorithms. Integrating these equations or finding ways to translate between them could lead to hybrid models that leverage the strengths of both approaches.

Visualization of Model Structures:

Visualization plays a crucial role in understanding complex models. Collaborators from different disciplines can share techniques for visualizing model structures, helping to make complex systems more interpretable and facilitating communication between experts.

Complementary Nature of Models:

Machine learning models excel at capturing patterns in large datasets, while mechanistic models provide a deeper understanding of the underlying biology. Combining these approaches may result in more robust models that leverage the strengths of both paradigms.

Efficiency in Drug Development:

Integrating machine learning and mechanistic modeling can streamline drug development processes. Machine learning can help identify potential drug candidates and predict their effects, while mechanistic models can provide insights into the specific mechanisms of action and potential side effects.

Optimizing Treatments for Individuals:

The collaboration between disciplines can lead to the development of personalized treatment strategies. Machine learning can analyze patient data to identify patterns and predict responses to treatments, while mechanistic models can provide a deeper understanding of individual patient characteristics.

Challenges and Opportunities:

While collaboration between disciplines holds immense potential, challenges such as data integration, model interpretability, and validation need to be addressed. Overcoming these challenges will open up new opportunities for innovation in drug development and healthcare.

- **ANN in medicine and biological research**

The increasing interest and application of Artificial Intelligence (AI), specifically Artificial Neural Networks (ANNs), in the field of medicine and biological research.

Rapid Advancements in Computer Technology:

The opening statement acknowledges the tremendous advancements in computer technology. This sets the context for the growing interest in utilizing AI, particularly ANNs, in the field of medicine and biological research.

Definition and Functionality of ANNs:

ANNs are described as mathematical algorithms generated by computers. They are characterized as learning from standard data and capturing knowledge contained in the data. Trained ANNs are suggested to approach the functionality of small biological neural clusters, serving as digitized models of the biological brain.

Capability to Detect Complex Relationships:

ANNs are highlighted for their ability to detect complex nonlinear relationships between dependent and independent variables in data. This is emphasized as a strength compared to the human brain, which may struggle to identify such relationships in complex datasets.

Widespread Use in Medicine:

ANNs are reported to be widely used in various disciplines of medicine, with a particular emphasis on cardiology. The applications mentioned include diagnosis, electronic signal analysis, medical image analysis, and radiology.

Modeling in Medicine and Clinical Research:

The passage notes that many authors have extensively applied ANNs for modeling in medicine and clinical research. This suggests a broad range of applications, indicating the versatility of ANNs in healthcare-related tasks.

- **Applications in Pharmacoepidemiology and Medical Data Mining:**

The use of ANNs in pharmacoepidemiology and medical data mining is highlighted, showcasing the expanding role of these algorithms in analyzing large-scale healthcare datasets and extracting meaningful patterns.

- **ANN as a statistical infrences**

an innovative approach using Artificial Neural Networks (ANNs) to overcome the challenge of making statistical inferences for a single individual, a scenario where traditional statistical methods may face limitations due to the absence of a sample population.

Individual Treatment with Group Statistics:

- Acknowledges the limitation of transforming a single individual into a group for statistical analysis.
- Proposes the opposite approach: treating a single individual with a group of statistics.

Use of Independent Classification Models:

- Suggests employing several independent classification models within ANNs.
- These models make different errors but exhibit a similar average predictive capacity on the same individual.

Training Multiple Neural Networks:

- Theoretically possible to train hundreds of neural networks using the same dataset.
- Results in a collection of ANNs with comparable average performance but variations in architecture, topology, learning laws, weights, training cycles, etc.

Variability for Individual Predictions:

- This variability allows the ensemble of neural networks to make different mistakes at the individual level.
- Each network in the ensemble processes independently and provides predictions for a diagnostic category, survival plausibility, or drug dosage level.

'Parliament of Independent Judges':

- Describes the ensemble of ANNs as a 'parliament of independent judges' acting simultaneously.
- Generates several hundred answers for a new patient, creating a nonparametric distribution of output values.

Statistical Inference for Single Individuals:

Challenges the dogma that statistical inference is not possible for a single individual.

Through the ensemble approach, statistical descriptors (mean, mode, median, variance, confidence interval, etc.) can be obtained for the output values.

- **ANNs in biomedical sciences**

The focus is specifically on the extensive application of NNs in biomedical systems, with a detailed analysis of their role in medical diagnosis. The passage emphasizes the strengths of Neural Networks (NNs) in identifying patterns and trends in data, highlighting their applicability in predicting and forecasting. The focus is specifically on the extensive application of NNs in biomedical systems, with a detailed analysis of their role in medical diagnosis. Here are key points from the passage:

Strengths of Neural Networks:

- NNs are described as being particularly adept at identifying patterns or trends in data.
- They are well-suited for prediction and forecasting tasks.

Application in Biomedical Systems:

The passage emphasizes the extensive application of NNs in biomedical systems, indicating their relevance in the medical field.

Motivation for Neural Network Applications in Medical Diagnosis:

An analysis is conducted to motivate the use of NNs in medical diagnosis. This suggests a focus on the advantages and effectiveness of NNs in addressing diagnostic challenges.

Special Note on Cancer Diagnosis:

The passage specifically highlights the efforts of neural networks in the field of cancer diagnosis. This may suggest a particular emphasis on the significance of NNs in detecting and diagnosing cancerous conditions.

Importance of Neural Networks in Medical Diagnosis:

The primary focus of the paper is underscored as the importance of applying NNs in the medical world, particularly in diagnosing various diseases. This indicates a recognition of the potential impact and benefits of NNs in healthcare.

Application of Technical Concepts:

Various technical concepts, including MLP (Multi-Layer Perceptron), SVM (Support Vector Machine), RBF (Radial Basis Function), CANFIS (Cooperative Adaptive Neuro-Fuzzy Inference System), TLRN (Three Layer Radial Basis Function Neural Network), PCA (Principal Component Analysis), SOM (Self-Organizing Map), and SNNS (Stuttgart Neural Network Simulator) are mentioned.

These concepts are applied for diagnosing various diseases using NNs, showcasing the diversity of techniques employed in medical applications.

- **ANNs for the use and diagnosis of cardiovascular system.**

Purpose of Neural Networks in Cardiovascular System Modeling:

- ANNs are used experimentally to model the human cardiovascular system.
- The primary goal is to diagnose medical conditions by building a model of an individual's cardiovascular system and comparing it with real-time physiological measurements taken from the patient.

Early Detection of Medical Conditions:

- Regularly performing the routine of modeling and comparing an individual's cardiovascular system with real-time measurements can lead to the early detection of potential harmful medical conditions.
- Early detection is emphasized as a means to facilitate the process of combating diseases.
- Physiological Variables in Cardiovascular Modeling:
- A model of an individual's cardiovascular system must capture the relationships among physiological variables such as heart rate, systolic and diastolic blood pressures, and breathing rate.
- The model should adapt to different physical activity levels to reflect the individual's physical condition accurately.

Adaptability of the Model:

- The model needs to adapt to the features of any individual without the supervision of an expert.
- This adaptability requirement is cited as a reason for employing neural networks in cardiovascular system modeling.

Sensor Fusion in Medical Modeling and Diagnosis:

- ANNs are chosen due to their ability to provide sensor fusion, which involves combining values from multiple sensors.
- Sensor fusion allows ANNs to learn complex relationships among individual sensor values, even if each sensor is sensitive only to a specific physiological variable.

Complex Relationships and Detection of Medical Conditions:

- ANNs, through sensor fusion, can detect complex medical conditions by analyzing data from individual biomedical sensors.
- This implies that even if each sensor is designed to detect a specific physiological variable, ANNs can uncover intricate

relationships that might be overlooked in individual sensor analyses.

LITERATURE SEARCH:

1. Jacques Bourquin et al.,(1996)7, This paper introduces the application of Artificial Neural Networks (ANN) in pharmaceutical sciences. It describes different types of ANN, including associating, feature-extracting, and nonadaptive networks, explaining their historical origins and computing concepts. ANN offers various modeling and analysis possibilities in pharmaceutical fields, such as clinical pharmacy, drug design, and analytical data interpretation. The few existing applications are promising, warranting further investigation.

2. Jacques Bourquin, et al.,(1996)11, The application of ANN in pharmaceutical development was assessed with theoretical and practical examples. ANN models showed better data fitting and predicting abilities compared to traditional statistical methods like Response Surface Methodology (RSM). Experimental data from a tablet compression study fitted well with different ANN models. ANN methodology shows promise for modeling pharmaceutical technology data sets.

3. Jacques Bourquin, et al.,(1997)1, The application of ANN in pharmaceutical development was assessed with theoretical and practical examples. ANN models showed better data fitting and predicting abilities compared to traditional statistical methods like Response Surface Methodology (RSM). Experimental data from a tablet compression study fitted well with different ANN models. ANN methodology shows promise for modeling pharmaceutical technology data sets.

4. Jacques Bourquin et al.,(1997)2, This paper introduces the application of Artificial Neural Networks (ANN) in pharmaceutical sciences. It describes different types of ANN, including associating, feature-extracting, and nonadaptive networks, explaining their historical origins and computing concepts. ANN offers various modeling and analysis possibilities in pharmaceutical fields, such as clinical pharmacy, drug design, and analytical data interpretation. The few existing applications are promising, warranting further investigation.

5. Kozo Takayama et al.,(1999)6, The study assessed O-ethylmenthol's impact (MET) on ketoprofen's percutaneous absorption from alcoholic hydrogels in rats (in vitro and in vivo). Addition of small MET quantities to the hydrogels significantly increased ketoprofen permeation compared to the control. Partitioning and drug diffusivity were also influenced by MET concentration. An innovative simultaneous optimization technique using an artificial neural network (ANN) was employed to design a ketoprofen hydrogel with MET. The ANN effectively represented nonlinear relationships between causal factors (ethanol and MET amounts) and response variables (penetration rate, lag time, and irritation score). The optimized hydrogel results closely matched predictions for effectiveness and safety.

6. S. Agatonovic-Kustrin et al.,(1999)3, Artificial neural networks (ANNs) are computer programs inspired by the human brain's information processing. They learn from data patterns and relationships, not from explicit programming. ANNs consist of interconnected artificial neurons or processing elements organized in layers, with weighted inputs and transfer functions. During training, the network's inter-unit connections are optimized to minimize prediction errors. ANN are effective for data sets with non-linear relationships, making them valuable in pharmaceutical processes. They require large training sets but can combine literature-based and experimental data for problem-solving. ANN applications include classification, prediction, and modeling, with potential uses in pharmaceutical sciences, from drug design to clinical pharmacy.

7. Antonio M. Rabasco Alvarez, ET AL.,(2000)39 This paper provides a concise review of lipid applications in the pharmaceutical domain. It covers various lipids utilized as excipients in cosmetics and medicines, ranging from vegetable oils like almond, apricot, and avocado oils to animal-source oils such as fish and bird oils. Fats and waxes also find application in cosmetic formulations. The versatility of phospholipids is explored, serving as vehicles for therapeutic substances like liposomes. The study delves into lipids' biological activity, highlighting their role as active substances in pharmaceuticals, cosmetics, and nutritional supplements. Carotenoids, retinoids, and tocopherols are discussed for their antioxidant properties, contributing to health and diagnostic medicine.

8. R. Burbidge, et al.,(2001)26, The support vector machine (SVM) classification algorithm shows promising potential for structure-activity relationship analysis. In a benchmark test comparing various machine learning techniques, SVM outperforms artificial neural networks, radial basis function networks, and a C5.0 decision tree in predicting dihydrofolate reductase inhibition by pyrimidines. The SVM is significantly better than most methods, except for a manually capacity-controlled neural network that takes longer to train.

9. A. Faure, et al.,(2001)30, This paper reviews the techniques for process control and scale-up of pharmaceutical wet granulation processes. It discusses specific methods based on liquid saturation and wet mass consistency for high-shear mixer granulation, which are related to granule deformability and particle size. For fluid bed granulation, moisture content in the bed is the key parameter to control, monitored using near-infrared or temperature probes. Computerized techniques like fuzzy logic, neural networks, and experimental design models are popular for fluid-bed process control. Additionally, particle size population balance modeling is under development for both fluid bed and high-shear granulation.

10. Kozo Takayama et al.,(2003)1, The content discusses the challenges in optimizing pharmaceutical formulations with multiple factors and responses. The traditional response surface method (RSM) using a second-order polynomial equation has limitations in predicting optimal formulations accurately. The review introduces the multi-objective simultaneous optimization technique, incorporating an artificial neural network (ANN). ANNs are increasingly used in pharmaceutical research to predict complex relationships between factors and responses, demonstrating superior performance in optimization through numerical examples.

11. Narayanaswamy Subramanian, et al.,(2003)21, The study aimed to optimize cytarabine liposome formulation using artificial neural networks (ANN) and multiple regression analysis with 33 factorial design (FD). Both methods were used to predict the percentage drug entrapment (PDE) based on formulation variables. The results showed that ANN provided more accurate predictions compared to multiple regression analysis, making it a valuable tool for pharmaceutical formulation optimization.

12. John C. Lindon, et al.,(2006)27, This minireview discusses the analytical and statistical techniques used in metabonomics, which involves the simultaneous determination of multiple metabolites in biofluids and tissues. Applications to pharmaceutical research, preclinical drug safety studies, disease diagnosis, and therapy monitoring are highlighted. The use of metabonomics in predicting an individual's response to treatment is exemplified. The advantages and challenges of the metabonomics approach are summarized

13. Yves Roggo, et al.,(2007)31, Near-infrared spectroscopy (NIRS) is a rapid and non-destructive analytical method, combined with chemometrics, making it powerful for the pharmaceutical industry. It is suitable for analyzing solid, liquid, and biotechnological pharmaceutical forms. NIRS can be used in pharmaceutical development, production for process monitoring, and quality control. This review covers chemometric techniques and various pharmaceutical NIRS applications, including qualitative analyses, quantitative methods, and on-line applications, with practical examples.

14. Antonei B. Csoka, et al.,(2008)28, The paragraph discusses epigenetics and its role in gene expression. It suggests that pharmaceutical drugs can cause persistent epigenetic changes, leading to potential side effects even after the drug is discontinued. The hypothesis proposes that some diseases may have an epigenetic basis. The paragraph calls for the incorporation of epigenetic assays into drug safety assessments and presents a new approach termed "pharmacoepigenomics." The impact of this approach could be significant in pharmacology and medicine.

15. Masato Nishikawa, et al.,(2008)10, Photocrosslinked polyacrylic acid hydrogel modified with 2- hydroxyethyl methacrylate (HEMA) is a promising adhesive for dermatological patches. The study investigated using this hydrogel with indomethacin (IDM) as an anti-inflammatory patch. Formulation factors influenced swelling, permeation rate, and lag time of IDM. A novel optimization method (RSM-S) achieved a highly functional anti-inflammatory patch with good adhesive properties and bioavailability. Photocrosslinked polyacrylic acid hydrogel offers customizable functions, making it an attractive candidate for dermatological patches.

16. Rade Injac,er al.,(2008)41 This study introduces a specific and accurate micellar electrokinetic capillary chromatography method for quantifying caffeine, theobromine, theophylline, paracetamol, propyphenazone, acetylsalicylic acid, salicylic acid, and codeine phosphate in real samples of food, beverages, natural products, pharmaceuticals, and cosmetics. Operating at 25°C and 25 kV, the method employs a 20mM phosphate buffer (pH 9.0), 80mM sodium dodecyl sulfate, and 7.5% (v/v) acetonitrile, with UV detection at 210 nm. It proves to be both specific and precise, demonstrating recoveries between 98.9% and 101.2%, linear response, and a relative standard deviation below 2.1%. The approach is successfully applied to quantitatively analyze these compounds in various real-world products, showcasing its adaptability across diverse sample types.

17. Panagiotis Barmpalexis, et al.,(2009)24, Artificial neural networks (ANNs) were used to optimize a nimodipine zero-order release matrix tablet formulation and compared to multiple linear regression (MLR) on an external validation set. ANNs with eight hidden units showed better fit for all responses compared to MLR models. Further simplification of the ANN by pruning preserved only two inputs. Optimal formulations based on ANN and MLR predictions were identified, and the similarity factor confirmed ANNs' increased prediction efficiency.

18. Faith Chaibva et al.,(2010)2, An artificial neural network was employed to optimize the release of salbutamol sulfate from hydrophilic matrix formulations. Model formulations were created using varying levels of input factors through a central composite design. In vitro dissolution time profiles were used as target data to train the neural network for optimization. The neural network with nine nodes in one hidden layer showed the best predictive ability. The model successfully optimized formulations with desirable release characteristics, showing agreement between predicted and manufactured formulations. This study demonstrates the potential of artificial neural networks for optimizing pharmaceutical formulations with desired performance traits.

19. K. JAYARAM KUMAR, et al.,(2011)35 This study optimizes the concentration of a fatty alcohol and internal phase for a stable oil-in-water (O/W) emulsion using artificial neural networks (ANNs). ANNs provide accurate predictions, allowing the quantification of input importance. Adjusting network topology and parameters led to a close alignment between predicted and experimental values. The comparison of the ANN model's predictions with actual outputs showed a high R2 value of 0.84, indicating robust modeling. Supported by a correlation coefficient of 0.9445, the study demonstrates the adequacy of the ANN-based optimization for stable O/W emulsion formulation. Keywords: O/W emulsion, emulsifier, fatty alcohol, back propagation network, optimization, stability.

20. Wan Sarah Samiun,et al.,(2013)40 This study focuses on encapsulating aripiprazole in a palm kernel oil esters nanoemulsion for efficient brain delivery through intravenous administration. Employing high shear and high-pressure homogenizers, the researchers formulated a stable nanoemulsion system using lecithin, Tween 80, and glycerol as emulsifiers. Artificial neural networks (ANNs) were utilized to model the nanoemulsion formulation and minimize particle size. The study considered various input factors, including palm kernel oil ester (PKOE), lecithin, Tween 80, glycerol, and water amounts, to predict particle size. Different training algorithms were tested, and the optimal ANN topology, determined by minimized root mean squared error (RMSE), was found to be QP-5-4-1. The results demonstrate the effectiveness of ANN models in predicting particle size for stable nanoemulsions suitable for intravenous drug delivery.

21. Aleksander Mendyk, et al.,(2013)14, The study aimed to develop a generalized in vitro-in vivo relationship (IVIVR) model using in vitro dissolution profiles and quantitative/qualitative composition of dosage formulations as covariates. Chemoinformatics software computed molecular descriptors, and artificial neural networks were used for modeling. The model accurately predicted in vivo profiles for 37.6% of the formulations, demonstrating its effectiveness for IVIVR. The approach is unique as it incorporates various active pharmaceutical ingredients and dosage forms into a single model, providing preliminary IVIVC/IVIVR without in vivo data.

22. Hamid Reza Akbari Hasanjani et al.,(2015)5, The study aimed to simultaneously estimate Fluoxetine and Sertraline in tablets using UV-Vis spectroscopy and Artificial Neural Networks (ANN). The absorption spectra of both components were recorded in the 200-300 nm wavelength range. Calibration models were evaluated using synthetic binary mixtures. Three layers feed-forward neural networks with back-propagation algorithm were used to build and test the models. The optimized parameters resulted in a precise and convenient method with Relative Standard Deviation (RSD) of 1.06 and 1.33 for Fluoxetine and Sertraline, respectively. The proposed procedure showed good agreement between true and predicted concentration values, making it suitable for the determination of these drugs in commercial tablets.

23. Hiromi Baba, et al.,(2015)33 This paper tackles crucial challenges in predicting human skin permeability for chemical compounds, crucial for advancing dermatological medicines and cosmetics. To surmount limitations in existing databases and modeling approaches, we meticulously assemble a new dataset under uniform experimental conditions. Leveraging machine learning methods, including support vector regression (SVR) and random forest (RF), we craft robust prediction models. The resulting nonlinear SVR model distinguishes itself with an impressive determination coefficient of 0.910, showcasing exceptional accuracy and reliability in external validation. Notably, this study introduces one of the most extensive datasets featuring experimental log kp values, providing valuable tools for screening active ingredients and investigating unsynthesized compounds in dermatological formulations.

24. Dimitar A. Dobchev, et al.,(2016)34 This review examines the widespread use of artificial neural networks (ANNs) in drug discovery, specifically within the quantitative structure-activity relationships (QSAR) framework. ANNs, pivotal in various scientific fields over the last two decades, are critically assessed for their efficacy in drug development. The authors analyze the pros and cons of integrating ANNs into the QSAR framework, citing recent studies across diverse diseases. Despite challenges like overtraining and interpretability, the authors contend that ANNs have largely met researchers' expectations, serving as excellent tools for nonlinear data modeling in QSAR. The review concludes by endorsing the ongoing significance of ANNs in future drug development initiatives.

25. Hesham G. Moussa, et al.,(2016)23, The study proposes using a Model Predictive Controller based on Neural Networks to maintain a constant release of chemotherapeutic agents at the cancer site using echogenic liposomes. The goal is to reduce multiple drug resistance (MDR) in cancer cells by ensuring therapeutic drug levels within the tumor. The simulation results indicate the viability and robustness of the nonlinear model in maintaining a constant drug release, potentially reducing cancer resistance to chemotherapy.

26. Malay K et al.,(2016)8, Artificial Neural Networks (ANNs) are computational models based on the brain's structure, capable of learning and pattern recognition. They operate through parallel processing and distributed memory, making them fault-tolerant. ANNs use learning rules to adapt to changing environments and discover useful knowledge from data. They have three learning methods: supervised, unsupervised, and reinforcement learning. ANNs are superior to conventional methods in formulation development and optimization due to their flexibility and ability to learn from data.

27. Munish Puri, et al.,(2016)12, Artificial Neural Networks (ANNs) are computational models inspired by biological neurons. Neurons compute output values from inputs using weighted sums and thresholds. In ANN, the collective behavior of interconnected neurons drives the network's evolution. The network learns from past experience using algorithms like feed- forward and backpropagation. ANN's parallel processing and learning capabilities make it suitable for processing large biological data and prognosis. It works through mathematical operations, mimicking biological neuron patterns. ANN is a powerful machine learning technique with applications in various fields.

28. Jayvadan Patel, et al.,(2016)16, Controlled release drug delivery systems (CRDDS) offer numerous advantages, but their formulation and optimization can be complex. Artificial neural networks (ANN) provide a promising approach to tackle the challenges in CRDDS development. ANNs can handle multiple variables, learn complex relationships, and predict formulation performance. They have shown superior fitting and predicting capabilities compared to traditional methods like response surface methodology (RSM). The use of ANN can improve the optimization of CRDDS and aid in predicting in vivo drug release profiles.

29. Mohammad Rafienia, et al.,(2016)18, Feed-forward neural networks (MLP, RBFN, GRNN) were utilized to predict drug release profiles of betamethasone and betamethasone acetate in in situ forming systems. The input vectors included drug concentration, gamma irradiation, additive substance, and drug type. Nonlinear principal component analysis extracted three features as outputs of the ANNs. MLP showed superior performance over GRNN and RBF networks in terms of reliability and efficiency for estimating drug release profiles.

30. GarreŠ B. Goh, et al.,(2018)36 This study introduces SMILES, a deep recurrent neural network (RNN) for autonomously learning features from SMILES representations in chemical databases to predict various properties. Through Bayesian optimization for architecture tuning, the optimized SMILES excels in predicting toxicity, activity, solubility, and solvation energy, outperforming engineered feature-based MLP neural networks. It pioneers interpretability with an explanation mask, showcasing its ability to identify crucial characters for predictions. Tested on a solubility dataset, SMILES achieves an 88% accuracy, aligning with established first-principles knowledge. This work establishes interpretable deep neural networks as a valuable tool for the chemical industry, offering technically accurate insights and state-of-the-art prediction accuracy.

31. Maurício da Silva Baptista, et al.,(2019)38 This chapter explores the versatile applications of fluorescence in pharmaceuticals and cosmetics, emphasizing toxicology, task-specific fluorescent materials, and advanced analytical and imaging methods. Fluorescence enables noninvasive bio-imaging, facilitating the observation of biological processes, drug delivery monitoring, and highlighting microscopic structures. The discussion includes emerging techniques related to fluorescence, offering a comprehensive overview of its pivotal role in transforming approaches to pharmaceuticals and cosmetics. Fundamental concepts in photo science are briefly introduced for completeness.

32. Ahmet Sureyya Rifaioglu,et al.,(2020)43 a novel drug-target interaction prediction system, employs deep convolutional neural networks with 2-D structural representations, providing highly accurate predictions for early-stage drug discovery. Trained on 704 target proteins, DEEPScreen outperforms state-of-the-art methods, validated through rigorous testing and molecular docking analysis. Notably, it identifies JAK proteins as new targets for Cladribine, experimentally confirmed in vitro. This system showcases potential applications in drug discovery and repurposing, offering valuable insights for experimental pursuit in the chemogenomic space.

33. Asad Majeed Khan et al.,(2020)4, The purpose of this study was to develop pH-dependent, uncoated mesalamine matrix tablets using dicalcium phosphate (DCP) and Eudragit-S100 to achieve targeted drug delivery for ulcerative colitis treatment. Wet granulation technique was used to compress mesalamine formulations with varying DCP and Eudragit-S100 compositions. Artificial neural network (ANN) optimization was employed to achieve the desired formulation. The compressed tablets met the required criteria for physicochemical properties. The in-vitro dissolution study showed that the optimized formulation released mesalamine gradually, with 12.09% released after 2 hours and 72.96% released after 12 hours, indicating a complex release mechanism. This DCP-Eudragit-S100 blend may offer better control of ulcerative colitis compared to commercially available.

34. Katarzyna Ewa Tyrak, et al.,(2020)15, The study aimed to develop and validate an artificial neural network (ANN) for predicting nonsteroidal anti-inflammatory drug (NSAID)-exacerbated respiratory disease (N-ERD) in asthma patients. The ANN model demonstrated a high sensitivity of 94.12% and accuracy of 85.00% for N-ERD prediction. While it cannot replace the goldstandard aspirin challenge test, the ANN could provide additional value in identifying patients with N-ERD. External validation in a larger cohort is necessary to confirm the results.

35. Dalia M. Rasheed, et al.,(2020)32, This review focuses on the analysis of aroma composition in scented plants and natural products, particularly for ensuring quality and safety in food or cosmetic products. The use of fast and effective analytical tools for essential oil analysis is essential, especially when dealing with complex mixtures or blends of several oils. Multidimensional chromatography coupled with selective detectors, such as mass spectrometers, enables high-throughput and comprehensive analysis of hundreds of metabolites in a single step. Different multidimensional setups, like GC × GC and LC-GC, along with chemometric approaches, are discussed in this review for essential oils analysis, including chemotyping, enantio-separation, quality control, and adulteration detection in various matrices.

36. Sambit Sarkar, et al.,(2020), et al.,(2020)37 This study investigates the extraction yield of chlorophylls and carotenoids from wet and heat-dried microalgal biomass (Chlorella thermophila) using ethanol, optimizing extraction parameters. Chlorophyll yield was 2.7 times higher from wet biomass, and carotenoid yield was 6.7 times higher compared to dry biomass. Optimal conditions for highest chlorophyll yield (~60 mg/g-dry biomass) included 6 minutes homogenization time, 10,000 rpm, 1 mg/mL solid-solvent ratio, and 58 °C solvent temperature from wet biomass. For carotenoids, the same conditions were optimal, except for a 4 °C solvent temperature. Artificial neural network (ANN) modeling was employed for the extraction process, offering potential insights for industrial-scale extraction processes.

37. Ixchel Ocampo, et al.,(2021)20, Artificial neural networks (ANN) and data analysis (DA) were used to predict liposome size (LZ) in a Dean-Forces-based microdevice. The ANN model achieved a higher correlation coefficient (0.97247) compared to the DA model (0.882), demonstrating its effectiveness in predicting LZ. This study represents a novel application of ANN in nanotechnology and liposome size prediction.

38. Shan Wang, et al.,(2022)13, Artificial Neural Networks (ANNs) are powerful tools for extracting key points from complex pharmaceutical formulation development. ANNs offer flexibility and address intricate questions in a parallel and distributed manner, resembling biological neural networks. They can replace numerous trial and error experiments by efficiently analyzing data. ANNs have been extensively used in pharmaceutics research since the 1990s, becoming a significant method in pharmaceutical science. This review focuses on the latest applications of ANNs in predicting, characterizing, and optimizing pharmaceutical formulations, providing valuable insights for interdisciplinary studies in pharmaceutics and ANNs.

39. Priyanka Katiyar, et al.,(2022)29,The study focuses on supercritical fluid extraction (SFE) of essential oil from turmeric root waste. The oil is found to be rich in oleic acids, suitable for pharmaceutical and cosmetics industries. Mathematical Modelling (MM) and Artificial Neural Network (ANN) are used to gain insights into the extraction process. MM shows a two-phase extraction with solid phase resistance dominating. ANN helps optimize conditions for maximum oil yield, considering factors like solute-solvent repulsion, volatility, and intra-cellular structures. The study establishes the significance of turmeric root oil, proposes an extraction method, investigates extraction physics, and suggests optimized parameters for extraction.

CONCLUSION:

Artificial Neural Networks (ANNs) have found numerous applications in healthcare, leveraging their ability to recognize patterns, learn from data, and make predictions. Here are some key applications of Artificial Neural Networks in healthcare:

Disease Diagnosis and Prediction:

ANNs are used for disease diagnosis based on medical imaging data such as X-rays, MRIs, and CT scans. They can detect patterns indicative of diseases like cancer, diabetes, and neurological disorders.

Prediction models using ANNs can estimate the risk of developing certain diseases based on patient data, contributing to early intervention and preventive measures.

Drug Discovery and Development:

ANNs are employed in drug discovery by predicting the potential efficacy and safety of new compounds. They can analyze molecular structures, predict biological activity, and assist in the identification of promising drug candidates.

Drug response prediction models can personalize treatment plans by considering individual patient characteristics.

Electronic Health Records (EHR) Management:

- ANNs contribute to the analysis of Electronic Health Records, helping in patient risk stratification, predicting readmission risks, and identifying potential complications.
- They assist in extracting meaningful information from large datasets, improving clinical decision-making and patient management.

Genomic Data Analysis:

- ANNs analyze genomic and genetic data to identify patterns associated with hereditary diseases, predispositions, and potential treatment responses.
- They play a role in genomic medicine by aiding in the interpretation of complex genetic variations.
- Telemedicine and Remote Monitoring:
- ANNs can be used in remote monitoring applications, predicting health outcomes, and assessing patient conditions based on data from wearables and other remote sensors.
- They contribute to telemedicine by facilitating remote diagnostic capabilities and personalized health monitoring.

Fraud Detection and Healthcare Billing:

- ANNs help in detecting healthcare fraud by analyzing patterns in billing data and identifying unusual or suspicious activities.
- They assist in streamlining healthcare billing processes and reducing errors.

Patient Outcome Prediction:

- ANNs can predict patient outcomes, including recovery rates after surgery, response to treatments, and likelihood of complications.
- These predictions aid healthcare professionals in making informed decisions about patient care.

Personalized Treatment Plans:

- ANNs contribute to the development of personalized treatment plans by considering individual patient characteristics, medical history, and response to previous treatments.
- Personalized medicine aims to optimize treatment efficacy and minimize side effects.

Clinical Decision Support Systems:

- ANNs are integrated into clinical decision support systems, providing healthcare professionals with real-time insights and recommendations based on patient data.
- They assist in evidence-based decision-making and improving overall patient care.

Healthcare Operations and Resource Management:

- ANNs are applied to optimize healthcare operations, such as predicting patient admission rates, resource allocation, and staff scheduling.

- They contribute to efficiency improvements and cost reduction in healthcare organizations.
- As technology continues to advance, the applications of Artificial Neural Networks in healthcare are expected to expand, contributing to more accurate diagnostics, personalized treatments, and improved overall healthcare outcomes.
- Artificial Neural Networks (ANNs) are also finding applications in the cosmeceutical industry, which combines cosmetics and pharmaceuticals. Here are some notable applications of ANNs in cosmeceuticals:

Formulation Optimization:

ANNs can be utilized to optimize cosmeceutical formulations by predicting the best combination of ingredients for specific skincare products. This includes achieving the desired texture, stability, and effectiveness of the product.

Ingredient Analysis:

ANNs are employed to analyze the effectiveness of different cosmetic ingredients, predicting their impact on skin health and appearance. This aids in selecting ingredients that address specific skincare concerns, such as anti-aging or moisturizing properties.

Personalized Skincare Recommendations:

ANNs can analyze individual skin types, preferences, and concerns to provide personalized skincare recommendations. This helps in tailoring cosmeceutical products to meet the unique needs of each consumer.

Skin Condition Diagnosis:

Neural networks can assist in diagnosing various skin conditions by analyzing images or data related to skin health. This includes the identification of issues like acne, pigmentation, or dehydration.

Product Development and Innovation:

ANNs contribute to the development of innovative cosmeceutical products by predicting trends, consumer preferences, and emerging skincare needs. This aids companies in staying ahead of market demands.

Texture and Sensory Analysis:

ANNs can be employed to predict the sensory attributes of cosmeceutical products, such as texture, fragrance, and feel on the skin. This ensures the development of products that offer a pleasant user experience.

Anti-Aging Solutions:

Neural networks are applied to predict the effectiveness of anti-aging formulations and ingredients. This includes analyzing the impact of compounds on collagen production, skin elasticity, and wrinkle reduction.

Market Research and Consumer Insights:

ANNs assist in analyzing market trends and consumer preferences by processing large datasets. This information helps in developing cosmeceutical products that align with current market demands.

Quality Control and Batch Consistency:

Neural networks are employed in quality control processes, predicting the quality and consistency of cosmeceutical batches. This ensures that each product meets specified standards.

Sunscreen Formulation Optimization:

ANNs can contribute to the optimization of sunscreen formulations by predicting the effectiveness of different UV filters and their combinations. This aids in developing products with optimal sun protection properties.

Marketing and Branding Strategies:

Neural networks analyze consumer behavior and responses to different marketing strategies. This information helps in tailoring marketing and branding approaches for cosmeceutical products.

Sensitivity and Allergenicity Prediction:

- ANNs can predict the likelihood of skin sensitivity or allergic reactions to specific cosmetic ingredients. This information is crucial for formulating products suitable for individuals with sensitive skin.

- The application of artificial neural networks in cosmeceuticals reflects the industry's commitment to innovation, customization, and addressing individual skincare needs. As technology continues to advance, the integration of neural networks is expected to play a significant role in shaping the future of cosmeceutical product development and marketing.

Strengths and limitations:

Strengths:

Comprehensive Scope and Search Strategy:

The review's comprehensive scope and the use of a well-designed search strategy involving multiple databases enhance the likelihood of capturing a wide range of relevant studies. This approach contributes to the robustness and inclusiveness of the review.

Alignment with Scoping Review Methods:

The selection of variables for data collection based on bodies of work with similar inquiry demonstrates a thoughtful and methodologically sound approach. Aligning with the principles of a scoping review allows for a broad exploration of the existing literature on the subject.

Inclusion of Novice Authors with Fundamental Understanding:

The inclusion of authors who were novice to the field of artificial neural networks but still managed to provide a fundamental understanding speaks to the accessibility and clarity of the review. This can make the information more approachable for a broader audience, including those new to the topic.

- **Limitations:**

Heterogeneity in Reporting Measures:

The acknowledgment that studies included in the review did not always use standardized reporting measures is a valid concern. Heterogeneity in reporting can introduce challenges in synthesizing findings and may affect the overall quality and reliability of the review.

Inclusion of Publications of Lower Quality:

The mention that the review may include publications of lower quality highlights a potential limitation. Assessing and addressing the quality of included studies is crucial for the overall validity of the review. It is important for the authors to discuss the potential impact of lower-quality studies on the review's conclusions.

Complex Nature of Artificial Neural Networks:

While the review's authors demonstrated a fundamental understanding of the complex nature of artificial neural networks, the inherent complexity of the topic could pose challenges in synthesizing and presenting information in a way that is accessible to readers who may be less familiar with the field.

Need for Clear Inclusion and Exclusion Criteria:

The review should ideally provide clear inclusion and exclusion criteria for study selection. This ensures transparency in the process and allows readers to understand the basis on which studies were included or excluded.

Potential Bias in Search Strategy:

While a comprehensive search strategy is a strength, it's important to acknowledge the potential for bias in the selection of databases and the inclusion of only English-language publications. This could limit the generalizability of the findings.

Approach to Overcome Limitations:

Evolutionary Algorithms (EAs): To address the limitation of non-informative variables, one sophisticated approach is to use evolutionary algorithms (EAs). These adaptive systems help define sub-groups of variables to be selected, enhancing the overall performance and accuracy of ANNs.

- **Advancements of ANNs in pharmaceuticals**

Drug Discovery and Design:

ANNs are used in the prediction of molecular properties and drug-relevant activities. They assist in the identification of potential drug candidates by analyzing vast datasets related to chemical structures, bioactivity, and pharmacological profiles.

Pharmacokinetics and Pharmacodynamics Modeling:

ANNs play a crucial role in modeling pharmacokinetic and pharmacodynamic profiles of drugs. They help predict drug absorption, distribution, metabolism, and excretion, as well as their effects on the body.

Predictive Toxicology:

ANNs are employed to predict the potential toxicity of drugs or drug candidates. By analyzing molecular structures and biological data, ANNs contribute to the early identification of compounds with potential safety issues, reducing the risk of adverse effects during clinical trials.

Personalized Medicine:

ANNs are used to analyze patient data, including genetic information, to predict individual responses to specific medications. This allows for the development of personalized treatment plans tailored to a patient's unique characteristics.

Disease Diagnosis and Monitoring:

ANNs are applied in disease diagnosis by analyzing complex datasets from various diagnostic sources. They help in identifying patterns indicative of specific diseases and contribute to the development of diagnostic tools for conditions such as cancer and neurodegenerative disorders.

Optimization of Formulations:

ANNs are utilized to optimize drug formulations, considering factors such as drug solubility, stability, and release profiles. This aids in the development of drug delivery systems that enhance efficacy and minimize side effects.

Quality Control in Manufacturing:

ANNs are employed in quality control processes during pharmaceutical manufacturing. They help in detecting deviations from expected product quality, ensuring the consistency and reliability of pharmaceutical products.

Bioprocess Optimization:

ANNs contribute to the optimization of bioprocesses in the production of biopharmaceuticals. They assist in monitoring and controlling parameters such as cell culture conditions, fermentation, and purification processes to improve efficiency.

Market Forecasting and Trend Analysis:

ANNs are used for market forecasting and trend analysis in the pharmaceutical industry. They analyze market data, including sales, pricing, and regulatory trends, to provide insights into market dynamics and guide strategic decision-making.

Drug Repurposing:

ANNs assist in identifying new therapeutic uses for existing drugs by analyzing biological and clinical data. This can accelerate the drug development process by repurposing known compounds for different medical indications.

- **Advancements of ANNs in cosmeceuticals**

Product Formulation and Optimization:

ANNs are utilized in the formulation and optimization of cosmetic products. They assist in predicting the most effective combinations of active ingredients, ensuring optimal product performance and desired cosmetic benefits.

Personalized Skincare Recommendations:

ANNs analyze individual skin characteristics and preferences to provide personalized skincare recommendations. By considering factors like skin type, sensitivity, and specific concerns, these systems suggest tailored skincare routines and product selections.

Skin Condition Assessment:

ANNs contribute to skin condition assessment by analyzing images and data related to skin health. They can evaluate factors such as wrinkles, pigmentation, and hydration levels, providing a more accurate and objective assessment compared to traditional methods.

Product Efficacy Prediction:

ANNs help predict the efficacy of cosmetic products based on their ingredients and formulations. This aids in the development of products with enhanced performance and ensures that marketing claims align with actual outcomes.

Customer Feedback Analysis:

ANNs analyze customer feedback, reviews, and social media sentiments related to cosmetic products. This information is valuable for companies to understand consumer preferences, improve existing formulations, and develop new products based on market demand.

Texture and Sensory Perception Modeling:

ANNs are used to model and predict the sensory aspects of cosmetic products, such as texture, fragrance, and overall user experience. This helps in designing products that not only deliver effective results but also offer a pleasant sensory experience.

Anti-Aging Product Development:

In the development of anti-aging cosmeceuticals, ANNs play a role in predicting the effectiveness of ingredients and formulations in addressing specific signs of aging. This includes the reduction of wrinkles, improvement of skin elasticity, and overall skin rejuvenation.

Customized Fragrance Formulation:

ANNs are employed in the formulation of customized fragrances based on individual preferences. By analyzing scent profiles and user feedback, ANNs assist in creating personalized fragrance blends for cosmetic products.

Market Trend Analysis:

ANNs analyze market trends, consumer behavior, and emerging preferences in the cosmeceuticals industry. This information helps companies stay informed about evolving market demands and adjust their product offerings accordingly.

Product Innovation and Research:

ANNs contribute to the innovation and research efforts in cosmeceuticals. By predicting potential interactions between ingredients and assessing their impact on skin health, ANNs support the development of novel products with advanced formulations

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