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USAGE OF NEURAL NETWORKS FOR ANALYSIS AND PROCESSING OF EXPERIMENTAL RESEARCH OF COMPOSITE MATERIALS

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Abstract. *Modern industrial development demands the creation of new materials to enhance the durability and operational lifespan of machines while reducing metal and energy consumption. Composite materials, particularly those based on polymers (reactoplasts), play a key role in achieving these goals. Neural networks, including CNNs, RNNs, LSTMs, GANs, and transformers, outperform traditional algorithms in pattern recognition tasks and are effective tools for analyzing macro- and microstructures of composite materials with predefined properties. Despite challenges in training deep models, requiring significant computational resources and energy, optimization methods like quantization and distillation help reduce costs. Integrating quantum computing further accelerates optimization processes. The importance of Explainable AI is emphasized to address the «black-box» nature of neural networks, ensuring their reliability for critical applications. These technologies are essential for advancing intelligent systems and creating next-generation materials for high-tech industries.*
Key words: *composite materials, neural networks, artificial intelligence, Explainable AI, optimization, quantum computing, advanced materials.*

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1. INTRODUCTION

Modern development of industry requires the development of new materials to enhance the durability and time between overhauls of various mechanisms and machines. The use of composite materials (CM) will also reduce the metal and energy consumption of the developed units when they are in operation. In this regard, the development of new materials and coatings based on both cermets and polymers, primarily reactoplastics, is a promising area. The development of composite materials involves the use of large amounts of experimental data. Among the many methods and models of processing experimental data, neural network technologies currently take a prominent place. It is important to note that neural networks are a key component in the development of artificial intelligence, which is capable of learning and recognising complex relationships between input and output data (patterns). The development of the concept of neural networks originates from the study of the nervous system, where neurons function as basic computing units. Being one of the most revolutionary achievements in the field of artificial intelligence, neural networks provide a wide range of opportunities for solving complex scientific and technical problems. Due to their ability to model non-linear dependencies and adapt to large amounts of data, neural networks have become a fundamental tool for creating intelligent systems of the next generation. In most cases, the developed modern neural networks are nonlinear models that are able to approximate arbitrary functions while performing tasks with high accuracy of processing a large amount of experimental data.

The aim of the study is to analyse and justify the choice of structure and type of neural networks for processing experimental data of composite materials to optimise their properties aimed at increasing the service lifespan and time between overhauls of machines and mechanisms.

2. ARCHITECTURE AND TYPES OF NETWORKS

All graphic materials of neural networks were taken as prototype diagrams for this article from the Internet. The presented pictures of neural networks were analysed and adapted for the needs of processing the results of experimental data of composite materials: physical and mechanical, structural characteristics, images of the interface, etc. We used the analysed and obtained networks to determine the parameters of the outer surface layers at the interface in the «filler-binder» system.

The websites used are provided in the text of the article.

To ensure the successful functioning of a neural network, an architecture consisting of a multitude of interconnected elements – neurons – which are organised into a system of layers is used (Fig. 1). The input, hidden and output layers provide successive information processing, where each neuron performs a linear combination of input data with the subsequent application of an activation function.

The input layer receives the initial input data, which is fed to the neurons as numerical values. The number of neurons in this layer is determined by the dimensionality of the input data.

The hidden layers are the main and important element of the network, as using activation functions they perform nonlinear transformation of the input data. The number of layers and neurons in them determines the computing power of the network.

The output layer generates the final processing result based on the calculations in the previous layers. This result can be represented by classes or probabilities. When processing experimental data, the numerical values of the studied quantities are usually used.

Each neuron in the hidden layers performs calculations as follows:

$$z = \sum_{i=1}^{n} (w_i \cdot x_i) + b,$$

where x_i are the input values, ω_i are the weights of the neural connections, and b is the offset. The use of the activation function f(z) allows us to take into account nonlinearity in the model. The most common functions:

- *ReLU (Rectified Linear Unit):* $f(z) = \max(0, z);$
- *Sigmoid:* $f(z) = \frac{1}{1+e^{-z}};$
- *Hyperbolic tangent:* $f(z) = \tanh(z).$

Activation functions, such as ReLU, sigmoid, or hyperbolic tangent, allow the network to model complex, non-linear relations in data.

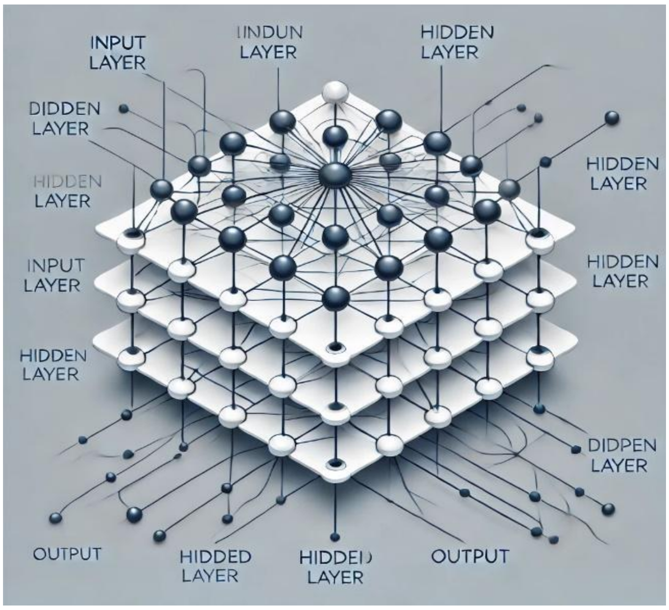


Figure 1. The basic architecture of a neural network. The main components of an artificial neural network: an input layer, several hidden layers, and an output layer. The nodes (neurons) and weight connections that calculate linear combinations of input signals are shown. (https://in.linkedin.com/in/mdaniq 45?trk=public_post_feed-actor-name)

The ability of machine learning of system during its processing is an important aspect of using neural networks when processing a large amount of experimental data. Machine learning (ML) is a sub-domain of artificial intelligence (AI) that allows a machine to automatically find (learn) the statistical structure of data and transform such representations (patterns) to bring them closer to the expected result. The learning process is improved through a feedback channel to compare expected and calculated results. It is based on the error backpropagation (feedback) mechanism [5–6], which optimises neuronal weights based on gradient descent (Fig. 2). The backpropagation algorithm calculates the derivatives of the loss function for each parameter, ensuring its gradual update. During training, a large amount of data is used, which allows the neural network to «learn» and generalise solutions for new examples.

Using deep learning systems, neural networks have been able to achieve new results in various fields, from pattern recognition and natural language processing to medical diagnostics and autonomous driving. This stage of network operation can be divided into three different possibilities based on the system’s feedback method: unsupervised learning, reinforcement learning, and supervised learning. Deep neural networks, which include dozens or hundreds of hidden layers, are able to extract hierarchical features that are critical for processing high-dimensional data. One of the most important architectures for data processing (Fig. 3) is convolutional neural networks (CNNs), which effectively process images, including structural formations in CM, using convolutional and summation operations. [7–10]. The basic idea is to find a formula or function that generates an output label yi using input functions Vi. The process of finding the predictor function f is often referred to as fitting or training the solution/model.

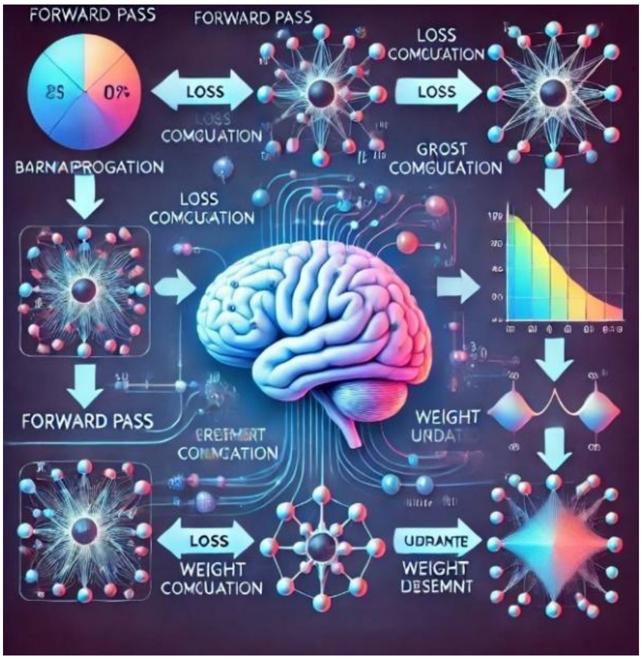


Figure 2. Feedforward data propagation, calculation of the loss function, backpropagation of gradients, and updating weights using gradient descent (https://in.linkedin.com/in/mdaniq45? trk=public_post_feed-actor-name)

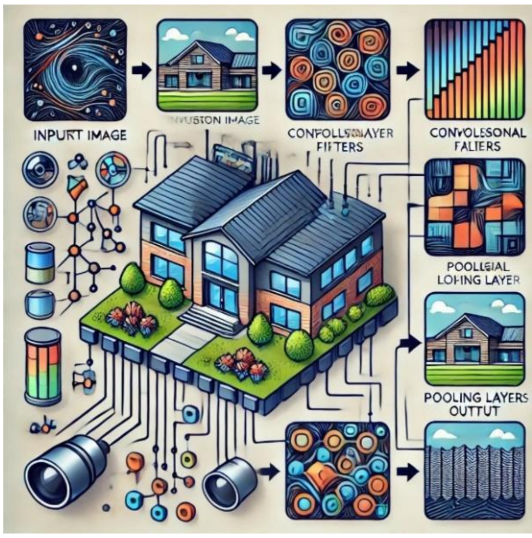


Figure 3. Convolutional neural network (CNN). The structure of a convolutional neural network that processes images. Convolutional layers with filters, max-pooling layers and a fully connected output layer for classification are shown. (https://solveforce.com/iot-sensors-and-actuators-the-dynamic-duo-powering-solveforce-innovations/)

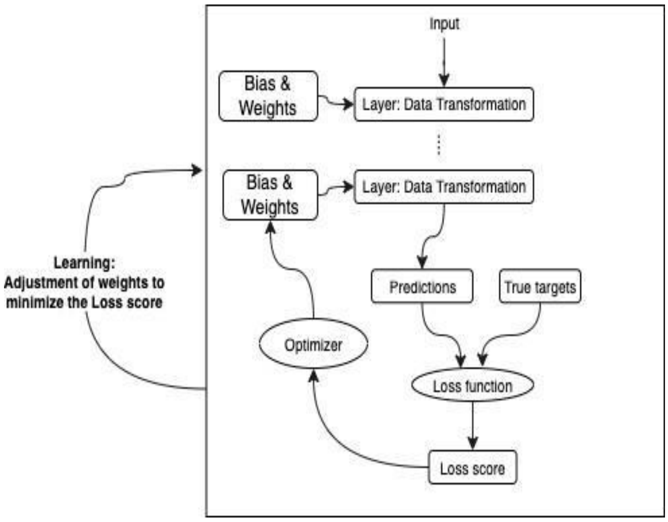


Figure 4. The learning cycle

Time series and sequence processing, recurrent (Fig. 5) neural networks (RNN) [11], and their improvements, such as LSTM (Fig. 6) and GRU, will allow for efficient analysis of data that depend on previous states [12–14]. Due to the mechanism of memory and control over time dependence, recurrent architectures allow to recognise new possibilities for processing experimental data as input parameters.

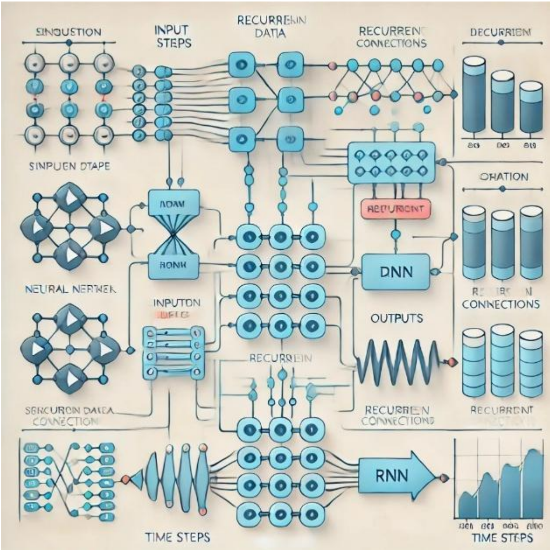


Figure 5. Recurrent neural network (RNN). The diagram shows the processing of sequential data in a recurrent neural network. Time steps, feedback between nodes and data flow from input to output are shown. (https://www.linkedin.com/in/irsath-ali/recent-activity/all/)

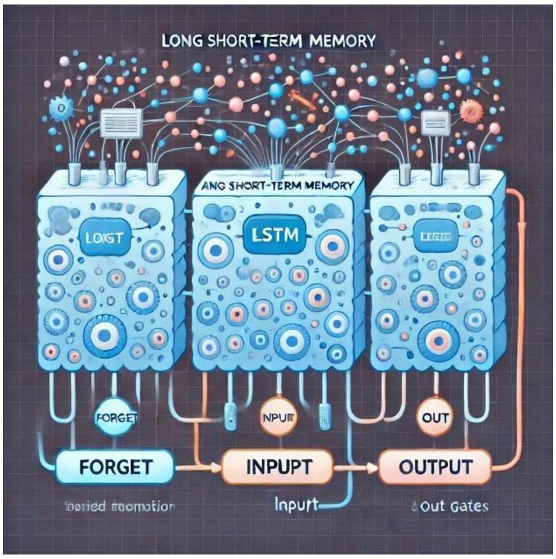


Figure 6. LSTM network. The figure illustrates the structure of an LSTM (Long Short-Term Memory) cell, including input, output, and forgetting gates. It shows how information is controlled at each time step.(https://in.linkedin.com/in/ mdaniq 45?trk=public_post_feed-actor-name)

When constructing neural networks, it is important to use the transformational architecture, which has revolutionised the processing of experimental data sets by replacing recurrent connections with a self-attention mechanism. Transformer-based models (Fig. 7), such as GPT and BERT, have shown the ability to understand semantic contexts with high accuracy [15–16]. Due to parallel data processing, transformers provide high performance even on large amounts of data.

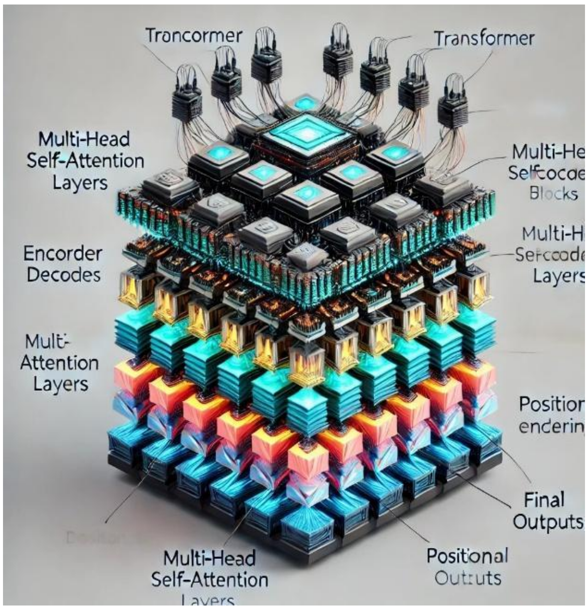


Figure 7. Transformer architecture. The Transformer model includes encoder and decoder units, multi-head self-attention, positional coding, and final outputs. (https://in.linkedin.com/in/ mdaniq 45?trk=public_post_feed-actor-name)

One of the most important aspects of research using neural networks is their interpretability and generalisability. It should be noted that despite their high efficiency, many modern neural network models function as “black boxes”, which makes it difficult to explain their decisions. The use of Explainable AI methods improves the efficiency of these systems and ensures their application for processing experimental data and subsequent analysis.

Another important issue is computational efficiency, as deep neural networks require computing resources and energy. Optimising neural networks, using quantum computing, and developing efficient training algorithms are important steps in overcoming these limitations.

Being a fundamental element of artificial intelligence, neural networks provide high efficiency in solving tasks related to classification, regression, segmentation and optimisation of experimental data. These systems are characterised by the ability to learn from the results, with subsequent processing and the ability to find dependencies in complex and highly interactive data sets. Artificial neural networks (ANNs) are the result of abstract modelling of neurons and synapses in the human brain, where each network element interacts to perform computational tasks.

Let’s take a closer look at different types of neural networks designed for specific tasks and data:

Convolutional neural networks (CNN). They are used to process macro and micro-level images with experimental data, such as the deformation of samples during testing. They are characterised by convolutional layers that allow for the detection of local features at different levels. Pulling operations (max-pooling or average-pooling) reduce the data dimensionality, ensuring efficient image processing of the structural characteristics of materials, including composites.

Recurrent neural networks (RNN). They are designed to analyse sequences and time series. Their structure provides for the preservation of “memory” of previous states through feedback. Modified RNNs, such as LSTM (*Long Short-Term Memory*) and GRU (*Gated Recurrent Unit*), solve the problem of gradient loss and provide better performance for long sequences.

Transformers. They are based on the self-attention mechanism, which allows to effectively consider the dependencies between all elements of the sequence. Due to parallel processing and scalability, transformers have replaced RNNs in a number of tasks.

Neural network training is an iterative process of optimising weights using gradient descent algorithms. Thus, by repeating the process several times, the system learns the most efficient way to perform a task in a given environment. Training a neural network requires a way to measure the performance of the «learner». In ANN learning, you can measure the cost function. The Cost function is the sum of the difference between the system’s output and the desired output. In this approach to ANN learning, the lower the cost, the closer the desired output is. And like any other learning, this is done by trial and error, gradually minimising the cost after several training cycles. The process includes:

Forward Propagation. The input data pass through all layers of the network until the output is obtained.

Calculation of the loss function. It determines the error of the result compared to the expected value.

Backpropagation. The error is propagated in the opposite direction to update the weights by the rule:

$$w_{new} = w_{old} - \eta \frac{\partial L}{\partial w},$$

where ω_{old} is a loss function, and $\eta \frac{\partial L}{\partial \omega}$ is learning speed.

By creating a feedback loop or backpropagation, these values can be automatically changed to the nearest desired value, thus minimising costs. In practice, this means that after each learning round of data, the ANN adds the adjusted values to the connections of each hidden layer, repeating one level in the opposite direction. After several training rounds, the network should be able to navigate between data it has never seen before. Thus, manual training is not required. The network can adjust the values automatically by moving backwards in the network. It should be noted that neural networks are a powerful tool for modelling complex systems. Their development requires further research to increase efficiency and resilience to new challenges.

3. ANALYSIS OF THE PROBLEMS OF BUILDING AND TRAINING ARTIFICIAL NEURAL NETWORKS

ANNs are the result of the continuous evolution of mathematical models that attempt to reproduce the adaptive properties of biological neural coding and information processing [17]. Their architectural principles are based on the ability to perform distributed parallel calculations, which can significantly improve the performance of systems in solving problems where classical algorithmic methods are ineffective. The main factor that distinguishes neural networks from traditional machine learning methods is the ability to independently identify significant features out of experimental data during training, which eliminates the necessity for preliminary manual programming of rules or deep pre-processing of information.

However, the real difficulty in the operation of a neural network lies in the dynamic adjustment of weighting coefficients that affect the contribution of each input signal to the final result. The conditions for optimal adjustment of these parameters are ensured during training, which involves iterative minimisation of the loss function using adaptive optimisation algorithms such as Adam, RMSProp, or SGD (Stochastic Gradient Descent). These algorithms use gradients to update the weights, thus providing a gradual reduction of the error in modelling the data processing process.

In deep neural networks, where there can be hundreds or even thousands of hidden layers, the computational complexity of training increases exponentially. The problem with the deep architecture is that the backpropagation of gradients encounters gradient damping or explosion, which leads to inefficient optimisation of the network. To solve this problem we introduced normalisation methods, such as Batch Normalisation, which stabilise the distribution of neuronal internal values and speed up the training process. Moreover, regularisation in the form of Dropout reduces the probability of information «overdose» by randomly disabling a certain percentage of neurons during each iteration of data processing [18].

Convolutional neural networks are a particularly important architectural innovation when constructing them, as they are adapted to process spatially structured data. Convolutional kernels that pass through the input image matrices allow the neural network to identify local and global features of objects, regardless of their location. This principle is especially effective when used in image recognition tasks by adding convolutional layers, pooling layers, normalisation layers, and fully connected layers between the input and output layers. Convolutional layers significantly reduce the computational power required to calculate all these accumulative weights and network biases. Building an ANN is highly dependent on trial and error, and therefore training an accurate neural network is a time-consuming process.

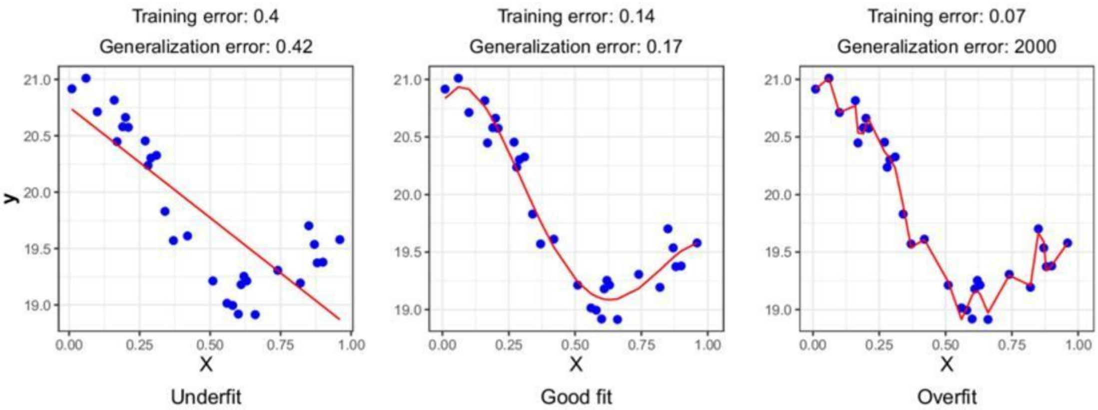


Figure 8. Display of under- and overfitting of the training curve. A good fit is represented by the corrected training curve (in the middle)

Recurrent neural networks (RNNs), which store information about temporal dependencies in data, are the basis for solving problems that require the processing of sequences. However, basic RNNs have the limitation that they have a short memory, which leads to the loss of context in long sequences. Modified structures, such as LSTM (Long Short-Term Memory) and GRU (Gated Recurrent Unit), use special cells to control the flow of information, allowing to effectively take into account both short-term and long-term dependencies.

4. DIRECTIONS AND PROSPECTS FOR THE DESIGN AND DEVELOPMENT OF NEURAL NETWORKS

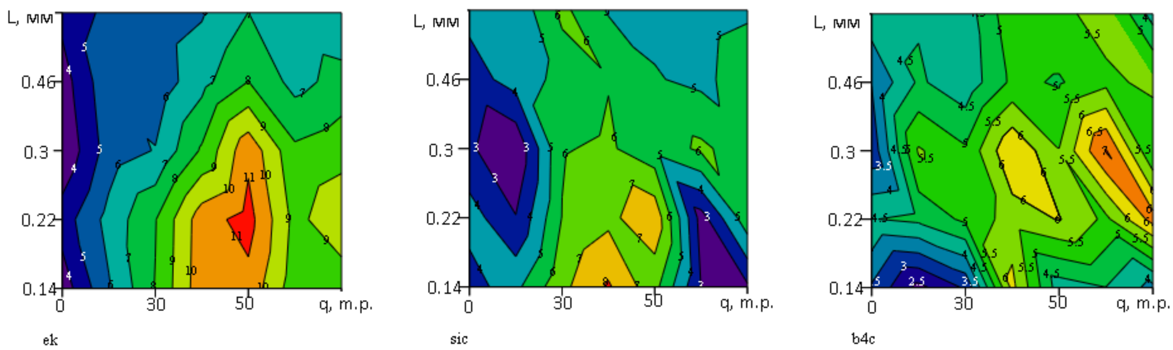
The emergence of (transformational) models is the next step in data processing, where the mechanism of self-attention allows us to take into account global dependencies in all elements of the sequence simultaneously. Unlike recurrent networks, transformers provide parallel processing, which reduces model training time. Well-known architectures such as GPT (Generative Pre-trained Transformer) and BERT (Bidirectional Encoder Representations from Transformers) have demonstrated exceptional results in text generation, automatic translation, and understanding of language semantics.

However, despite technological advances, the effectiveness of neural networks may be limited by the following factors. In particular, power consumption in the process of training models for processing large data sets is a critical factor that limits their practical application in real time. In this regard, considerable attention is being paid to the development of quantum computing methods and optimised neural networks that reduce computational costs. The problem of trust in AI solutions remains relevant, as in many cases neural networks cannot explain how they came to a particular conclusion. The development of Explainable AI methods is essential for the widespread adoption of these technologies.

In modern approaches to neural network development, the usage of hybrid architectures is promising. Different types of networks are combined to achieve optimal performance for solving problems of multifactor environments. Combining convolutional neural networks (CNNs) with recurrent architectures (RNNs or LSTMs) allows simultaneous processing of spatial and temporal dependencies, which is especially useful for video analysis, where objects have to be recognised and their dynamics tracked. Hybrid models prove to be effective in image recognition for the analysis of structural parameters, including composite materials [19–20].

A study of micrographs of thin films of epoxy composites modified by the introduction of dispersed filler particles was carried out. A prerequisite for obtaining composites with high technological and operational characteristics is to ensure a strong and long-term bond between the active centres on the filler surface and the binder macromolecules. Physical methods of controlling the structure and properties of polymer composites are based on the influence of the filler's composition and nature on the structure formation processes and the degree of crosslinking of the epoxy matrix, which determine the performance characteristics of the materials. Residual stresses are one of the key factors that affect the properties of materials during their use. They significantly affect the strength of adhesive joints, wear resistance and maintainability of composite coatings used to protect the surfaces of parts. It should be noted that most epoxy-based materials are used mainly in the form of coatings [21–22]. The use of artificial neural networks to study residual stresses, which are key to the mechanical and operational properties of epoxy composites, is an important area of modern materials science [23–27]. Particular attention should be paid to the analysis of the dependence of internal stresses of materials on the coating thickness and filler content.

The dependence of the predicted value of internal stresses on the thickness of the epoxy composite film and filler content is shown in Fig. 9. These figures make it possible to visually assess the dependence of internal stresses on the coating thickness.



a b c

Figure 9. Diagrams of dependencies of CM residual stresses on the coating thickness L and filler content q of stresses: (a) alumina, (b) silicon carbide, (c) boron carbide

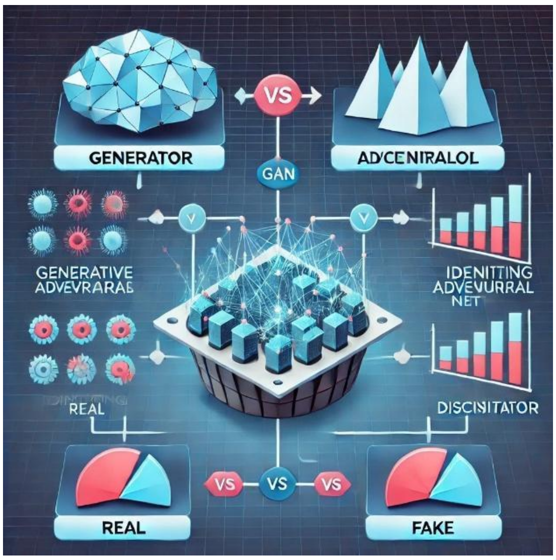


Figure 10. Generative Adversarial Network (GAN). Interaction "adversarial process" between the generator, which creates synthetic data, and the discriminator, which tries to distinguish fake data from real data. (https://www.researchgate.net/figure /Neural-network-architecture-for-multimodal-repr esentation-learning-with-self-supervision_fig2_33 5141438)

BGenerative Adversarial Networks (GANs) are an important area of neural networks in generative models. GANs (Fig. 10) consist of two networks – a generator and a discriminator – that interact with each other during training. The generator creates synthetic data that has the maximum similarity to real data, while the discriminator tries to recognise them. This interaction allows GANs to generate high-quality macro- and microstructure images.

Autoencoders are an important subcategory of neural networks, used to reduce data dimensionality and extract hidden features (Fig. 11). Autoencoders learn to reconstruct the input data at the output, in this case, keeping the most significant information in the hidden layers. This principle makes it possible to solve the problems of data compression, anomaly detection, and generation of new examples from the latent space. Variational autoencoders (VAEs) are a further development of autoencoders that combine the advantages of probabilistic models to create smooth and continuous latent representations.

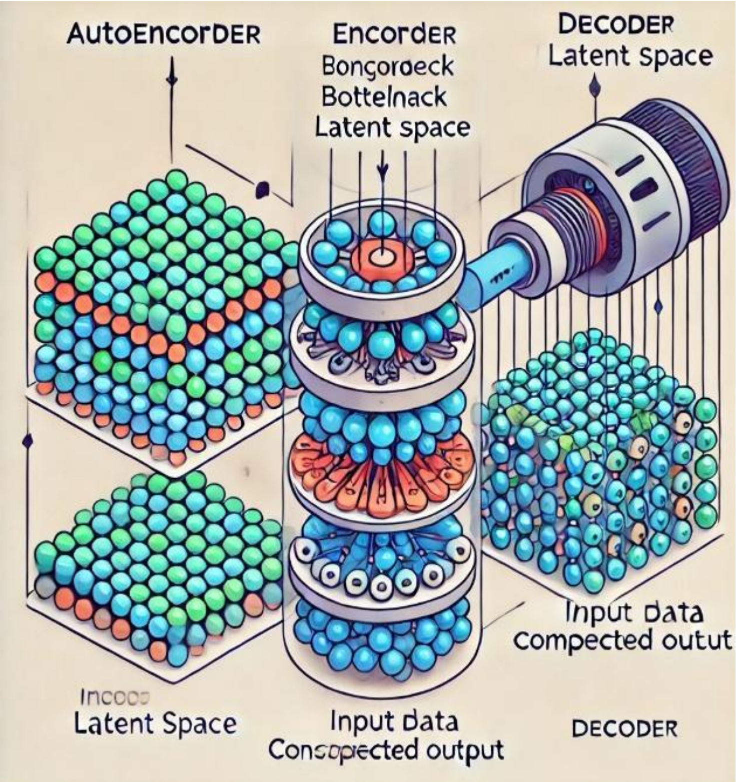


Figure 11. An autoencoder. The encoder (compresses the input data into the latent space) and the decoder (reconstructs the output based on the received features). (https://beast1251.tistory.com /245#google_vignette)

Over the past few years, neural networks have been widely used in the field of Big Data. The massive amounts of structured and unstructured data generated by modern systems require efficient approaches to their processing and analysis. Neural networks, in particular architectures based on *graph neural networks (GNNs)*, demonstrate high efficiency when data is represented in the form of graphs (Fig. 12). This is especially relevant for processing data where the structure of CMs, for example, based on epoxy materials, where the topological structure is represented in the form of spatial graphs[28–30].

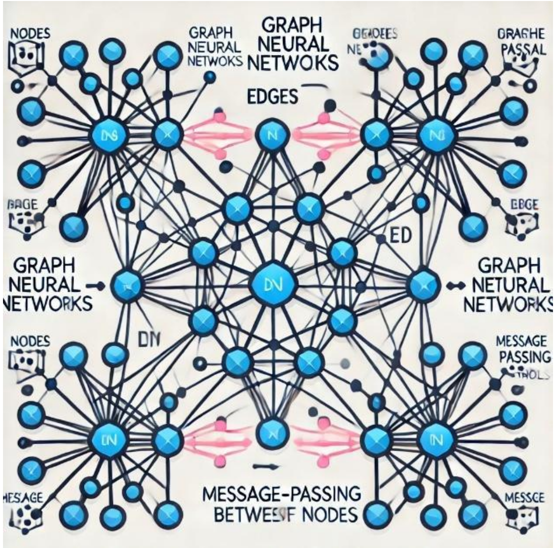


Figure 12. Graph Neural Network (GNN). Processing of graph-structured data in GNN. It shows nodes (vertices), edges. (https://kumo.ai/resources/blog/why-are-shallow-embeddings-important-in-recommendations/)

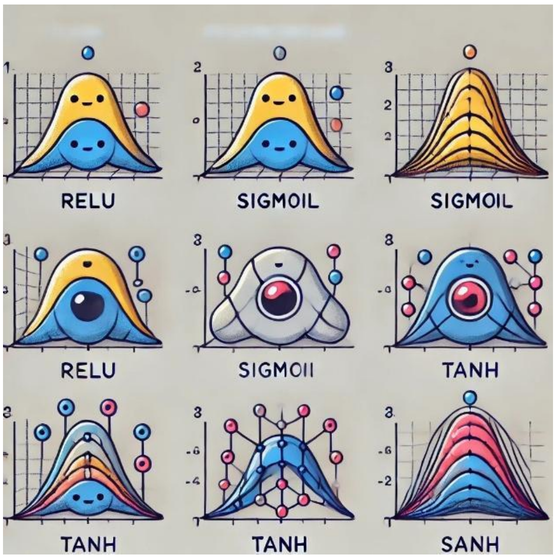


Figure 13. Comparison of popular activation functions (ReLU, Sigmoid, Tanh, and Swish). Shows the dependence of the output value on the input signal (https://www.linkedin.com/in/helinyigit/?originalSubdomain=tr)

The next step in the development of modern neural networks is accompanied by research in quantum computing, which has the potential to revolutionise learning processes. Quantum neural networks (QNNs) use the principles of quantum superposition and entanglement to simultaneously process a huge number of states, which can significantly speed up optimisation and the search for global minimums in loss functions.

In the context of the globalisation of modern systems, neural networks are becoming a central component of digital systems that combine cloud computing and data analytics. Deep learning networks are used to control distributed sensor networks, predict system behaviour in real time, and automate infrastructure solutions in the complex research and development of composite materials. The growth in computational costs that are associated with training large models stimulates the development of quantisation and low-level programming methods that reduce hardware resource requirements. Knowledge Distillation methods allow transferring information from large neural networks to smaller models that operate with lower power consumption but maintain high performance in processing input data.

Thus, today, neural networks are a high-tech tool that in the process of analysing and processing large data sets takes into account engineering, research and development aspects. The further development of neural networks will depend on their ability for generalisation, adaptation and interpretability in the face of dynamic chances of input data.

5. CONCLUSIONS

The article substantiates the efficiency of using artificial neural networks for processing the results of experimental research. It is established that the modern architecture of networks, which include convolutional neural networks (CNN), recurrent networks (RNN), LSTM, GAN and transformers, provide performance that exceeds traditional algorithms in pattern recognition tasks and is a very effective tool for analysing macro- and microstructures in the creation of composite materials for various functional purposes with predictable properties.

The article substantiates the efficiency of using artificial neural networks for processing the results of experimental research. It is established that the modern architecture of networks, which include convolutional neural networks (CNN), recurrent networks (RNN), LSTM, GAN and transformers, provide performance that exceeds traditional algorithms in pattern recognition tasks and is a very effective tool for analysing macro- and microstructures in the creation of composite materials for various functional purposes with predictable properties.

The limitations associated with the complexity of deep model training, which requires significant resources, in particular graphics processing units (GPUs) and energy, are analysed. It is established that the application of optimisation methods, such as model quantisation and distillation, can reduce computational costs without losing performance. The integration of quantum computing into neural networks significantly speeds up the optimisation process.

The importance of interpretability of solutions is established, since most modern neural networks function as «black boxes». The development of approaches to the explainable process using artificial intelligence (Explainable AI) is important for the application of neural networks in research related to the recognition of structural organisations in composite materials.

Thus, neural networks are a tool that not only expands the boundaries of scientific achievements, but also creates new challenges that boost the development of modern science and engineering in the field of experimental data processing. Solving the challenges associated with interpretability and computational costs will allow them to unlock their full potential. Therefore, the research and implementation of neural networks remains a priority area to ensure the next step towards the creation of composite materials with predefined characteristics for advanced industries.

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ВИКОРИСТАННЯ НЕЙРОННИХ МЕРЕЖ ДЛЯ АНАЛІЗУ ТА ОБРОБКИ ЕКСПЕРИМЕНТАЛЬНИХ ДОСЛІДЖЕНЬ КОМПОЗИТНИХ МАТЕРІАЛІВ

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Резюме. *Сучасний розвиток промисловості потребує створення нових матеріалів, які забезпечують підвищення ресурсоздатності та збільшення міжремонтного періоду роботи машин і механізмів. Використання композитних матеріалів сприяє зниженню метало- та енергоємності розроблених агрегатів. Одним із перспективних напрямків є розроблення матеріалів та покриттів на основі полімерів, а саме, реактопластів. Застосування композитів вимагає опрацювання великих масивів експериментальних даних, де провідну роль відіграють нейронні мережеві технології. Встановлено, що сучасна архітектура нейромереж, зокрема згорткові нейронні мережі (CNN), рекурентні мережі (RNN), LSTM, GAN та трансформери, забезпечує продуктивність, яка перевершує традиційні алгоритми у завданнях розпізнавання образів. Ці мережі є ефективними інструментами при аналізі макро- та мікроструктур композитних матеріалів з наперед заданими функціональними властивостями. Отримано результати залежностей залишкових напружень КМ від товщини покриття L та вмісту наповнювача q напружень. Разом із тим дослідження виявили певні обмеження, пов'язані зі складністю навчання глибоких моделей, що потребують значних обчислювальних ресурсів, таких, як графічні процесори (GPU), та значного енергоспоживання. Використання методів оптимізації, зокрема квантування моделей і Knowledge Distillation, дозволяє знижувати обчислювальні витрати без втрати продуктивності. Інтеграція квантових обчислень у нейронні мережі значно прискорює процеси оптимізації. Особливу увагу приділено важливості інтерпретованості рішень. Більшість сучасних нейромереж функціонують як «чорні скриньки», що ускладнює їх використання в критичних задачах. Розвиток Explainable AI сприяє підвищенню довіри до нейронних мереж та їх ефективному застосуванню для дослідження структурних організацій композитних матеріалів. Таким чином, нейронні мережі є не лише інструментом, що розширює межі наукових досягнень, а й викликом, який стимулює розвиток сучасної науки та інженерії. Подолання викликів, пов'язаних із інтерпретованістю та обчислювальними витратами, відкриває нові можливості для створення інтелектуальних систем і композитних матеріалів із наперед заданими характеристиками для передових галузей промисловості.*

Ключові слова: *композитні матеріали, нейронні мережі, штучний інтелект, реактопласти, Explainable AI, квантові обчислення, оптимізація моделей, інтелектуальні системи.*

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