INTELLIGENT INFORMATION TECHNOLOGIES TO SUPPORT DECISION-MAKING WHEN APPLYING THE CAD/CAM/CAE SYSTEM OF DESIGN AND USING ADDITIVE TECHNOLOGIES

ANTON PANDA1, KOSTIANTYN DYADYURA2, ANDREY SMORODIN3, DMITRIY DMITRISHIN4, SVETLANA ANTOSCHUK5

1Faculty of Manufacturing Technologies with a seat in Presov, Technical University of Kosice, Slovak Republic
2Department of Biomedical Engineering, Odessa Polytechnic National University, Shevchenka Ave, 1, 65044 Odessa, Ukraine
3Department of Applied Mathematics, Odessa National Polytechnic University, Odessa, 65044, Ukraine
4Department of Applied Mathematics, Odessa National Polytechnic University, Odessa, 65044, Ukraine
5Odessa National Polytechnic University, 1, Ave. Shevchenko, Odessa, 65044, Ukraine

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e-mail: anton.panda@tuke.sk

The direction of research is the development of principles and methods for making scientifically based decisions in the design and additive manufacturing of bone substitutes based on apatite-biopolymer composites with functional properties depending on the nature of the localization of the cavity bone defect and its size. The relevance is due to the fact that the development of an intelligent decision-making support system based on neural network modeling, the development of methods for their training, tabagato-criterion optimization of design processes, will allow the creation of three-dimensional solid models of defects taking into account their spatial structure and bone substitutes for the synthesis of biomaterials with controlled composition, porosity and mechanical strength, which are optimal for a specific area of bone replacement, which will increase the effectiveness of treatment and prosthetics in orthopedics and traumatology. A set of methods for analyzing images of bone tissue, taking into account its spatial structure, which are obtained by sensors of different physical nature, with the use of neural network models, development of methods of their design, optimization, and training is proposed. A modification of the method of learning neural networks based on gradient descent, based on the application of the theory of nonlinear dynamics, is proposed. Corresponding theoretical provisions have been developed.

KEYWORDS
Medical devices, 3D printing, Nonlinear dynamic, Tissue engineering, Bone scaffolds, Additive manufacturing, Convolutional neural networks, Medical imaging, Artificial neural networks

1 INTRODUCTION
The production of bone substitutes with functional properties that take into account the patterns of new formation of bone tissue became possible thanks to the application of the CAD/CAM/CAE design system and the use of additive technologies [ISO/IEC 3532-1:2023, Top 2021]. Currently, the use of additive technologies for the production of bone substitutes determines the effectiveness of the latest methods of treatment and prosthetics in traumatic surgery, oncology, cranio-maxillofacial surgery, dentistry, etc. However, problems in the production of bone substitutes using additive technologies are related to both the complexity of the structure of the bone tissue itself and the accuracy of the reproduction of the spatial image of the hollow defect for the construction of its 3D model [Kuznetsov 2020, Celard 2023, Kumar 2024]. Despite the existence of a significant variety of apatite-biopolymer composites, which differ in composition, porosity and, accordingly, strength, until now there is no differentiated approach to the selection of a bone substitute depending on the nature and localization of the cavity bone defect, its size and loading conditions [Barnik 2019]. Making informed decisions in the design of bone substitutes for their additive manufacturing, taking into account all risks, is possible only on the basis of the results of image analysis that are highly effective in terms of accuracy and speed, obtained using modern methods of radiography, computer and magnetic resonance imaging, etc. At the heart of these methods are various geometric or pixel transformations that can allow the generation of images similar to the original [Karrach 2020].

For the additive manufacturing of bone substitutes with controlled composition, structure, porosity and strength, depending on the nature and localization of the cavity bone defect, its size and loading conditions, a complex of interconnected methods and means of analysis, clustering, segmentation and classification of objects in the images is proposed [Vasko 2021]. Digital Imaging and Communications in Medicine (DICOM) is a standard for transmitting and managing information about medical images and related data [ISO/IEC 3532-1:2023]. At the same time, the analysis of medical images is considered a difficult [Kumar 2023] and time-consuming task [Iqbal 2023], especially for young doctors and specialists who do not have sufficient experience. One of the important stages of processing is the search for the content of the medical image, the selection of features of the relevant content of the image for effective medical application. Solid medical models are typically created from composite two-dimensional images obtained from medical imaging systems. The accuracy of the final model depends on the resolution and accuracy of the original image data. Major factors affecting accuracy are image resolution, amount of image noise, contrast between tissues of interest, and artifacts inherent to the imaging system. Additional errors may be caused by the process of converting DICOM or PACS data into computational formats used in segmentation editing software and saving the STL 3D grid format for use in additive manufacturing systems [Zaborowski 2007, Adamcik 2014, Svetlik 2014, Olejarova 2017 & 2021, Sedlackova 2017, Celas 2018, ISO 10993-1:2018, Labun 2018, Gamec 2019, Kuznetsov 2019, Murcinkova 2019, Pollak 2019 & 2020, ISO 10477-2020, ISO/ASTM TR 52916:2022, Straka 2021 & 2022, Vagaska 2021, Rimar 2024]. When saving the customized STL file, all metadata defining the color, material and texture of the surface are lost. The lack of accuracy and precision of 3D data from scanning systems, software for editing and modeling can reduce the quality of a medical device made by additive technologies. More slices require physicians to review even more image material, especially with the increasing use of high-resolution medical
The role of artificial intelligence (AI) in the field of medicine is constantly expanding [Top 2021, Cerald 2023]. Artificial intelligence includes various technologies based on advanced algorithms and learning systems. Various terms are used in connection with AI, such as machine learning, deep learning (DL), and conventional neural networks [Kumar 2023, Kumar 2024]. DL approaches have already proven their ability to surpass human capabilities in medical applications, particularly in the diagnosis and prediction of disease development. DL approaches represent key techniques for several medical applications, including decision making, disease stage tracking, disease detection, disease diagnosis and analysis, etc. [Krenicky 2022]. Deep Convolutional Neural Networks (DCNNs) are the most widely used deep learning systems for sequence identification applications in images. By constantly changing its parameters with a learning algorithm, a DCNN can be trained to autonomously extract appropriate features from training instances for a specific field. A CNN model does not require explicitly generated features as input because feature representations are discovered during training. The main motivation for reviewing and explaining how artificial neural networks (NNs) and deep generative models work in medical imaging is to encourage their use in the medical field. Regarding generative models, Zhai et al. [Monkova 2013, Michalik 2014, Panda 2014 & 2021, Baron 2016, Mrkvica 2016, Balara 2018, Chaus 2018, Duplakova 2018, Sukhodub 2018a, Zhai 2018, Flegner 2019 & 2020, Harnicarova 2019, Pandova 2020] consider numerous variants of autoencoders, while Kazeminia et al. [Kazeminia 2020] focus on the application of GANs for medical image analysis. In medicine, it is often impossible to collect a sufficient number of images and prepare a high-quality set of data certified by doctors. This required the creation of a special architecture that requires a smaller amount of data for the task of semantic segmentation – U-Net [Smorodin 2020]. In addition to the task of object segmentation, it is often necessary to solve the task of identifying individual instances of objects. For these purposes, the R-CNN network (regional convolutional network) [Smorodin 2021] was developed, which simultaneously solves the tasks of localization and semantic segmentation of objects. Its Faster R-CNN extension uses a regional proposal network to determine the region of interest (Region of Interest) and find a rectangle that contains the required object in itself.

An important scientific and practical task, which is solved during the creation of a software product for intelligent decision-making support in the design of a bone substitute, is the design of architectures and ensuring the reduction of the training time of deep neural networks by improving the optimization methods used for this purpose. The conducted analysis showed that one of the effective ways to solve this problem is to reduce the time spent on learning neural networks, which can be achieved by finding new and improving existing optimization methods used in learning NM. The most common in deep AI training are a number of methods based on the gradient optimization method. However, they all have a common drawback in the conditions of multi-objective, multi-modal and noisy function - "slow" convergence, which significantly increases the learning time. To eliminate it, a modification of AI training methods based on gradient descent, based on the application of the theory of nonlinear dynamics, is proposed, and relevant theoretical provisions for the implementation of the methods are developed. The purpose of the research: development of methodology, principles and approaches to the creation, implementation and use of intelligent information technologies to support decision-making in the application of the CAD/CAM/CAE design system and the use of additive manufacturing technologies of bone substitutes with functional properties from the collection of anatomical data to the final model, which takes into account patterns of bone tissue neoplasms [Dyadyura 2017, Sukhodub 2019].

2 MATERIALS AND METHODS

The scientific approach that is implemented in the project is based on the use of system-wide evolutionary transdisciplinary models. To create a decision-making support system, clinical information is systematized according to the research topic and objectives. Methods of research: general clinical, X-ray, computer, densitometric, electron microscopic. The learning process is performed using back-propagation to update the internal values of the network and reduce losses, offering more accurate predictions. In the training cycle, the chosen optimization method is used, which depends on the learning speed of the neural network. Optimization consists in finding the local minimum of a complex and multidimensional function. Therefore, the speed of the learning process directly depends on the speed of optimization. The analysis showed that the gradient descent methods and their modifications are the most common when learning neural networks. The well-known gradient descent method is one of the first optimization algorithms. As the complexity of the data and the number of training cases increases, it also becomes more difficult to find the minima and the computational cost. Given this fact, many optimization algorithms have emerged over the years. Stochastic gradient descent (SGD) is an iterative algorithm that follows a function until it finds its lowest point as gradient descent. The only difference is that SGD updates the internal network parameters based on random examples instead of processing them all. The process is computationally cheaper, but the parameters have higher variance and larger oscillation steps. The impulse algorithm aims to reduce the fluctuation and variance of SGD by using a parameter stored at each iteration that affects the next update in a way similar to acceleration [Dmitrishin 2021a,b]. Previous optimizers use a constant learning rate, which is a problem when gradients are sparse or small. Algorithms such as [Dmitrishin 2019] and its variants such as [Pandova 2018, Kivimaa 2019] or [Jurko 2011] introduce a parameter to change it, achieving a variable learning rate. These options aim to mitigate the drop in learning rate that AdaGrad suffers from by using exponential moving averages of past gradients [Macala 2017]. The method of gradient descent, which in the mini-batch training mode formally looks as follows:

$$\Theta_{t+1} = \Theta_t - \frac{1}{\tilde{n}} \cdot \psi_{\gamma} \cdot \sum_{i=1}^{\tilde{n}} L(f(x_i; \Theta_t), y_i)$$  \hspace{1cm} (1)$$

where $\Theta_t$ neural network parameters at time $t$; $B$ is the number of elements in one mini-packet of training data; $L(f(x_i; \Theta_t), y_i)$ is loss function reflecting the error between predicted values $f(x_i; \Theta_t)$ and expected results $y_i$; $f(x_i; \Theta_t)$ is a function denoting the corresponding transformations performed by a neural network with internal parameters $\Theta_t$ and input parameters $x_i$; $\gamma$ is learning rate.

If you enter an additional function from the $\Theta$ parameter:

$$G(\vartheta) = \vartheta - \frac{1}{\tilde{n}} \cdot \psi_{\gamma} \cdot \sum_{i=1}^{\tilde{n}} L(f(x_i; \vartheta), y_i)$$

Then expression (1) can be represented as a classical discrete dynamical system.

$$\Theta_{t+1} = G(\Theta_t)$$  \hspace{1cm} (2)$$

The expression (2) allows us to present the method of gradient descent in the form of DDS, to which the provisions of nonlinear dynamics can be applied. Such a representation allows for the
development of modifications of the discrete dynamic system (2) taking into account the feedback with delay and the predictive feedback. Taking into account (1) and (2), a modification of the gradient descent method is proposed, taking into account the feedback with a delay in the discrete dynamic system:

$$\Theta_{t+1} = (1 - \lambda) \cdot G \left( \sum_{j=1}^{N} a_j \cdot \Theta_{t-1} + \frac{2}{\eta} \cdot \sum_{i=1}^{N} b_i \cdot \nabla \Phi(\Theta_t) \right) + \lambda \cdot G \left( \Theta_t \right) \cdot u_t$$

(3)

where parameters $a_j$ and $b_j \sum_{j=1}^{N} a_j = \sum_{j=1}^{N} b_j = 1, \forall \lambda \in \mathbb{R}$.

Taking into account (1) and (2), a modification of the gradient descent method is proposed, taking into account the predictive feedback in the discrete dynamic system

$$\Theta_{t+1} = G(\Theta_t) + u_t$$

(4)

where is the predictive feedback:

$$G(\Theta) = \sum_{i=1}^{N} a_j \cdot \Theta_i$$

In practice, they use a set of loss functions (objective functions), specially created for different classes of tasks. The task of neural network training is reduced to finding the minimum of the loss function. So, the entire learning process can be imagined as a standard optimization problem that can be solved by known optimization methods. Many of these methods can be divided into two large classes: first and second order. The difference between the classes lies in the degree of the derivative of the objective function used for optimization.

The proposed method of searching for parameters is implemented in the following sequence:

Stage 1. Solution of the optimization problem on the class of complex polynomials.

Stage 2. Numerical modeling using variations of admissible parameters, in order to determine the parameters $a_j, b_j, \lambda$ of the improved method of gradient descent (3), (4).

Stage 3. Experimental verification of the found parameters for various tasks. The method of finding parameters for the proposed modifications of the gradient descent method, taking into account feedback with a delay and predictive feedback in a discrete dynamic system based on the solution of optimization problems on the class of complex polynomials, which allows to ensure their implementation for a wide range of optimization problems, has been developed.

To conduct a comparative experiment to check the performance of new modifications of the gradient descent algorithm, a multilayer perceptron of the following architecture was implemented (Fig. 1).

The selection of the number of hidden levels and neurons at each of these levels was based on the analysis of a large number of numerous experiments with different values of these hyperparameters. At the same time, the optimization was in depth, as the great depth of the architecture led to an increase in training time, and also required a larger volume of data.

Cone beam computed tomography (CBCT) was used in the work. The result of the operation of these devices are digital flat images of high resolution (Fig. 2). He software of the scanner allows you to glue images as you move the scan around the head (Fig. 3). Within the framework of this study, an intelligent information system for the recognition of CT images for the maxillofacial was developed (Fig. 4). Training a deep neural network.

To use it, you need to perform the following steps:

1. Choose the structure of the neural network;
2. Create a database of CT images;
3. Training a neural network;
4. Carry out validation and testing.

$$\left( N + 1 \right) \cdot \cos(N + 1) \cdot \vartheta + \left( N + 1 \right) \cdot \cos(N + 3) \cdot \vartheta = 0$$

The algorithm for calculating the coefficients of the extremizer is given.

3. In the class of polynomials with $T$ is circular symmetry $F_N^{(T)} = z \cdot \sum_{j=1}^{N} a_j \cdot z^{-j+1}$ to find the asymptotic estimate of the value $\max_{x \in \mathbb{D}} F_N^{(T)}(z)$. The extreme asymptotic value at $N \to \infty, \max_{x \in \mathbb{D}} F_N^{(T)}(z) \to \frac{1}{2} \cdot \frac{\pi}{\sqrt{3}} \cdot N^{2/7}$, where $c_T = \pi^{-1} \cdot 2^{1/7}$.

$$\Gamma^2 \left( \frac{1}{2} + \frac{1}{7} \right), \Gamma(z) \text{ is the gamma function.}$$

The Extremizer

$$F^{(0)}(z) = z + \sum_{j=2}^{N} a_j \cdot z^{-j+1}, e\text{, such a problem is considered on the class of unifoliate functions defined on the extended complex plane.}$

$$\sum_{j=1}^{N} a_j = 1, k \in \mathbb{N}$$

The solution boils down to solving extremal problems for which there are extremal values and extremizers. The solution boils down to solving extremal problems for which there are extremal values and extremizers.

Such a problem is considered on the class of unifoliate functions and typical-real functions according to Rogozinsky. Applied definitions: $C$ is extended complex plane; $D$ is a closed central unit circle, the inversion operation is indicated by an asterisk

$$(z) = \frac{1}{z} \text{ a function } \Phi(z) = (1 - \lambda) \cdot \frac{z^j - \sum_{j=1}^{N} a_j \cdot z^{-j+1}}{z^{-j+1} - \sum_{j=1}^{N} a_j \cdot z^{-j+1}}$$

The solution boils down to solving extremal problems for which there are extremal values and extremizers.

1. For the polynomial $F(z) = \sum_{j=1}^{N} a_j \cdot z^j$ with real coefficients and schlicht normalization $a_1 = 1$. Find

$$\sup_{a_2, \ldots, a_N} \left\{ \Phi(F(z)) : \Phi(F(z)) = 0 \right\}$$

The extreme value is as follows $- \frac{1}{4} \cdot \sec^2 \frac{\pi}{N+2}$ and the corresponding extremizer

$$F(z) = \frac{1}{u_0^2 \cdot \cos \frac{\pi}{N+2}} \cdot \sum_{j=1}^{N} U^j_{n+1} \cdot \left( \cos \frac{\pi}{N+2} \cdot U_{j-1} \cdot z \right)$$

(5)

$$\text{is unique and monofoliate, } U_{j}(x) \text{ is Chebyshev polynomials of the second kind.}$$

2. In the class $T_N$ of all typically real polynomials of degree $N$ schlicht, by normalizing $a_1 = 1$, find the value

$$J_N = \max_{p \in \mathbb{T}, \frac{1}{z} \in \mathbb{D}} \left\{ |F(\frac{1}{z})| \right\}$$

The extreme value is defined as

$$J_N = \begin{cases} \frac{1}{4 \cdot \sin^2 \theta} \cdot \frac{\pi}{2N+2}, & N \text{ is odd} \\ \frac{1}{8 \cdot \sin^2 \theta} \cdot \frac{\pi}{2N+2}, & N \text{ is even} \end{cases}$$

(6)

Where $\Theta$ is the minimum positive root of the equation

$$\left( N + 3 \right) \cdot \cos(N + 1) \cdot \vartheta + \left( N + 1 \right) \cdot \cos(N + 3) \cdot \vartheta = 0$$

The algorithm for calculating the coefficients of the extremizer is given.
The development and training of neural networks was carried out on a computer with 64 GB of RAM and an Nvidia Quadro RTX 3000 graphics accelerator. This accelerator is equipped with 6 GB of video memory that can be used for training neural networks. All the software was built on the basis of the OpenSource library of the Facebook company: PyTorch. The stages of training the neural network for testing different training methods are shown in Figure 5. The training process includes the following steps:

- collect the required number of CT images and mark them;
- generate a set of CT images using data augmentation methods;
- divide the received set into 3 parts: training, test, and verification;
- choose the best architecture of the neural network, that is, the one that will show the best result on the test data set.

The surface digitization procedure begins with the generation of actually measured surface points (or their conversion, for example, to STL format), which are the measured digitization data. In most digitization systems, the measured points are mathematically processed using such operations as:

- agreement
- filtering
- weighing
- selective deletion
- smoothing, etc.

Data augmentation methods were used to generate a training sample of CT images. In the work, the initial amount of data was limited to 54 CT images. Each of the images was a black and white image with 256 shades of gray in JPG format. The size of each of the images was 3000 by 1500 pixels.

All images were pre-denoised by image processing techniques and several medical professionals labeled the images, highlighting each tooth and the corresponding binary mask. Each mask is an image where the intensity of each pixel reflects the probability of belonging to the corresponding tooth (value 1) or background (value 0). In our case, the neural network will have about 18 million parameters, including about 50% requiring training.
Therefore, methods of so-called data augmentation or, in other words, expansion, are used. To generate such a large amount of data, a specialized software environment was developed with the ability to distribute the load between several GPUs and between different servers in the cluster. The first part of the task was solved with the help of the common library Albumentations [Smorodin 2021]. After preparing the raw data, the main part of the system was built based on the new Pytorch Lightning library [Smorodin 2020], developed based on PyTorch to facilitate development and research in deep learning. The advantage of this library is its ability to parallelize the training process not only between several cores of the same processor and/or several graphic accelerators on the same server but also to use different architectures of distributed computing (including "cloud" solutions of Amazon, Azure, and Google).

Figure 5. Stages of neural network training

3 RESULTS AND DISCUSSION

To create a decision support system, clinical information is systematized (Fig. 6) in accordance with the topic and tasks of the study. On the basis of the obtained metadata, reconstruction is performed using 3D visualization (Fig. 7, 8) to extract the data of the region of interest. In this process, medical imaging technology, imaging conditions and data conversion process will continue to influence the production of medical supplements.

Figure 6. Patient B. Diagnosis: Osteoblastoclastoma of the mandible

Figure 7. 3D modeling and printing of the model for preoperative preparation

Figure 8. 3D modeling and printing of an implant

Figure 9. Control study after surgery

Porous biomaterials, including those with a nanoscale structure, based on calcium-deficient hydroxyapatite (cdHA) with a Ca/P molar ratio ranging from 1.5 to 1.67 are used to restore bone tissues in combination with biodegrading polymer biomolecules, as well as the necessary drugs for their dosed release in the area of the defect during the regenerative cycle [Sukhodub 2018b, Harnicarova 2019]. The training process was performed on a computer with an integrated GPU and took an average of about one hour for each optimizer. To get an initial idea of the learning characteristics for a given neural network architecture and generated training data, the recommended Adam algorithm was applied with a learning factor of 0.0001. Several runs for 100 epochs showed that the network stops learning quite quickly, which means that it does not make sense to spend so much time and resources, so it was suggested to limit ourselves to 50 epochs for comparison. The generation of 2000 images from a
small training set led to a stabilization of the learning process after 5 epochs. Another 5 were added, in case there is a flat area next to the local minimum or one of the algorithms is stuck in a trough. It remained possible to stay on the plane or in the abyss for a long time, but limited resources and time did not allow to expect too long an improvement in accuracy. Training was forced to stop if there was no noticeable improvement within 5 epochs.

The analysis of the results showed that the best learning results were shown by the Adagrad and Adam algorithms (0.0502 and 0.0474, respectively). Moreover, Adam, as the most common of the existing “default” algorithms today and recommended for the initial approach to the local extremum, outperformed Adagrad throughout the entire training, and only around 10 epochs did both algorithms approach each other in terms of results. It is also possible to emphasize the clear advantage in speed of the new algorithm concerning SGD without moment and Nesterov and its slight lag behind SGD with moment and Nesterov at the very beginning of training with the next small advantage. It follows that the new modification with defined coefficients has already achieved better values of the loss function between the first and second epochs than those achieved by the SGD only at the 4th epoch. This indicates a double advantage in terms of learning time (fastness). In the training process, additional information was collected, which allows to evaluate the real use of GPU resources for various optimization algorithms without evaluating the complexity of the source code of the algorithms themselves. The minimum value of the loss function was achieved by the Adam algorithm, but the best result on the validation (test) data set was obtained by the developed gradient descent algorithm.

The minimum value of the loss function was achieved by the Adam algorithm, but the best result on the validation (test) data set was obtained by the developed gradient descent algorithm. The last interesting parameter of computational complexity is the number of iterations per unit of time. According to this parameter, it makes sense to evaluate only three algorithms: SGD, Adam, and the new algorithm. The Pytorch Lightning library shows the learning rate at the end of each run. For the three analyzed algorithms, these values are 38.55 it/s, 39.0 it/s, and 39.42 it/s, respectively. It follows that even taking into account the additional calculation of the gradient of the loss function, the new algorithm allows the learning process to have the same speed as other algorithms. The obtained results made it possible to accelerate the learning processes of several neural network architectures, which were developed as part of the software of Artefakt AI companies. Such acceleration made it possible to carry out a wide search for optimal hyperparameters for each of the network architectures, using the limited resources of the computing cluster. A 20% acceleration of the learning process is obtained, and as a result, the neural network can work both as the core of a personal application and as the main part of a hardware extension for CT scanners.

CONCLUSIONS

The application of new learning models of deep neural networks based on theoretical provisions of nonlinear dynamics using gradient descent algorithms to support multi-criteria decision-making in the design of a bone substitute with controlled composition, porosity and strength and the subsequent selection of additive technology for its production from apatite-polymer biomaterials, including with a nanoscale structure, allows to improve the existing approaches. A new optimization method during training has been developed, which will allow to reduce the training time of various adapted types of neural network architectures compared to methods and means of recognizing changes in object properties based on images based on artificial neural networks. Data augmentation methods were used to generate the training sample. Complex analysis of images obtained by sensors of different physical nature will allow to obtain complete and reliable information regarding the design of a bone substitute, depending on the nature and localization of the cavity bone defect, its size and loading conditions. Modification of the method taking into account feedback with a delay and predictive feedback in a discrete dynamic system allows it to be applied both in the training of neural networks in order to reduce the training time and for solving other optimization problems.

In future research, a software product will be developed for an intelligent decision-making support system for studying the dynamics of changes in bone tissue after war injuries during various stages of the post-traumatic period and designing bone substitutes based on the analysis of images obtained by sensors of different physical nature, which will allow effective correction of the structure and mineral composition of bone tissue in order to restore the mechanical and functional properties of bone. The obtained results are a new theoretical and practical information material that will contribute to more effective treatment and prosthetics of bone tissue in case of military and civilian injuries, thanks to the design and manufacture of bone substitutes with controlled composition, structure, porosity and mechanical strength depending on the nature and localization of the cavity bone defect, its dimensions and load conditions.

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