

Article

Smart Web Service of Ti-Based Alloy's Quality Evaluation for Medical Implants Manufacturing

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Abstract: The production of biocompatible medical implants is accompanied by technological and time costs. As a result, to be used in the human body, such a product must be of the highest quality. Assessing the quality of biomedical implants made of titanium alloys is relevant given their impact on the health and life of their wearer. In the case of the production of such implants by additive technologies, an important task is to evaluate the properties of the alloys from which it is made. The modern development of Artificial Intelligence allows replacing traditional assessment methods with machine learning methods for such assessment. Existing machine learning methods demonstrate very low classification accuracy, and existing hybrid systems, although increasing classification accuracy, are not sufficient to apply such schemes in practice. The authors improved the hybrid PNN-SVM system to solve this problem in this paper. It is based on the combining use of PNN, Ito Decomposition, and SVM. The PNN's summation layer outputs were used as additional attributes to an initial dataset. Ito decomposition was used to nonlinearly model relationships between features of an extended dataset. Further classification is carried out using SVM with a linear kernel. The proposed approach's modeling is performed based on a real-world dataset using the smart web service designed by the authors. Experimentally found an increase in the classification accuracy by 6% of the proposed system compared to existing ones. It makes it possible to use it in practice. Designed smart web service, in which the authors implemented both improved and existing hybrid classification schemes allows to quickly, easily, and without high qualification of the user to implement and explore in more detail chosen classification scheme when classification tasks in various fields of industry.

Keywords: smart technologies; web service; modified PNN; SVM; PNN-SVM scheme; small data approach; machine learning; medical manufacturing; medical implants

Citation: Izonin, I.; Tkachenko, R.; Duriagina, Z.; Shakhovska, N.; Kovtun, V.; Lotoshynska, N. Smart Web Service of Ti-Based Alloy's Quality Evaluation for Medical Implants Manufacturing. *Appl. Sci.* **2022**, *12*, 5238. <https://doi.org/10.3390/app12105238>

Academic Editors: Volker Wesling and Kai Treutler

Received: 7 May 2022

Accepted: 20 May 2022

Published: 22 May 2022

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1. Introduction

It is known that the method of powder metallurgy is one of the best ways to obtain products from pure metals and alloys based on them [1]. According to a pre-developed algorithm, the corresponding microstructure can be constructed (design) [2]. It considers the size and quantitative ratio of phases, the proportion of pores of a specific size, their shape, and the nature of the distribution of the cross-section of the product. Thus, the

functional properties of products from these alloys can also be predicted. Intensive research is underway in this direction [3–5], which indicates the relevance of the aim set in this paper. It is primarily due to the biofunctionalization of titanium alloys due to the unique set of corrosion-mechanical properties compared to alternative biomaterials such as polymers and ceramics.

Therefore, one of the most critical stages of powder metallurgy is making powders, their machining, alloying, heat, or chemical treatment [6]. It makes it possible to control the shape and size of the powder particles, which directly determines their value. The particles' size and shape in the powder affect the number and size of the macropores formed during pressing [7,8]. The decrease in porosity with decreasing powder size is determined by the surface energy level per unit volume. A higher energy level characterizes smaller particles with a high specific surface area, and therefore they sinter better. The porosity during the sintering of spherical particles is about 50%, and the shape of the pores formed in this case is non-spherical [5,9]. Thus, the use of powdered titanium alloys with a particular morphology of the location of the pores is based on the principle of structural homogeneity, which ensures a uniform distribution of pores of the same size and shape [10,11].

Creating a multifactorial process of microstructure design of biocompatible materials should consider changes in material properties (corrosion resistance, adhesive strength, levels of passivation with bone tissue, etc.) depending on their structure. This became possible due to precise studies of titanium powder alloys of different alloying systems [10] and modern neural network modeling methods [12]. However, traditional research methods of powder alloys require large material resources [13], and the use of the existing machine learning methods [14] does not provide sufficient accuracy for their use in industrial systems.

In addition, many problems accompany the use of artificial intelligence tools by materials scientists. It includes the lack of basic skills in data preprocessing and data analysis; lack of the necessary qualification when working with machine learning methods for the development, configuration, and use of artificial intelligence tools in solving applied problems of Materials Science, etc.

Therefore, this paper aims are to improve the hybrid intelligent diagnostic system, which would increase the accuracy of work when solving the Ti-based alloy's quality evaluation task for medical implants manufacturing, as well as develop a simple, intuitive and fast smart web service of the quality assessment of sintered alloys for the manufacture of biomedical products.

The main scientific results of this paper are the following:

- we have generalized the approach to preprocessing small-sized and middle-sized datasets for further use by an arbitrary classifier. It is based on the different use of the output signals of the summation layer of the modified version of the Probabilistic Neural Network (PNN), the outputs of which form a complete system of events;
- we have improved the hybrid PNN-SVM system by additional modeling the relationships between all attributes of the extended dataset by PNN summation layer outputs based on the Ito decomposition;
- we have developed a smart web service for Ti-based alloy's quality evaluation for medical implant manufacturing which is based on different options for preprocessing a given dataset using the outputs of a PNN's summation layer with subsequent analysis of the obtained dataset by the SVM classifier.

The practical significance of each of the above scientific results obtained during this study, as well as the possibility of their further use, can be described as follows:

- The modified variant of realization of a PNN provides an increase in classification accuracy compared to the basic variant of realization of this ANN. In addition, the use of the neural network's summation layer outputs provides the possibility of fur-

ther use of the obtained set of probabilities belonging to each class of the task to replace the initial inputs of the problem (reduce dimension) or expand the attributes of the initial dataset to build comprehensive diagnostic systems;

- advanced hybrid PNN-SVM system provides a significant increase in classification accuracy compared to both existing and single models, which form it when solving the task of predicting the properties of the material for the manufacture of biocompatible titanium implants for various applications;
- designed smart web-service of Ti-based alloy's quality evaluation for medical implant manufacturing implements three different data mining options based on PNN-SVM classifier and provides flexibility, high accuracy, and high speed, which significantly reduces human, material, and time resources when solving the stated problem.

The structure of the paper is as follows: in Section 2, an overview and critical analysis of existing approaches are conducted. Section 3 is devoted to a detailed description of the improved hybrid PNN-SVM system, algorithms for its training and application, and the developed smart web service. Section 4 presents the results of experimental studies on the accuracy of all hybrid systems implemented in the smart web service to solve the stated task. The fifth section compares the improved system's results with existing ones and describes its advantages and disadvantages.

2. State-of-the-Arts

The modern production of biomedical implants, in particular from titanium alloy powders, is based on the development of additive technologies. Such implants have many advantages [15], but studying the properties of alloys sintered as a result of 3D printing is an urgent task [16,17]. They affect the biocompatibility and other essential characteristics of the product from such alloys, which is vital for the non-rejection of the implant by the human body during operation [18].

Experimental studies by traditional methods are pretty common in the scientific literature [19–23]. However, they require a lot of material resources to purchase powders, human and time resources for their processing, expensive equipment for their research and analysis, and so on. The modern development of Data-driven Materials Science provides an opportunity to use artificial intelligence tools to solve such tasks. It is made possible by the large amount of data accumulated over the years that can be analyzed. One of them is to predict the properties of titanium alloy before it is sintered by 3D printing. This section of the paper is devoted to reviewing and analyzing existing works that use machine learning methodology [24] to solve the stated task.

In [25], the principles of creating expert systems that can accumulate expert knowledge to solve complex tasks in powder metallurgy are considered. In particular, the authors consider the basic principles of using artificial neural networks for solving the design, materials, and process optimization tasks in powder metallurgy. In [14] considers the effectiveness of traditional machine learning methods (Logistic Regression, AdaBoost, SVM, SGD, MLP) to solve the task of predicting the properties of titanium alloys. Experimentally, it has been established that classical machine learning methods do not provide high accuracy. The highest accuracy was obtained for the SVM with *rbf*-kernel. It reaches 76%. This result is explained by the features of this algorithm and the dimension of the processed dataset (small data). However, this result is not satisfactory for using this methodology in practice.

In [26], the problem of powder selection and process parameters for Powder Metallurgy was investigated. The authors used an apparatus of artificial neural networks, which provided much higher accuracy compared to statistical simulations. The input parameters of the neural network during the powder selection task's solution were only the powder's mechanical properties. However, such powders are characterized by many

other critical properties that must be taken into account by the artificial intelligence model to obtain satisfactory results.

In [27], the problem of obtaining high-quality powders of the set sizes was solved. To solve it, the authors used an approach based on Bayesian optimization [28]. The accuracy of determining the number of parameters of the process of obtaining powders reached 77%, which is satisfactory when solving such a task. However, its increase will significantly improve the quality of powder alloys for manufacturing various products.

In [29], the collection and preliminary processing of data of titanium alloy powders were performed. Each vector of the resulting set was marked. Four classes of Ti-based alloys conformity are allocated. To solve the Ti-based alloys classification task, the authors used a Probabilistic Neural Network. This type of Artificial Neural Network (Figure 1) does not require implementing the training procedure and has several advantages when processing short datasets.

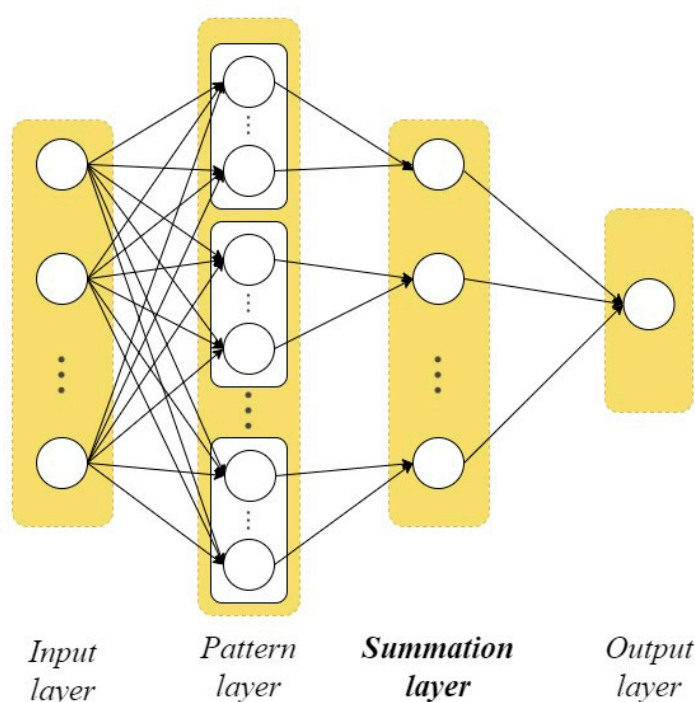


Figure 1. Topology of the classical PNN.

The authors obtained a classification accuracy of 80%. It is much higher than the accuracy of the classical machine learning methods from [14]. However, it is not sufficient to use the proposed approach in practice. One of the reasons may be that the authors did not select the optimal value of the smooth factor. Since the importance of this parameter significantly affects the accuracy of the PNN.

The authors [29] used the feedforward neural network approach to predict material properties. They perform the feature selection procedure and use this neural network type to solve prediction tasks based on a significantly reduced dimension preprocessed dataset. The advantage of this step is to increase the prediction accuracy and, in part, the speed of the training procedure. However, the iterative nature of the training algorithm requires significant time to implement this model.

In [12], the authors solved the task of predicting the properties of titanium alloys using a hybrid scheme. It involves a combination of PNN and machine learning algorithms. This approach is due to the very low accuracy of classification using existing machine learning methods [14]. One of the reasons for this is that the dataset used contains many independent attributes that can reduce the accuracy of the classifier [30]. Therefore,

the authors proposed an approach to reduce data dimensionality with their subsequent classification. The paper's main idea is to use the Probabilistic Neural Network as a tool for data preprocessing, mainly to reduce the dimension of the input data space of the task. In this case, it was implemented through the outputs of the summation layer of the PNN. It forms a vector of probabilities of belonging of each observation to each of the predefined classes of the task. Thus, the study's main goal was to transform the vectors of the entire dataset and replace the original dataset with the resulting dataset. Further classification based on the new dataset was performed using Logistic Regression. The flowchart of the proposed approach is shown in Figure 2 [12].

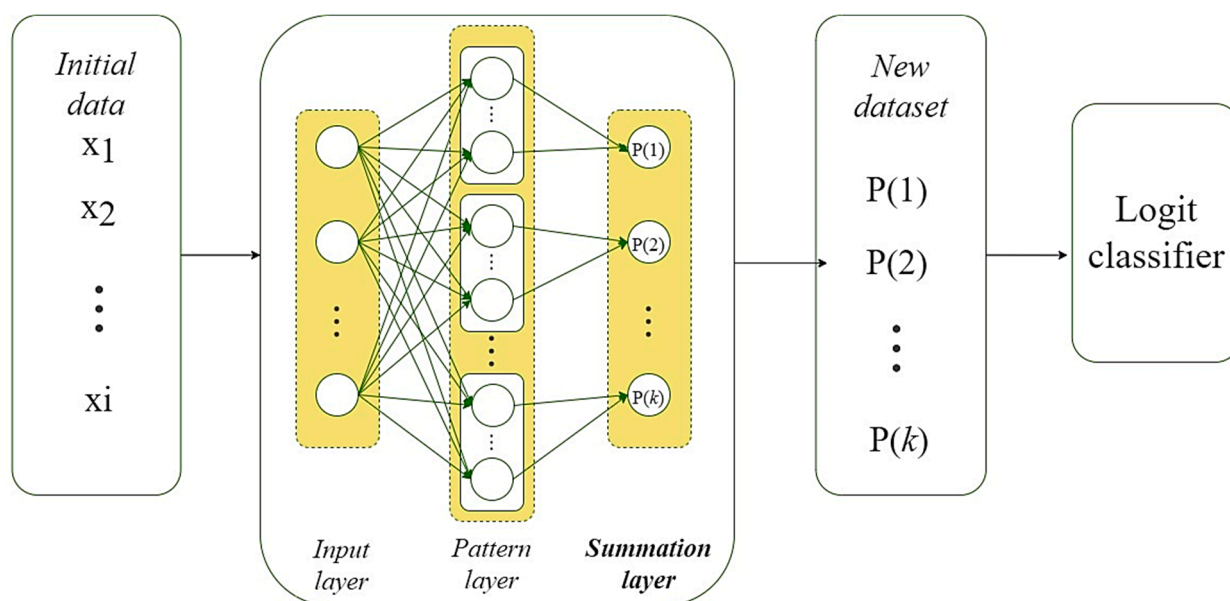


Figure 2. Flowchart of the PNN-Logit system that used PNN-based dimensionality reduction.

As a result of experimental research, the authors found that the classification based on the initial and modified datasets differs significantly. In particular, in the first case, the accuracy was close to 64% (logit classifier) and 88% (classical PNN classifier), and in the second—90% (PNN + logit classifier). That is, the proposed hybrid PNN-Logit scheme provided an increase in accuracy by 24% compared to the logit classifier and an increase of 2% compared to the classical PNN classifier.

The advantage of this approach, in addition to a significant increase in accuracy, is a significantly smaller dimension of the input data space required for the effective operation of the classifier based on machine learning [31]. However, if there are a small number of predefined classes of the task (e.g., 2 or 3), the probability vector of each class will contain a small number of elements (e.g., 2 or 3). It may undermine the proposed approach's effectiveness, particularly accuracy.

To increase the hybrid system's accuracy for intellectual data analysis of the problem with a few labeled classes, the authors in [12] proposed a modification of this approach. The modified PNN-Logit schema also uses a PNN-based preprocessing procedure. However, the main difference of this scheme was the nonlinear expansion of the input data space instead of reducing the dimensionality, as in the previous case. The method was to use the outputs of the PNN summation layer to replace the initial dataset and further expand the new dataset space using Ito decomposition [32]. Further classification of the dataset expanded in this way was carried out using Logistic Regression. The flowchart of the proposed approach is shown in Figure 3 [12].

Ito decomposition (Kolmogorov-Gabor Polynomial) is increasingly used to approximate nonlinear dependences with high accuracy [33–35]. For the classification problem, such an approach is substantiated by Cover's theorem [36]. It was the main reason for its

use to modify the scheme from Figure 2 [37]. Mathematically, Ito decomposition can be represented as follows,

$$Y(x_1, \dots, x_n) = \theta_i + \sum_{i=1}^n \theta_i x_i + \sum_{i=1}^n \sum_{j=i}^n \theta_{i,j} x_i x_j + \sum_{i=1}^n \sum_{j=i}^n \sum_{l=j}^n \theta_{i,j,l} x_i x_j x_l + \dots$$

$$\dots + \sum_{i=1}^n \sum_{j=i}^n \sum_{l=j}^n \dots \sum_{z=k-1}^n \theta_{i,j,l,\dots,z} x_i x_j x_l \dots x_z \quad (1)$$

where n is a number of features x_1, \dots, x_n , and k is the Ito decomposition degree, θ is the Ito decomposition coefficient.

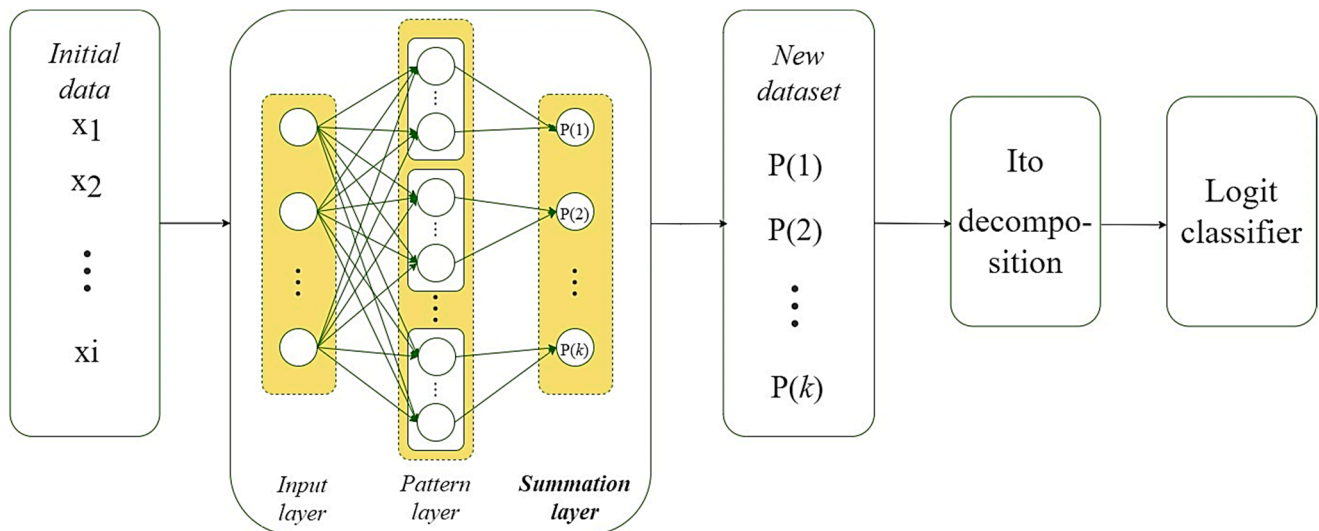


Figure 3. Flowchart of the PNN-Ito-Logit system.

According to experimental studies, a modified approach using Ito decomposition increased accuracy up to 2% (from 90% for the scheme of Figure 2 to 92% for the scheme of Figure 3).

Despite the relatively high accuracy of the two approaches described above, an error of 8% is significant, especially in the case of solving the tasks of diagnosing the properties of the alloy from which biomedical implants will be made. In addition, in the case of a few labeled classes, particularly for a two-class problem, they will not be as effective because the actual classification is based on PNN-derived probabilities (only two attributes).

The authors of [38] investigate the problem of machine learning methods processing short sets of data in the Materials Science domain. The authors proposed an intuitive scheme to expand the input data space of the problem to improve the prediction accuracy. It consists of adding to the initial dataset additional attributes that are essentially a “rough estimate” of the material’s properties. This approach is also based on Cover’s theorem and should increase the accuracy of classifiers or regressors. The authors have shown a significant increase in the accuracy of the proposed method compared to existing ones. However, the main problem here is the need for a “rough assessment” of the material’s properties as a scheme to expand the space of input features of a given dataset. An expert should do it. Therefore, in such a model appears a human factor. Secondly, the expert’s opinion may be subjective, which will significantly affect the data in the form of outliers or anomalies—and consequently, the accuracy of the machine learning method. Third, for medium-sized datasets, such an approach will require significant time and human resources in the form of expert work on each vector of the specified dataset.

To avoid such shortcomings, Ref. [39] developed a new smart system. It is also based on PNN summation layer outputs, but the fundamental difference here is that they are included as additional features to the initial dataset. The dataset expanded in this way is

fed to the selected classifier. The flowchart of the proposed approach is shown in Figure 4 [39].

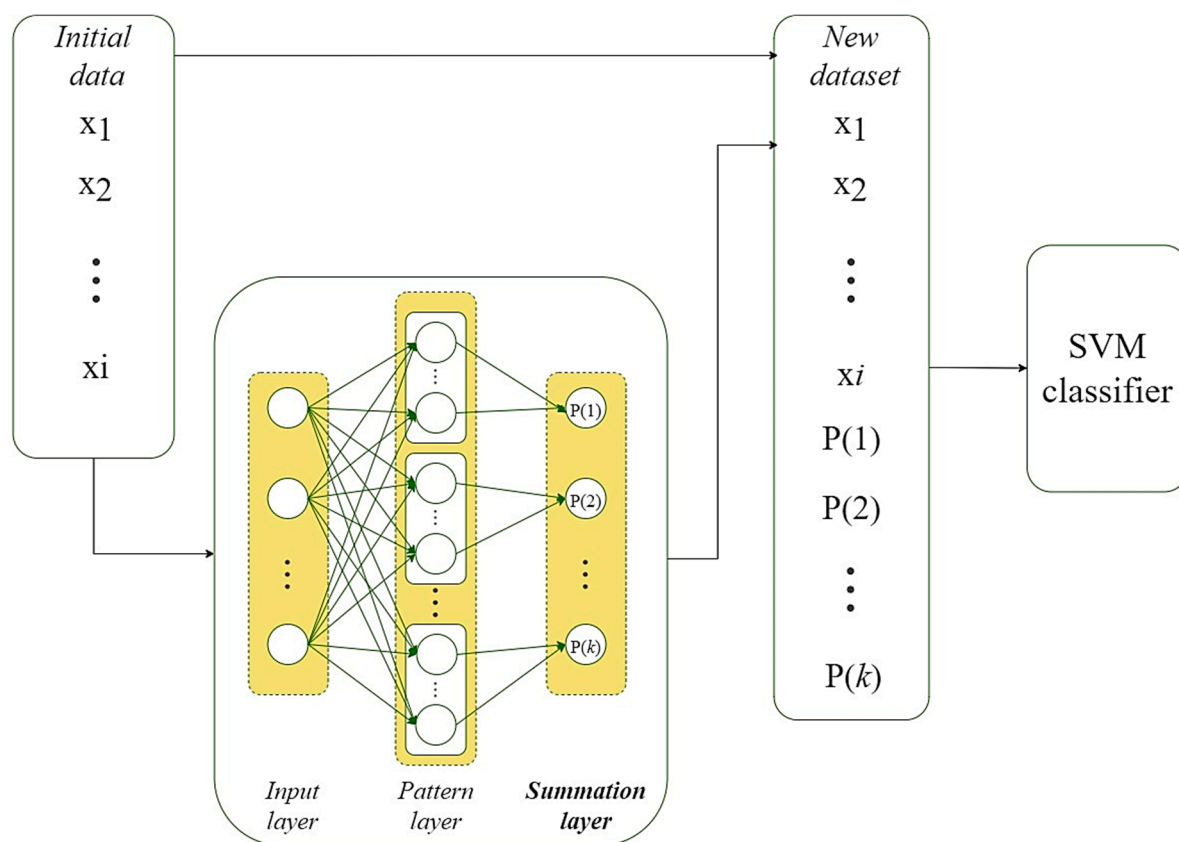


Figure 4. Flowchart of the PNN-SVM system.

In [39], SVM was used by the authors as a classifier. This machine learning algorithm demonstrates the highest accuracy of existing machine learning methods to solve the stated task [13]; allows the process of short datasets efficiently, and provides a high-speed training process. In the case of creating a hybrid system, where the element is a neural network without training, the latter factor plays an essential role in developing an algorithm for learning the entire hybrid scheme.

Experimental studies were based on SVM with *rbf*-kernel. This approach for nonlinear input expansion significantly increases the classification accuracy. The results showed that the proposed scheme provides a 15% higher accuracy (91%) than a single SVM with *rbf*-kernel (74%). However, this scheme did not increase accuracy compared to the scheme in Figure 2.

This paper proposed an advanced PNN-SVM smart system that will provide the best classification accuracy. In addition, the paper proposed a user-friendly smart web service that implements all of the above methods.

3. Materials and Methods

In the previous section, we summarized existing research on the development of intelligent systems of Ti-based alloy's quality evaluation for medical implant manufacturing. Most of them are based on various approaches to preprocessing small-sized and middle-sized datasets based on PNN outputs.

The use of PNN is explained by the fact that this ANN provides the ability to obtain the output signal in the form of the value of the class to which the current observation belongs. In addition, PNN allows acquiring a set of probabilities belonging to each of the predefined classes of the task. Such signals are formed in the PNN summation layer. The

latter advantages provide the possibility of comprehensive preprocessing of medical datasets to reduce the dimensionality or expand the space of input data of the stated task. As shown above, both approaches are justified, particularly in improving the accuracy of the work compared to the basic option of using PNN in the classification tasks.

Other advantages of PNN include the lack of training procedure as such, high speed when processing small-sized and middle-sized datasets, high efficiency of processing data with outliers, and others [40]. They provided a relatively widespread use of these neural networks in biology and medicine [41].

Let us consider the realization of PNN and its modification in more detail.

3.1. Modified PNN

Lets assume that the number of vectors equal to represents the sample of tabular data N . Each i -th vector \bar{x}_i ($i = 1, N$) belongs to one of the K classes. Accordingly, the vectors \bar{x}_{i_k} from N will belong to the k -th class, where $k = 1, K$. In addition, denote the current vector as \bar{x}_p .

To implement the PNN, it is necessary to perform several following steps:

1. Calculate the Euclidean distances d_{p,i_k} from the current vector \bar{x}_p to each vector of a given dataset \bar{x}_{i_k} , ($i_k = 1, N$), which belong to the corresponding k -th class ($k = 1, K$) according to the formula:

$$d_{p,i_k} = \sqrt{\sum_{i_k=1}^N (x_{i_k} - x_p)^2} \quad (2)$$

2. Calculate Gaussian functions φ_{p,i_k} from d_{p,i_k} according to the formula:

$$\varphi_{p,i_k} = \exp\left(-\frac{d_{p,i_k}^2}{\sigma^2}\right), \quad (3)$$

where σ is the scope parameter of the Gaussian function (smooth factor). It should be noted that this is the only PNN parameter to be configured for each specific task.

3. Calculate the probabilities of belonging of the \bar{x}_p vector to each predefined classes k , $k = 1, K$ based on (3) according to the expression:

$$P(k) = \frac{\sum_{i_k=1}^{N_k} \varphi_{p,i_k}}{N_k}. \quad (4)$$

The main problem of expression (4) is that the sum of the obtained probabilities of belonging to each of the k , $k = 1, K$ classes of the task is not equal to 1. This can significantly affect the accuracy of complex diagnostic systems that include PNN as one of the elements.

To avoid this shortcoming, we propose to use a different one approach to calculate the probabilities $P(k)$ of the current vector \bar{x}_p belonging to each of the predefined classes k , $k = 1, K$ of the task:

$$P(k) = \frac{\sum_{i_k=1}^{N_k} \varphi_{p,i_k}}{\sum_{k=1}^K \sum_{i_k=1}^{N_k} \varphi_{p,i_k}}, \quad (5)$$

Thus, we obtain a different from the basic algorithm of the formation of the output signals of the summation layer PNN, which will form for the current vector \bar{x}_p the vector of probabilities belonging to each of the $k, k = 1, K$ classes of the task. The sum of these probabilities in each new vector will be equal to 1. That is, (5) describes the formation of a complete system of events. This approach will increase the accuracy of the proposed version of the PNN implementation, which will increase the accuracy of the complex system as a whole, which is based on the use of this neural network without training.

The scheme of realization of both variants of PNN is given in Figure 5

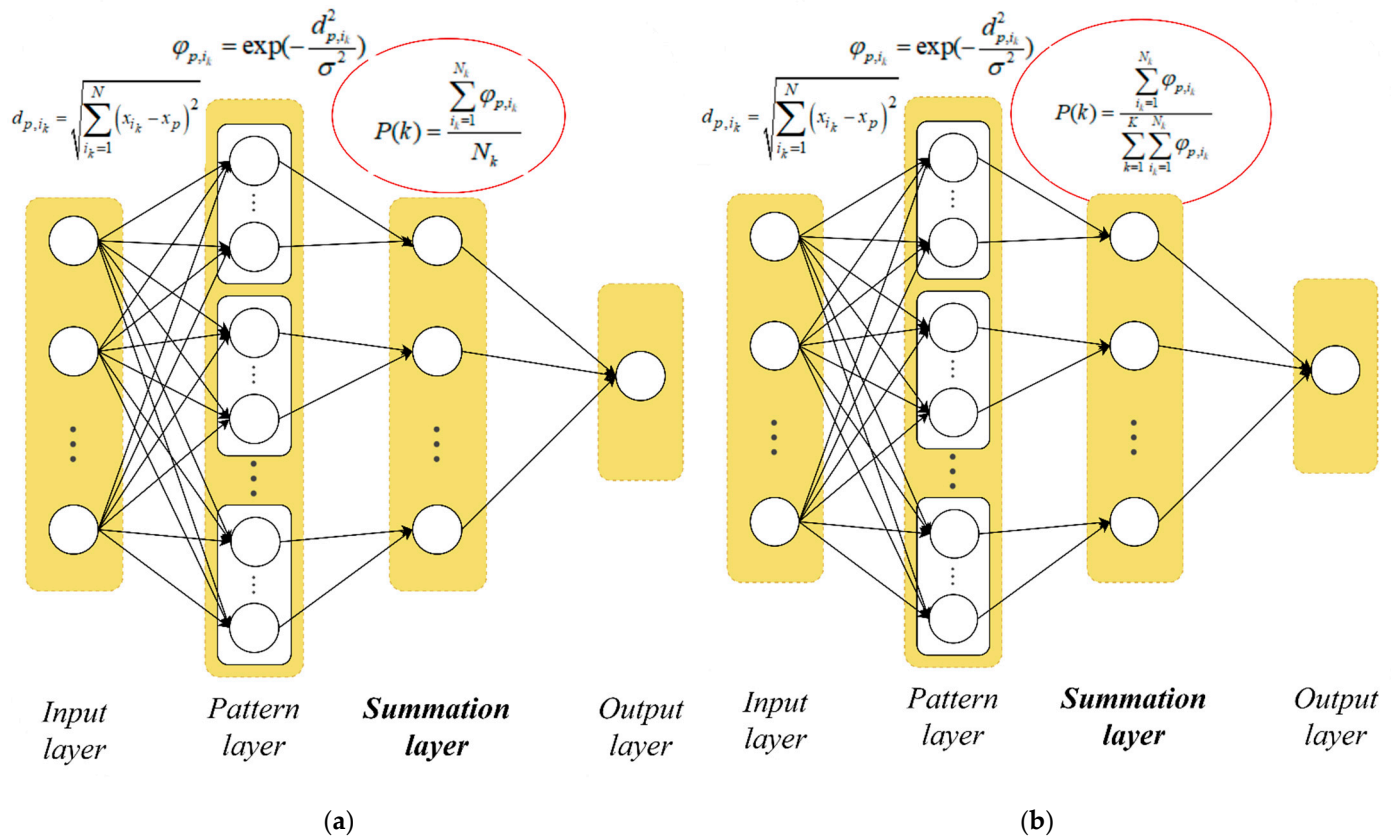


Figure 5. Probabilistic Neural Network: (a) classical version; (b) a modified version.

3.2. Improved PNN-SVM System

This paper proposes improving the PNN-SVM system, demonstrating its effectiveness in solving Ti-based alloy's quality evaluation task for medical implant manufacturing. The basic version of the system is presented in [39].

The existing system is based on the principle of preprocessing data using PNN and expanding the initial dataset with the PNN-based outputs to improve the accuracy of solving the classification task by the SVM method. The use of SVM here is explained by the highest accuracy of this method among the classifiers based on machine learning methods that are studied in [14]. The proposed system is based on additional modeling of relationships between all attributes of the extended due to the outputs of the PNN summation layer dataset based on the use of the second-degree Ito decomposition. Theoretically, the use of such an approach is fully justified by Cover's theorem on the separation of images [42].

A flowchart of the improved smart PNN-SVM system is shown in Figure 6.

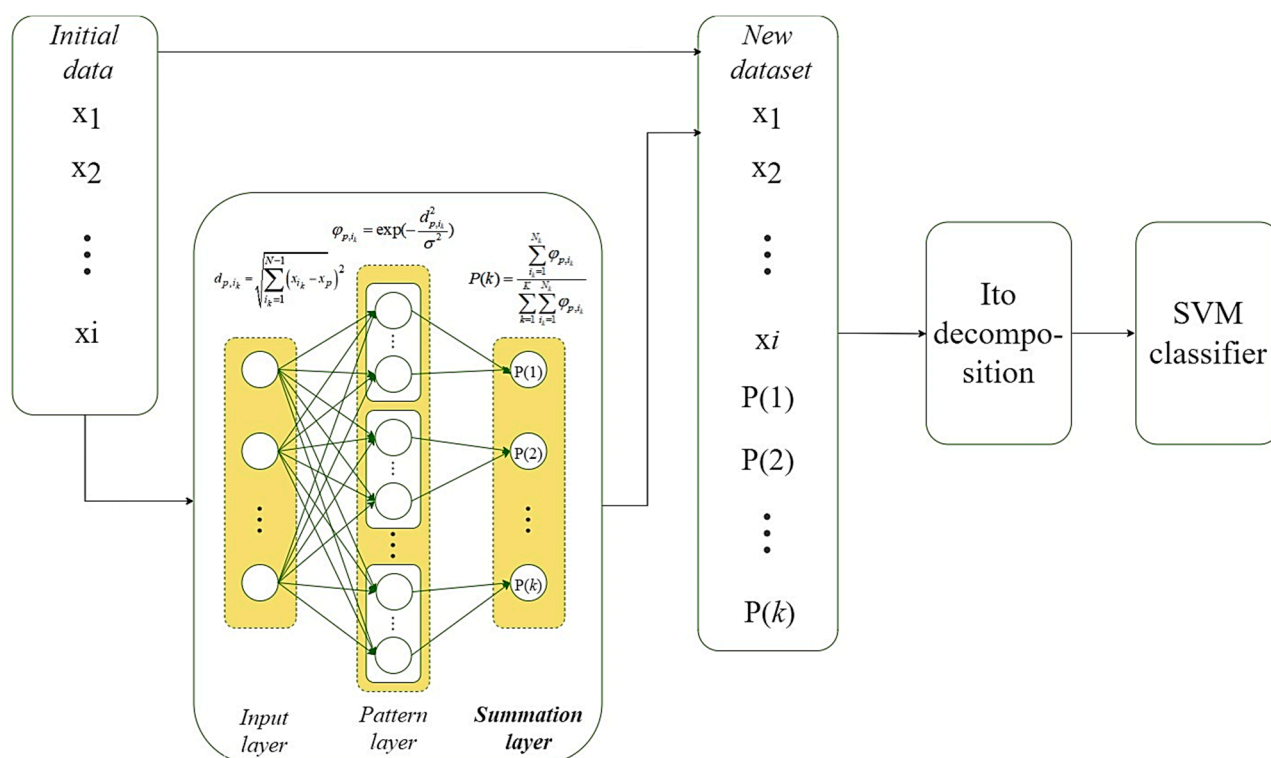


Figure 6. Flowchart of the improved PNN-SVM smart system.

Since PNN does not require a training procedure, but it is necessary to implement SVM, the proposed smart system based on a combination of these two machine learning methods provides procedures for both training and application.

The training procedure for the improved smart system is as follows:

- prepare and apply a modified PNN to obtain a set of probabilities of belonging of each observation from the training set to each of the defined classes of the stated task;
- form a new set of training data by combining the initial dataset with the corresponding probability vectors obtained in the previous step;
- perform nonlinear expansion of a new dataset using the second-degree Ito decomposition according to (1);
- perform SVM-based linear classifier training using the extended training dataset in the previous step.

Accordingly, the main steps of the testing procedure for a pre-trained improved smart system are as follows:

- apply the prepared PNN to the current vector to obtain the vector of probabilities of its belonging to each of the defined classes of the stated task;
- form a new vector by combining the current vector with the probability vector obtained in the previous step;
- perform the second-degree Ito decomposition on the extended vector to model the relationships between the input attributes of a given vector and the probabilities of its belonging to each of the defined classes of the stated task;
- perform classification using pre-trained SVM with the linear kernel;
- get the result of the system work.

3.3. Smart Web-Service

For developing a smart web service, the authors have selected optimal tools for working with machine learning [43–46]. Let's consider the main components of the practical implementation of the system.

The main programming language is Python. Machine learning requires constant data processing, and Python has built-in libraries and packages for almost every task [47]. It helps machine learning engineers reduce development time and increase productivity when working with complex artificial intelligence programs [48]. The following libraries were used for development: Scikit-learn; NumPy; Pandas; Matplotlib.

The logical structure of the system consists of separate modules, the functionality of which is combined in the main file of the project, which also implements the user interface—main.py. The implementation of the probabilistic neural network is contained in the pnn.py file.

The file implements the PNN class, which contains several methods for creating and working with the network. PNN modifications described in the previous section are also implemented here.

The Streamlit library was used to build the user interface. This library has a wide range of interface components and allows the creation of smart web applications for machine learning and data analysis. The authors have developed a clear, intuitive, and not overloaded with details graphical interface, which is shown in Figure 7.

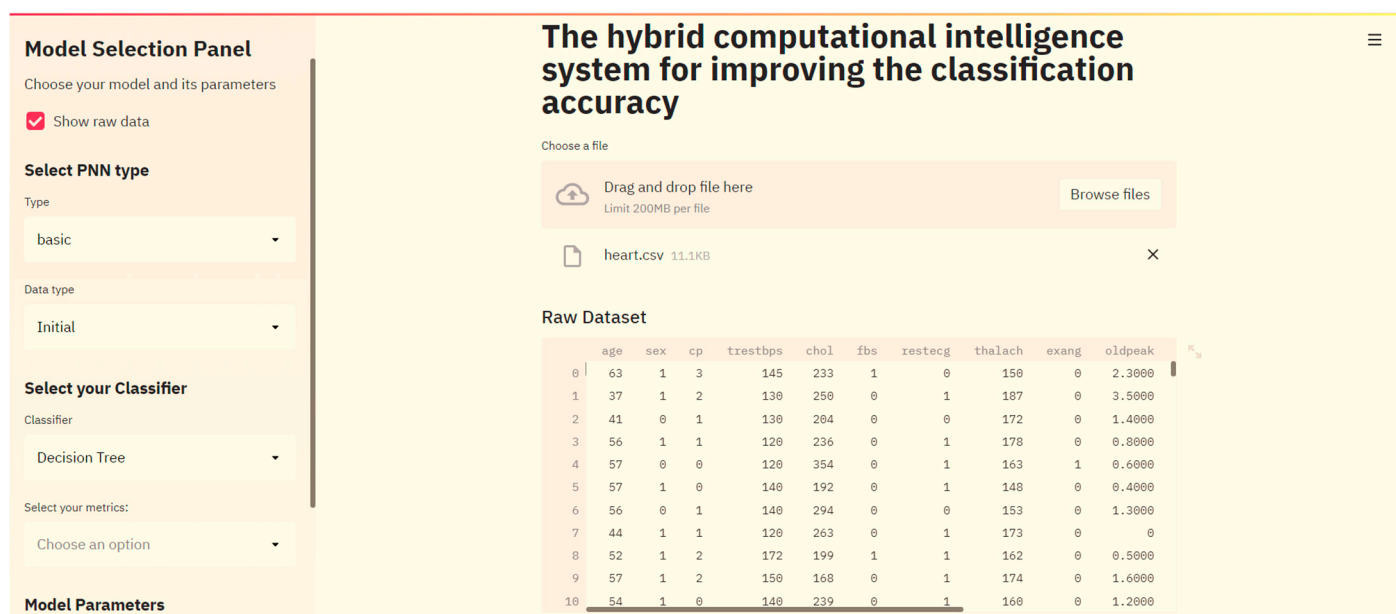


Figure 7. Smart web-service's user interface.

The user interface consists of two main areas:

- Panel for selecting machine learning models and their parameters (Figure 8)
- The main window for downloading and displaying a dataset, presentation, and visualization of machine learning models (Figure 9).

×

Model Selection Panel

Choose your model and its parameters

☒ Show raw data

Select PNN type

Type

modified ▾

Data type

Expanded with PNN results ▾

Select your Classifier

Classifier

Logistic Regression ▾

Select your metrics:

Confusion Matrix ×

Precision-Recall Curve ×

⊕ ▾

Model Parameters

C (Regularization parameter)

0,01 − +

Maximum number of iterations

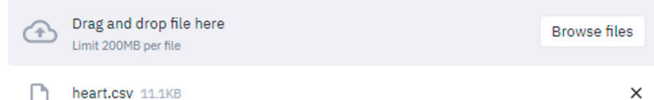
100 ● 100 500

☐ Classify

Figure 8. Panel for selecting machine learning models and their parameters.

The hybrid computational intelligence system for improving the classification accuracy

Choose a file



Raw Dataset

	age	sex	cp	trestbps	chol	fbs	restecg	thalach	exang	oldpeak
0	63	1	3	145	233	1	0	150	0	2.3000
1	37	1	2	130	250	0	1	187	0	3.5000
2	41	0	1	130	204	0	0	172	0	1.4000
3	56	1	1	120	236	0	1	178	0	0.8000
4	57	0	0	120	354	0	1	163	1	0.6000
5	57	1	0	140	192	0	1	148	0	0.4000
6	56	0	1	140	294	0	0	153	0	1.3000
7	44	1	1	120	263	0	1	173	0	0
8	52	1	2	172	199	1	1	162	0	0.5000
9	57	1	2	150	168	0	1	174	0	1.6000
10	54	1	0	140	239	0	1	160	0	1.2000

PNN Results

Accuracy: 84.0 %

Precision: 0.84

Recall: 0.84

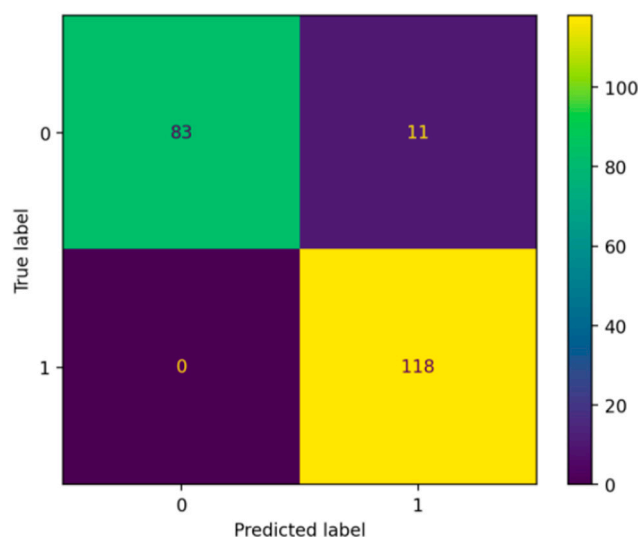
Logistic Regression Results

Accuracy: 95.0 %

Precision: 0.91

Recall: 1.0

Confusion Matrix



(a)

(b)

Figure 9. The panel of results of the smart web service: (a) window for downloading and displaying the dataset; (b) a window for presenting and visualizing the results of machine learning models.

To start working with the application, the user should click on the file's download button located in the main window and open the dataset file to be processed, or drag this file to the button area. By clicking on the "Show raw data" check box in the left panel, you can display the dataset as a table in the main window.

After downloading the file, a section of work with a PNN will be available on the panel, where a drop-down menu with the possibility of selecting the PNN type will be presented. Option "Basic" uses a neural network that does not describe a complete system of actions, and option "Modified" uses a neural network with a complete system of events.

Selecting the PNN type (classical and modified) activates the progress bar, showing how close the program is to complete the network preparation process. When the indicator is filled with blue, a section will appear with the selection of the classifier, namely: "Classifier"—a drop-down menu with different options of classifiers; "Data type"—a drop-down menu with data options on which to set the classifier, according to Table 1. "Metrics"—a multi-choice drop-down menu, with options for visualization of metrics [49] to assess the optimality of the algorithm—confusion matrix, ROC curve, etc. After selecting the above parameters, the section for selecting classifier hyperparameters appears. Finally, a button appears to start the classification and visualization process with user-selected parameters.

Table 1. The results of the modeling of the improved PNN-SVM smart system.

Performance Indicator	Improved PNN-SVM Smart System	
	Train Mode	Test Mode
Total accuracy	0.99	0.97
Precision	0.98	0.97
Recall	0.99	0.97
F1-score	0.99	0.97

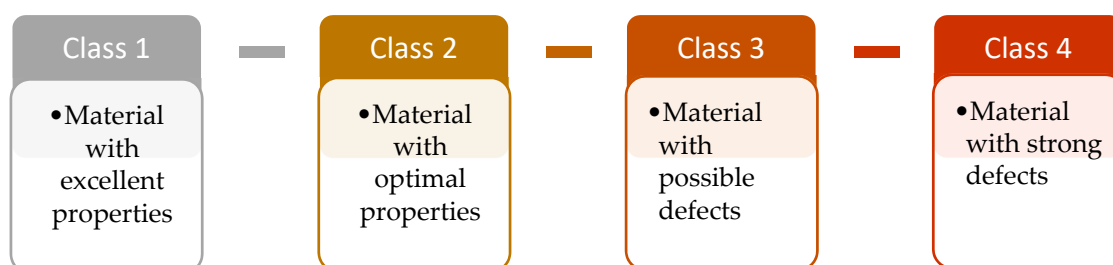
4. Modeling and Results

The multiclass classification task was investigated in this paper. Modeling of the improved PNN-SVM smart system was conducted using the smart web service developed by the authors. It is implemented in Python. Among the performance indicators, the authors use well-known indicators: Total accuracy, Precision, Recall, and F1-score [50]. All experimental studies were performed using the developed smart web service.

4.1. Dataset Description

The improved PNN-SVM smart system modeling was performed using a real-world dataset to solve the Ti-based alloy's quality evaluation task for medical implant manufacturing. It was collected at the Materials Science and Materials Engineering Department of Lviv Polytechnic National University and placed in a public repository [51].

The problem was assigning the observation with 20 attributes to one of the four classes presented in Figure 10. Each observation's main classes of attributes should be distinguished chemical and phase composition, size and form of parts, polydispersity, and satellite composition.

**Figure 10.** Classes of the Ti-based alloy's quality evaluation task for medical implants manufacturing.

The training dataset contained 384 observations, and the test dataset had 96 observations. A more detailed description of the dataset used for modeling can be found at [29].

In addition to all of the above, the authors used the second-order Ito decomposition (1) to model the relationships between all attributes of a given dataset:

$$Y(x_1, \dots, x_n) = \theta_i + \sum_{i=1}^n \theta_i x_i + \sum_{i=1}^n \sum_{j=i}^n \theta_{i,j} x_i x_j, \quad (6)$$

This approach is explained because the task has 20 attributes and four classes. As a result, we obtain 24 attributes for which simulations should be performed using this decomposition scheme. A significant increase in the degree of Ito decomposition will significantly affect the system's operating time, as the input data for the operation of SVM will become more and more. In addition, as shown in [12], high degrees of this decomposition can provoke overfitting, which will not provide satisfactory results for the smart system [52].

4.2. Improved PNN-SVM System Results

The results of modeling of the improved PNN-SVM smart system from Figure 6 based on a given dataset are shown in Table 1

It should be noted that these results were obtained with the optimal value of the smooth factor ($\sigma = 0.12$) for PNN and SVM with *linear* kernel. Practical experiments have shown that the nonlinear *rbf*-kernel, which demonstrates the highest accuracy among other kernels when using a simple SVM [14], in the proposed system provides significantly lower accuracy (93% vs. 97%). This is due to the additional modeling of input data before submission to the SVM based on the Ito decomposition, which is provided by the improved PNN-SVM system. According to Cover's theorem [42], nonlinear expansion of the input data space, in this case, based on this decomposition type, increases the probability of correct classification by linear models. That is why the linear kernel for SVM here demonstrates the highest accuracy among other kernels

As can be seen from Table 1, the improved PNN-SVM smart system provides high classification accuracy according to all performance indicators.

4.3. Results of All Other Variants of the Investigated Smart System

In this paper, also other existing approaches based on PNN are used that are implemented in the designed smart web service, in particular:

- Classical PNN;
- Modified PNN;
- PNN-Logit system from [12] that used PNN-based dimensionality reduction;
- Modified PNN-Ito-Logit system proposed in [12] that used PNN-based dimensionality reduction;
- PNN-SVM system that used PNN-based dimensionality reduction;
- Modified PNN-Ito-SVM system that used PNN-based dimensionality reduction;
- PNN-SVM system proposed in [39].

The results of all studied approaches using the developed web service are summarized in Table 2.

It should be noted that assessing the results of different systems adequately, additional modeling of PNN-Logit and PNN-Ito-Logit (approaches that used PNN for dimensionality reduction) systems was performed by replacing the Logistic regression with an SVM classifier. As a result, Table 2 presents two new systems for comparison, one of which demonstrated the highest accuracy among those considered. It indicates the effectiveness of using the SVM in all considered variants of the smart system in solving the stated task.

Table 2. The results of the studied smart systems.

Investigated Smart System	Total Accuracy	Precision	Recall	F1-Score
Classical PNN ($\sigma = 0.04$) **	0.88	0.84	0.91	0.85
Modified PNN ($\sigma = 0.12$) **	0.90	0.92	0.85	0.88
PNN-Logit (where PNN used for dimensionality reduction) ($\sigma = 0.12$) **	0.90	0.90	0.90	0.90
PNN-SVM (where PNN used for dimensionality reduction) * ($\sigma = 0.12$) **	0.91	0.91	0.91	0.90
Modified PNN-Ito-Logit (where PNN used for dimensionality reduction) ($\sigma = 0.12$) **	0.92	0.92	0.92	0.91

Modified PNN-Ito-SVM (where PNN used for dimensionality reduction) *	0.92	0.93	0.92	0.92
($\sigma = 0.12$) **				
PNN-SVM system	0.91	0.91	0.91	0.90
($\sigma = 0.12$) **				

* modeling conducted for the existing approaches from [12] that used SVM instead Logit. ** optimal value of the smooth factor that provide highest classification accuracy.

Comparing Tables 1 and 2 shows the highest classification accuracy by using an improved PNN-SVM smart system.

5. Comparison and Discussion

The authors compared the performance of the improved version of the PNN-SVM system with other systems based on the use of PNN as a tool for data preprocessing. To do this, use all the methods described in Section 4.1.

In addition, the authors compared their work with classical machine learning methods, in particular:

1. Logistic Regression Classifier;
2. SVM with *linear* kernel Classifier;
3. SVM with *rbf* kernel Classifier.

These methods were chosen because they can be used as optimal classifiers for the second part of the improved system. The results of all investigated methods based on the Total accuracy indicator are presented in Figure 11.

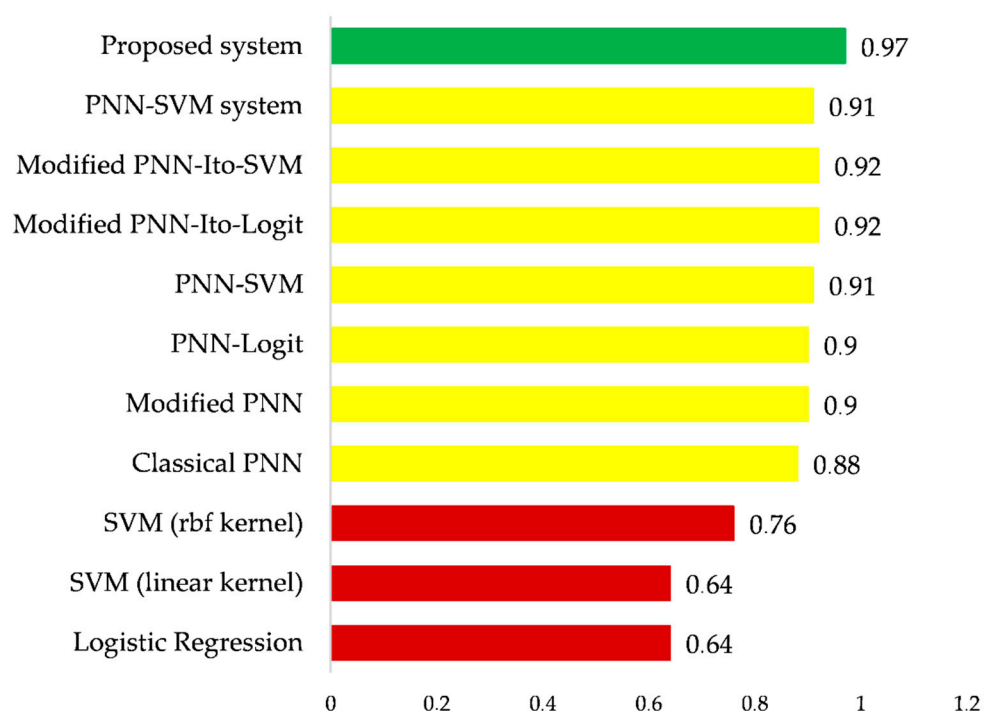


Figure 11. Total accuracy values for all investigated methods.

To facilitate the analysis of the results for all the studied methods, the histogram in Figure 11 is conditionally divided into three areas. The red area indicates unsatisfactory results of applying the machine learning methods for solving the Ti-based alloy's quality evaluation task for medical implant manufacturing. The second is the yellow area, in which the combined set of hybrid approaches indicates the permissible level of accuracy

of solving the classification task according to [14]. The green bar graph determines the highest accuracy when solving the stated task.

From the results presented in Figure 11 it can state the following:

1. Classical machine learning methods (red bars of the histogram), both linear and non-linear, do not provide a satisfactory level of accuracy in solving the multiclass classification task;
2. Probabilistic Neural Network without training, as well as its modification, provide satisfactory but insufficient accuracy for their practical use;
3. All considered hybrid intelligent systems provide an increase of accuracy in comparison with the basic classifiers which form them;
4. Systems where PNN is used to reduce the dimension of the input data space of the task provide a slight increase in accuracy, although significantly reduce the duration of training procedures for such systems;
5. PNN-based systems for expanding the input data space of the task increased the accuracy of linear classifiers, which is fully justified by Cover's theorem. However, high enough accuracy is not obtained here;
6. The highest classification accuracy in solving the stated task is obtained using the improved system proposed in this paper. In particular, due to additional modeling of the attributes of the extended dataset based on the Ito Decomposition, it was possible to increase the system's accuracy by more than 6% compared to the existing implementation of the system.

The last point provides a significant advantage when using the improved system to solve the classification tasks. In particular, a classification accuracy of 97% will ensure a proper assessment of Ti-based alloy's quality for the defect-free production of biocompatible titanium implants for various purposes.

Among the disadvantages of the proposed approach that should be noted is a significant increase in the duration of the training procedure of the improved system compared to the basic option. This is due to the considerable increase in the number of attributes of the extended dataset, which is fed to the SVM classifier [53,54]. However, the following should be noted here:

- the improved system is based on preprocessing of data based on an Artificial Neural Network without training, which will eliminate this shortcoming in the case of processing small-sized and middle-sized datasets [55,56];
- a linear SVM is selected as the basic classifier, which is quite fast [57]. The processing of nonlinear extended inputs also provides significantly higher classification accuracy than other kernels of this method. In addition, the optimal implementations of this method, which are laid down in the Scikit-learn library and its was used in this paper, provide high performance of this machine learning method;
- in Materials Science tasks, large datasets are challenging to collect [38,58]. That is why combining the above methods will provide high-speed processing of available data.

In case it is necessary to process large datasets, the authors implemented other approaches in the designed smart web service, particularly the system based on PNN's dimensionality reduction, which will significantly reduce the computational load and the duration of the training procedure by the selected classifier.

Created smart web service allows you to quickly, easily, and without great qualification of the user to implement and explore in more detail the chosen classification scheme when solving both the stated and other classification tasks in various industries.

6. Conclusions

Evaluating the properties of biocompatible products is an essential task that depends on both the health and even the life of the carrier of such products. Modern 3D printing technologies provide the opportunity to significantly reduce the costs and the time of production of medical implants, in particular from titanium alloys. Avoiding the additional

costs of producing a defective material is possible by evaluating its properties before sintering by 3D printing (in particular based on a set of different properties of titanium alloy powders). The best option for implementing such an approach is to use artificial intelligence tools.

Existing machine learning methods provide low accuracy in solving this task. Hybrid variants increase classification accuracy, but it is still not sufficient for their use in practice. In this paper, the authors have proposed improving the hybrid scheme of multiclass classification based on the combined use of improved PNN, Ito decomposition, and SVM with linear kernel. It is implemented in the form of smart web service.

The improvement consists of additional modeling of all extended attributes of the dataset due to the PNN's outputs based on the Ito decomposition. According to Cover's theorem, such nonlinear modeling of relationships between attributes of a given dataset provides an opportunity to increase the accuracy of linear classification. That is why the last step of the improved system is to use SVM with a linear kernel.

The operation of the advanced hybrid PNN-SVM system was modeled using a real-world dataset to solve the Ti-based alloy's quality evaluation task for medical implant manufacturing. The authors found the high efficiency of the improved version of the system. In particular, the level of classification accuracy reaches 97%, which is a significantly higher figure (as much as 6%) than all other considered methods. It provides an opportunity to use this hybrid scheme when solving the stated task.

Among the shortcomings of the developed system, a significant increase in the duration of the training procedure should be noted. However, since most materials science tasks are characterized by small amounts of data intended for analysis, this shortcoming can be ignored.

Further research will be conducted in the direction of application and study of the effectiveness of both the improved scheme and all schemes implemented by the authors in the form of smart web services in solving other applied classification tasks. In addition, it is planned to use a non-iterative SGTm neural-like structure as a linear classifier (instead of SVM with a linear kernel) to decrease the training time and increase the total accuracy of the proposed system.

Author Contributions: Conceptualization, R.T. and I.I.; methodology, I.I.; software, N.S. and I.I.; validation, Z.D., V.K. and N.L.; formal analysis, N.S. and V.K.; investigation, I.I.; resources, R.T. and N.L.; data curation, Z.D.; writing—original draft preparation, I.I.; writing—review and editing, I.I.; visualization, N.L.; supervision, R.T.; project administration, V.K.; funding acquisition, I.I. All authors have read and agreed to the published version of the manuscript.

Funding: The National Research Foundation of Ukraine funded this research under project number 2021.01/0103.

Data Availability Statement: The data that support the findings of this study are openly available in ResearchGate at [51].

Conflicts of Interest: The authors declare no conflict of interest.

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