Neural Network modeling of Thin Films Deposition Processes in the Master’s Degree Programs “Electronics and Nanoelectronics” and “Nanoengineering”

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Abstract. In this paper we consider the application of artificial neural networks in the Master’s degree programs. Nowadays neural network models have become a powerful tool of scientific research for engineers and students. Besides successful research depends on confided usage of common methods and algorithms of statistical community special attention in degree programs is given to data analysis and modeling methods. Students study modern neural networks software products, methods of data preparing, designing and training neural network and then apply neural networks algorithms in practice. The neural networks modeling plays a significant role in students education. During it students learn to create, tune and train their own neural networks and get full and detailed understanding of research in computer vision. Neural Networks models are successfully presented in graduation works. In this paper a few examples of how neural networks are used in thin films deposition processes modeling are presented.

1 Introduction
Successful economic development is impossible without nanotechnology. Nowadays there is an increasing demand worldwide for specialists knowledgeable in nanotechnology (Panfilov, Kolesnik, Ryabov & Sidorova, 2017). In conformity on modern requirements of the third generation standard in highest professional education and Master’s Degree Programs “Electronics and Nanoelectronics” and “Nanoengineering” (Bauman Moscow State Technical University, Educational plans and programs, 2019) student's scientific work is an obligatory part of education in the Chair of Electronic Technologies in Mechanical Engineering of Bauman Moscow State Technical University. For four semesters students of Masters's degree studies under the guidance of scientific supervisor work on a specific scientific problem such as investigation and development of modern technologies, engineering of technical processes and equipment. Students can, depending on their background and interests, choose the research fields such as processing techniques, specialized equipment and key materials of electronics, nanoelectronics and nanoengineering: vacuum technics (Vasilev, Malevannaya & Moiseev, 2017), vacuum (Kolesnik, Zhuleva, Predtechenskiy, Kyaw & Phyo, 2017) and colloidal (Kuleshova, Panfilova & Prohorov, 2018) thin films deposition, various lithographic and etching processes, etc.

The nature of nanoscience is cross-disciplinary and students specialize not only in nanoelectronics...
and nanoengineering, but in chemistry, nanophysics, quantum mechanics, etc. Besides successful research depends on confined usage of common methods, algorithms and tools of statistical community special attention in degree programs is given to modern, current and demanded data analysis and modeling methods. Master’s degree program include the course “Neural Network modeling of Complex Technical Systems”. It is taught in the third semester of the Master’s programs “Electronics and Nanoelectronics” and “Nanoengineering”.

2 Methodology of Education

Neural networks can be used in technological process control, code sequence prediction, failure analysis, machine vision, signal identification, nonlinear modeling, etc (Moroz, Cheremisin, Cherkashina & Kholod, 2016; Rene, Lópe, Kim & Park, 2013; Huo, He, Su, Xi, & Zhu, 2013). A neural network is a computing model whose layered structure copies the structure of neurons in the brain, with layers of several connected single processing elements, called neurons. The neurons are connected by weights. These weights are tuning in during learning or training until the error becomes minimum. Neural networks are training over many examples. Training data is a specific number of observations, for each of which values of several variables are indicated. Most of these variables are set as inputs and the network will learn to find a match between the values of the input and known output variables. To train the artificial neural network, data is required to be divided into three datasets as training, validation and test data. The mathematics of neural networks is well developed and many computer programs are available to create, train and exploit neural networks.

Every neural network application is special, but developing the network follows these steps:

- preparing the data,
- creating the neural network,
- training the neural network,
- validating the network’s results,
- tuning the neural network,
- integrating the neural network into a project.

According to the steps of networks development the course consists of five parts. The first part of the course discusses applications of neural networks to practical engineering problems in technological and analytical equipment, sensor and control systems, pattern recognition, clustering. The second part of the course is devoted to accessing and preparing the data. The third part of the course gives an introduction to basic artificial neural network architectures. It provides a clear and detailed survey of fundamental neural network types - multilayer perception, radial basis function network, probability neural networks and Kohonen neural network (Gurney, 2014). Students learn how to construct a set of simple elements - artificial neurons. The fourth part of the course discusses training of neural networks, optimisation algorithms and learning rules: backpropagation and several variations of backpropagation, such as the conjugate gradient, Levenberg-Marquardt algorithm, gradient descent and gradient descent with adaptive learning rate (Sapna, Tamilarasi & Kumar, 2012). At the fifth part of the course students learn how to validate the network’s results and final-tune network parameters. Figure 1 shows the course structure.

Seminars are devoted to the software products: Statistica Neural Networks (Statistica Automated Neural Networks, 2019), Neural Network Toolbox for MATLAB (now - Deep Learning Toolbox) (Deep Learning Toolbox, 2019) and NeuroShell (NeuroShell 2, 2019). During the homework students learn to create, tune and train their own neural networks and get full and detailed understanding of research in computer vision.
After completing the study of the discipline “Neural Network modeling of Complex Technical Systems” the student are expected to:

- understand neural networks algorithms;
- know modern neural networks software products;
- be capable to prepare data;
- be capable to design, train, tune and test neural network;
- be capable to apply neural networks algorithms in practice.

3 The Results of Education and Discussion
Since the course has rather practical than theoretical nature, it plays an important role in student’s research work and development of their graduation works. It is advised to use the homework for solving scientific technical tasks in individual research projects.

There are a few examples of how neural networks are used in students projects in this article:

- modeling of the metal islands thin films growth while vacuum evaporation process using multilayer perception,
- forecasting the properties of photonic band colloidal thin films using radial basic function neural network.

Regression models (Dreiseitl & Ohno-Machado, 2002) are used in students research most often. They describe the relationship between a response (output) variable and predictor (input) variables of technological process, equipment, product or material. Here are a few examples from homeworks and graduation works.

Typical homework report includes abstract, introduction, description part, designing part, results of neural network modeling, discussion and conclusion. Investigating system or process, its input and output parameters and available statistical data are presented and analyzed in description part. The designing part contains the rationale for choosing inputs and outputs, the type of neural network, transfer and error functions and learning algorithm for network training. Description of neural network training, validating and application are presented as a results of modeling. New understanding of the problem, interpreting the findings and the prospects of using modeling results are presented in the discussion section. In conclusion section the arguments involved in the body paragraphs are summarized. The results of neural networks modeling are showed not only in homework reports but special time is reserved for students presentation. Thus homework’s neural networks modeling is a
completed work. It plays a significant role in student’s research and therefore homework reports are widely used as a part of grading works.

Figure 2 illustrates the modeling of colloidal photonic crystal (Armstrong & O’Dwyer, 2015) film deposition process. The films were deposited by vertical lifting method. It has gained great interest because of its simplicity and ability to vary the conditions. To predict the wavelength and reflectance at photonic band gap (PBG) of film the following initial data was necessary: colloidal particles size and material, colloidal solution concentration and lifting velocity. All data were determined directly from the results of the series of reflectance measurements of the polystyrene and silica particles films at various velocities (Kuleshova et al., 2018). The obtained reflectance spectrum shows that the wavelength and reflectance of PBG are in dependence on the lifting velocity, colloidal concentration and particles size for both materials. But self-assembly processes that occur during vertical deposition have been characterized by uncontrolled formation of defects over larger length scales.

The radial basic function (RBF) neural network was used in the simulation as the most precise for the task of predicting nonlinear relation. The RBF neural network model with 4 input neurons, one hidden layer with 20 neurons and 2 output neurons has been created. It describes the relationship between the wavelength and reflectance at PBG (output variable) and colloidal particles size and material, colloidal solution concentration and lifting velocity (input variables).

Neural network was used to optimize the effect of the above-mentioned factors. The revealed dependences allowed to determine the optimal conditions for obtaining high photonic crystalline quality of opal film: the highest values of the relative area of ordered structure and reflectance at the PBG. Obtained at optimal conditions opal film has closest packed structure consisting of hexagonal close packed layers and high reflectance. The results of modeling can be used for various applications of photonic crystal films: nanophotonics, laser technics, luminescence microscopy of biological objects, plasmonics, sensory, etc.

![Modeling of Colloidal Photonic Crystal Film Deposition](image)

**Fig. 2.** Modeling of the colloidal photonic crystal film deposition by vertical lifting process.

Figure 3 shows an example of modeling of metal islands film growth (Sidorova, Pronin & Isaeva, 2018). Multilayer perception (MLP) with two hidden layers was used in the simulation because of it extrapolation ability (Hettiarachchi & Minns, 2005). The best way to determine the number of hidden neurons is to train several networks. Preliminary option analysis included two MLP and two RBF
neural networks. It was revealed that a few number of hidden neurons result in a higher training error and too many hidden neurons results in a higher validation and testing error.

**Fig. 3.** Modeling of the metal islands thin films growth while vacuum evaporation process.

The modeling approach described in the course “Neural Network modeling of Complex Technical Systems” allows to get useful information for effective student’s scientific investigation. Neural network models help students understand the thin films deposition processes dependencies.

### 4 Conclusion

The principles of artificial intelligence is applied with the help of neural networks (Rene & Saidutta, 2008; Russell & Norvig, 2016). For engineers and nanoscientists neural network models have become a powerful tool of scientific research and machine learning. The concept of neural network modeling has widespread applications in the field of applied science and engineering, in particular, in nanotechnology. The minimum value of errors, the high level of objectivity in the results of output predicting and real-time control are the advantages of neural networks in comparison with other methods.

The results acquired with neural network models for the experimental study of nanotechnological processes show that the application of neural networks is sufficient. Neural Networks models are successfully used in students scientific and research projects and presented in Master’s and Specialist’s graduation works. The aim of the course is not only to introduce students to the neural network modeling, and also to develop self-learning abilities (Siriwongs, 2015; Cheng & Chau, 2013).

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