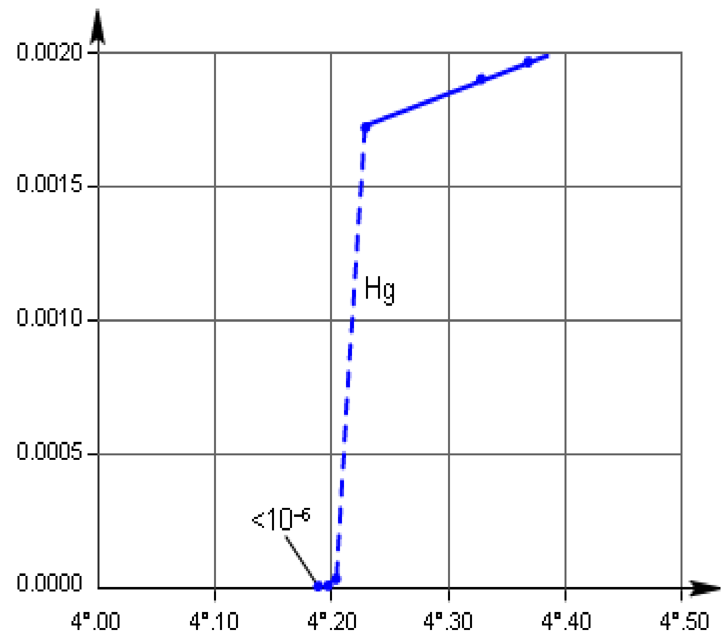

Figure 1. Dependence of the specific resistance of mercury on temperature. Retrieved from: https://xreferat.com

United Nations Educational, Scientific and Cultural Organization

Junior Academy of Sciences of Ukraine

THE MACHINE LEARNING MODELS FOR PREDICTION SUPERCONDUCTING PROPERTIES OF MATERIALS

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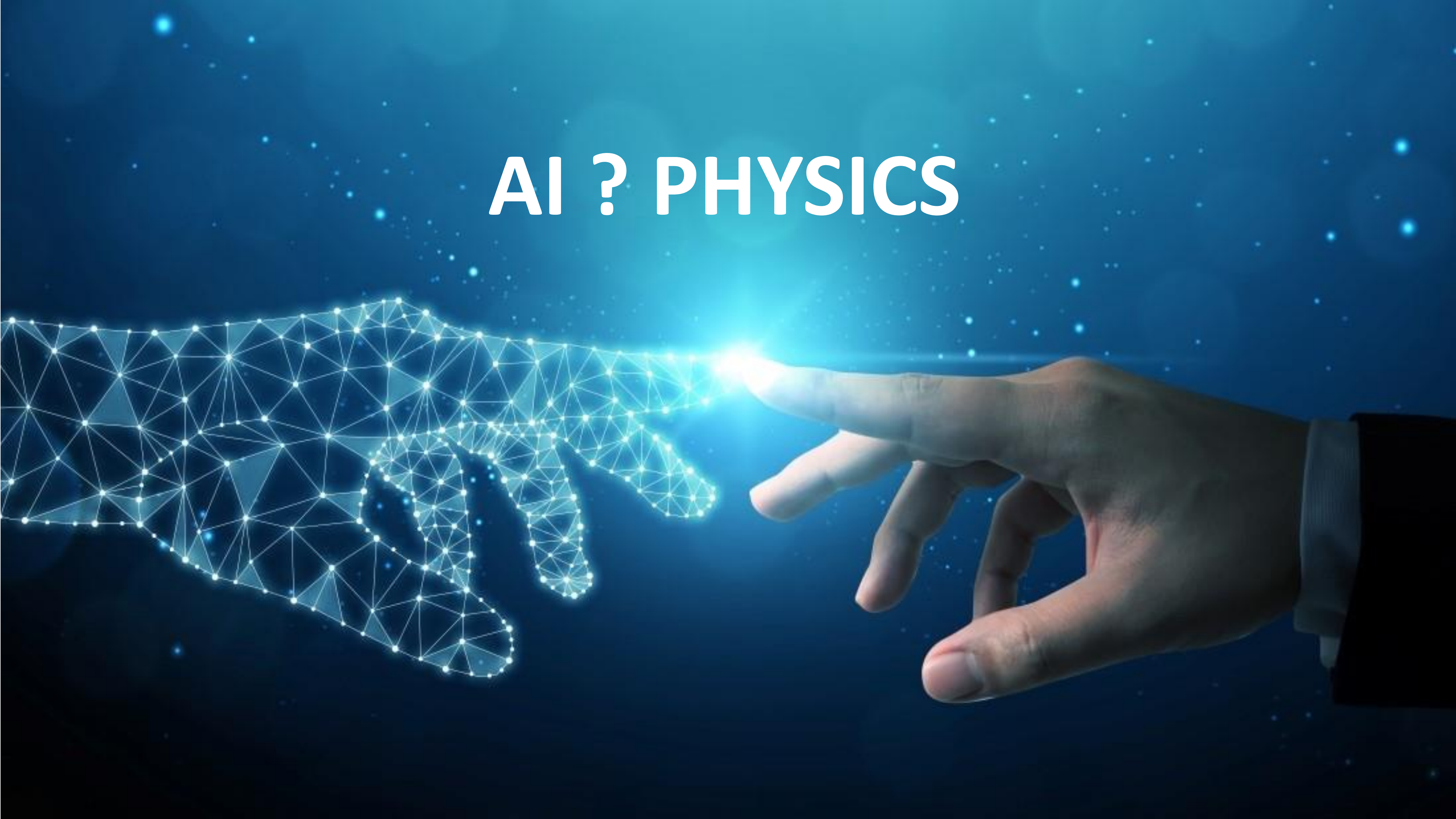
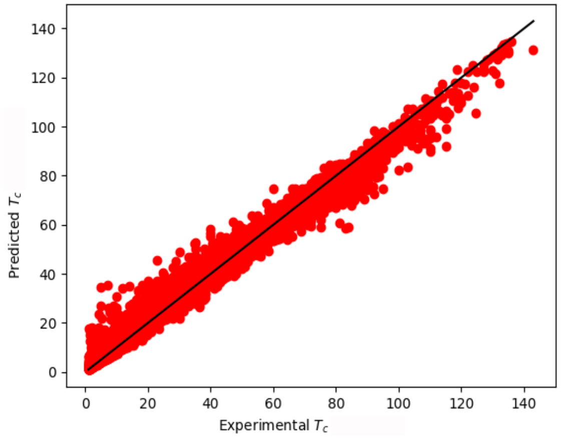

AI ? PHYSICS

Map of the project

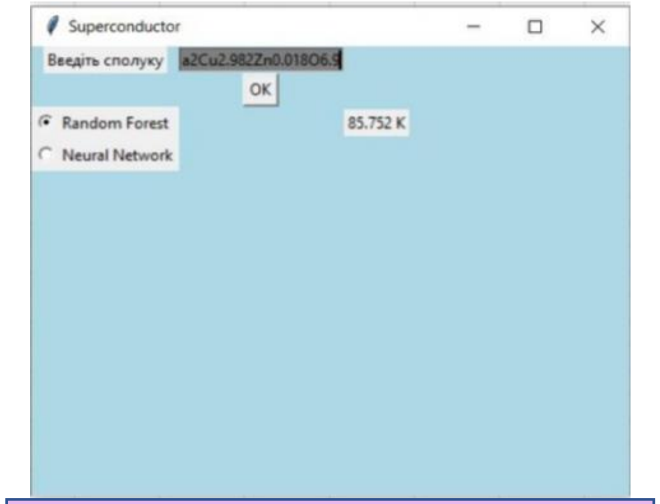
collecting information from available databases

preliminary processing according to methods used in the industry machine learning

select only those characteristics that most affect superconductivity



modeling based on various types of regression analysis, decision trees and neural networks.



creation a graphical interface

A random forest was created for high-temperature and low-temperature superconductors. R2_score (coefficient of determination) indicates whether successfully obtained traces confirm the model.

To create these Decision trees, it was necessary to divide the entire database into the corresponding critical temperatures:

Up to 2K for low-temperature and higher for high-temperature superconductors.

Training Set R-Square= 0.93

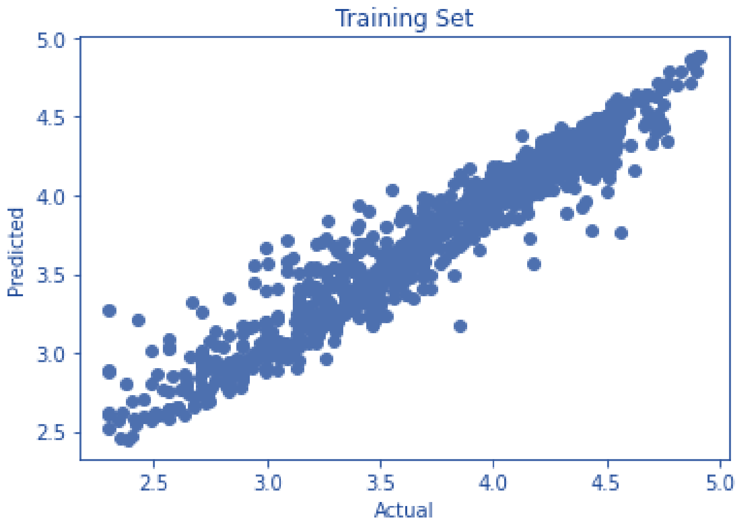


Figure.2 Training set of random forest for “high-Tc” superconductors

Training Set R-Square= 0.95

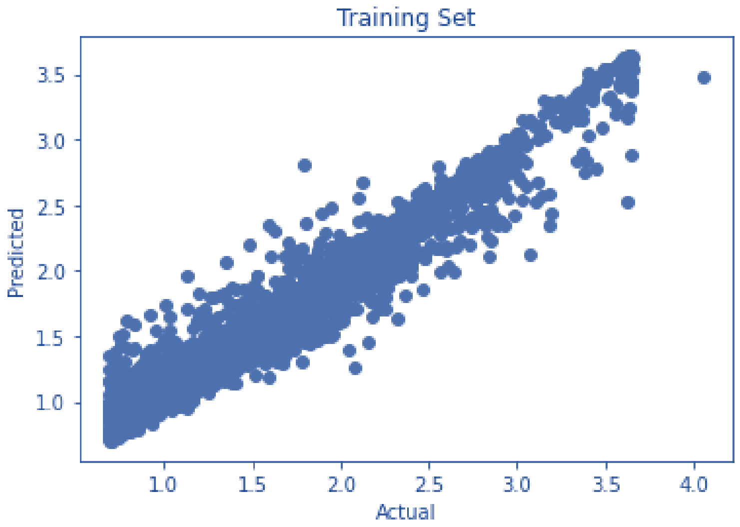


Figure 3 Training set of random forest for “low-Tc” superconductors

Neural Network

To predict the critical temperature of new potential superconductors of any type, a neural network was created.

The process of model training is shown in figure 4, from which you can make a conclusion about the convergence of the model.

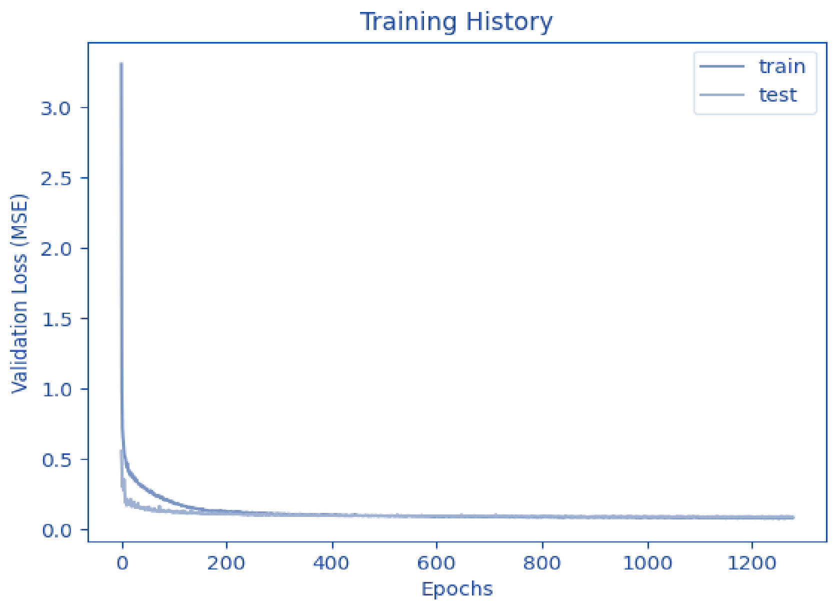


Figure 4

When the neural network trains, the dataset splits on three parts: training, testing and validation sets. These figures show accuracy of training and testing neural network.

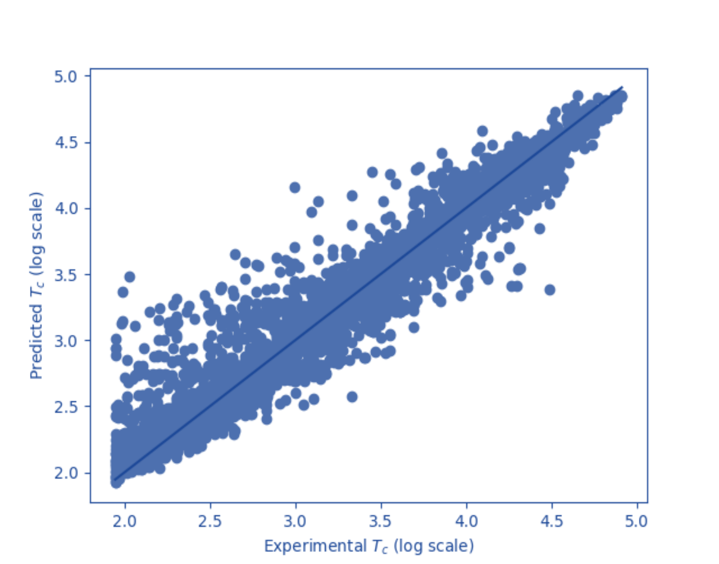


Figure 5

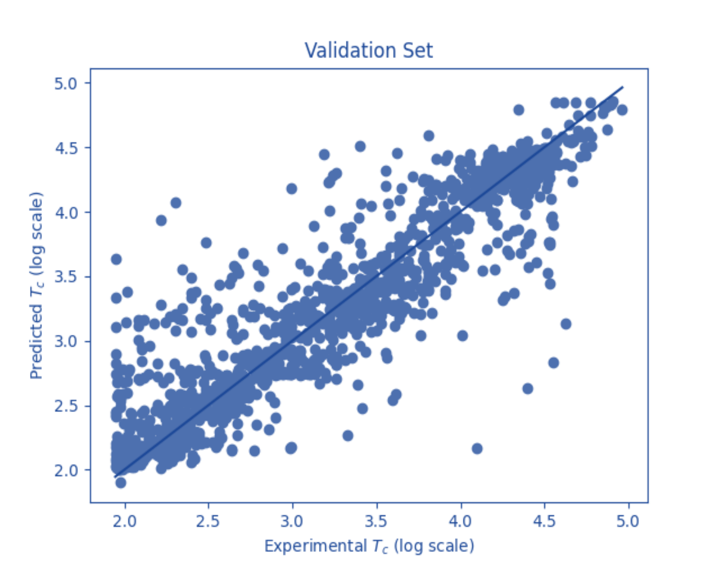


Figure 6

Figure 7

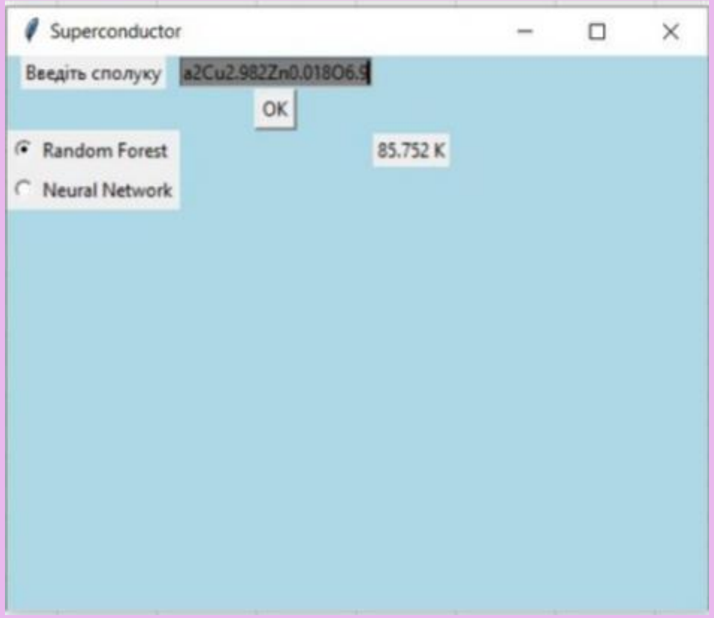


Figure 8

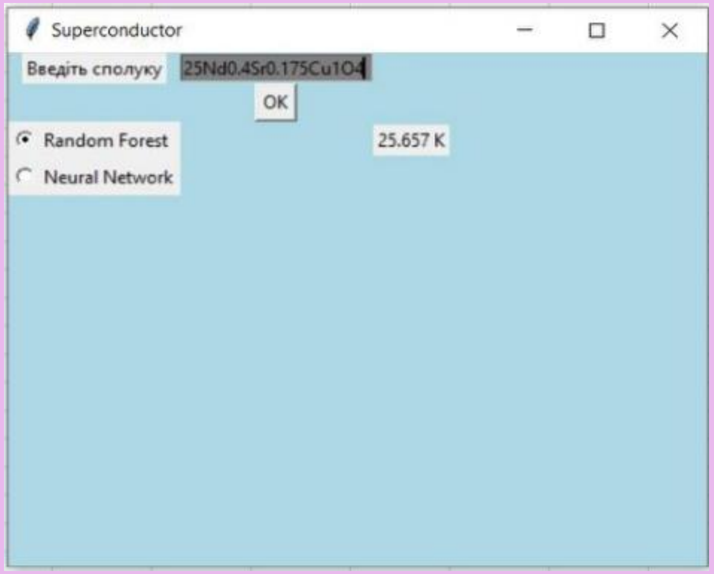
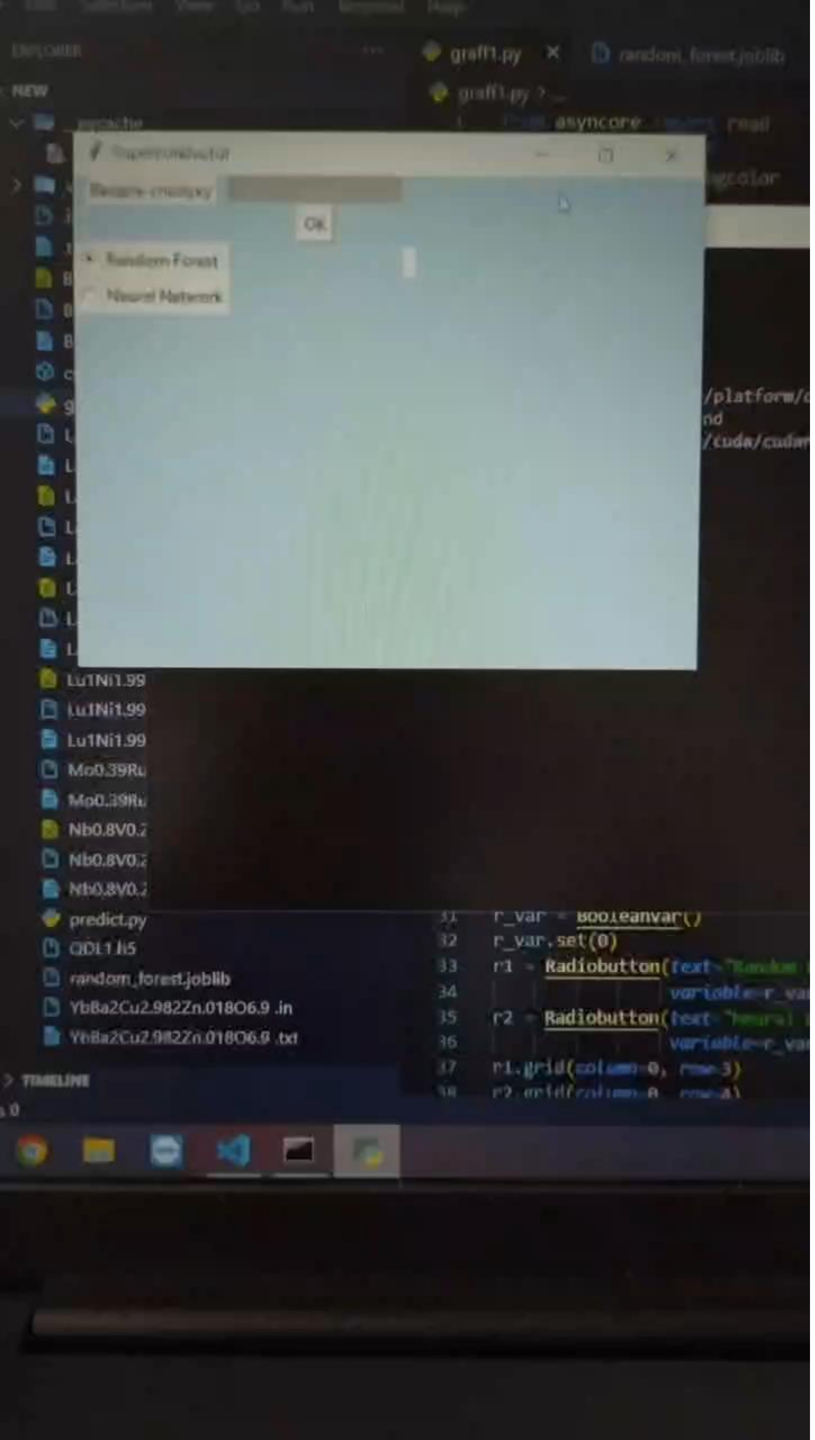


Figure 9

The true critical temperature of a substance:

YbBa2Cu2.982Zn.018O6.9 = 85.1K

La.425Nd4Sr175Cu104 = 25 K



Parameters most important for formation of superconducting properties (according to this model):

- mean_CovalentRadius
- frac_sValence
- mean_NsValence
- frac_dValence
- mean_NdValence
- mean_NUnfilled
- Comp_L2Norm
- mean_MendeleevNumber


Why it is necessary?

Problems which happened

Linear regression

Unfortunately, the correlation coefficient appeared to be small, which means that linear regression is not suitable for prediction the critical temperature of superconductors.

The highest coefficient was obtained for high-temperature superconductors:

Y['Tc'].corr(X['mean_NUnfilled’]):

-0.4663574740436221

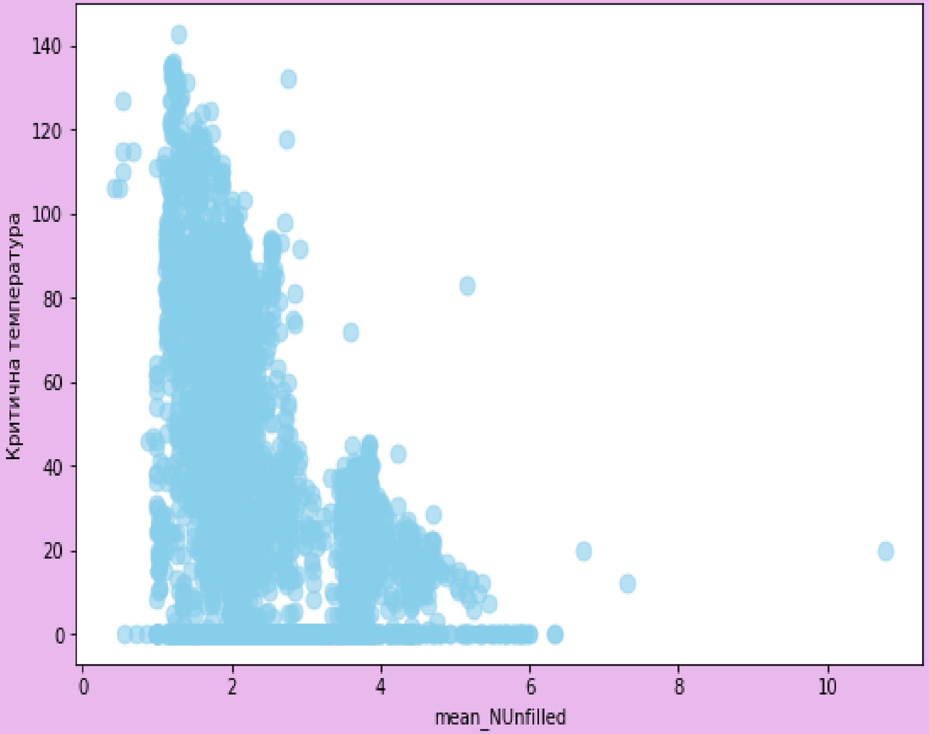
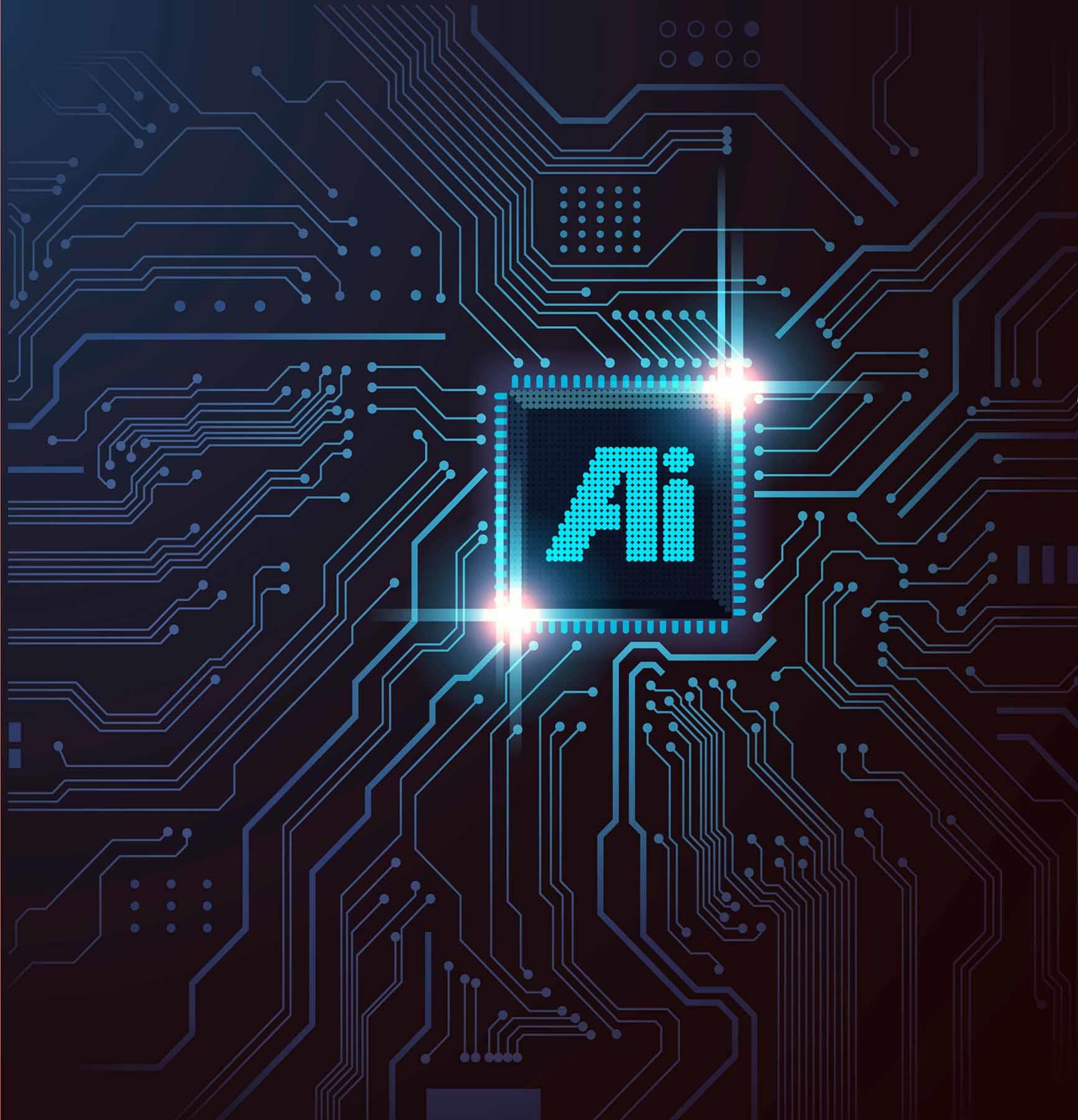


Figure 10

Conclusions

The work deals with one of the most promising materials - superconductors. The result of the project was a set of machine learning models (linear regression, random forest, neural network), which allow determining the influence of various physical properties of compounds on the temperature of the superconducting transition with the possibility of predicting this characteristic based on the chemical composition and crystal structure of the compound.

This approach makes it possible to significantly accelerate the search for materials with superconducting properties.



Thank you for attention!
You are welcome with questions