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MACHINE LEARNING MODELS TO FIND UNOBSERVABLE CENTRALITY-RELATED PARAMETER VALUES IN COLLISIONS OF DIFFERENT NUCLEI IN THE INITIAL ENERGY RANGE FROM 40 TO 200 GEV

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Abstract. This paper continues studies in machine learning models capabilities aimed to finding the best way to predict the values of unobservable quantities that characterize centrality, based on experimental data for observable quantities: the number of charged particles and the number of neutrons produced in ultrarelativistic nuclear interactions. The sought-for unobservable quantities were the number of wounded nucleons involved in the interaction and the number of binary nucleon-nucleon collisions. A decision tree, a random forest, and a multilayer perceptron (MP) were tested as machine learning models. The prediction accuracy of the models was characterized by the coefficient of determination R^2. Dependences of R^2 values on initial energies (40–200 GeV) for different systems of colliding nuclei were obtained. The MP model was found to be able to predict the values of unknown quantities in a wide range of initial energies for different systems of nuclear interactions with good accuracy.

Keywords: machine learning, nuclei collisions, initial energy, *R*-squared, multilayer perceptron

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МОДЕЛИ МАШИННОГО ОБУЧЕНИЯ ДЛЯ НАХОЖДЕНИЯ ЗНАЧЕНИЙ НЕНАБЛЮДАЕМЫХ ПАРАМЕТРОВ, ОПИСЫВАЮЩИХ ЦЕНТРАЛЬНОСТЬ, ПРИ СТОЛКНОВЕНИЯХ РАЗЛИЧНЫХ ЯДЕР В ЭНЕРГЕТИЧЕСКОМ ДИАПАЗОНЕ ОТ 40 ДО 200 ГЭВ

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Аннотация. Данная работа продолжает исследования возможностей моделей машинного обучения, направленные на поиск оптимального пути предсказания значений ненаблюдаемых величин, характеризующих центральность, основываясь на экспериментальных данных для наблюдаемых величин: числа заряженных частиц и числа нейтронов, рождающихся во взаимодействии ультрарелятивистских ядер. Искомыми ненаблюдаемыми величинами были число раненых нуклонов, участвующих во взаимодействии, и число бинарных нуклон-нуклонных столкновений. В качестве моделей машинного обучения были протестированы дерево решений, случайный лес и многослойный перцептрон (МП). Точность предсказания моделей характеризовалась коэффициентом детерминации (R^2). Получены зависимости значений R^2 от начальных энергий (200 − 40 ГэВ) для разных систем сталкивающихся ядер. Установлено, что модель МП способна с хорошей точностью предсказывать значения искомых величин в широком диапазоне начальных энергий для различных систем ядерных взаимодействий.

Ключевые слова: машинное обучение, столкновение ядер, начальная энергия, коэффициент детерминации, многослойный перцептрон

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Introduction

Algorithms based on machine learning methods have long yielded good results in various fields of science and technology, often surpassing standard algorithms [1]. In fiew of this, it seems reasonable to apply machine learning to physics of ultrarelativistic collisions of nuclei.

This paper intends to continue and expand the studies in [2]. This initial study applied machine learning methods to determine the values of unobservable experimental quantities from the observed ones. The former include the number of binary nucleon–nucleon collisions N_{coll} in a nucleus–nucleus collision at a given initial energy and the number of wounded nucleons N_{part} produced in a nucleus–nucleus collision. The latter are the number of charged particles N_{ch} and the number of neutrons N_{neut} produced in each individual nucleus–nucleus interaction.

We have found that three models, namely, a decision tree, a random forest and a multilayer perceptron, are capable of predicting the values of N_{coll} and N_{part} with good accuracy in a wide range of collision systems [2].

However, the above-mentioned study was limited to considering the applicability of the models only for a given initial center-of-mass energy $\sqrt{s_{NN}} = 200$ GeV.

As the next stage in our research, we intend to find out whether these models are applicable for varying values of the initial energy $\sqrt{s_{NN}}$. In fact, the initial energy can determine the nature of the processes occurring during the collision of nuclei [3].

This paper analyzes the applicability of machine learning models to predicting the number of wounded nucleons N_{part} involved in the interaction and the number of binary nucleon–nucleon collisions N_{coll} (parameters characterizing centrality) at initial energies in the range of 40–200 GeV.

The basis for the models are the quantities observed experimentally: the number of charged particles and the number of neutrons produced in each individual nucleus–nucleus interaction for various systems of colliding nuclei.

Computational technique

The input parameters of the models (decision tree, random forest and multilayer perceptron) are the multiplicities of charged particles N_{ch} and neutrons N_{neut}.

The multiplicity of charged particles was set in the range of pseudorapidities $3 < |\eta| < 4$, and the number of neutral particles in the range of pseudorapidities $5 < |\eta| < 8$. These ranges were selected based on the experimental data from [4]. Additional input parameters of the models were the number of protons and neutrons in colliding nuclei and the center-of-mass energy $\sqrt{s_{NN}}$ [5]. These parameters allow simulating collisions of nuclei of different nature at different initial energies.

We considered collision events for a wide variety of nuclei used by researchers in a large number of very diverse experiments [4]. These nuclei are hydrogen H (protons) p, helium He, copper Cu, xenon Xe, gold Au, lead Pb and uranium U.

The models were trained on the following binary systems, randomly selected from the above nuclei:

$$p + \text{Cu}, p + \text{U}, \text{He} + \text{Xe}, \text{He} + \text{U}, \text{Cu} + \text{Cu}, \text{Cu} + \text{Xe}, \text{Xe} + \text{Pb}, \text{Au} + \text{Au}.$$

The predictions of the models were verified on the following binary systems:

$$p + \text{Pb}, p + \text{Xe}, p + \text{Au}, \text{He} + \text{Cu}, \text{He} + \text{Au}, \text{He} + \text{Pb}$$
(light-heavy collision systems);

$$\text{Cu} + \text{Au}, \text{Cu} + \text{Pb}, \text{Cu} + \text{U}, \text{Xe} + \text{U}, \text{Au} + \text{Pb}, \text{Au} + \text{U}, \text{Pb} + \text{U}$$
(asymmetric heavy collisions)

$$\text{Xe} + \text{Xe}, \text{Pb} + \text{Pb}, \text{U} + \text{U}$$
(symmetric heavy collision systems).

The selected initial energies $\sqrt{s_{NN}}$ lay in the range from 40 to 200 GeV [4].

The models were trained at energies in the range of 40–200 GeV with a step of 40 GeV, and verified in the extended energy range of 20–260 GeV with a step of 20 GeV. The tables below give only part of the data obtained (not for all selected initial energies) for space considerations.

The same as in [2], training of the models and verification of their prediction accuracy were preceded by simulation (generation) of the above-mentioned binary collisions, but at different initial energies (see above). The PYTHIA8/Angantyr 8.307 software was used to generate collisions [5]. The number of generated events was 100,000. Numerical values of wounded nucleons N_{part} and binary nucleon–nucleon collisions N_{coll} were obtained from each event, as well as multiplicities of charged particles and neutrons (reference values).

The decision tree [6], random forest [7] and multilayer perceptron [8] were considered as machine learning models, as in the previous study [2], where these models produced the best results.

The model parameters that the program did not determine during training (hyperparameters) was selected with the Tree Parzen Estimators algorithm [9] from the Optuna library [10].

The details of the simulation were as follows. The decision tree model had a depth of 63. The random forest model included 37 estimators with a maximum depth of 84 each. The multilayer perceptron consisted of 7 input neurons, 5 hidden layers of 512 neurons each, with a ReLU activation function and an output layer of two neurons with a linear activation function. The number of epochs for training was 45, and Adam was chosen as the gradient descent optimizer [11].

The prediction accuracy provided by the models for N_{coll} and N_{part} was characterized by the determination coefficients R^2_{Ncoll} and R^2_{Npart} [12], which are determined by the following formula:

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{N} y_i^2},$$

where R^2 includes R^2_{Ncoll} or R^2_{Npart}; y_i *are* the reference values of the given quantities; $\hat{y}_i$ *are* the values predicted by the model; N is the number of values [2].

The prediction accuracy of the parameters N_{coll} and N_{part} was characterized by the arithmetic mean R^2 of R^2_{Ncoll} for N_{coll} and R^2_{Npart} for N_{part} [13]:

$$\overline{R}^2 = \frac{R_{N_{coll}}{}^2 + R_{N_{part}}{}^2}{2}.$$

The closer R^2 to unity (the maximum value), the closer the computational values to the reference ones.

Confidence intervals and errors of the determination coefficient R^2 were found by the bootstrap method [14].

Computational results and discussion

Tables 1–9 present the computational results for the determination coefficients R^2 depending on the initial energy of colliding nuclei $\sqrt{s_{NN}}$, for three classes of collision systems on which the verification was performed.

The models that gave the best results are considered (see [2]): a multilayer perceptron, a decision tree and a random forest.

As follows from analysis of the data presented in the tables, all models used yield good results for any systems of colliding nuclei at initial energies of 40, 80, 120, 160 and 200 GeV (on which the models were trained), since the values of $R^2 > 0.95$.

Because one of our goals was to analyze the results of model predictions at points interpolated and extrapolated by energy, the tables show the determination coefficients at energies of 20, 60, 180 and 220 GeV.

Table 1

Determination coefficients of multilayer perceptron model as function of initial energies $\sqrt{s_{NN}}$ for light-heavy collision systems

$\sqrt{s_{NN}}$, GeV	Determination coefficient $\bar{R}^2$ for collision system				
	p + Xe	p + Au	p + Pb	He + Au	He + U
20	0.742±0.019	0.706±0.023	0.789±0.024	0.902±0.023	0.895±0.022
40	0.954±0.022	0.956±0.025	0.954±0.028	0.984±0.023	0.988±0.025
60	0.967±0.025	0.965±0.025	0.932±0.025	0.983±0.025	0.983±0.023
80	0.951±0.026	0.967±0.028	0.969±0.024	0.987±0.026	0.988±0.026
160	0.957±0.025	0.957±0.021	0.965±0.027	0.989±0.025	0.989±0.026
180	0.957±0.027	0.960±0.026	0.961±0.026	0.989±0.024	0.990±0.024
200	0.955±0.029	0.948±0.026	0.959±0.026	0.987±0.027	0.990±0.024
220	0.952±0.027	0.949±0.023	0.951±0.029	0.983±0.025	0.988±0.030

Table 2

Determination coefficients of multilayer perceptron model as function of initial energies $\sqrt{s_{NN}}$ for asymmetric heavy collision systems

$\sqrt{s_{NN}}$, GeV	Determination coefficient $\bar{R}^2$ for collision system						
	Cu + Au	Cu + Pb	Xe + Pb	Xe + U	Au + Pb	Au + U	Pb + U
20	0.860± ±0.023	0.846± ±0.021	0.725± ±0.019	0.733± ±0.018	0.679± ±0.014	0.689± ±0.019	0.685± ±0.016
40	0.978± ±0.023	0.978± ±0.024	0.988± ±0.023	0.994± ±0.023	0.999± ±0.024	0.998± ±0.028	0.999± ±0.029
60	0.969± ±0.028	0.949± ±0.024	0.995± ±0.026	0.951± ±0.024	0.980± ±0.025	0.971± ±0.025	0.975± ±0.028
80	0.993± ±0.029	0.990± ±0.026	0.998± ±0.025	0.993± ±0.028	0.998± ±0.027	0.994± ±0.024	0.994± ±0.028
160	0.996± ±0.028	0.994± ±0.023	0.999± ±0.025	0.998± ±0.027	0.998± ±0.025	0.998± ±0.031	0.998± ±0.030
180	0.995± ±0.030	0.994± ±0.028	0.999± ±0.022	0.998± ±0.033	0.999± ±0.026	0.998± ±0.028	0.998± ±0.023
200	0.994± ±0.024	0.994± ±0.024	0.999± ±0.024	0.997± ±0.025	0.999± ±0.035	0.998± ±0.026	0.998± ±0.029
220	0.996± ±0.028	0.993± ±0.030	0.999± ±0.027	0.997± ±0.028	0.999± ±0.026	0.998± ±0.025	0.998± ±0.028

Table 3

Determination coefficients of multilayer perceptron model as function of initial energies $\sqrt{s_{NN}}$ for symmetric heavy collision systems

$\sqrt{s_{NN}}$, GeV	Determination coefficient $\bar{R}^2$ for collision system		
	Xe + Xe	Pb + Pb	U + U
20	0.840±0.022	0.682±0.020	0.627±0.020
40	0.960±0.028	0.998±0.025	0.998±0.023
60	0.899±0.024	0.985±0.026	0.972±0.027
80	0.972±0.026	0.998±0.027	0.993±0.028
160	0.992±0.026	0.998±0.026	0.998±0.028
180	0.993±0.026	0.999±0.032	0.998±0.025
200	0.993±0.029	0.999±0.027	0.999±0.028
220	0.992±0.028	0.999±0.029	0.999±0.024

Table 4

Determination coefficients of decision tree model as function of initial energies $\sqrt{s_{NN}}$ for light-heavy collision systems

$\sqrt{s_{NN}}$, GeV	Determination coefficient $\bar{R}^2$ for collision system				
	p + Xe	p + Au	p + Pb	He + Au	He + U
20	0.399±0.009	0.151±0.004	0.251±0.007	0.228±0.006	0.328±0.008
40	0.978±0.025	0.978±0.027	0.986±0.025	0.975±0.028	0.983±0.029
60	0.577±0.014	0.672±0.019	0.454±0.014	0.502±0.013	0.611±0.019
80	0.969±0.034	0.973±0.026	0.964±0.023	0.972±0.025	0.970±0.027
160	0.985±0.026	0.995±0.028	0.988±0.027	0.983±0.030	0.997±0.024
180	0.971±0.024	0.983±0.024	0.985±0.026	0.964±0.026	0.980±0.036
200	0.982±0.027	0.980±0.029	0.989±0.029	0.966±0.028	0.969±0.030
220	0.993±0.028	0.988±0.031	0.980±0.027	0.974±0.026	0.953±0.029

Table 5

Determination coefficients of decision tree model as function of initial energies $\sqrt{s_{NN}}$ for asymmetric heavy collision systems

$\sqrt{s_{NN}}$, GeV	Determination coefficient $\bar{R}^2$ for collision system						
	Cu+Au	Cu+Pb	Xe+Pb	Xe+U	Au+Pb	Au+U	Pb+U
20	0.260± ±0.008	0.268± ±0.008	0.359± ±0.008	0.304± ±0.008	0.361± ±0.015	0.398± ±0.010	0.364± ±0.010
40	0.966± ±0.023	0.976± ±0.027	0.981± ±0.028	0.994± ±0.033	0.996± ±0.024	0.992± ±0.027	0.989± ±0.028
60	0.293± ±0.008	0.173± ±0.004	0.027± ±0.001	0.557± ±0.016	0.685± ±0.018	0.732± ±0.022	0.782± ±0.021
80	0.989± ±0.027	0.980± ±0.026	0.997± ±0.026	0.994± ±0.024	0.996± ±0.027	0.991± ±0.027	0.988± ±0.025
160	0.982± ±0.026	0.973± ±0.026	0.990± ±0.028	0.996± ±0.028	0.989± ±0.028	0.986± ±0.026	0.978± ±0.023
180	0.966± ±0.027	0.968± ±0.028	0.978± ±0.024	0.983± ±0.025	0.990± ±0.027	0.976± ±0.027	0.978± ±0.030
200	0.980± ±0.025	0.986± ±0.026	0.983± ±0.024	0.994± ±0.027	0.996± ±0.027	0.988± ±0.023	0.982± ±0.027
220	0.976± ±0.026	0.984± ±0.028	0.964± ±0.026	0.987± ±0.024	0.988± ±0.025	0.979± ±0.028	0.978± ±0.024

Table 6

Determination coefficients of decision tree model as function of initial energies $\sqrt{s_{NN}}$ for symmetric heavy collision systems

$\sqrt{s_{NN}}$, GeV	Determination coefficient $\bar{R}^2$ for collision system		
	Xe + Xe	Pb + Pb	U + U
20	0.275±0.007	0.383±0.010	0.329±0.009
40	0.983±0.025	0.996±0.029	0.983±0.027
60	0.169±0.005	0.715±0.020	0.757±0.021
80	0.981±0.027	0.994±0.028	0.970±0.025
160	0.965±0.023	0.994±0.026	0.965±0.025
180	0.971±0.025	0.984±0.028	0.973±0.027
200	0.978±0.025	0.995±0.023	0.978±0.025
220	0.979±0.023	0.989±0.028	0.977±0.028

Table 7

Determination coefficients of random forest model as function of initial energies $\sqrt{s_{NN}}$ for light-heavy collision systems

$\sqrt{s_{NN}}$, GeV	Determination coefficient $\bar{R}^2$ for collision system				
	p + Xe	p + Au	p + Pb	He + Au	He + U
20	0.311±0.008	0.098±0.002	0.205±0.006	0.192±0.006	0.302±0.009
40	0.979±0.026	0.980±0.024	0.985±0.025	0.980±0.025	0.980±0.025
60	0.628±0.016	0.705±0.015	0.508±0.012	0.589±0.016	0.661±0.019
80	0.973±0.024	0.989±0.032	0.988±0.028	0.983±0.025	0.979±0.030
160	0.990±0.023	0.991±0.029	0.987±0.025	0.981±0.027	0.992±0.028
180	0.989±0.028	0.994±0.031	0.993±0.025	0.990±0.029	0.992±0.032
200	0.994±0.029	0.993±0.027	0.997±0.025	0.984±0.02	0.984±0.030
220	0.986±0.030	0.994±0.027	0.990±0.030	0.980±0.027	0.970±0.024

Table 8

Determination coefficients of random forest model as function of initial energies $\sqrt{s_{NN}}$ for asymmetric heavy collision systems

$\sqrt{s_{NN}}$, GeV	Determination coefficient $\bar{R}^2$ for collision system						
	Cu+Au	Cu+Pb	Xe+Pb	Xe+U	Au+Pb	Au+U	Pb+U
20	0.270± ±0.007	0.274± ±0.007	0.343± ±0.012	0.290± ±0.007	0.338± ±0.010	0.378± ±0.010	0.352± ±0.008
40	0.983± ±0.027	0.986± ±0.026	0.992± ±0.029	0.995± ±0.027	0.994± ±0.024	0.972± ±0.025	0.967± ±0.028
60	0.501± ±0.012	0.393± ±0.011	0.282± ±0.007	0.709± ±0.018	0.754± ±0.020	0.793± ±0.021	0.806± ±0.020
80	0.988± ±0.025	0.984± ±0.028	0.997± ±0.026	0.994± ±0.028	0.992± ±0.031	0.974± ±0.025	0.968± ±0.025
160	0.988± ±0.031	0.987± ±0.024	0.996± ±0.033	0.998± ±0.025	0.995± ±0.028	0.985± ±0.031	0.981± ±0.026
180	0.985± ±0.027	0.984± ±0.027	0.983± ±0.026	0.995± ±0.023	0.992± ±0.025	0.984± ±0.027	0.983± ±0.027
200	0.986± ±0.025	0.988± ±0.025	0.983± ±0.024	0.997± ±0.028	0.993± ±0.028	0.987± ±0.024	0.983± ±0.029
220	0.977± ±0.026	0.980± ±0.024	0.962± ±0.026	0.987± ±0.026	0.984± ±0.027	0.976± ±0.028	0.975± ±0.023

Table 9

Determination coefficients of random forest model as function of initial energies $\sqrt{s_{NN}}$ for symmetric heavy collision systems

$\sqrt{s_{NN}}$, GeV	Determination coefficient $\bar{R}^2$ for collision system		
	Xe + Xe	Pb + Pb	U + U
20	0.277±0.008	0.379±0.010	0.311±0.008
40	0.986±0.023	0.990±0.029	0.947±0.027
60	0.456±0.014	0.759±0.022	0.768±0.022
80	0.977±0.030	0.986±0.030	0.952±0.027
160	0.985±0.026	0.995±0.029	0.968±0.027
180	0.986±0.032	0.991±0.028	0.977±0.027
200	0.988±0.027	0.992±0.025	0.973±0.025
220	0.978±0.028	0.981±0.029	0.971±0.027

Comparing the data obtained, we can conclude that the multilayer perceptron model showed the best results compared to the others with an interpolated initial energy of 60 GeV, since its R^2 values are closest to unity. We should also note that the value of R^2 for the decision tree and random forest models is noticeably less than unity (within the errors given in the tables).

Further analysis of these tables suggests that all models show good results for extrapolating the given values towards higher energies (220 GeV), $R^2 > 0.9$. However, all models proved incapable of fully describing the considered dependences at energies lower than the ones on which the training was conducted (20 GeV). The determination coefficient R^2 is much less than unity for all three models considered in this study. This is due to excessively low multiplicities of charged particles N_{ch} and neutrons N_{neut} at an initial energy of 20 GeV. Because of the strong differences in the values of N_{ch} and N_{neut} at 20 GeV, as well as at the energies on which the training was conducted, none of the models turned out to be capable of correctly predicting the required values of N_{coll} and N_{part}.

Conclusion

The studies carried out allowed to establish an optimal machine learning model capable of predicting the number of wounded nucleons N_{part} and the number of binary nucleon collisions N_{coll} characterizing the collision centrality, which are not observed in the experiment, based on the experimentally observed multiplicity of charged particles N_{ch} and the number of neutrons N_{neut} produced in the collision for a wide variety of collision systems with the initial energies $\sqrt{s_{NN}}$ ranging from 40 to 200 GeV.

We established for the initial conditions and the selected parameters (the energies and collision systems on which the training was conducted, as well as the energies of the interpolated and extrapolated points) that the multilayer perceptron model gives the best results compared to the decision tree and random forest models. Moreover, the multilayer perceptron can predict the values of N_{coll} and N_{part} with high accuracy ($R^2 > 0.9$) in collisions at higher (extrapolated) initial energies: 220, 240 and 260 GeV.

Intel® Core™ i9-9980XE processor, NVIDIA GeForce RTX™ 2080 Ti graphics card and 64 GB RAM were used for the computations.

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