

## NUCLEAR PHYSICS

Original article

DOI: <https://doi.org/10.18721/JPM.16210>

### **MACHINE LEARNING MODELS TO DETERMINE UNOBSERVABLE CENTRALITY-RELATED PARAMETER VALUES FOR A WIDE RANGE OF NUCLEAR COLLISIONS AT THE ENERGY OF 200 GeV**

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**Abstract.** In the paper, a comparative analysis and a search for the optimal machine learning model have been conducted. The model should predict the values of unobservable centrality-related quantities based on the experimental data for observable quantities, namely, the number of charged particles and the number of neutral ones born in the interactions of both heavy and light ultrarelativistic nuclei. The sought-for unobservable values were the numbers of wounded nucleons involved in the interactions and of the binary nucleon-nucleon collisions. Linear and polynomial regressions of various degrees, a decision tree (DT), a random forest (RF), and a multilayer perceptron (MP) were chosen and considered as machine learning models. The prediction accuracy of the models was characterized and tested by the coefficient of determination. The DT, RF, and MP models were found to predict the desired values with the highest accuracy, i.e., they gave equally good results.

**Keywords:** machine learning, nuclei collisions, regression, decision tree, random forest, multilayer perceptron

**Citation:** Lobanov A. A., Berdnikov Ya. A., Mitrankov Iu. M., Machine learning models to determine unobservable centrality-related parameter values for a wide range of nuclear collisions at the energy of 200 GeV, St. Petersburg State Polytechnical University Journal. Physics and Mathematics. 16 (2) (2023) 111–120. DOI: <https://doi.org/10.18721/JPM.16210>

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Научная статья  
УДК 539.12  
DOI: <https://doi.org/10.18721/JPM.16210>

## МОДЕЛИ МАШИННОГО ОБУЧЕНИЯ ДЛЯ ОПРЕДЕЛЕНИЯ ЗНАЧЕНИЙ НЕНАБЛЮДАЕМЫХ ПАРАМЕТРОВ, СВЯЗАННЫХ С ЦЕНТРАЛЬНОСТЬЮ, ДЛЯ ШИРОКОГО СПЕКТРА ЯДЕРНЫХ СИСТЕМ ПРИ ЭНЕРГИИ 200 ГЭВ

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**Аннотация.** В работе проведен сравнительный анализ и поиск оптимальной модели машинного обучения, которая позволила бы предсказывать значения ненаблюдаемых величин, характеризующих центральность, основываясь на экспериментальных данных для наблюдаемых величин: числа заряженных частиц и числа нейтральных частиц, рождающихся во взаимодействии как тяжелых, так и легких ультрарелятивистских ядер. Искомыми ненаблюдаемыми величинами были число раненых нуклонов, участвующих во взаимодействии, и число бинарных нуклон-нуклонных столкновений. В качестве моделей машинного обучения были выбраны и рассмотрены линейная и полиномиальные регрессии различных степеней, дерево решений (ДР), случайный лес (СЛ) и многослойный перцептрон (МП). Точность предсказания моделей характеризовалась и проверялась коэффициентом детерминации. Установлено, что модели ДР, СЛ и МП с наибольшей точностью предсказывают искомые значения, т. е. дают одинаково хорошие результаты.

**Ключевые слова:** машинное обучение, столкновение ядер, регрессия, дерево решений, случайный лес, многослойный перцептрон

**Ссылка для цитирования:** Лобанов А. А., Бердников Я. А., Митранков Ю. М. Модели машинного обучения для определения значений ненаблюдаемых параметров, связанных с центральностью, для широкого спектра ядерных столкновений при энергии 200 ГэВ // Научно-технические ведомости СПбГПУ. Физико-математические науки. 2023. Т. 16. № 2. С. 111–120. DOI: <https://doi.org/10.18721/JPM.16210>

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### Introduction

There is much interest towards machine learning methods, as they yield good results in diverse fields ranging from speech models to image generation.

For this reason, it seems worthwhile to apply existing machine learning algorithms in nuclear physics, elementary particle physics and high-energy physics, as well as develop new algorithms.

The physics of ultrarelativistic heavy-ion collisions is a fascinating field of research, holding immense potential for exploring the unusual state of matter that is quark-gluon plasma [1].

The high-energy interactions of nuclei are generally studied in collider experiments, measuring the characteristics of particles produced in ion beam collisions [2].

The energy of an ion beam is commonly expressed by the amount of energy per nucleon. This allows comparing the nucleus–nucleus collisions with proton-proton ones; it is assumed that the moving nuclei are a nucleon beam, while the collision of nuclei is a combination of nucleon pair collisions from different nuclei.



It was established in [3] that an important property of nucleus–nucleus collisions is a significant increase in the average multiplicity (calculated per colliding nucleon pair inside the nucleus) relative to the average multiplicity observed in a collision of free nucleon pairs (outside the nucleus).

The number of interacting nucleon pairs  $N_{coll}$  and the number of wounded nucleons  $N_{part}$  in nucleus–nucleus collisions characterizes the collision centrality [4]. Centrality determines the overlap volume of colliding nuclei and is related to the impact parameter of the collision (Fig. 1).

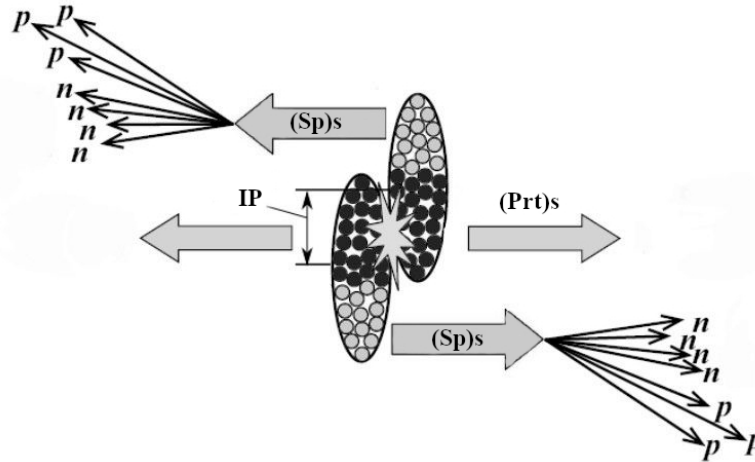


Fig. 1. Schematic representation of nuclear reaction: spectators (Sp)s; participants (Prt)s; impact parameter IP  
Interacting nucleons (black circles) and non-interacting nucleons (gray circles) are shown;  $p$  are protons,  $n$  are neutrons

The overlap volume is in turn related to the number of nucleons participating in the interaction  $N_{coll}$  and the number of wounded nucleons  $N_{part}$  located in this volume and experiencing inelastic scattering. The values of  $N_{coll}$  and  $N_{part}$  cannot be determined experimentally for each collision of nuclei (event). However, even earlier data obtained at the RHIC (Relativistic Heavy Ion Collider) and SPS (Super Proton Synchrotron) accelerators [5, 6] showed that the multiplicities of particles (or their total transverse energies) are directly proportional to  $N_{coll}$  and  $N_{part}$ . This means that  $N_{coll}$  and  $N_{part}$  can be determined for the given multiplicities (or total transverse energies).

The goal of this study was to develop an optimal machine learning model allowing to predict the unobservables characterizing centrality.

These unobservable quantities are the number of wounded nucleons involved in the interaction and the number of binary nucleon–nucleon collisions.

The prediction should be based on the quantities observed in the experiment: the number of charged particles and the number of neutrons generated in each individual nucleus–nucleus interaction.

### Simulation and computational technique

The machine learning model should predict the number of wounded nucleons  $N_{part}$  and the number of binary nucleon–nucleon collisions  $N_{coll}$  in a nucleus–nucleus collision at a given initial energy. The numbers of charged and neutral particles in each event in the pseudo-rapidity ranges  $3 < |\eta| < 4$  and  $5 < |\eta| < 8$ , respectively, were chosen as the model parameters. The ranges were selected based on the experimental data, taken close to those used in experiments [2, 7]. The number of protons and the number of neutral particles in interacting nuclei were added to the above parameters to extend the functionality of the model for various collision systems.

Because it is impossible to determine the quantities  $N_{part}$  and  $N_{coll}$  experimentally,  $N_{part}$  and  $N_{coll}$  taken for training were preliminarily obtained in this study using the PYTHIA8/Angantyr 8.307 Monte Carlo generator [8].

The center-of-mass energy per nucleon pair was chosen equal to  $\sqrt{s_{NN}} = 200$  GeV for all nucleus–nucleus collisions considered. This energy is used in a large number of experiments at the RHIC collider [2].

The number of nucleus–nucleus collisions generated was 100,000.

From the standpoint of machine learning, prediction of  $N_{part}$  and  $N_{coll}$  depending on the multiplicity of charged particles  $N_{ch}$  and neutrons  $N_{neut}$  is a regression problem [9] (supervised training). For this reason, the methods most commonly used for this type of problems were selected and considered as machine learning models: linear regression [10], polynomial regressions of different degrees [10], decision tree [11], random forest [12] and multilayer perceptron [13].

Hyperparameters of the models (the parameters that are not determined during training) were selected using the Optuna library [14]. Tree Parzen Estimators was chosen as the algorithm [15].

The determination coefficient  $R^2$  [16] characterized the prediction accuracy of the models, following the expression

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

where  $y_i$  are the reference values (for example,  $N_{coll}$ ),  $\hat{y}_i$  are the values of  $N_{coll}$  predicted by the model,  $N$  is the number of values.

The maximum value of the determination coefficient  $R^2$  is equal to 1. The closer it is to 1, the closer the values obtained using the model are to the reference values. The model's prediction quality for  $N_{coll}$  and  $N_{part}$  was characterized by the arithmetic mean of their determination coefficients (since we intended to predict the values of two quantities).  $R^2$  refers to this arithmetic mean from now on.

The confidence intervals and errors of the determination coefficient  $R^2$  were found by the bootstrap method [17].

This numerical method allows to analyze statistical distributions. It is based on repeated Monte Carlo generation based on the available sample (introduced in 1977 by Bradley Efron and consisting in generating an empirical distribution [18] based on the available sample). Using the empirical distribution as a theoretical probability distribution allows generating a large number of pseudo-samples of arbitrary size via a random number generator. The resulting set of pseudo-samples is used to estimate the mean value and the error, constructing a confidence interval for the considered random variable with a confidence probability  $p = 0.997$ .

$N_{coll}$ ,  $N_{part}$ ,  $N_{ch}$  values can be obtained for each nucleus–nucleus interaction (100,000 collisions generated in PYTHIA8/Angantyr were taken). This is used to construct the dependence of  $N_{coll}$ ,  $N_{part}$  on the multiplicity of charged particles  $N_{ch}$  for the collision of gold nuclei (Au + Au) at an energy  $\sqrt{s_{NN}} = 200$  GeV (initial data).

Fig. 2,*a* shows the dependence of  $N_{coll}$  on  $N_{ch}$ , obtained in the manner described here. Evidently,  $N_{coll}$ ,  $N_{ch}$  have certain distributions that occur during simulation in the PYTHIA8/Angantyr package. To accelerate the training and optimize the performance of the models, these distributions of quantities were divided into 50 intervals, each characterized by a specific average value of a physical quantity. Fig. 2,*b* shows such an averaged dependence for the number of nucleon–nucleon collisions  $\langle N_{coll} \rangle$  on the average multiplicity of charged particles  $\langle N_{ch} \rangle$ .

The resulting 50 intervals were randomly divided into 80% for training the models and 20% for testing them.

A similar computational pattern appears for the dependence of  $N_{part}$  on  $N_{ch}$ .

### Comparison of linear and polynomial machine learning models for predicting the dependence $N_{coll}(N_{ch})$ in Au+Au collisions

As mentioned above, the following machine learning models were used: linear regression, polynomial regressions of various degrees, decision tree, random forest and multilayer perceptron.

**Linear and polynomial regression.** Let us start our consideration with the simplest of the above models. Quadratic and cubic functions were chosen as models of polynomial regression to avoid overfitting the model at higher degrees of the polynomial [19]. For comparison, a collision system of gold nuclei (Au+Au) was considered at the interaction energy  $\sqrt{s_{NN}} = 200$  GeV.

Fig. 2,*a* shows the dependence of the number of nucleon–nucleon collisions on the multiplicity of charged particles approximated by linear, quadratic and cubic functions. Fig. 2,*b* shows the dependence of the average number of wounded nucleons  $\langle N_{coll} \rangle$  on the average multiplicity of charged particles  $\langle N_{ch} \rangle$  approximated by the same three functions.

Analyzing the data in Fig. 2, we can conclude that the approximation by a linear function systematically overestimates the number of wounded nucleons at high multiplicities of charged particles. For this reason, we only consider the computational results for polynomials of the 2nd and 3rd degrees.

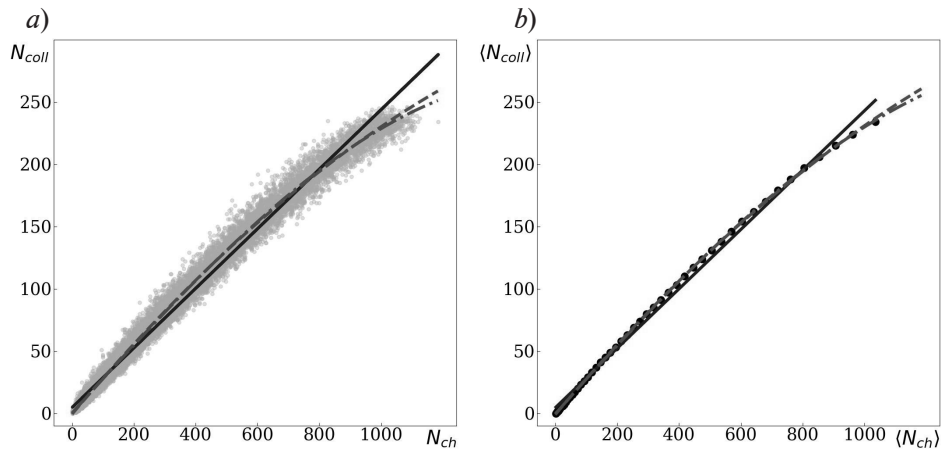


Fig. 2. Initial (gray area) (*a*) and averaged (symbols) (*b*) computational dependences for the number of nucleon–nucleon collisions of gold nuclei versus the initial (*a*) and averaged (*b*) multiplicity of charged particles; data approximation by various functions: linear (solid lines), quadratic (dashes) and cubic (dash-dotted lines)

### Predictions made by machine learning models for the $N_{coll}$ ( $N_{ch}$ ) dependence for heavy ion collisions

To estimate the capabilities that the models have for generalizing the dependences and determining them, let us consider training on symmetric collision systems: copper (Cu + Cu), xenon (Xe + Xe), gold (Au + Au), lead (Pb + Pb) and uranium (U + U), subsequently testing them on asymmetric systems (see Table 1).

Here we give a dependence of  $R^2$  for various models and various collisions systems on which the models were not trained. As follows from analysis of the data in Table 1, the results produced by the 3rd degree polynomial dependence are noticeable worse for most heavy ion collision systems, and differ from those given by other models. The determination coefficient  $R^2$  in many systems is significantly less than unity for such a model. Therefore, it seems ill-advised to further consider this model.

The obtained values of the determination coefficient coincide within the error for all models (except for the 3rd degree polynomial) within the same system (see Table 1). An exception is observed for polynomial regression of the 3rd degree, for which the value of  $R^2$  is statistically significantly different from other models.

### Predictions for collisions of light-heavy nuclei

This section considers training of the models on light-heavy ion collisions

$$p + Au, p + Cu, d + Au, d + Cu, He + Au, He + Cu,$$

where  $p$  are protons,  $d$  are deuterium nuclei.

The models are also verified on asymmetric systems given in Table 2. This situation is interesting as it allows to carry out further generalization to various (different from the ones previously considered) collision systems and to check how well the models can perform in this case.

Table 1

**Determination coefficients for various models and non-symmetric collision systems**

Collision system	Determination coefficient $R^2$				
	Polynomial		Decision tree	Random forest	Multilayer perceptron
	2nd degree	3rd degree			
Cu + Xe	0.990±0.025	0.175±0.005	0.979±0.030	0.981±0.021	0.967±0.023
Cu + Au	0.986±0.023	-2.301±0.328	0.963±0.024	0.969±0.028	0.934±0.025
Cu + Pb	0.984±0.026	-0.087±0.442	0.960±0.027	0.963±0.026	0.926±0.024
Cu + U	0.982±0.029	0.460±0.769	0.960±0.026	0.961±0.031	0.921±0.024
Xe + Au	0.997±0.028	0.155±0.004	0.991±0.027	0.992±0.030	0.987±0.029
Xe + Pb	0.996±0.026	-0.284±0.013	0.990±0.026	0.991±0.027	0.984±0.029
Xe + U	0.996±0.028	-0.224±0.119	0.987±0.029	0.989±0.026	0.977±0.022
Au + Pb	1.000±0.031	0.999±0.025	0.998±0.024	0.999±0.026	0.999±0.030
Au + U	0.999±0.024	0.901±0.024	0.998±0.030	0.998±0.027	0.996±0.027
Pb + U	0.999±0.027	0.963±0.026	0.998±0.027	0.998±0.031	0.997±0.028

Note. Data are given for verification of the models for collision systems on which the models were not trained.

Table 2

**Determination coefficients for four models and for systems of light-heavy ion collisions**

Collision system	Determination coefficient $R^2$			
	2nd degree polynomial	Decision tree	Random forest	Multilayer perceptron
$p + U$	0.511±0.016	0.988±0.031	0.965±0.026	0.953±0.026
$p + Xe$	0.978±0.029	0.990±0.028	0.973±0.026	0.947±0.026
$d + Pb$	0.856±0.022	0.996±0.028	0.987±0.027	0.983±0.027
$d + U$	0.507±0.015	0.996±0.023	0.983±0.027	0.983±0.026
$d + Xe$	0.990±0.031	0.988±0.024	0.982±0.024	0.973±0.022
He + Pb	0.863±0.023	0.996±0.033	0.990±0.026	0.991±0.024
He + U	0.597±0.016	0.993±0.026	0.977±0.026	0.992±0.024
He + Xe	0.989±0.030	0.989±0.026	0.982±0.024	0.983±0.023

Note. Data are given for verification of the models for collision systems on which the models were not trained.

Table 2 shows the dependence of the determination coefficient for the models considered in this paper and various nuclear systems on which the models were not trained. It follows from the data in the table that the 2nd degree polynomial dependence gives noticeably worse (statistically validated) results, unlike other models. The determination coefficient for this model is significantly different from unity in many systems. As in the first case, it seems impractical to consider it further.

The obtained values of the determination coefficient coincide within the error for all other models (except for the results for the 2nd degree polynomial) within the same system.

**Generalized case**

It is of the greatest interest to apply the models to interactions of both light-heavy and heavy-heavy nuclei. The models were trained for such situations on a range of collision systems of both light and heavy nuclei, considered in the previous two sections:





Cu + Cu, Xe + Xe, Au + Au, Pb + Pb, U + U;

$p + Au, p + Cu, d + Au, d + Cu, He + Au, He + Cu.$

The prediction accuracy was verified on the collision systems listed in Table 3. The Table also gives values of  $R^2$  for different models, depending on the collision system. Analyzing the obtained results, we can conclude that all models yield similar values of the determination coefficient within the error.

Table 3

**Generalized computations of determination coefficients for three models and various collision systems that did not participate in the training**

Collision system	Determination coefficient $R^2$		
	Decision tree	Random forest	Multilayer perceptron
$p + U$	0.984±0.030	0.954±0.026	0.955±0.026
$p + Xe$	0.984±0.029	0.960±0.024	0.956±0.025
$d + Pb$	0.996±0.027	0.982±0.024	0.990±0.026
$d + U$	0.990±0.024	0.974±0.025	0.987±0.025
$d + Xe$	0.984±0.022	0.971±0.023	0.971±0.026
He + Pb	0.997±0.026	0.985±0.024	0.991±0.029
He + U	0.993±0.026	0.981±0.029	0.990±0.030
He + Xe	0.985±0.024	0.987±0.032	0.987±0.026
Cu + Xe	0.980±0.025	0.982±0.031	0.990±0.027
Cu + Au	0.969±0.023	0.965±0.025	0.983±0.023
Cu + Pb	0.965±0.027	0.961±0.025	0.981±0.029
Cu + U	0.959±0.024	0.959±0.023	0.980±0.027
Xe + Au	0.991±0.023	0.992±0.029	0.996±0.024
Xe + Pb	0.991±0.027	0.991±0.029	0.995±0.028
Xe + U	0.988±0.026	0.987±0.025	0.993±0.026
Au + Pb	0.999±0.027	0.999±0.027	0.999±0.023
Au + U	0.997±0.028	0.998±0.026	0.998±0.025
Pb + U	0.998±0.025	0.999±0.030	0.999±0.028

### Conclusion

We carried out a comparative analysis of machine learning models to determine the optimal algorithm for obtaining experimentally unobservable parameters characterizing the collision centrality, specifically, the number of wounded nucleons and the number of binary nucleon collisions, based on observable quantities, i.e., the multiplicity of charged particles and the number of neutrons produced in the collision. We adopted models of polynomial regression of different degrees, decision tree, random forest and multilayer perceptron.

It was established in the analysis that the decision tree, the random forest and the multilayer perceptron predict the values of  $N_{part}$  and  $N_{coll}$  with the greatest accuracy ( $R^2 \gtrsim 0.95$ ), which is to say that these models yield equally good results (within uncertainty) for a fixed initial energy.

We propose an additional parameter that is the initial energy of colliding nuclei  $\sqrt{s_{NN}}$  to be introduced as a natural continuation of this study to expand the applicability range of the considered models to an arbitrary range of initial energies.

The computations were run on an Intel® Core™ i9-9980XE processor and an NVIDIA GeForce RTX™ 2080 Ti video card. RAM was 64 GB.

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*Received 18.01.2023. Approved after reviewing 30.01.2023. Accepted 31.01.2023.*

*Статья поступила в редакцию 18.01.2023. Одобрена после рецензирования 30.01.2023. Принята 31.01.2023.*