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Application and Challenges of Machine Learning Techniques in Mining Engineering and Material Science

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Abstract

The ultimate objective of modern engineering applications in mining and material science is to develop good quality novel materials with desirable qualities. Machine Learning (ML) is used in the mining industry to provide solutions to complex problems of the mining industry and improve the efficiency of the overall system. ML methods are increasingly being used by materials scientists to uncover hidden trends in data and generate predictions. Furthermore, data centric techniques can provide useful insights into the basic processes that influence material behaviour while simultaneously reducing human labour in large data processing. The ability of persons to find new materials and infer complex relationships is important for the development of new materials. Large amounts of machine-readable data must be available to use statistical methodologies to speed materials research. In mining engineering, ML can be used for analyzing geographical data, assessing the risk of rock fall, predicting equipment failures and impact of mining activities on the environment etc. Material science data may be used in a variety of ways, including property prediction, the search for new materials and discovering synthesis methods. Selecting proper machine learning techniques to provide solutions is very important and that is discussed here. The purposes of this paper are to provide a comprehensive list of different ML techniques which are applied for the mining and material science domain.

Keywords: *AI, Data Science, Engineering, Machine Learning, Material Science, Mining*

1.0 Introduction

As innovation goes higher than application of that new technology in industry also goes next level with new direction. Artificial Intelligence (AI) is one of the prominent areas which are used in many fields to achieve high efficiency with less human interventions. Machine learning methods may be used to apply AI to a range of industries. Machine Learning (ML) techniques are applied in different techniques like medical diagnosis and medicine recommendation, crop recommendation in agriculture, marketing, supply chain management, self-driving cars, speech reorganization, mining engineering, material science, fraud detection and prevention etc. For a variety of applications, machine learning techniques are used in mining and material science in that most common one is prediction of quality of mined metal, equipment failures and impact of mining activities on environment

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Figure 1. Machine learning in mining[2].

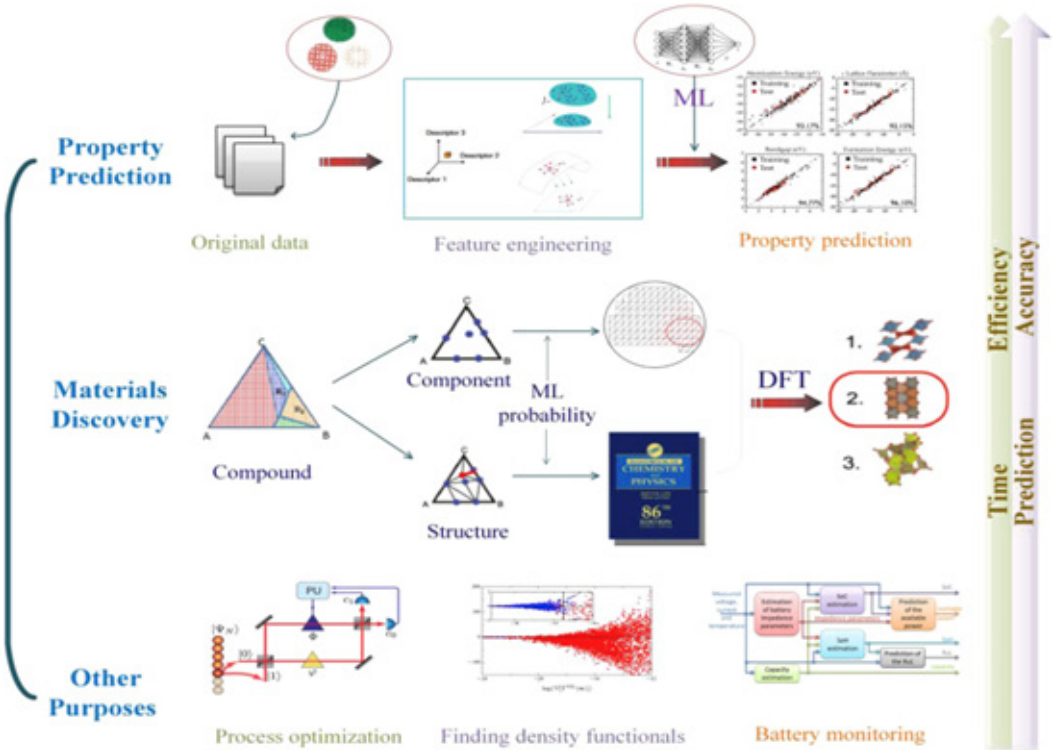

Figure 2. Application's of the ML in materials science domain[5].

and materials properties with the goal of finding new materials. Since 2018, there has been significant activity in using machine learning in the mining industry, particularly in the field of mineral exploration, primarily driven by the abundance of available data[1]. Figure 1[2] shows an overview of machines in the mining industry. The mining industry is characterized by its dynamic nature as well as where frequent fluctuations are common, which are accompanied by uncertainties regarding resource prices, volatile resource fields, and the management of large projects throughout their entire life cycles. Mining companies have profited from the application

of ML techniques in discovering valuable minerals for extraction. Many review articles give overviews about this[3,4].

Repeating theoretical and experimental characterisation investigations are generally extensive and it takes a long time to find new materials. As shown in Figure 2, novel (new) materials research is divided into different stages and various scientific teams are involved in it. Even though skilled people are involved in every phase, but limited possibilities are there for reutilizing the input between earlier and later phases but if we do so we can accelerate the overall process[5]. Presently, numerous outstanding review papers which give information on materials science research using machine learning[6]. The review paper[7] gives an outline of the state-of-the-art in the subject of continuous materials mechanics in terms of machine learning and statistical learning methodologies. A wide range of relevant investigations are presented in paper[8], demonstrating that ML may be applied to construct efficient as well as accurate materials. There are a variety of challenges that exist when we use data and data analytics methods in material science research[9,10] and article[11] presents a future materials innovation ecosystem in a forwarded direction of data informatics.

In recent years the area of ML expanded in material informatics[12]. Given the quick pace of change in this industry, it's difficult to grasp both the scope of opportunities and the best techniques for implementing them. In this paper tried to deliver a summary of the areas in which ML had a significant impact in materials science domain and evaluation metrics used in ML models. Finally try to explore a few of the potential problems and challenges that the materials society has in effectively utilising machine learning's capabilities.

ML applications in discovery of materials and design fall into three categories: prediction of material properties, new material innovation, etc. The primary idea behind this is to find novel materials to perform better.

2.0 Machine Learning Approaches

Applications of ML and AI to materials science are now common. Applying machine learning techniques involves many steps. i.e., shown in Figure 3.

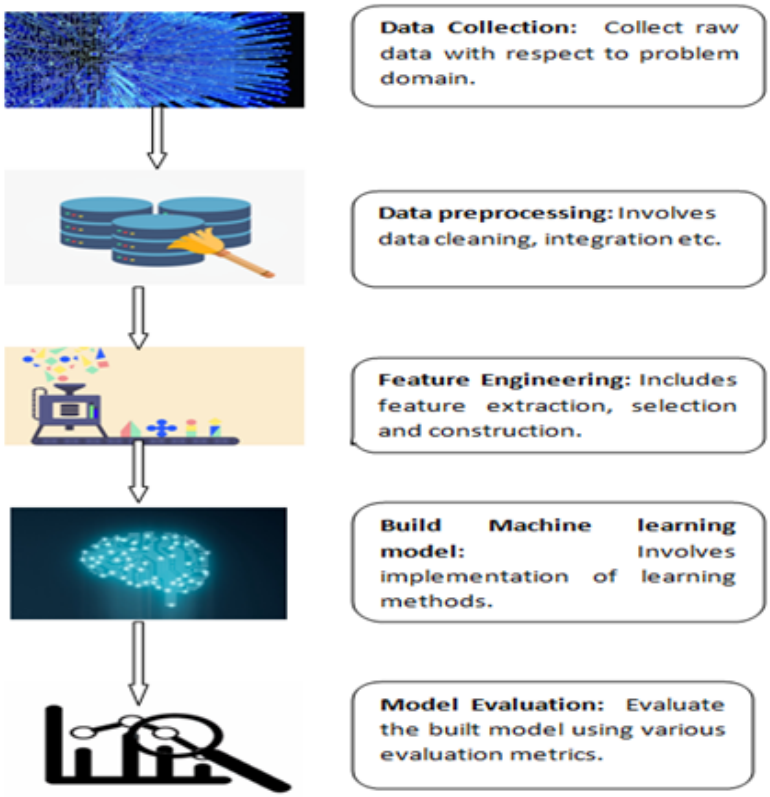

Figure 3. Basics process of machine learning.

2.1 Data Collection

Data collection is an important step of ML and that rests on "quality" and "quantity" of the data and collection of such types of data is a major challenge in material informatics. Quality and quantity of the datasets used for the training the ML algorithms plays an important role in order to create precise ML models. Identification of training experience is the first step of the ML model. This identification or gathering or creation of the training dataset mainly depends on how we want to train our model. The data was obtained from either publicly accessible open sources or individually collected for private data. There are a variety of datasets freely available for generic purposes in different platforms such as Kaggle[13] and UC Irvine Machine Learning Repository[14].

The use of ML techniques in the mining industry evolved tremendously due to large availability of the data. The mining data set is available through various resources like data.world[15], which provide data related to the number of mineral mines, agricultural minerals, ferrous metal mines, mines and mineral resources, global mining location data, nonferrous metal processing plants, etc. Spatially explicit estimates of the area utilized for surface mining on a global level are provided by Global Mining Areas and Validation Datasets. This dataset comprises over 21,000 polygons representing mining activities, primarily focused on coal and metal ores. Multiple data sources were combined to determine the approximate locations of active mines between 2000 and 2017[16]. The dataset[17], provides comprehensive data on the global extraction of coal and metal ores at the level of individual mines. It encompasses information from 1171 mines across 80 countries, detailing production figures for 80 different materials between the years 2000 and 2021. Kaggle provides a dataset for quality prediction of mining process[18], though this percentage % of silica in the iron ore concentrate can be predicted.

There are a variety of datasets accessible in the materials sciences. In that many of them are free and other need a paid membership to use part or all of their services. In that few datasets are focusing on structural evidence and some on chemical/ physical attributes of materials. University of BATH[19] provides various engineering science data. In that material science data is also available with respect to computational materials research, nanotechnology related data and electronic-structure data from density-functional theory. Open dataset is available for a variety of materials[20]. The ubiquitous Cambridge Structural Database (CSD)[21], contains millions of crystal structures dataset and inorganic crystal information available in Inorganic Crystal Structure Database (ICSD)[22], COD[23] and ICDD[24], and many others also available for chemical systems, such as GDB7[25] for small organic molecules and ZINC8[26] virtual screening of compounds. Figshare contains 3 types of datasets i.e. dilute solute diffusion, pervoskite stability of perovskite materials and metallic glasses dataset[27]. The majority of these databases provide both a web front-end and an Application Programming Interface for easy exploration and visualisation of data.

2.2 Data Pre-processing

When it comes to enormous datasets, we need to remember "four V's," i.e. volume, variety, veracity and velocity of data. As a result, data must be normalised and cleansed before being used. Before proceeding further, handling missing or inconsistent data is very important to get accurate results.

2.3 Feature Engineering

Using statistical or machine learning methodologies, feature engineering transforms raw data into desired features. Material science research features must be capable of capturing all essential data like properties of materials. The amount of processing required strongly depends on the algorithms which we use. The extraction of features not required for deep learning approach[28]. Naturally, the optimum representation relies on the target extent as well as the diversity of the occurrence space. Descriptors should ideally be uncorrelated, as many correlated characteristics might reduce the model's efficiency and accuracy. Further feature selection is required to avoid the dimensionality reduction[29]. When it comes to image data, there are four categories of characteristics: geometric features, statistical features, texture features, and colour features need to be extracted[30].

2.4 ML Model Design

Machine learning models are designed to perform various tasks like prediction, classification etc. ML algorithms are

mainly categorized into three groups i.e., Unsupervised, Supervised and Reinforcement learning.

2.4.1 Unsupervised Learning

It refers to using the AI concept to group the patterns in the data without using training dataset and this is applied when no class labels are obtainable or used when we don't know exactly what you're looking for. Principal component and cluster analysis are the two main methods which are used in machine learning applications. It takes an enormous amount of time to evaluate today's rapidly expanding datasets in the manufacturing industry and make inferences from them. Engineering materials are grouped together based on material similarity. In this experiment, the K-means algorithm was applied for clustering[31]. Research article presents unsupervised learning algorithms such as k-means and CLARA. These algorithms are used to group mine planning blocks into clusters based on their similar grades, but with dissimilar processing destinations[32]. Machine learning techniques are utilized to address numerous challenges in surface lignite mining operations. In this context unsupervised machine learning is applied to mineral exploration and enhancing mine planning through image analysis. Specifically, unsupervised machine learning proves valuable in interpreting satellite images for both deposit exploration and assessing the environmental impact[33]. Predictive model of materials depends on the features selected and clustering can be used for selection of optimal feature set. In this experiment K-Means, agglomerative, and density-based clustering is used to categorize clusters in a diverse set of 425 silver nanoparticles[34]. Understanding the trends, associations, and linkages in material data sets, as well as presenting conclusions to others, depends heavily on data visualization. In an experiment, self-organizing maps or Kohonen networks are used to help visualize the nanoparticles of silver and platinum grounded on structural similarities and to uncover hidden patterns. Both approaches may be used with computational data as well as experimental results, and they may be helpful in identifying patterns related to more complex combination, processing, or operational settings[35].

2.4.2 Supervised Learning

This learning algorithm is mainly used for classification and prediction tasks. In supervised learning, the first model is trained with known data (Training Data) and tested with unknown data (Test Data). "Cross-entropy" and "negative log-likelihood" are the most prevalent loss functions for classification tasks, whereas "root mean squared error" and "root mean absolute error" are frequently employed for regression assignments. Many works done on mineral exploration in the mining industry using ML techniques based on geological data. Where geochemical survey data and deep learning techniques are used[36]. This article[37] presents a study comparing the effectiveness of different machine learning techniques for perceiving geochemical irregularities allied to mineralization. The techniques evaluated include an incongruity gauge, a semi-administered classifier, and a managed classifier, completely built on the KNN algorithm. To evaluate their effectiveness in accurately identifying geological rock types in an area with complete ground validation information, several ML algorithms such as Naïve Bayes, k-nearest neighbor, random forest, and support vector machines are compared[38]. ML is used in mineral processing and also used in mineral processing for prediction and potential difficulties of separation and the identification of minerals[39,40]. For mineral studies, Support vector machine, random forest, and artificial neural networks are frequently used supervised learning algorithms[41]. In the research paper, PSO-ELM used for prediction rockbrust and obtained good result which shows direction for future study in this field[42]. In recent research paper for rockbrust prediction SVM, BP, RBF, RF, ELM and global optimization algorithm is used also achieved good result[43].

ML is used in the material science in material classification, large-scale simulations and calculations, construction of DFT functional, and property prediction and material design have gotten a lot of attention[44-46]. Mechanical material qualities must be properly anticipated and well-ordered because which are closely connected to and influenced by progression constraints and microstructures[47]. These data-driven techniques in materials science have a lot of potential. ML presentations for metallic material representation

are discussed in the following review. Many factors relating to material processing and structure have an impact on the qualities and performance of produced components[48]. The practice of administered ML to foresee the mechanical characteristics of materials depending on their microstructural pictures is investigated[49]. ML models are used to foresee the mechanical characteristics of graphene-armoured metal matrix nanocomposites, experiment out of many ML models, G-SVM gives the furthermost precise result although it comes at a greater computational cost[50]. The mechanical properties of fibre composites were predicted using supervised ML approaches, and the observed ML model was capable of correctly predicting the homogenised characteristics of random microstructures correctly[51]. The UTS of a material is the extreme force it can bear beforehand failure. For the ultimate tensile strength of the material, ANN and K-nearest-neighbor method were used, and it was discovered that ANN performs better[52]. The effects of composition and processing factors on the strength, impact toughness, and ductility of API grade micro alloyed channel steel is investigated in article[53]. The link between composition and processing factors and mechanical qualities is determined using ANN models, which are adept of likelihood and diagnostics in nonlinear and multifaceted systems. The function of different aspects in building pipeline steel with such increased performance was successfully studied with respect to various parameters. Locally weighted regression algorithm was fruitfully applied in determining the tensile power of steel is a hot-rolled concept[54,55].

From "chemical composition, heating, rolling, and chilling temperature" various 18 parameters were chosen as inputs. The output variable and these factors have a definite physical contributory link. In addition, least squares SVMs are effective methods for predicting materials' elastic modulus and yield stress. Machine learning algorithms have been identifying connections and patterns from enormous volumes of complicated data for decades. The materials science society has recently begun to participate in these approaches in order to excerpt information and intuitions from collected data. Many advancements in computational methods, such as DFT[56], have occurred. DFT has been used in atomic, molecular, and chemical systems, as well as extended solids, surfaces, defects, and 0D, 1D, and 2D systems. Structure, electronic/transport, thermal, electron–phonon, optical, catalytic, magnetic, topological, and other features have all been investigated[57]. Thermodynamic Permanence prediction of solids materials DFT and ML is one of the important areas where many works are going on. Work started with analysing a data set that comprises DFT intentions of around 250,000 cubic perovskite systems. The findings imply that by narrowing the space of important chemical compositions, machine learning may be utilised to rapidity up extraordinary-amount DFT computations (by at minimum a factor of 5) without sacrificing accuracy[58]. Different prediction models of machine learning algorithms like NN, KNN, RF, SVM, DT and AdaBoost" classifiers are recognised to expect thermodynamic stability[59].

Materials property prediction helps in novel resources discovery. The use of ML algorithms to aid the discovery of record-breaking supplies is demonstrated in article[60]. Despite their failure to discover novel chemistries, the models are quite good at recognising the unusual (extraordinary) compositions in the dataset we used. The identification of new ternary compounds can be considerably accelerated using an iterative mix of ML approaches and first-principles computations[61]. This research[62] highlights the critical need to improve the exploratory capacity of present ML algorithms for novel material discovery. Introduced a set of k-fold-m-step Forward Cross-Validation (kmFCV) techniques as a novel way to evaluate machine learning algorithms for exploratory prediction. Modern chemistry and materials research rely heavily on atomic and automated assembly replications created on quantum theoretical computations. Simulations may be speed up using machine learning models, allowing for greater period and span scales. Their productivity of the developed exemplary be contingent strongly on the proposal and dataset cast-off for the process. In this area many research work happened by using ML techniques and in article[63] tried to consolidate such works. Many supervised machine learning algorithms are used in material science in recent years i.e Artificial Nueral Network[65,66], Naïve bayes[67,68], CART[69], SVM[70,71,72], bagging, AdaBoost, and RF regression[73].

2.4.3 Reinforcement Learning (RL)

RL is a different type of learning than supervised or unsupervised learning. An RL agent will get rewards when he moves from one state to another. The agent performs an activity that has an influence on the environment and results in a new state based on the present state. The scoring function evaluates the completed action, and the agent learns if this activity leads to a reward in the present state of the environment based on the reward.

A self-learning AI framework was proposed for copper mining operations, specifically for analyzing drilling machines and processing mill sensor data. This framework shows its practicality for real-time production planning with incoming new information in mining complexes[74]. Chemical species adapted to highly specific demands are produced through molecular discovery. In this article, researchers introduce ORGANIC, a context built on Objective-Reinforced GAN that may produce a spreading across molecular space that corresponds to a certain set of necessary metrics. A model that combines a GAN to generate non-repetitive sensible molecular species and RL to bias this generative distribution to some attributes[75]. RL is applied to microstructure optimizations with the goal of identifying the underlying physical processes of improved functionality. According to this work, RL is a potential machine learning technique for problems involving material design optimization and for improving comprehension of the dynamics of microstructural simulations[76].

2.5 Model Evaluation

As previously stated, the basic purpose of ML algorithms is to train and develop an effective learned model that makes correct predictions. Calculated accuracy helps to

Table 1. Performance evaluation metrics

Evaluation Metric	Formula
Coefficient of Determination(R^2)	$R^2 = \frac{SSR}{SST}$
Mean Square Error(MSE)	$MSE = \frac{1}{N}\sum_{i=1}^{N}(Y_i - \dot{Y}_i)^2$
Root Mean Square Error(RMSE)	$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(Y_i - \dot{Y}_i)^2}$
Mean Absolute Error (MAE)	$\mathrm{MAE} = \frac{1}{\mathrm{N}}\sum_{i=1}^{n}\lvert Y_i - \dot{Y}_i\rvert$
Accuracy	$Acy = \frac{TP + TN}{TP + TN + FP + FN}$
Precision	$\mathrm{P} = \frac{TP}{FP+TP}$
Recall	$F1 = 2 * \frac{P * R}{P + R}$
F1-Score	$R = \frac{TP}{TP + FN}$

Note: SSR is "Sum of Squared Regression" and SST is "Sum of Squared total".

ensure that the model works accurately or not. While handling ML models, we need to know about how to handle the underfitting and overfitting of data. It's critical to strike a balance between underfitting and overfitting by adjusting the hyper parameters to build an ideal model. This crucial phase of fine-tuning hyper-parameters to get the best result is not always straightforward, since it takes efficient explorations, time and tolerance. To measure the performance of ML algorithms various statistical approaches are used, in that some listen with mathematical formulas in Table 1. These techniques display how the model fits with given data. They may also be used in sensitivity analysis to highlight the significance of each input variable in the prediction process. Statistical metrics may be used to analyze the success of machine learning approaches as well as to compare the effectiveness of various algorithms. To evaluate the overall performance of the classification model accuracy metrics is used.

3.0 Challenges

Machine learning is increasing its role in the mining and material science engineering field day by day due to requirements and demand. A mining industry contributing a large to global economy and mining sustainability, and achieving high efficiency is a challenging task due to environment and other external factors. ML are rapidly emerging as game-changing factors in the mining industry and this have the power to completely transform mining operations, enhancing efficiency, safety, and sustainability. A Materials informatics has evolved from a marginal field of research to a well-established subject, with different frontiers and finest practices for applying ML to materials development.

3.1 Data Collection

However, having a huge data volume is not simply advantageous; dealing with massive volumes of data may also be difficult. Due to significant advancements in sensors and data collection methods on the one hand, and storage technologies on the other, data are becoming increasingly easy to obtain and store. Many domains nowadays have no concerns about collecting massive volumes of data without understanding how they will be examined. The explosion of data may be seen with respect to total samples gathered in a given time, but also amount of attributes, or features, that are assessed instantaneously throughout the process. Now data is growing from single dimension to n-dimensions and dealing with that data also throws up lots of challenges. In the mining industry, the availability of historical data may be limited, particularly for newer mining sites or unconventional methods. This can impact the performance of the training model. Ensuring the efficiency of ML models relies deeply on the quality of data.

3.2 Feature Engineering

The use of feature engineering is important in supervised algorithms. The feature must be accessible, applicable, and machine-readable. The accuracy and computation time of the model are determined by choosing the proper feature vector. Underfitting may result from fewer features, whereas more features may increase computing costs. Therefore, choosing appropriate and pertinent elements from the real-world environment in the field of mining and material science is a difficult issue. Deep learning may be used in this way to improve outcomes from features without relying much on human input for feature building or feature selection.

3.3 Selection of Appropriate Algorithm

There is no prior rule that any algorithm works better for mining and material science research. Efficiency of the algorithm depends on the problem domain and dataset. We always need to work on various algorithms and then choose which algorithm gives the best solution to our concerned problem. So, selecting an appropriate algorithm is another challenging task.

In most cases, computers using ML/AI tools are superior to people at tasks like analyzing mining geographical data, predicting mine operation expenses, mineral analysis, material prediction, etc. But in between, human intuition will continue to be valuable for sanity checks and mistake reduction.

4.0 Conclusion

This paper comprises generic methodologies as well as their application to interpreting the complicated

interactions along the mining metals quality prediction, resource estimation, ore sorting and quality checking, geotechnical engineering in mining industry and in material science field composition, processing, structure and mechanical characteristics using machine learning techniques. This article outlines fundamental ideas of machine learning and each stage of the workflow with aims to provide a comprehensive list of different ML techniques which are applied for the mining and material science domain and challenges which need to be faced during mining and material science research. This paper has explained the problems regularly associated with applying machine learning and has provided appropriate guidelines for its effective application. Advanced ML and geospatial intelligence can create a huge impact on future research on mining engineering, which promotes sustainability with increased efficiency with effective handling of resources. ML techniques help the future scientists to work on material property prediction and molecular simulation.

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