

Machine Learning and Nanotechnology: How do they contribute to each Other

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Abstract

It is undoubtedly of great impression how some of the areas of evolving Computational Sciences, such as Machine Learning and the great and vast nanotechnology domain, can contribute to all-world research. Some examples are nanotoxicology in medicine and food regulation, using predictive models to study the biological activity of nanomaterials, characterization of nanoparticles, and against COVID-19, with the development of vaccines and nanosensors. The relationship between nanotechnology and machine learning was investigated through bibliometric analysis using articles registered in the Scopus database. The keywords “Machine Learning” and “Nanotechnology” were searched in the Scopus database to develop this work. Two hundred sixty-seven scientific articles were gathered using the number of publications per year, area of knowledge, and countries as search criterions. Then, the titles and abstracts of these papers were stored in Research Information Systems (RIS) format and went through automatic analysis by the software “Visualization Of Similarities Method” (VOS viewer) version 1.6.18., which gave us a notion of link strength produced by their intercorrelation network with maps of Clusters, which was followed by a numerical criterion. Due to the limitation of VOSViewer to integrate and process the data in tables, tree maps, or graphics, Python can import and filter the data. So, it is possible to create new forms of visualizing data and the relationship between them using Python software. The trendline that describes the volume of publications as a function of the year assumes a third-order polynomial behavior, with $R^2=0.9716$. Furthermore, the present work inferred the ten countries with the highest volume of publications that intersect the two areas between researched years. The United States, China, and the United Kingdom lead the volume of publications, with a significant difference between the amount of US publications and the subsequent ones.

Keywords: Machine Learning, Nanotechnology, Computer Science, Algorithms, Data Mining, Visualization Of Similarities Method, Python.

1. INTRODUCTION

Throughout the years, humankind has been living in the age of data. Today, everything is connected to a data source and digitally recorded. Extracting insights from these data can build intelligent applications in various relevant domains, such as Machine Learning and Nanotechnology.

Machine Learning (ML), an essential field in Artificial Intelligence, has been a critical factor in digital solutions. In ML, a computer program is requested to develop some tasks, and it is said that the machine has learned from its experience if its measurable performance improves as it gains more and more experience in executing these tasks. So, the machine makes decisions and predictions/forecasting based on data [1,2].

The essence of most ML algorithms is to build up, optimize models and learn the parameters in the objective function from the given data. The effectiveness and efficiency of numerical optimization algorithms dramatically influence the popularity and application of ML models [1,2].

According to the available technique with human supervision, they are classified as: “Supervised Learning”, “Unsupervised Learning”, “Semi-supervised Learning”, and “Reinforcement Learning” [2].

With regards to supervised learning, it requires prior knowledge of a training dataset to learn a link between the input as well as the expected output. The goal is to construct a classifier or regressor that can estimate the output value for previously unseen inputs. An excellent example of supervised learning is each training example of input data (color, shape, odor, etc.) paired with its known classification label (apple or orange) [3]. It allows the learner to deal with similarities and differences when the objects to be classified have many variable properties within their classes but still have fundamental qualities that identify them. Most importantly, the successful learner should be able to recognize an apple or an orange that it has never seen before. Examples of supervised learning techniques include Neural Network (NN), Supporting Vector Machine (SVM), Decision Trees (DT), etc [3,4].

In unsupervised learning, on the other hand, no specific output value is provided. Instead, one tries to infer some underlying structure from the inputs. For instance, in unsupervised Clustering, the goal is to infer a mapping from the given inputs (e.g., vectors of real numbers) to groups such that similar inputs are mapped to the same group [5,6]. Other examples of unsupervised learning include Self Organizing Maps (SOMs), Principal Component Analysis (PCA), and Probabilistic Latent Semantic Analysis (PLSA) [5-7].

Semi-supervised learning is the branch of machine learning concerned with using labeled and unlabelled data to perform specific learning tasks. Conceptually situated between supervised and unsupervised learning, it allows harnessing the large amounts of unlabelled data available in many situations combined with typically smaller sets of labeled data [7,8]. The main objective of semi-

supervised learning is to understand how combining labeled and unlabeled data may change the learning behavior and design algorithms that take advantage of such a combination. [8,9]

As is the case for machine learning in general, most of the research on semi-supervised learning is focused on classification. Semi-supervised classification methods are particularly relevant to scenarios where labeled data is scarce. In those cases, constructing a reliable supervised classifier may not be easy. [9,10] Semi-supervised learning models include self-training, mixture, co-training, and multiview learning [10].

Reinforcement Learning (RL) is the assignment of getting an “agent” that can observe the environment, select and perform actions, and obtain rewards in return (or penalties in the form of negative rewards). The agent then learns by itself what is the best strategy, called a “policy,” to get the most rewards over time; the policy defines what action the agent should choose when a particular situation is given [11].

In other words, it studies the systems that can be represented by an agent interacting with a dynamic environment by taking different actions to maximize its cumulative reward. The so-called agent has a specific state that belongs to a set of limited legal, possible states known as the “state space”. After choosing an action from the legal actions (actions set), the agent receives a reward (a numeric value) that depends on the chosen action and its current state. The environment determines state space and action set. RL systems might have more than one agent; in this case, it is called a Multi-Agent RL (MARL). Generally, RL systems can be formulated by using the Markov Decision Process (MDP) and the more generic form of it: Partially Observable Markov Decision Process (POMDP) [12].

In particular, it optimizes scientific discovery in various fields such as physics, chemistry, and biology. Moreover, physical systems, particularly quantum systems, may allow for more efficient reinforcement learning protocols to facilitate access to quantum states [13].

Machine learning is transforming all areas of science. The complex and time-consuming calculations in molecular simulations are particularly suitable for an ML revolution and have already been profoundly affected by the application of existing ML methods [14].

However, the model is just one component of the ML pipeline, which spans data collection, model selection, training algorithms and procedures, model evaluation, and deployment. One remarkably under-explored aspect of the evaluation and deployment components of the pipeline is the interpretability of performance metrics, such as accuracy, precision, or recall. This facility can help physicians to anticipate future events at an expert level, drawing from information well beyond the individual physician’s practice experience. [15,16]

Via an exploratory analysis, Yin and collaborators observed that after observing a model’s accuracy in practice, people are more likely to increase their trust in the model if the model’s observed

accuracy is higher than their accuracy [17]. Also, a meta-analysis using ML to predict sepsis in hospitals shows its accuracy and importance for other areas [18].

These results highlight the need for designers of ML systems to clearly and responsibly communicate their expectations about model performance, as this information shapes the extent to which people trust a model, both before and after they can observe and interact with it in practice.

Nanotechnology refers to any technology implemented at the nanoscale and has applications in the real world by controlling or restructuring matter at the atomic and molecular levels, in a size range of about 1 to 100 nm in at least one of their dimensions [19].

This field is recognized as an emerging enabling technology for the 21st century, besides the already established areas of information technology and biotechnology. This recognition is due to the scientific convergence of physics, chemistry, biology, materials, and engineering, allowing the control of matter in almost all technologies [20].

Nanotechnology is concerned with the development and utilization of structures and devices with organizational features at the intermediate scale between individual molecules where novel properties occur, such as physicochemical compared to bulk materials which imply the capability to build up tailored nanostructures and devices for given functions by control at the atomic and molecular levels. The material, therefore, might be nanostructured to increase performance or provide a specific performance in their properties [20,21].

In approximately half a century, nanotechnology has become the basis for remarkable industrial applications and exponential growth. For example, in the pharmaceutical communities of practice, nanotechnology has profoundly impacted medical devices such as diagnostic biosensors, drug delivery systems, and imaging probes. In the food and cosmetics industries, the use of nanomaterials has increased dramatically for improvements in production, packaging, shelf life, and bioavailability [22].

Adapting some computational tools, methodologies, and algorithms to some particular needs in nanotechnology brings a better understanding of potential adverse effects, interactions in biological and environment, properties, and ways to reduce or improve them. Some examples of its use are projects NanoSolveIT & NanoCommons [23].

NanoSolveIT is developing a nanoinformatics framework that includes innovative multiscale methods, tools, and systems developed to exploit available and emerging data on NMs physicochemical, fate and transformation, release & exposure, and (eco) toxicological properties, including mechanistic insights gained from systems biology approaches. At the same time, NanoCommons builds the European nanotechnology community informatics platform. In order to reach even larger scales and biological events, the approach being developed is to combine physics-based multiscale modeling for the calculation of advanced descriptors and properties of NMs with

nanoinformatics methods for the evaluation of their complex properties and functionalities [23,24].

For a better understanding of the relationship between Machine Learning and Nanotechnology, the terms presented in the titles and abstracts of articles found in the Scopus database were analyzed using the VOSViewer (Visualization of Similarities (VOS)) software [25].

VOS viewer is a software tool for building and visualizing 2D bibliometric maps. It allows the creation of networks of citation relationships, bibliographic coupling, co-citation, or co-authorship; the software shows the total link strength between the nodes of each Cluster generated, as well as the relevance and occurrence of terms [25].

The closer the nodes, the more correlations they have with each other. VOSviewer map and network files are tab – delimited text files for storing a network. A map file contains information about the items in a network. Items are characterized by attributes. A network file contains information about the links between items. Each line in a network file corresponds to a link. If a network file contains multiple links between the same pair of items, VOSviewer will merge these links into a single combined link. The strength of the combined link will be equal to the sum of the strengths of the individual links [25].

Due to the limitation of VOSViewer to integrate and process the datas in tables, tree maps or graphics, Python can be used to import the datas and filters them. So, it's possible to create new forms of datas visualization and the relationship between them using a software made in Python language.

The search in the Scopus database using the term “VOSViewer” returned 3183 documents, of which 2038 were articles. The first publication is from 2009. Besides, the bibliometric mapping regarding VOSViewer covers large areas of science, such as Social Sciences (14.8%), Medicine (12.8%), Computer Science (10.2%), Business, Management, and Accounting (8.4%), Engineering (8.1%), Environmental Science (8.1%), Energy (4.4%), Arts and Humanities (3.5%), Biochemistry, Genetics and Molecular Biology (3.3%), Agricultural and Biological Sciences (3.2%) and others (23.2%).

The search data shows that VOSViewer is a multidisciplinary tool and can be used in diverse areas, including Nanotechnology. Among the three countries that most used this software, China leads with 942 documents, followed by India with 342 and the United States, which contributed with 237 documents.

So, the study aims to export the data from the Scopus database in RIS format, create bibliometric maps using the keywords “Nanotechnology and Machine Learning.”; and process those maps and network files from VOSviewer using Python software. And then look for the relationship between nanotechnology and machine learning and how they contribute to each other.

2. METHODS

A search using the keywords nanotechnology and machine learning was performed in the Scopus database using the key TITLE-ABS-KEY ("nanotechnology") AND "machine learning" AND (LIMIT-TO (DOCTYPE, "ar")). This search returned 267 articles used for bibliometric analysis by VOSViewer software. Then, the gathered information was classified by the number of publications per year, area of knowledge, and country using the Scopus Database tools.

Then, the RIS file from Scopus was processed using the VOSviewer software, v. 1.6.18 [25], producing a Clustering map from which the two most prominent nodes of the two biggest Clusters were used in a second Scopus search without document type limitation. The bibliometric classification was made in the "overlay" and "network" modes. Additionally, the files were exported as NET and MAP for average publication time (overlay map) and subjects (Cluster map) classification, respectively. Data from MAP files were sorted by Cluster size and total link strength. The top-five nodes for each Cluster were selected and plotted.

3. RESULTS AND DISCUSSION

Nanotechnology profoundly impacted recent developments in several areas of science and industry. The possibility of controlling matter at the nanometer scale continues to significantly boost innovation in areas such as electronics, physics, and medicine [26, 27].

The development of new materials with unique characteristics, new and more effective drugs in fighting diseases and new sensors for more optimized toxicity assays are some examples of recent progress enabled by nanotechnology. However, mastering the control of this scale is a significant challenge [28]. This challenge resides in the physical limitations and the manifestation of complex quantum phenomena on this scale, which are not yet been completely elucidated. In this context, artificial intelligence techniques, such as machine learning, have helped the development of nanotechnology by allowing both the overcoming of physical limitations associated with experimental research and the progressive elucidation of complex physical phenomena [29].

The study of parameters associated with nanosystems by machine learning also allows time optimization associated with research and its costs by reducing the minimum number of experiments and the need for skilled labor [30].

The relationship between nanotechnology and machine learning was investigated through bibliometric analysis using articles registered in the Scopus database. The growing interest in the contributions of nanotechnology and machine learning can be seen from the graph of the volume of publications per year relevant to these two areas. The search for the keywords "Nanotechnology" and "Machine Learning" in the Scopus database results in 267 articles and shows an upward trend between 2004 and 2022, with significant growth from 2018 onwards, as **Figure 1** shows. The

trendline that describes the volume of publications as a function of the year assumes a third-order polynomial behavior, with $R^2=0.9716$.

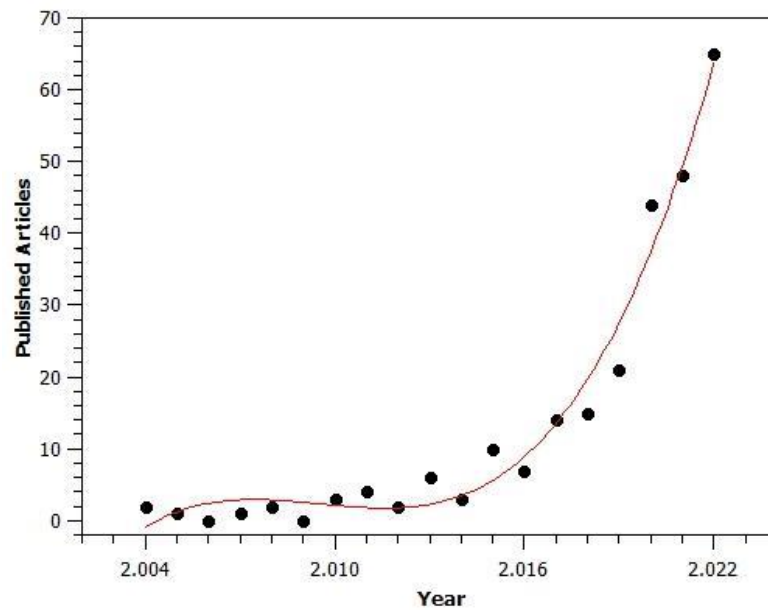


Figure 1.Published articles containing the keywords “nanotechnology” and “machine learning” per year (2004-2022).

Furthermore, **Figure 2** shows the ten countries with the highest volume of publications that intersect the two areas between 2004 and 2022. The United States, China, and the United Kingdom lead the volume of publications, with a significant difference between the amount of US publications and the subsequent ones.

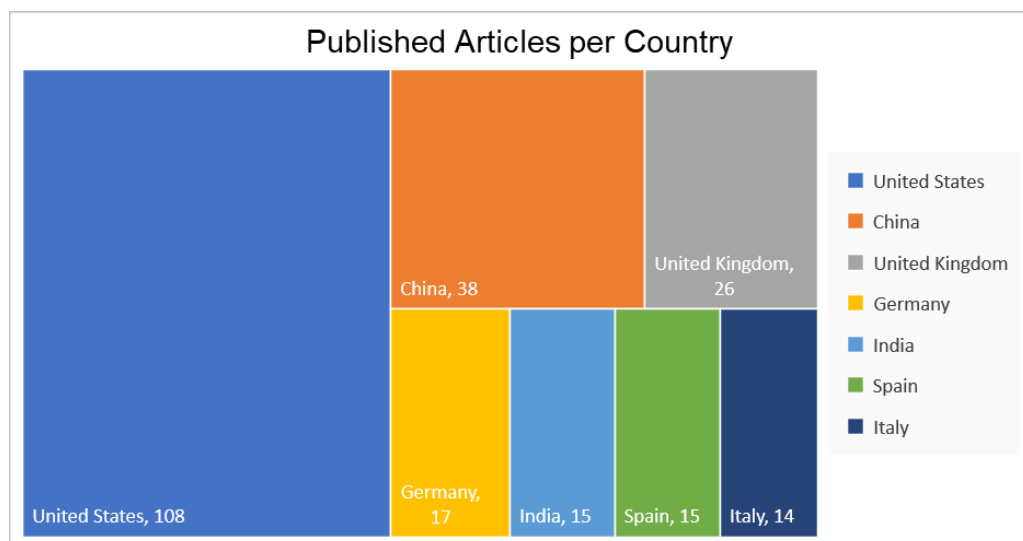


Figure 2.Published articles containing the keywords “nanotechnology” and “machine learning” per country.

In turn, the number of articles published by subject area is shown in **Figure 3**. Engineering, Materials Science, and Physics are the main areas of interest for nanotechnology and machine learning applications. As an example of research that converges engineering and materials science,

SINGH et al. (2021) [31] sought to evaluate the in vitro nanotoxicity related to cell-nanomaterial interactions, using machine learning algorithms to predict the phenotype and polarity functions presented by cells in interaction with several nanomaterials. In physics, BALLARD et al. (2017) [32] developed a framework using machine learning that allows the design of portable and low-cost plasmonic nanosensors based on a refraction index prediction model.

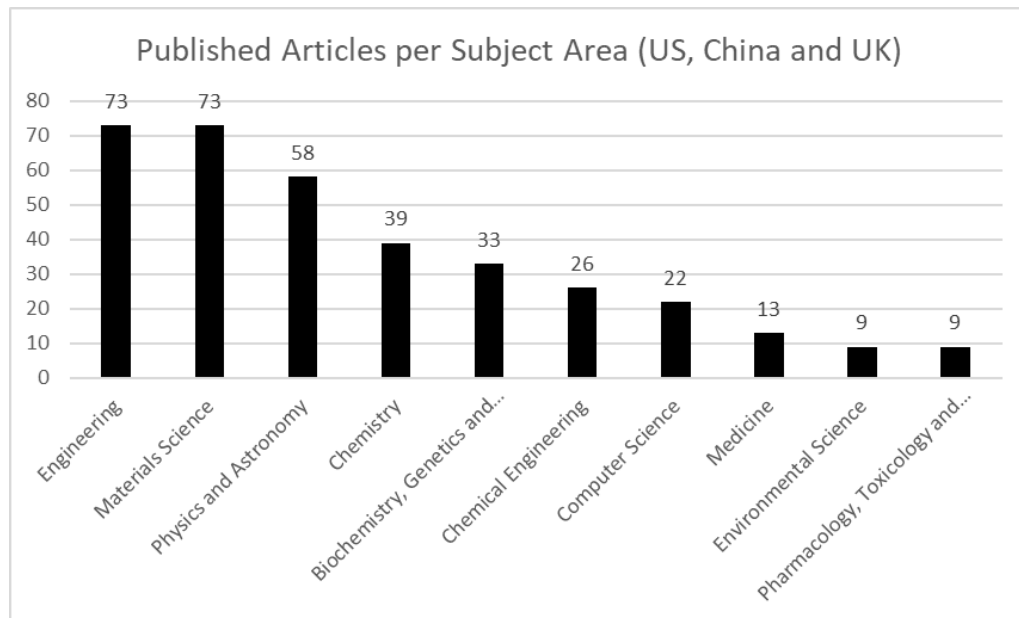


Figure 3. Published articles containing the keywords “nanotechnology” and “machine learning” per subject area.

Figure 4 allows the visualization of the mapped network formed from the search limited to articles of the main keywords "nanotechnology" and "machine learning". Five Clusters were found, and each Cluster's two most prominent nodes were highlighted. These Clusters contain the words "accuracy" and "machine learning" (red Cluster); "model" and "machine" (green Cluster); "property" and "technique" (yellow Cluster); "data" and "nano" (blue Cluster) and, finally, "approach" and "size" (purple Cluster).

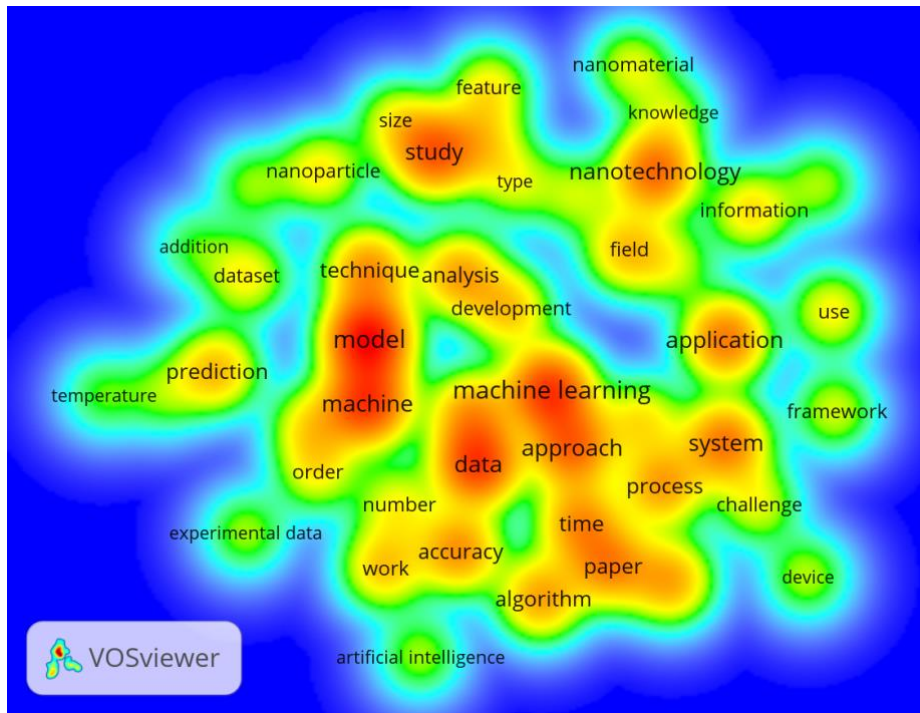


Figure 6 .VOS density map of titles, abstracts and keywords related to “model” and “data”.

Visualization of Similarities

With the help of some libraries such as Pandas and Plotly, three treemaps were generated, respectively Figures 7, 8, and 9.

The first tree map, as shown in Figure 8, demonstrates the top five nodes per Cluster, differentiating Clusters by color, number of occurrences, and year of publication.

In Cluster 1, represented by the blue color, shows that the words “technology”, “accuracy”, “analysis”, “application” and “machine learning” had their respective occurrence numbers: 61, 64, 69, 74 and 110. All the occurrences between 2018 and 2019. In Cluster 2, represented by the red color shows the words “parameter”, “work” “technique”, “data”, “model”, with their respective occurrence numbers: 41, 52, 74, 84 and 100 between the years 2018 and 2020.

Cluster 3 represented by the green color shows the words “effect”, “feature”, “number”, “algorithm” and “process”, with their respective occurrence numbers: 35, 38, 40, 59, 61 between the years 2019 and 2020. The fourth Cluster represented by the purple color shows the words “experiment”, “performance”, “paper”, “system” and “machine”, with their respective occurrence numbers: 37, 47, 58, 87 and 114 between the years 2018 and 2019.

The last one (Cluster 5) represented by the orange color shows the words “structure”, “property”, “nanotechnology”, “approach”, “study”, with their respective occurrence numbers: 48, 49, 79, 80 and 82, between the years 2018 and 2019.

Treemap: Top five nodes per cluster (Cluster, Occurrences, Label & Avg. pub. year)



Figure 7. Tree map: Top five nodes per Cluster

The second tree map established by Figure 8, shows the Top-five link strength between items (LSBI). This one was generated from the NET database showing the comparison between terms and their nodes in each Cluster.

Treemap: Top five Link strength between items (LSBI) (LSBI, Terms, Cluster nodes, Years, & Eucli



Figure 8. Tree map: Top five link strength between items (LSBI)

The terms do not follow any color criterion in this tree map. With lowest LSBI is “machine vs. machine learning” in the red Cluster with a numerical quantity of 40, followed by the comparisons “machine learning vs. system” and “machine vs. model” in the blue Cluster with a numerical quantity of 43. The green Cluster has the terms “data .vs model” with numerical quantity 44, and the last one with the highest LSBI is in the purple Cluster with the terms “machine learning .vs model” with numerical quantity 45. The code made another comparison between terms, and the tree map shown in Figure 9 presents the top five most recent nodes in all the articles analyzed by VOSviewer.

Like the last tree map, this one does not have any color criterion. All the Clusters show terms in papers between 2020 and 2021. In the five most recent nodes, the node “pressure” (n.66) interconnects with all the Clusters, as shown in **Diagram 1**, the term most cited recently.

Treemap: Top five most recent nodes (LSBI, Terms, Cluster nodes, Years, & Euclidean distance)

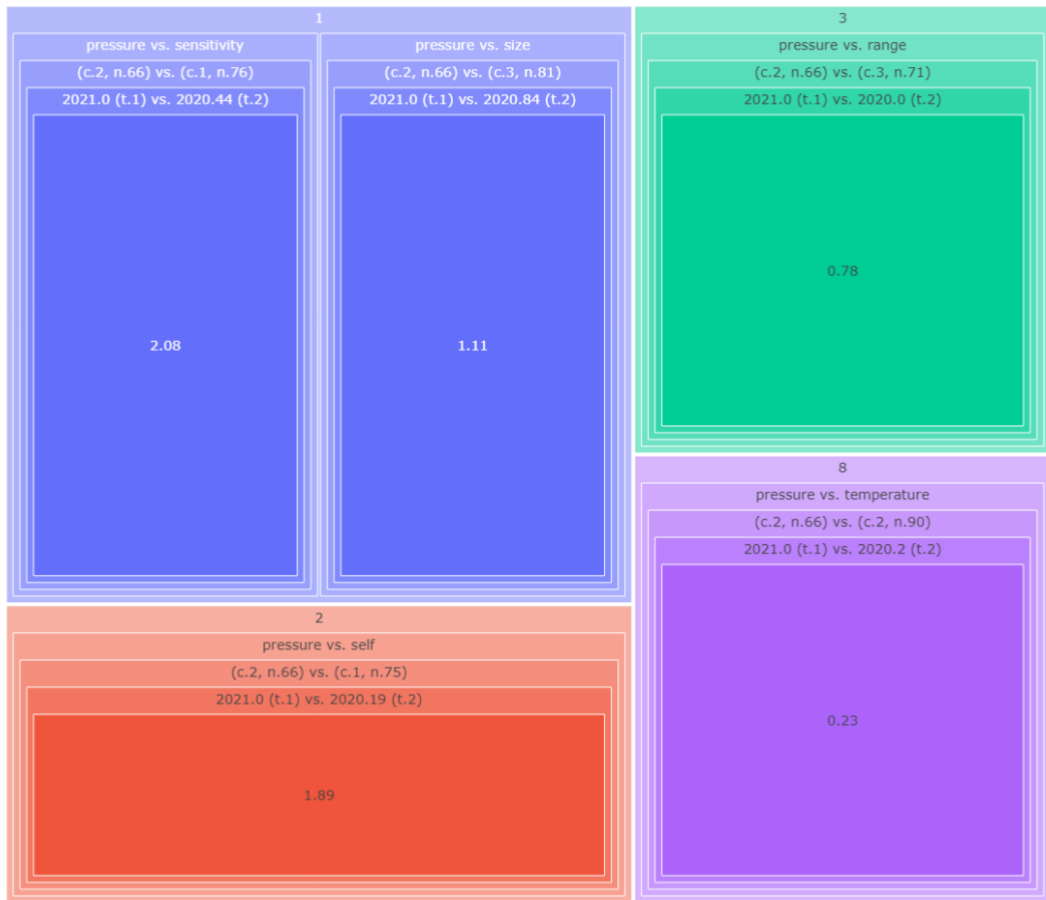


Figure 9 . Tree map: Top five most recent nodes

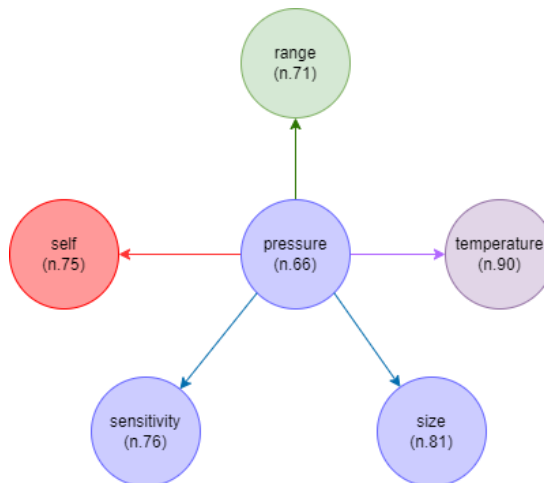


Diagram 1- Interconnection between nodes in the blue Cluster

Results from software analyses prove that all the most recent nodes communicate mainly through node 66 (term "pressure"), meaning that in all analyzed papers, the terms nanotechnology and Machine Learning have a great tendency to analyze parameters such as pressure interconnected with other parameters such as temperature variation, size, and sensitivity in nanoscale materials. So it can be deduced that the use of Machine Learning for predicting parameters is increasingly being used for the evolution of studies in nanotechnology.

4. CONCLUSION

The production of scientific articles has been happening more frequently year after year. With the countless volumes of information comes the challenge of understanding the means used during the advance of research on specific topics, which has consequences, such as relevant data inserted in these documents that go unnoticed during academic readings. From this, creating strategies to visualize advances and understand the topics of interest is of great importance for the excellence of scientific work.

This work used scientific data from the Similarity Visualization Method and Python. In this study, 2038 scientific articles from Scopus were analyzed. Tools such as VOSViewer and Python allowed the mapping of publications containing the terms "Machine Learning" and "Nanotechnology", revealing that in the last ten years, the theme growth grew exponentially from 2016 to 2022 compared to previous years.

The areas of study with a more significant relation to the themes were "Engineering", "Materials Science" and "Physics and Astronomy", with the United States as the most extensive academic contributor, followed by China and the United Kingdom. The analysis made from the VOS exposed the presence of 5 Clusters demonstrating the evolution of interests over the years. VOS density maps were obtained from filters using the keywords "accuracy" and "machine learning", and then "machine" and "model", revealing the behavior between the keywords with a more significant presence in nanotechnology and machine learning publications.

The map generated from the "accuracy" and "machine learning" filters showed a lower degree of separation between the keywords found in the second map, composed of the "machine" and "model" filters. The organization of keywords and their intensity in the first density map allows highlighting the general objectives of research articles that seek to converge the areas of nanotechnology and machine learning. In contrast, the second map highlights the individual contributions of nanotechnology and machine learning to each other.

The Python software shows the main Clusters and the 5 in the primary ones, listing the strength between the links and the most recent associated terms in the academic environment. Using acronyms and abbreviations generates duplicity in the results, which are analyzed and discarded at

the end. Machine Learning and nanotechnology are relatively recent fields of study, being fundamental and relevant issues in current studies with increasing growth trends.

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