IJCRT.ORG ISSN : 2320-2882

INTERNATIONAL JOURNAL OF CREATIVE RESEARCH THOUGHTS (IJCRT)

An International Open Access, Peer-reviewed, Refereed Journal

A Review On Probabilistic Graphical Models For Anticipating Characteristics Of Novel Materials Derived From Their Composition And Structure

Sangeetha S A [1], Yamuna H S [2], Manjula P H [3]

[1] Senior Scale Lecturer, Department of Ceramics Technology, S J (Government) Polytechnic Bengaluru, Karnataka, India.

[2] Selection Grade Lecturer, Department of Chemical Engineering, S J (Government) Polytechnic Bengaluru, Karnataka, India.

[3] Selection Grade Lecturer, Department of Mechanical Engineering, Government Polytechnic Chintamani, Karnataka, India.

ABSTRACT

Probabilistic graphical models, often known as PGMs, provide a strong framework for modelling intricate interactions between various components. Through the incorporation of data about the elemental composition and structural characteristics, these models make it possible to deduce the attributes of materials from a probabilistic point of view. This technique bears promise attempts towards expediting the design of materials discovery, as it makes it easier to predict the characteristics of a wide variety of materials, including their electrical and mechanical properties, as well as their thermal and optical behaviour. The use of PGMs in the field of materials science is an example of a sophisticated approach that is used to harness data-driven insights in order to direct the discovery of novel materials that have specific functions. The objective of this study is to conduct a literature review with the intention of examining the possible applications of data science ideas, big data, and machine learning in the context of the production of artificial intelligence. This is a strategy that involves reviewing the existing literature in order to get an understanding of the use and application of computational intelligence in the cutting-edge research and innovation in materials science. Using machine learning to solve complex chemical issues that would otherwise be intractable is shown by the results of this study. Predicting the characteristics of novel materials based on their composition and structure may be accomplished via the use of PGMs, which provides a potential route within this field.

Keywords: Novel Materials; Composition and Structure; PGMs; Design of Materials.

1. INTRODUCTION

The search for new materials with desirable characteristics has been a continuous difficulty in materials research. Conventional approaches used over the years to identify new materials, such empirical trial and error and the density functional theory (DFT)-based methods are unable of keeping up with the fast pace of the development of new materials today because of their long development cycles, low efficiency, and high cost [1]. Applied for the prediction of material characteristics, acceleration of simulations, design novel structures, for the prediction synthesis pathways of new materials [2], machine learning has been a subject of interest in many industrial disciplines including material science and chemistry. Among the quickly expanding class of machine learning models are PGMs [3]. Because they directly deal with graph or structural representations of molecules and materials as such having complete access to crucial information necessary to describe materials [4], they are often employed in chemistry and materials research. Materials scientists are always working to improve their capacity for understanding, prediction, and enhancement of materials characteristics [5]. To grasp and forecast materials characteristics throughout the last years, materials scientists have mostly depended on simulation and modelling approaches. Scientists have developed new approaches to forecast and enhance materials qualities more reasonably priced and less time-consuming as the conventional trial-and-error technique in materials research is imitated in certain aspects.

Data-driven approaches like machine learning have lately been embraced to anticipate novel materials, therefore transforming the field of materials science research [6]. Considered the fourth pillar of research, next to the experiment, theory, and simulations, machine learning and data science have grown to be a major component of natura science. From the database screening, finding first candidate materials property predictions, for material designs, for the prediction of the synthesis conditions and automated experimental data analysis as well as experimental planning, machine learning techniques are progressively used in all stages of the materials development cycle [7]. From a broad spectrum of traditional machine learning algorithms including decision trees, convolutional neural networks, and probabilistic graphical models, machine learning approaches employed in material science span.

Because of its ability to forecast the properties of newly developed materials depending on their inherent composition and structural features, PGMs have attracted great interest. Particularly well-suited for uses in chemistry and materials science, PGMs are a fast-changing family of machine learning models [8]. Their natural capacity to run directly on graph or structural models of molecules and materials provides them complete access to relevant data essential for material characterization. PGMs provide a sophisticated knowledge of many features spanning electrical and mechanical properties to thermal and optical behaviour by harnessing the intricate interactions between various material components, hence enabling probabilistic inference of material attributes [9], [10].

Among many disciplines, including bioinformatics, social science, control theory, image processing, marketing analysis, among others [11], [12], the graphical models have been used extensively. Still, structure learning for graphical models presents a difficult problem as one must manage a combinatorial search over the space of all potential structures.

Materials research has always been challenged in its search for new materials with particular and desired qualities. Discovering new materials has always mostly depended on empirical trial and error techniques, which were driven by intuition and a limited knowledge of the fundamental ideas controlling materials behaviour [13]. But as materials science has developed, the need for methodical and systematic ways to hasten the identification and design of novel materials has been even more apparent. Predicting materials propertied by modelling the behaviour of atoms and electrons within materials depended much on density functional theory (DFT) and other theoretical approaches in the last decades. These approaches had several limits, including being computationally costly, which limited their use to quite small-scale and hampered their capacity to keep pace with the fast-changing scene of materials development [14], [15]. Although they offered insightful analysis.

Materials science underwent a paradigm change as machine learning (ML) methods became available. Described by its capacity to identify trends and associations within big datasets, ML offers a potential path for material property prediction, fast simulation acceleration, and design guidance for novel materials [16]. Starting with hidden relationships between materials composition, structure, and characteristics enabling for more informed and effective exploration of the large materials space, researchers began using ML algorithms. Within the field of machine learning, PGMs become a sophisticated and flexible instrument for material property prediction [17]. PGMs are ideal for illustrating complicated interactions in materials as they provide a structure for expressing and evaluating ambiguous knowledge. PGMs provide a special benefit in retrieving pertinent information vital for material characterisation; they directly deal with graph or structural representations of molecules and materials [18].

PGMs' capacity to combine many information sources, evaluate uncertainty, and enable probabilistic inference of materials characteristics has helped them to become popular in material sciences science. This method allows the prediction of a wide range of characteristics, including electrical, mechanical, and thermal [19], thus enabling a sophisticated knowledge of the complex interaction among many material components.

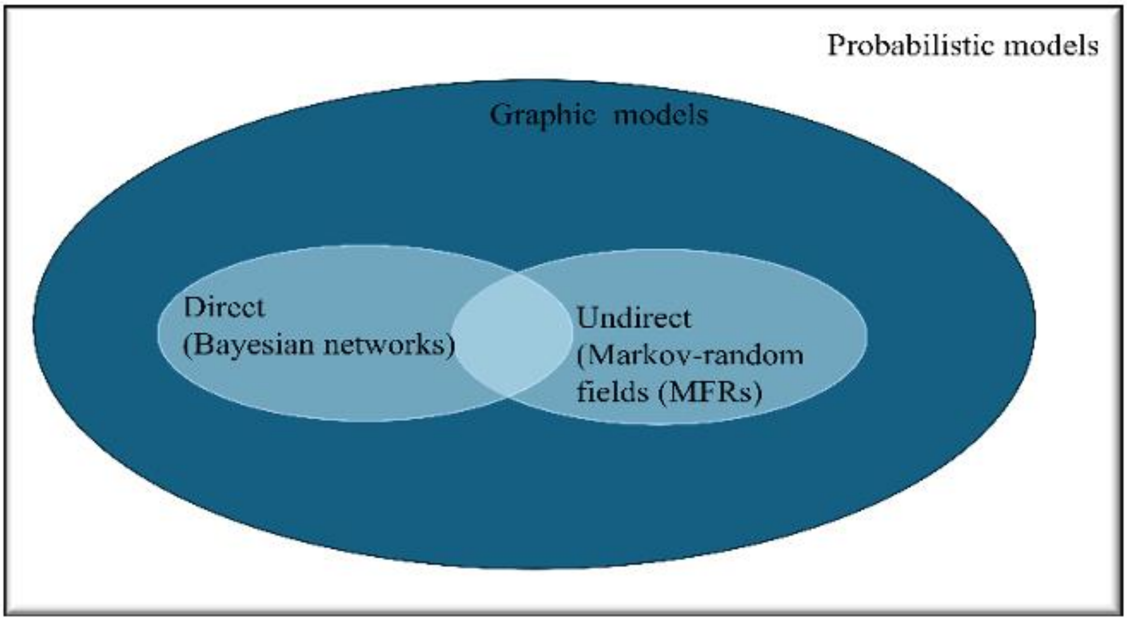

Fig. 1. Flavours of probabilistic graphical models

Figure 1 presents the two sub-categories of the probabilistic graphical models: (i). both direct and indirect graphic models. The direct graphic models are characterized as Bayesian networks often referred to as belief networks. Representing a collection of variables and their conditional dependencies using a direct acrylic graph (DAG), they are probabilistic graphical models. Every node in a Bayesian network is a random variable; the directed edges connecting the nodes capture probabilistic dependencies, therefore expressing the casual interactions among the variables.

Described as Markov networks, the undirected graphic models form a collection of variables with pairwise Markovian dependencies using an undirected graph. Every node in a Markov random field (MRF) stands for a random variable; however, the lack of direct edges suggests that the link between the variables is undirected and usually denotes the concept of local interactions or spatial closeness [20]. We provide in this work a thorough review of the current structure learning methods. This work intends to use PGMs' intrinsic probabilistic character to decode complex interactions among structural characteristics, material compositions, and consequent properties. This work aims to build and improve PGMs able to precisely forecast material properties by combining many datasets including material compositions, structural configurations, and related attributes. Such prediction algorithms might hasten the creation and research on novel materials. Notwithstanding this introduction, this work consists of four additional parts: technique, data collecting, suggestions, and conclusion.

2. METHOD

An illustration of the number of sources that were examined may be seen in Figure 2. The terms "PGMs for prediction of materials properties" and "machine learning for prediction of materials properties" were used as search criteria in order to extract information from the Materials project, the Open Quantum materials database, journals of materials science, computational materials science, journals of chemical information and modelling, and the American Chemical Society's applied materials and interfaces. This comprises conferences, journals, early access publications, and magazines that were chosen for use in this study because they were selected.

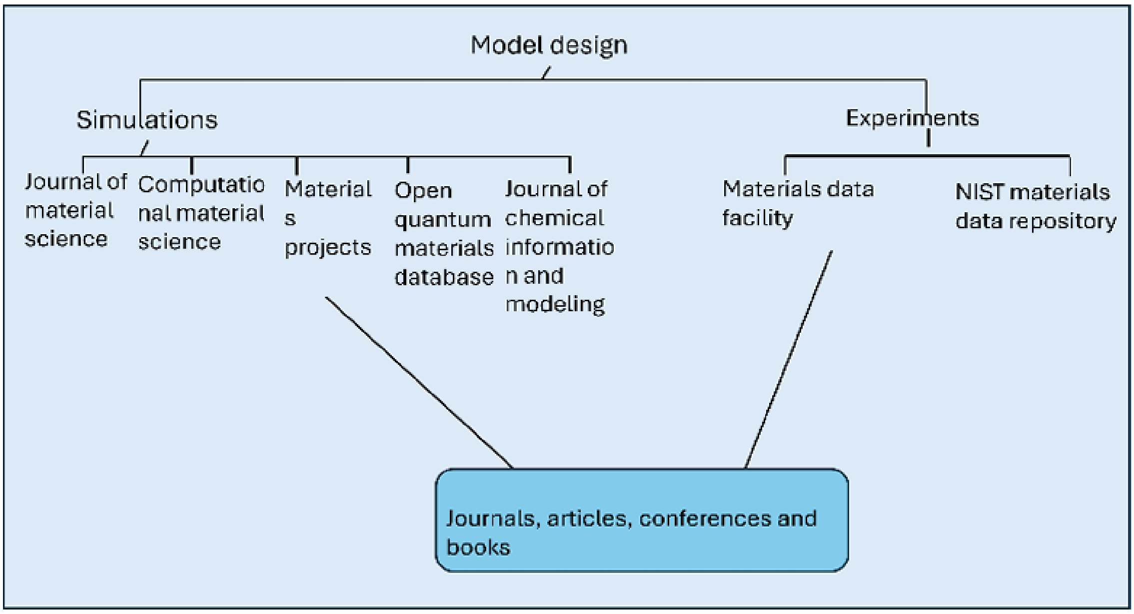

Fig. 2. Different sources used to conduct this work

While a significant amount of research has been conducted on the use of data-driven and machine learning techniques for the purpose of predicting the characteristics of materials, only a small amount of study has been conducted on the utilization of PGMs for the purpose of predicting or designing new materials for certain functions. The need for the development of unique material characteristics for certain capabilities is a difficulty that is faced by a large number of researchers in a variety of fields, including medical, aerospace, computer and communication, and energy, among others. It would be beneficial for researchers from a variety of fields to collaborate in order to maximize their potential, improve the shortcomings of forecasting new features of materials, and make the process more efficient and less expensive. Materials project, Open Quantum materials database, journals of materials science, computational materials science, journals of chemical information and modelling, and ACS applied materials and interfaces were the sources that were consulted and used in the process of carrying out this study. This collection of materials included a complete abstract and citation database that was meticulously maintained by experts. Data and academic publications from a broad variety of fields have been enhanced as a result of this innovation. It delivers a wider variety of outcomes than other methods.

3. RESULTS AND DISCUSSION

In the field of materials science, researchers in the fields of chemistry and engineering often use data-driven models and machine learning in order to make predictions about the characteristics of materials. There were no research publications that yielded findings for the use of PGMs for the purpose of predicting the properties of materials; however, there were over a million results identified for the use of machine learning and data-driven models for the purpose of predicting the characteristics of materials. Random forest, Support Vector Machines, Convolutional Neural Networks, Gradient Boosting Machines, and Gaussian Process Regression are the machine learning techniques that are used the most often for the purpose of predicting the qualities of materials. While a significant amount of literature has been written on probabilistic graphical models and the influence they have had on the area of materials science, there has been a very little amount of research conducted to actually utilize these models to forecast the characteristics of any materials. It is necessary to do more study in order to investigate the potential of PGMs for application in the prediction of the characteristics of materials. Our investigation has led to the development of a number of suggestions that may be implemented in order to enhance the use of probabilistic graphical models (PGMs) in the process of forecasting the characteristics of novel materials. The encouragement of data exchange and cooperation among academics is of the utmost importance, first and foremost. Within the community of materials scientists, open-access repositories and collaborative platforms have the potential to promote the interchange of data pertaining to materials and further the development of multidisciplinary cooperation. In addition, it is vital to make investments in the development of user-friendly software tools and platforms for the purpose of constructing, training, and deploying PGMs. This will enable researchers to properly exploit the potential of these models. In addition, the provision of training and educational resources may provide researchers with the knowledge and abilities necessary to make the most of the potential of PGMs in the field of materials science research. For the purpose of ensuring that all investigations are rigorous and comparable to one another, it is necessary to create standardized methodologies and standards for verifying the efficacy of PGMs in predicting material attributes. It is possible to improve the reliability and accuracy of material property predictions via the collaboration of computational and experimental researchers in order to combine PGMs with improved experimental methodologies. In addition, when it comes to developing the profession, it is essential to take into account to take into account ethical issues, long-term financing and support, and collaboration with stakeholders from academia, business, government, and the wider community. Through the adoption of these suggestions, the community of materials scientists has the potential to accelerate the use of PGMs toward the discovery of creative discoveries and breakthroughs in the design and engineering of materials.

4. CONCLUSIONS

One of the most interesting new directions in the field of material science research is the investigation of PGMs for the purpose of predicting the characteristics of new materials based on their composition and structure respectively. PGMs provide a diverse framework for modelling the relationships between material components, ranging from Bayesian networks to Markov random fields. This allows for a better understanding of the underlying processes that drive the behaviour of materials. PGMs make it possible to forecast a wide range of material properties, including those in the electrical, mechanical, thermal, and optical domains. This is accomplished by combining information on the composition of elements, structural motifs, and ambient conditions. It should come as no surprise that the use of PGMs for the purpose of speeding the discovery and design of materials offers immense potential. Through the use of data-driven insights and computational intelligence, researchers are able to investigate novel materials that possess individualized functions, therefore propelling progress in a variety of scientific fields and industrial sectors. When looking into the future, the future of PGMs in the field of materials science resides in their continuing refining and application to new possibilities and difficulties that are just emerging.

Investigating potential future research avenues in the field of PGMs for the purpose of forecasting new characteristics of materials presents an exciting opportunity for investigation. The creation of dynamic graphical models that are able to capture temporal dependencies and changes in material characteristics over time is one of the options that might be pursued. This is especially significant for materials that are exposed to variable environmental circumstances or that are experiencing phase transition. It is possible to examine the hierarchical modelling technique in order to represent the multiscale aspect of material behaviour, which ranges from the atomic and molecular scale to the qualities of the material at the macroscale. This would provide insight into the complex material systems. The incorporation of uncertainty quantification methodologies into PGMs would make it possible for researchers to measure and integrate uncertainty into model predictions, hence improving the resilience and reliability of predictions about the properties of materials. The path that research will take in the future has the potential to increase the capacities of PGMs to make predictions and to promote innovation in the fields of materials science and engineering.

REFERENCES

1. Wei, J., Chu, X., Sun, X.Y., Xu, K., Deng, H.X., Chen, J., Wei, Z. and Lei, M., 2019. Machine learning in materials science. Info Mat, 1(3), pp.338-358,
2. Wang, A.Y.T., Murdock, R.J., Kauwe, S.K., Oliynyk, A.O., Gurlo, A., Brgoch, J., Persson, K.A. and Sparks, T.D., 2020. Machine learning for materials scientists: an introductory guide toward best practices. Chemistry of Materials, 32(12), pp.4954-4965.
3. Mueller, T., Kusne, A.G. and Ramprasad, R., 2016. Machine learning in materials science: Recent progress and emerging applications. Reviews in computational chemistry, 29, pp.186-273.
4. Butler, K.T., Davies, D.W., Cartwright, H., Isayev, O. and Walsh, A., 2018. Machine learning for molecular and materials science. Nature, 559 (7715), pp.547-555.
5. Morgan, D. and Jacobs, R., 2020. Opportunities and challenges for machine learning in materials science. Annual Review of Materials Research, 50, pp.71-103.
6. El-Shafie, M., 2023. Hydrogen production by water electrolysis technologies: A review. Results in Engineering. Natural gas, 240, p.48.
7. Koller, D. and Friedman, N., 2009. Probabilistic graphical models: principles and techniques. MIT press.
8. Reiser, P., Neubert, M., Eberhard, A., Torresi, L., Zhou, C., Shao, C., Metni, H., van Hoesel, C., Schopmans, H., Sommer, T. and Friederich, P., 2022. Graph neural networks for materials science and chemistry. Communications Materials, 3(1), p.93.
9. Bhadeshia, H.K.D.H. 1999. Neural networks in materials science. ISIJ international, 39(10), pp.966-979.
10. Ferguson, A.L., 2017. Machine learning and data science in soft materials engineering. Journal of Physics: Condensed Matter, 30(4), p.043002.
11. Sucar, L.E., 2015. Probabilistic graphical models. Advances in Computer Vision and Pattern Recognition. London: Springer London. doi, 10(978), p.1.
12. Pernkopf, F., Peharz, R. and Tschiatschek, S., 2014. Introduction to probabilistic graphical models. In Academic Press Library in Signal Processing (Vol. 1, pp. 989-1064). Elsevier.
13. Martin, D. Schmidt, M.W. and Hillerbrand, R. Implementing AI Ethics in the Design of AI-assisted Rescue Robots", 2023 IEEE International Symposium on Ethics in Engineering, Science, and Technology (ETHICS), West Lafayette, IN, USA, i2023, pp. 1-1.
14. Bagayoko, D., 2014. Understanding density functional theory (DFT) and completing it in practice. AIP Advances, 4(12).
15. Burke, K. and Wagner, L.O., 2013. DFT in a nutshell. International Journal of Quantum Chemistry, 113(2), pp.96-101.
16. Jordan, M.I., 2003. An introduction to probabilistic graphical models.
17. Larrañaga, P., Karshenas, H., Bielza, C. and Santana, R., 2012. A review on probabilistic graphical models in evolutionary computation. Journal of Heuristics, 18, pp.795-819.

18. Frey, B.J. and Jojic, N., 2005. A comparison of algorithms for inference and learning in probabilistic graphical models. IEEE Transactions on pattern analysis and machine intelligence, 27(9), pp.1392-1416.
19. Ankan, A. and Panda, A., 2015. Probabilistic graphical models using python. In Proceedings of the 14th python in science conference (scipy 2015) (Vol. 10). Citeseer.
20. Bernardo, J.M. and Smith, A.F., 2009. Bayesian theory (Vol. 405). John Wiley & Sons.
21. Li, Stan Z. "Markov random field models in computer vision." In Computer Vision—ECCV'94: Third European Conference on Computer Vision Stockholm, Sweden, May 2–6 1994 Proceedings, Volume II 3, pp. 361-370. Springer Berlin Heidelberg, 1994.