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Review

Machine Learning Approaches in Predicting Chemical Reactions: A Comprehensive Review

Hossein Tarahomi Ardakani[1], Hamid Reza Hanif[2], Mohsen Katebi Jahromi[3,*]

[1] Department of Computer Science, Payame Noor University (PNU), Tehran, Iran.

[2] Department of Mathematics and Computer Science, Iran University of Science and Technology

[3,*] Department of Electrical Engineering, Safashahr Branch, Islamic Azad University, Safashahr, Iran.

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ABSTRACT

The rapid advancement of machine learning (ML) techniques has significantly transformed the landscape of chemical research, particularly in predicting chemical reactions. This review provides a comprehensive overview of the various machine learning approaches utilized in the prediction of reaction outcomes, mechanisms, and kinetics. We begin by discussing the foundational concepts of machine learning and its relevance to chemistry, highlighting key algorithms such as neural networks, support vector machines, and decision trees. The paper systematically categorizes existing methodologies based on their application: reaction outcome prediction, reaction mechanism elucidation, and kinetic modeling. We delve into the datasets commonly employed for training ML models, emphasizing the importance of high-quality, curated chemical data. Furthermore, we explore the integration of quantum chemical calculations with machine learning to enhance predictive accuracy. Challenges such as data sparsity, model interpretability, and the need for generalizability across diverse chemical spaces are critically examined. Finally, we discuss future directions for research, including the incorporation of transfer learning, active learning, and the development of user-friendly software tools to democratize access to these powerful predictive techniques. This review aims to provide a valuable resource for chemists and data scientists alike, fostering collaboration and innovation at the intersection of chemistry and artificial intelligence.

Keywords: Machine Learning, Chemical Reactions, Prediction Models, Data-Driven Approaches

*Corresponding author email address: mo.katebi@iau.ac.ir

Introduction

The field of chemical reactions is at the heart of numerous scientific and industrial endeavors, ranging from drug discovery and material science to environmental chemistry and energy production [1]. Understanding and predicting chemical reactions have traditionally relied on rigorous experimental studies and theoretical modeling, often requiring significant time, resources, and expertise. However, with the advent of advanced computational tools and the exponential growth of data availability, machine learning (ML) has emerged as a transformative technology in the realm of chemistry [2]. This review paper delves into the burgeoning intersection of machine learning and chemical reaction prediction, providing a comprehensive overview of the methodologies, applications, and future directions in this exciting field. Chemical reactions are inherently complex processes governed by intricate quantum mechanical and thermodynamic principles [3]. The sheer diversity of chemical species, reaction pathways, and environmental conditions makes the prediction of reaction outcomes a challenging task. Traditional approaches, such as quantum chemistry calculations and molecular dynamics simulations, have made significant strides in elucidating reaction mechanisms [4]. However, these methods are often computationally expensive and scale poorly with the increasing size of chemical systems. This is where machine learning offers a compelling alternative by leveraging data-driven algorithms to uncover patterns and relationships within large datasets of chemical reactions [5].

The application of machine learning in chemistry is not entirely new; its roots can be traced back to the early use of statistical models for quantitative structure-activity relationships (QSAR) in drug design [6]. However, recent advancements in ML algorithms, coupled with the availability of high-performance computing infrastructure and extensive chemical datasets, have catalyzed a paradigm shift in how chemists approach reaction prediction. Techniques such as deep learning, natural language processing, and reinforcement learning are now being employed to tackle problems that were once deemed intractable. From predicting reaction yields and selectivity to exploring reaction mechanisms and retrosynthetic pathways, machine learning has demonstrated remarkable potential across a wide spectrum of applications [7]. One of the key drivers behind this progress is the growing repository of chemical data generated through experimental studies, computational simulations, and high-throughput screening methods. Publicly available databases such as Reaxys, PubChem, and the Cambridge Structural Database provide a wealth of information on chemical structures, reaction conditions, and outcomes [8]. Additionally, advancements in cheminformatics have enabled the efficient representation of chemical information through formats like SMILES (Simplified Molecular Input Line Entry System) and molecular graphs. These representations serve as the foundation for training ML models to learn complex relationships between reactants, products, and reaction conditions [9]. Another critical factor contributing to the success of machine learning in chemical reaction prediction is the interdisciplinary collaboration between chemists, computer scientists, and data engineers. While chemists bring domain expertise and an understanding of reaction mechanisms, computer scientists contribute advanced algorithmic techniques and optimization strategies [10]. This synergy has led to the development of tailored ML models that address specific challenges in chemistry, such as handling imbalanced datasets, interpreting model predictions, and ensuring generalizability across diverse chemical spaces. Despite these advancements, several challenges remain in fully realizing the potential of machine learning for chemical reaction prediction. The quality and diversity of training data play a pivotal role in determining model performance [11].

Machine Learning Approaches for Chemical Reaction Prediction

Data Representation in Chemistry

The ability of machine learning (ML) models to accurately predict chemical reactions is profoundly influenced by the way chemical data is represented, as the chosen representation directly impacts the model's capacity to understand and process molecular information. Several common approaches have been developed to represent chemical data effectively, each tailored to capture specific aspects of molecular and chemical properties [12]. One widely used method involves **Molecular Descriptors**, which are numerical values designed to encode various chemical properties of molecules. These descriptors capture essential features such as the types of atoms present, the types of bonds connecting them, and the overall topology or three-dimensional arrangement of the molecule. Examples of molecular descriptors include Extended Connectivity Fingerprints (ECFP), which are highly informative for tasks like molecular similarity and substructure searching, and RDKit descriptors, which provide a rich set of computed chemical features that are useful for predictive modelling [13]. Another powerful representation method involves **Graph Representations**, where molecules are modeled as graphs, with atoms serving as nodes and bonds acting as edges. This approach mirrors the natural connectivity of molecules and allows models to work directly with molecular structures. Graph Neural Networks (GNNs) are a class of ML models specifically designed to leverage these graph-based representations, enabling them to learn complex relationships and patterns inherent in molecular graphs. Additionally, **SMILES Strings**, or Simplified Molecular Input Line Entry System strings, offer a compact and linear textual representation of molecules [14]. These representations are particularly well-suited for sequence-based machine learning models, such as recurrent neural networks (RNNs) or transformers, which can process and learn from the sequential nature of SMILES strings. Finally, there is the use of **Reaction Templates**, which are predefined sets of rules or patterns that describe specific types of chemical reactions. Template-based methods depend on these reaction patterns to predict the outcomes of chemical processes, leveraging prior knowledge about reaction mechanisms to enhance predictive accuracy. Together, these diverse representation methods form the foundation for modern ML-driven approaches in computational chemistry, enabling researchers to model, analyze, and predict chemical behavior with unprecedented precision and efficiency [15].

Supervised Learning Methods

Supervised learning is a fundamental approach in machine learning that involves training a model on labeled data to enable it to make predictions about reaction outcomes or properties. This method is particularly valuable in the field of chemistry, where understanding and predicting the results of chemical reactions is crucial for numerous applications, including drug discovery, materials science, and process optimization [16]. Among the various tools and techniques used in supervised learning, deep learning methods have emerged as powerful solutions for tackling complex reaction prediction tasks. Deep learning encompasses a variety of architectures, each offering unique advantages for processing different types of data and extracting meaningful patterns. One prominent category of deep learning models is neural networks, which are designed to mimic the structure and function of the human brain. Within this category, feedforward neural networks and convolutional neural networks (CNNs) have been widely applied to reaction prediction challenges [17]. Feedforward neural networks are composed of layers of interconnected nodes that process input data and learn hierarchical representations to make predictions. Convolutional neural networks, on the other hand, excel at processing spatially structured data, such as images [18]. A notable example of CNN application in chemistry is Chemception, a model that utilizes CNNs to analyze molecular images. By converting chemical structures into image-like inputs, Chemception can predict reaction outcomes with impressive accuracy, leveraging the spatial relationships encoded in the molecular representations [19].

Beyond traditional neural networks, graph neural networks (GNNs) have gained significant attention in recent years due to their ability to handle graph-structured data, which is particularly relevant for chemistry. Chemical molecules are naturally represented as graphs, with atoms as nodes and bonds as edges [20]. GNNs, such as Message Passing Neural Networks (MPNNs) and Graph Convolutional Networks (GCNs), are specifically designed to operate on such graph-structured data. These models learn to encode the structural and chemical properties of molecules by iteratively updating node representations through message-passing mechanisms. By analyzing the molecular graphs of reactants and products, GNNs can effectively predict reaction outcomes, identify reaction mechanisms, and even suggest potential reactants for desired products [21]. Their ability to capture complex interactions within molecular structures has made them a powerful tool in computational chemistry. Another innovative approach to reaction prediction involves sequence-to-sequence (Seq2Seq) models, which were originally developed for natural language processing tasks like machine translation. Seq2Seq models have been adapted for chemical reactions by leveraging SMILES (Simplified Molecular Input Line Entry System) strings, a text-based representation of chemical structures [22]. In this framework, chemical reactions are treated as translation tasks, where the input sequence represents the reactants' SMILES strings and the output sequence corresponds to the products' SMILES strings. Transformer-based architectures, which have revolutionized natural language processing with their attention mechanisms, have demonstrated remarkable performance in this domain [23]. These models excel at capturing long-range dependencies and contextual relationships within sequences, enabling them to predict reaction products with high accuracy. The adaptability of Seq2Seq models to chemical data highlights their potential for advancing reaction prediction and facilitating the design of novel compounds [24].

In summary, supervised learning has become an indispensable tool for predicting chemical reaction outcomes and properties [25]. The integration of advanced deep learning techniques, including feedforward neural networks, convolutional neural networks, graph neural networks, and sequence-to-sequence models, has significantly expanded the capabilities of computational chemistry. Each of these approaches brings unique strengths to the table, whether it's processing image-like molecular representations with CNNs, analyzing graph-structured molecular data with GNNs, or translating SMILES strings with Seq2Seq models. Together, these methods are driving progress in chemical research and enabling scientists to tackle increasingly complex challenges in reaction prediction and molecular design [26].

Unsupervised and Semi-Supervised Learning

Unsupervised learning methods, which play a crucial role in the field of data science and machine learning, are widely employed to uncover hidden or latent patterns in reaction data when explicit labels are not available [27]. These methods are particularly valuable because they enable researchers to extract meaningful insights from datasets that lack predefined categories or annotations. By leveraging the inherent structure of the data, unsupervised learning techniques can identify clusters, trends, and relationships that might otherwise remain obscured. On the other hand, semi-supervised learning approaches provide a powerful alternative for scenarios where labeled data is scarce or expensive to obtain [28]. These approaches effectively combine the strengths of both labeled and unlabeled data, allowing models to learn more robustly and improve their performance even in situations where only a small portion of the dataset is annotated. This hybrid learning paradigm is especially advantageous in domains like chemical informatics, where creating labeled datasets can be time-consuming and resource-intensive [29].

Among the most commonly used techniques in unsupervised learning are clustering and dimensionality reduction, which have found widespread application in analyzing chemical datasets. Clustering methods, such as k-means clustering, are employed to group similar reactions based on shared characteristics or properties [30]. This helps researchers identify reaction families or categorize chemical processes with similar behaviors. Dimensionality reduction techniques, such as principal component analysis (PCA), address the challenges posed by high-dimensional datasets, which are often encountered in chemical research. By reducing the complexity of these datasets while retaining their most important features, PCA enables scientists to visualize and interpret the data more effectively [31]. Together, clustering and dimensionality reduction provide powerful tools for exploring and organizing complex chemical information. Another innovative approach that has gained significant attention in recent years is the use of variational autoencoders (VAEs). VAEs are a type of generative model designed to learn compact and meaningful latent representations of data, such as molecules or chemical reactions. These latent representations capture the underlying structure of the data in a lower-dimensional space, making them highly useful for a variety of applications. For instance, VAEs can be used for reaction prediction, where the goal is to forecast the outcomes of chemical reactions based on their input conditions. Additionally, VAEs have proven to be a valuable resource for novel reaction discovery, as they can generate new molecular structures or reaction pathways that align with desired properties or objectives. By bridging the gap between data representation and generative modeling, VAEs open up exciting possibilities for advancing research in chemistry and related fields [32].

Reinforcement Learning

Reinforcement learning (RL), a powerful machine learning paradigm, has increasingly been applied to a wide range of scientific and industrial challenges, including the optimization of chemical reaction pathways and the design of entirely novel chemical reactions. By leveraging the principles of trial and error, RL frameworks enable models to autonomously learn how to make decisions by interacting with a simulated environment [33]. In the context of chemistry, this environment is often designed to mimic the complex and dynamic nature of chemical systems, providing a virtual space where the RL model can explore various reaction conditions, pathways, or molecular transformations. The ultimate goal of this interaction is to maximize a predefined reward signal that reflects the success or desirability of the outcome. For instance, in reaction optimization tasks, the reward signal might be tied to critical metrics such as reaction yield, which measures the efficiency of converting reactants into products, or selectivity, which evaluates the preference for producing a specific desired product over unwanted byproducts [34]. By iteratively exploring different strategies and receiving feedback in the form of rewards, the RL model gradually hones its ability to identify optimal conditions or pathways that achieve superior performance. This approach holds immense promise for accelerating the discovery of innovative chemical processes, reducing experimental costs, and enhancing our understanding of complex reaction mechanisms [35].

Hybrid Approaches

In the field of machine learning, the combination of multiple techniques has proven to be a highly effective strategy for addressing complex tasks, particularly in areas such as reaction prediction, where the challenges often involve intricate patterns and multifaceted data representations. By leveraging the strengths of different machine learning models and integrating them into a unified framework, researchers and practitioners can significantly enhance the performance, accuracy, and generalization capabilities of their systems [36]. For instance, hybrid modeling approaches have gained considerable attention in recent years due to their ability to merge diverse methodologies tailored for specific aspects of the problem at hand. A notable example of this is the integration of graph neural networks (GNNs) and sequence-to-sequence (Seq2Seq) models for tasks related to chemical reaction prediction. GNNs are particularly well-suited for processing molecular graphs, which represent chemical compounds as nodes (atoms) connected by edges (bonds), enabling the model to capture the structural and relational information inherent in molecular configurations [37]. On the other hand, Seq2Seq models excel at handling sequential data, making them ideal for translating between different representations such as SMILES (Simplified Molecular Input Line Entry System) strings, which are linear notations used to describe molecular structures. By combining these two approaches, hybrid models can simultaneously exploit the graph-based representation of molecules for structural insights and the sequential representation for tasks like translation or prediction. This synergy allows for a more holistic understanding of the data and leads to improved performance in predicting chemical reactions, which often involve complex transformations that require both structural and sequential reasoning. As a result, such hybrid systems have emerged as powerful tools in computational chemistry and drug discovery, offering new opportunities to tackle challenging problems with greater precision and efficiency [38].

Applications of ML in Chemical Reaction Prediction

Machine learning (ML) has emerged as a transformative tool in the field of chemistry, offering innovative solutions to long-standing challenges. One of the most prominent applications of ML in this domain is reaction outcome prediction. This involves predicting the products that will result from a given set of reactants, a task crucial for both research and industrial applications. Advanced models like the Molecular Transformer have demonstrated exceptional accuracy in this area, leveraging sophisticated attention mechanisms that allow the model to focus on the most relevant portions of the input data. This capability has made these models invaluable for chemists seeking to understand and predict chemical behavior. However, the utility of ML in chemistry extends far beyond merely predicting the outcomes of reactions. For instance, ML models are also being employed for reaction yield prediction, where they estimate the efficiency or yield of a reaction under specific conditions [39]. This application is particularly valuable for optimizing industrial processes and laboratory experiments, where maximizing yield is often a critical objective. By providing reliable yield estimates, these models enable chemists to make more informed decisions about how to proceed with their work.

Another significant application of ML in chemistry is reaction condition optimization. Here, ML algorithms are used to recommend the best possible reaction conditions—such as temperature, solvent, or catalyst—to achieve a desired outcome, whether it be maximizing yield, enhancing selectivity, or minimizing waste. This capability is especially useful in contexts where trial-and-error experimentation would be time-consuming and resource-intensive. By narrowing down the range of conditions to test, ML can save both time and materials, making chemical research and production more efficient. Beyond these forward-looking applications, ML also plays a crucial role in retrosynthesis planning. Retrosynthesis is the process of determining a sequence of reactions that can synthesize a target molecule from readily available starting materials. Traditionally, this has been a labor-intensive task requiring significant expertise and manual effort. However, ML models have been developed to automate this process, dramatically reducing the time and effort required [40]. These models can analyze vast datasets of chemical reactions to identify plausible synthetic routes, providing chemists with valuable insights and enabling them to focus on refining and executing the most promising pathways. In summary, ML is revolutionizing the field of chemistry by addressing key challenges in reaction outcome prediction, yield estimation, condition optimization, and retrosynthesis planning. These advancements not only accelerate the pace of discovery and innovation but also enhance the efficiency and sustainability of chemical research and production. As ML technologies continue to evolve, their applications in chemistry are likely to expand even further, unlocking new possibilities and driving progress in this vital scientific discipline.

Challenges and Limitations

Machine learning (ML) approaches hold immense promise for advancing the field of chemical reaction prediction, offering the potential to revolutionize the way chemists understand, design, and optimize chemical processes. However, despite their significant potential, these approaches face a variety of challenges that need to be addressed to fully realize their capabilities. One of the primary hurdles is the issue of data quality and availability. High-quality labeled datasets are a cornerstone for training robust and reliable ML models. Unfortunately, in the context of chemical reactions, obtaining such datasets is far from straightforward. The data available is often limited in scope, noisy, or biased toward specific reaction types, which can hinder the ability of ML models to learn effectively [41]. This limitation is exacerbated by the fact that chemical reaction data is typically derived from experimental results, which may vary in accuracy and reproducibility depending on the conditions under which they were obtained. Additionally, proprietary concerns and intellectual property restrictions in the chemical industry further limit access to comprehensive datasets, creating a bottleneck for researchers seeking to develop and refine ML models. Another significant challenge lies in the interpretability of ML models. Many state-of-the-art models, particularly those based on deep learning architectures, function as "black boxes," producing predictions without offering clear insights into how these predictions were derived [42]. While these models may achieve high accuracy, their lack of transparency makes it difficult for researchers to trust their outputs or to extract meaningful chemical principles from their predictions. This opacity poses a major barrier to their adoption in practical settings, where understanding the rationale behind a prediction is often as important as the prediction itself. Furthermore, interpretability is crucial for ensuring that ML models align with established chemical knowledge and do not inadvertently propagate errors or biases present in the training data.

Generalization is another area where ML approaches for chemical reaction prediction encounter difficulties. Models trained on specific datasets often struggle to generalize to unseen reactions or novel chemical spaces that differ significantly from the training data. This limitation arises because chemical reaction spaces are vast and diverse, encompassing countless combinations of reactants, solvents, catalysts, and conditions. As a result, a model trained on a narrow subset of reactions may fail to capture the broader patterns and principles that govern chemical reactivity. This lack of generalization can severely restrict the utility of ML models in real-world applications, where predicting reactions involving novel compounds or under unexplored conditions is often required. Finally, computational costs represent a significant challenge in deploying ML approaches for chemical reaction prediction. Training complex ML models, particularly those involving deep learning techniques, demands substantial computational resources, including high-performance hardware such as GPUs or TPUs. These requirements can be prohibitively expensive and may not be accessible to all researchers or institutions, particularly those with limited funding or infrastructure. Moreover, the computational demands do not end with training; deploying these models for large-scale predictions or iterative optimization tasks can also be resource-intensive. This creates an additional barrier to entry for researchers who wish to leverage ML techniques but lack access to the necessary computational tools. In summary, while ML approaches for chemical reaction prediction offer exciting possibilities for advancing the field of chemistry, several challenges must be addressed to unlock their full potential. Issues related to data quality and availability, model interpretability, generalization capabilities, and computational costs all pose significant obstacles that require innovative solutions. Overcoming these challenges will likely involve interdisciplinary collaboration among chemists, data scientists, and computer scientists to develop methods that are not only accurate but also transparent, generalizable, and accessible to a broad range of researchers. By addressing these hurdles, the field can move closer to realizing the transformative impact of ML on chemical reaction prediction and beyond.

Future Directions

Transfer learning and the use of pretrained models represent a transformative approach in machine learning, particularly in the context of chemistry and related scientific fields. By leveraging models that have already been trained on large, diverse datasets, transfer learning allows researchers to fine-tune these models for specific tasks or datasets of interest, even when data availability is limited. This capability is especially valuable in fields where data scarcity is a persistent challenge, as it enables researchers to overcome this limitation while improving the generalization capabilities of the models. Pretrained models, therefore, serve as a powerful foundation that can be adapted to specialized applications, ultimately enhancing the efficiency and accuracy of predictions in chemistry-related problems. Moreover, the adoption of explainable artificial intelligence (AI) is another crucial advancement that holds significant promise for the field. By focusing on the development of interpretable machine learning models, researchers can provide clearer insights into the underlying chemical principles and mechanisms that drive model predictions. Such transparency not only fosters trust in AI-driven tools but also facilitates their acceptance among chemists, who often seek to understand the rationale behind computational outputs. Explainable AI bridges the gap between complex algorithms and domain expertise, making it a vital area of focus for future advancements. Furthermore, the integration of machine learning models with experimental workflows has the potential to revolutionize research processes. By seamlessly incorporating computational predictions into experimental designs, researchers can accelerate the validation of hypotheses and foster a collaborative environment between computational and experimental chemists. This synergy ensures that predictions are not only theoretically sound but also practically applicable, leading to more efficient discovery and innovation. Additionally, the expansion and curation of reaction databases play a pivotal role in advancing machine learning applications in chemistry. Larger and more diverse datasets enable the development of robust and versatile models capable of capturing a wide range of chemical phenomena. Efforts to compile comprehensive reaction databases will not only enhance model performance but also open new avenues for exploration and discovery in chemical research. Together, these advancements—transfer learning, explainable AI, integration with experimental workflows, and expanded reaction databases—represent key pillars for leveraging machine learning to address complex challenges in chemistry and beyond.

Conclusions and Future Perspectives

In conclusion, the application of machine learning (ML) in predicting chemical reactions has emerged as a transformative approach, offering significant advancements over traditional computational and experimental methods. This review highlights the diversity of ML techniques, ranging from supervised and unsupervised learning to deep learning and reinforcement learning, which have been successfully applied to predict reaction outcomes, reaction pathways, and reaction kinetics. The integration of ML with quantum chemistry, cheminformatics, and automated synthesis platforms has further expanded the scope of chemical research, enabling the discovery of novel reactions and the acceleration of drug development. Despite these achievements, several challenges remain. The quality and quantity of training data are critical for building accurate and generalizable models, yet chemical reaction datasets often suffer from issues such as data sparsity, noise, and bias. Additionally, the interpretability of ML models remains a key concern, as many approaches function as "black boxes," making it difficult to derive mechanistic insights. Addressing these limitations will require the development of more robust data curation techniques, the adoption of explainable AI methods, and the creation of standardized benchmarks for model evaluation. Looking forward, the future of ML in chemical reaction prediction is highly promising. Advances in natural language processing (NLP) could enable the extraction of vast amounts of reaction data from scientific literature, while innovations in generative models may facilitate the design of entirely new reactions with desired properties. Furthermore, the integration of ML with high-throughput experimentation and robotics has the potential to revolutionize reaction optimization and catalyst discovery. Collaborative efforts between chemists, computer scientists, and data engineers will be essential to harness these opportunities effectively. As computational power continues to grow and algorithms become more sophisticated, we anticipate that ML will play an increasingly central role in chemical research, driving progress toward a more predictive and data-driven paradigm. Ultimately, by addressing current challenges and embracing interdisciplinary collaboration, ML approaches will not only deepen our understanding of chemical reactivity but also pave the way for breakthroughs in materials science, pharmaceuticals, and sustainable chemistry.

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