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Engineering and Design of Molecular Systems

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Introduction

The application of deep learning to various research problems has accelerated progress in many fields and brought traditional paradigms into a new era of intelligence. Like the role of instruments in the old chemical revolution, we emphasize the need to integrate deep learning into engineering and molecular systems design as a catalyst for change in the next chemical revolution. To meet such research needs, we summarize the progress and progress of several key elements of molecular systems: molecular characterization, property estimation, characterization learning, and synthesis planning. Additionally, we emphasize the latest developments and promising directions of various deep learning optimization architectures, methods, and platforms. Our point of view is of interest to both computational and experimental researchers because it aims to chart a way forward for interdisciplinary cooperation, synthesize knowledge from available chemical data, and guide experimental work.

Theory

Chemicals not only play a central role in finding solutions too many pressing problems, but they also play a central role in the sustainable development of the global economy. Various chemical inventions have had a profound impact on our lives, such as the key role of synthetic fertilizers and industrial catalysis in the relationship between our food energy and water [1]. However, many developments in the past stem from accidental or rule-based heuristic experiments, subject to time and resource constraints, and a small class of molecular structures. From a chemical engineering perspective, another complex aspect of new chemical development lies in the multi-scale nature of chemical products and processes. Since chemicals provide hope for solving urgent needs, insisting that current design difficulties are simply the result of molecular complexity can result in global environmental efforts falling short of the 2,030 targets [2]. As you can see, the current paradigm shift requires new drivers of chemical product and process innovation to gain a foothold. The deep neural network architecture has surpassed many traditional and artisan AI methods, and continues to maintain the most advanced performance on many complex learning tasks. As deep learning algorithms become more and more complex in processing complex information, their applications have been extended to chemical engineering, including molecular design, control, and optimization. In particular, deep learning has overcome decades of theoretical and experimental work, predicting its 3D structure from the gene sequence of a protein, thus making a breakthrough in biological research. Facts have proved that the potential for transformational paradigm shift in deep learning chemical engineering has never been more accessible and urgent than it is today.

In the ongoing development of deep learning algorithms and architectures, significant progress in multiple learning tasks is attributed to attention-based neural network architecture. Since its first use in language tasks in 2017, the application of transformers has moved to visual tasks, and this development has appeared in the supervised learning framework of deep learning. The self-supervised learning framework has recently demonstrated the gathering of deeper knowledge in different fields. It also extends to integrated platforms in autonomous driving laboratories and to model interpretation due to medical and scientific applications. We hope that the latest advancements in deep learning will provide opportunities for the rapid and exciting development of new chemicals and process designs [3]. This development can be achieved most effectively by integrating knowledge from the fields of science and engineering to determine molecular representation, modeling, and physical limitations. Here, we first present the state of the application of deep learning in chemical design, namely, molecular characterization, property estimation, characterization learning, and synthesis planning. Then we discuss and describe new trends related to deep learning-based chemicals. And open path research, process design. Finally, the article summarizes the perspectives for future directions and recommendations.

Molecular Systems is the core of the molecular design learning task. Popular statements in molecular design and discovery fall into two categories: two-dimensional and three-dimensional. The correct choice of molecular representatives depends on the domain knowledge of the problem being discussed and the deep learning framework used. However, the choice of the best-performing representation for a learning task is not always clear. Stick to open research channels in computer chemistry. The choice of molecular representation (input) implemented by the deep learning method has a significant impact on their performance [4]. Therefore, designing generative models that support successful deep learning applications consumes most of the work of creating a molecular design framework. The original molecular representation is usually converted into a numerical representation through multiple neural networks, from which the original molecular representation can also be reconstructed. In the optimization process of these networks, the upper and lower level features represented by the molecules are encoded in the so-called latent or hidden space. In space, each molecular structure corresponds to a potential representation, which is usually a real-valued vector.

Attribute estimation models can help guide the design of molecular solutions because such models are designed to capture the underlying behavior of molecular systems controlled by thermodynamics. The purpose of this type of model is to reduce the time and cost associated with experimental screening, while significantly expanding the size of the design space [5]. When learning quantitative structural attribute relationship functions, deep learning algorithms systematically search the hypothesis space and find complex relationships; otherwise these relationships will be too complex to be conceptualized by experts. The synthesis plan (reverse synthesis) is the process of determining a series of chemical reactions to produce target molecules from available precursors [6]. The combination problem can also be solved from the backward approach by recursively selecting the precursor of the target molecule. Molecular design efforts have long been devoted to measuring the accessibility of candidate molecules from the perspective of synthesis through the routine use of expert-set synthetic accessibility scores and rules. Another approach is deep learning, which has brought about a

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successful paradigm shift, by using deep learning-based models to learn to classify potential precursors, which surpasses the traditional efforts of the past 6 years.

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