Through Graphical Models to Address out-of-Distribution Ways

Zexuan Lin*

GCTB-Northeastern State University (Tahlequah), USA Joint Institute of Technology, Guangzhou college of technology and business, Foshan, Guangdong province, China

Abstract. Out-of-distribution (OOD) generalization in deep learning models remains one of the significant challenges in artificial intelligence research. This article will systematically discuss the issue of OOD generalization, including the current primary solutions, comparative analysis of various methods and the future development directions in this field. The article first introduces the issues related to OOD generalization in the autonomous driving field, and then categorizes the mainstream methods for enhancing the OOD generalization ability of models nowadays. The system introduces methods for learning from data without labels, a structure-aware method and uncertainty-aware graph structure learning (UnGSL). Then these methods will be compared and summarized, and their respective advantages and disadvantages will be analyzed and contrasted. Finally, future research directions and plans for enhancing the OOD generalization ability of the model are also proposed. The article aims to provide a clearer and more comprehensive understanding of some breakthrough methods in current research on OOD generalization ability, and promote the application of these methods in actual fields.

1 Introduction

The issue of Out-of-distribution (OOD) generalization in deep learning models is a significant problem. The generalization ability of the model is weak, meaning that the parameters learned for a specific task are difficult to transfer to other tasks. This severely limits its adaptability in multi-task learning scenarios or real-world environments, resulting in incorrect answers or decreased accuracy in data prediction. Meanwhile, there is an urgent demand for this application in reality, such as in the field of autonomous driving. The behavioral decision-making module plays a kid role in connecting the high-level perception module with the low-level planning and control module. It provides a firm guarantee for the realization of safe and efficient autonomous driving technology. Lane-changing decision-making is a core issue in behavioral decision-making that requires a comprehensive analysis of the positions, speeds and other information of all vehicles within the observable environment, and making decisions based on observational data [1]. Nowadays, mainstream lane-changing decisions based on rules lack adaptability and generalizability to a complex environment. It is also reflected in the medical field, like a model for detecting emotional

* Corresponding author's email: lzx200606112025@outlook.com

stress that can be used for daily portable monitoring of people's emotional changes. However, due to the differences in signals among individuals, the OOD generalization problem in stress detection [2]. Therefore, the enhancement of generalization ability plays a crucial role in many fields.

This method quotes methods that vary samples and collect large-scale datasets that are both representative and diverse. This can make samples from various scenarios and allows for a better understanding of the model's output, effectively enhancing the model's generalization ability; in addition, by expanding the training data and performing random rotations and flipping of images. That can generate more image samples from different angles, thereby increasing the diversity of the training data[3]. These methods by increasing and training the dataset, allowing the model to generate output across a broader range of datasets, it can improve the model's OOD generalization ability.

In light of these methods, this paper also systematically reviews and compares other methods that enhance the OOD generalization ability. And then the latest methods have been proposed, this paper discusses the major challenges that exist today and the research directions to focus on in the future.

2 Research Background

2.1 The basic research background of the topic

With the application of AI in autonomous driving and the medical industry, if the generalization ability of the model leads to harmful results, the result would be unimaginable. This is also a breakthrough in the development of AI today, and effectively addressing this issue, which will be the essential path for the popularization of AI in critical infrastructure applications. This topic is a summary of methods to improve the OOD generalization of models.

2.2 The significance of the review

The problem of OOD generalization of models has always been a pressing concern in the development of AI. This review focuses on previous research that emphasized the diversity and quantity of datasets used to train models. Nowadays, some newly proposed methods, such as ingeniously defining structural embeddings and further integrating their properties into invariant learning. Research on OOD generalization ability has made breakthrough methods. By reviewing these, researchers can gain a clearer understanding of current breakthrough methods, thereby facilitating the innovation of subsequent methods.

2.3 Main overview of the OOD generalization problem in deep models

The OOD generalization means that machines in a deep learning model, the ability to perform on unknown predictions that are distributed differently from the training dataset. With a daily analogy, consider a student who understands basic chemical principles and concepts. No matter how complex or novel the questions are, the student can apply its core principles to solve the problem. This shows the student's OOD generalization ability is strong. Therefore, if a model has strong OOD generalization ability, the accuracy of the answers given by the machine will be higher.

3 Methods for OOD Generalization of Models

3.1 Invariant representation learning and label-free method

3.1.1 Necessary and sufficient causal information for invariant representation learning

For invariant representation learning, the general goal is to find all possible causalities, minimize the invariant risk. For example, these methods related to invariant risk generally assume that the generation process of data X is composed of causal features C and V(C or V, like environmental features or stylistic features). The goal of the method is to conclude the causal representation in the data through the model, just like how X can be judged to have two features C and V based on X. In the problem of OOD generalization, there are three common data generation assumptions shown in Figure 1. The arrows denote the causal generative direction and the dashed line connects the spurious correlated variables. In every assumption, the relationship between causal information C and data label Y remains unaffected by domain information V. Therefore, in order to improve the model's OOD generalization ability, and need to enhance the accuracy of labels and add some essential features that ensure the accuracy of causal information. Researchers divide label information into two types of features: necessity and sufficiency. Necessity describes the label as not true if the features disappear and sufficiency describes the presence of a feature that helps us determine the correctness of the label[4]. In invariant representation learning, environmental labels are necessary for model training. The called environmental labels refer to a set of samples with specific feature distributions. Every environment has a unique data distribution and the requirement for the model to be trained in multiple environments can enhance its generalization ability.

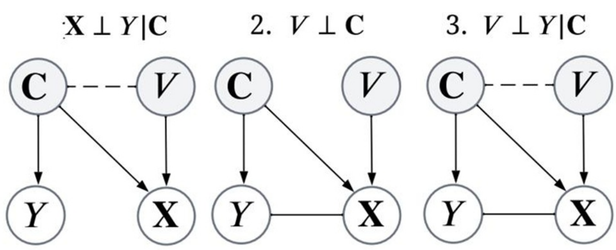

Fig. 1. Causal graph [4].

3.1.2 Self-supervised method without label

Invariance representation learning requires environmental labels to train the model, so it is important to have sufficient and necessary causal information and to grasp this causal information. However, not all causal information is the most crucial in generalization tasks. If incorrect key causal information is found, it is highly likely to mislead the model, resulting in erroneous prediction outcomes, which limits the application of such methods in academic research and practical scenarios. Self-supervised methods that do not require labels can solve the problem of poor generalization ability caused by incorrect labels.

With the continuous increase in data volume nowadays, the cost of manually annotating data labels for model training is also escalating. Unlabeled methods leveraging their unique characteristics can also enhance the learning efficiency and generalization ability of models. The principle of the unlabeled self-supervised learning method is based on the variational autoencoder. That can make the model automatically infer environmental labels from the training dataset during deep learning. The variational autoencoder can leverage the inherent structure within the dataset to generate pseudo-labels, thereby obtaining accurate environmental labels during the environmental inference phase[5]. Like in the medical field, analyzing medical scan images poses a challenge due to the impracticality of obtaining a vast amount of detailed medical image information, which also incurs high costs. Therefore, Self-supervised method without labels can classify with limited data, which can enhance the accuracy and efficiency of medical image model analysis.

3.2 Structure-aware method

In the previous invariant learning, researchers overlooked the constraints inherent to the unique structure of graph data, while the structure-aware method precisely embeds the graph structure into invariant learning. Like the Structure-aware Invariant learning framework for Node-level Graph OOD generalization (SING), the approach focuses on the regularization term of the specific structural invariance of the graph, and performs invariant learning under the constraints of aggregation patterns. Specifically, develop the invariance constraint regularization terms during the optimization of augmentations. Additionally, they define the structure embedding to elucidate the structural property and design the structure embedding alignment loss to optimize the augmentations and the invariant representations. By introducing the structure information, further integrate the unique structural property into invariant learning[6]. This not only enhances diversity across different environments but also enables the model to predict labels. The method also emphasizes node-level training, training the model's graph data through the commonalities and connections between nodes[7]. Like nowadays, graph neural networks (GNN) are used this way, which constructs a diverse graph by modifying nodes. Making it a graph enhancement technique for multiple training environments to solve the out-of-distribution generalization problem[8]. For deep learning on graph data, these models can effectively learn the structural information of graph data through the message passing mechanism between nodes in graph data and have achieved success in various types of tasks related to graph data. However, like this method, due to the interconnected nature of the graph structure, samples are not independent, which complicates the specific nature of node distribution bias. Identifying training environment information becomes challenging, variations in the feature, structural distributions between training and testing nodes can also lead to a decline in model performance. Graph data is also very common in daily life, such as dynamic graphs used in financial transactions and transportation networks. The nodes of these graphs are relatively complex, so the model's OOD generalization for such graph datasets is relatively weak**.**

3.3 Uncertainty-Aware Graph Structure Learning (UnGSL)

3.3.1 The basic principles of graph structure learning

The previously mentioned structure-aware method encounters difficulties in training node information within graph data. This method uses embedding node information in graph data for unchanged learning. This method reutilizes the uncertainty of node information, ignoring some node information that is irrelevant to the final model output. This allows for adaptive aggregation of information, thereby reducing the impact of such irrelevant node information[9].

Just like in some graph information, such as noisy connections and incomplete information, due to the inherent complexities and inconsistencies in data collection, which can conversely act as interference. Graph structure learning involves analyzing the node information of a graph and extracting the main information to generate answers. However, this method tends to overlook the rich relationships among the majority of unlabeled nodes.

3.3.2 Uncertainty-Aware graph structure learning (UnGSL)

This method was proposed in 2025, this type of method is an improvement on existing graph structure learning. UnGSL does not directly use the similarity of node information embeddings to learn the structure of symmetric graphs. This way focuses on the quality of node information and conducts a theoretical analysis of this node information. Blindly aggregating information from low-quality nodes can degrade the performance of uncertainty-aware nodes. UnGSL estimates the uncertainty of node information and utilizes it to adjust the strength of directional connections, where the influence of nodes with high uncertainty is adaptively reduced. This method utilizes the learnable values of each node to distinguish between high-quality and low-quality node information[10]. This also enhances the efficiency of model output and significantly improves OOD generalization, also avoiding the impact of low-quality node information. However, if the distribution exceeds the correlation between node uncertainty and node structure quality, the model's ability to generalize beyond the distribution is significantly limited.

4 The Connections and Comparisons among the Three Methods

Table 1. Three methods to enhance the ability of OOD generalization.

The name of the method	Self-supervised method without labels	Structure-aware method	Uncertainty-Aware Graph Structure Learning
Advantage	Reduced the cost of learning with labeled models	The introduction of graph data structures meets are current needs	Pay attention to the consideration of uncertainty in node information
Disadvantage	Lack of graph data	That cannot effectively handle node information in a complex graph	Rely on uncertainly nodes and node quality

There is relative progress among these three methods. In the first method, the unsupervised approach that doesn’t require labels, for example, as mentioned in Table 1. It frees the model from its dependence on labels. Some models require environmental labels to produce output results, which also makes causal information and environmental labels crucial. However, the cost of these manual labels is high and the efficiency is low. If the model labels are incorrect, it will greatly reduce the model's OOD generalization ability.

In the second method, the structure-aware method, it embeds the graph data structure into the invariant learning process. By leveraging the commonalities and connections between nodes, the graph data of the model is trained. Additionally, nodes can be modified to construct multiple graph datasets, which can enhance the model's OOD generalization ability of graph data within the model. However, these methods are not yet fully developed in grasping complex node information, such as that in dynamic graphs.

In the third method, the Uncertainty-Aware Graph Structure Learning, this type of method is relatively new and focuses on uncertainty node information. In the uncertainty node, information. Firstly, node information is classified to reduce the interference of irrelevant information during model output. This way also enhances the model's OOD generalization ability. However, this information is limited to the uncertainty of the nodes, if it exceeds the model's capacity, it may not be able to produce satisfactory output. Therefore, for these three methods, there are both relative advantages and disadvantages that need improvement. Future research on OOD generalization methods for models should also focus on these issues.

5 Conclusion

This paper sorts out the currently popular problem of OOD generalization ability of models, presenting three representative methods. These methods have significantly enhanced the OOD generalization ability of models to a certain extent, but they also possess drawbacks that need to be improved in the future. It is not difficult to find the problem of OOD generalization in real-life scenarios. If a model in deep learning overly focuses on unessential details, its accuracy will significantly decrease. In the medical field, machine models cannot fully cover all the special situations of patients. Like some rare diseases may have similar symptoms to common diseases in their early stages, which makes the model difficult to distinguish between them, potentially leading to misdiagnosis and other issues. Therefore, in order to apply AI models to more fields in the future. The researchers need to continue research and experimentation to address OOD generalization, which can enhance the generalization ability of these AI.

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