VR-GNN: Variational Relation Vector Graph Neural Network for Modeling both Homophily and Heterophily

Fengzhao Shi$^{1,2}$*, Ren Li$^{1,2}$*, Yanan Cao$^{1,2}$†, Yanmin Shang$^{1,2}$, Lanxue Zhang$^{1,2}$, Chuan Zhou$^{3}$, Jia Wu$^{4}$ and Shirui Pan$^{5}$

$^1$Institute of Information Engineering, Chinese Academy of Sciences
$^2$School of Cyber Security, University of Chinese Academy of Sciences
$^3$Academy of Mathematics and Systems Science, Chinese Academy of Sciences
$^4$Macquarie University
$^5$Griffith University

{shifengzhao, liren, caoyanan, shangyanmin, zhanglanxue}@iie.ac.cn, zhouchuan@amss.ac.cn, jia.wu@mq.edu.au, s.pan@griffith.edu.au

Abstract

Graph Neural Networks (GNNs) have achieved remarkable success in diverse real-world applications. Traditional GNNs are designed based on homophily, which leads to poor performance under heterophily scenarios. Current solutions deal with heterophily mainly by mixing high-order neighbors or passing signed messages. However, mixing high-order neighbors destroys the original graph structure and passing signed messages utilizes an inflexible message-passing mechanism, which is prone to producing unsatisfactory effects. To overcome the above problems, we propose a novel GNN model based on relation vector translation named Variational Relation Vector Graph Neural Network (VR-GNN). VR-GNN models relation generation and graph aggregation into an end-to-end model based on Variational Auto-Encoder. The encoder utilizes the structure, feature and label to generate a proper relation vector for each edge. The decoder achieves superior node representation by incorporating the relation vectors into the message-passing framework. VR-GNN can fully capture the homophily and heterophily between nodes due to the great flexibility of relation translation in modeling neighbor relationships. We conduct extensive experiments on eight real-world datasets with different homophily-heterophily properties and verify the effectiveness of our method.

1 Introduction

Graph Neural Networks (GNNs) have revealed superior performance on various real-world graph applications, ranging from social networks [Wang et al., 2019], citation networks [Veličković et al., 2018] to biological networks [Sanyal et al., 2020]. Graph Convolutional Network (GCN) [Kipf

*Equal contribution
†Corresponding author

Figure 1: Passing signed message and relation vector translation. The nodes B and C are the neighbors of A. Different colors of nodes represent different classes. The $B_{pos}$ (or $C_{pos}$) and $B_{neg}$ (or $C_{neg}$) represent the negative message and message transformed by relation vector of node B (or C) respectively. $R_b$ (or $R_c$) represents the relation vector of node B (or C). Dash lines with arrows represent aggregation operation.

and Welling, 2017] and its variants [Klicpera et al., 2018; Chen et al., 2020] learn node representations via smoothing the features between neighbor nodes. The smoothing operation is suitable for homophilic graphs [McPherson et al., 2001], where connected nodes tend to possess similar features and belong to the same class. However, on heterophilic graphs [Lim et al., 2021] where connected nodes have dissimilar features and different labels, the traditional GCNs suffer from poor performance and even underperformance Multi-layer Perceptron (MLP) that completely ignores the graph structure [Li et al., 2018].

Recently several efforts have been proposed to achieve heterophily-based GNNs. The algorithms can be mainly divided into two families based on designing methodologies: mixing high-order neighbors [Pei et al., 2019; Li et al., 2022b] and passing signed messages [Bo et al., 2021; Chien et al., 2020]. The approach of mixing high-order neighbors expects to aggregate more homophilic nodes and
remove heterophilic nodes. However, its performance is limited by the structure extracted and priors used [Suresh et al., 2021], which makes it more likely to produce a loss of information compared to directly modeling original graph [Ekabaram, 2014]. The approach of passing signed messages uses positive and negative signs to modify neighbor information. Under this type of method, the neighbors of different classes send negative messages to each other for dissimilating their features, and those of the same class pass positive messages for assimilation. However, the single numerical sign suffers from limited expressing capacity, which causes the modeling to be inflexible and insufficient. As shown in figure 1 (a), the heterophilic neighbors B and C deliver their negative messages $B_{\text{neg}}$ and $C_{\text{neg}}$ to A. However, the scalar weight (normally within $[-1, 1]$ to maintain numerical stability during message passing [Bo et al., 2021]) restricts $B_{\text{neg}}/C_{\text{neg}}$ to moving along the dotted line, hence the new aggregated representation of A is confined to the blue shaded part, which does not have the desired effect on extending distance between heterophilic neighbors.

To overcome the above problems, we introduce relation vectors into the message-passing framework. Inspired by the relation idea of knowledge graphs (KGs) [Hogan et al., 2021], we consider the connections also serve as the relationship between nodes. The message passing between nodes could be described by the added translation of the relation vector, which is similar to the form of TransE, a classical translation model for KG embedding [Bordes et al., 2013]. The demonstration is shown in figure 1 (b), neighbors B and C translate their features to $B_{\text{ref}}$ and $C_{\text{ref}}$ by the relation vector $R_{\text{B}}$ and $R_{\text{C}}$. Then after aggregating, central node A could obtain a more preferred representation in the red area to dissimilate with B and C. Compared with signed scalar weights, relation vectors are more flexible and expressive for modeling homophily and heterophily between nodes, which helps to achieve more adaptive message-passing algorithm.

Based on the above idea, we present a novel method named Variational Relation Vector Graph Neural Network (VR-GNN) for short). VR-GNN builds the framework based on Variational Auto-Encoder (VAE) [Kingma and Welling, 2013]. The encoder of VR-GNN treats relation vectors as hidden variables and adopts variational inference to generate it based on the graph structure, feature and label, which involve homophily and heterophily at different aspects [Suresh et al., 2021; Yang et al., 2021; Zhu et al., 2021]. The decoder incorporates generated relation vectors into the message-passing mechanism, where messages are computed by translating neighbors along connections. Because relation vectors have encoded the homophily/heterophily property of each edge, the translation could produce a suitable assimilation/dissimilation effect between neighbors. Finally, the model takes the output node representation to perform the downstream classification task and achieves SOTA performance on eight various datasets.

In summary, our main contributions are as follows:

- We propose a new message passing mechanism grounded on relation vector translation, for modeling both homophilic and heterophilic connections in graphs. Compared to previous approach of singed message passing, relation vectors are more flexible and possess a more expressive capacity.
- We propose a novel method named Variational Relation Vector Graph Neural Network (VR-GNN). VR-GNN builds the framework based on Variational Auto-Encoder (VAE), and provides an effective end-to-end solution for both relation vector generation and relation guided message passing.
- Through extensive experiments on eight common homophilic and heterophilic datasets, we demonstrate the validity of our introduced relation vector concept and VR-GNN method.

## 2 Preliminary

### 2.1 Problem Definition

A graph can be denoted as $G = (V, E)$ with a set of nodes $V = \{v_1, v_2, \ldots, v_N\}$ and a set of edges or connections $E$. The connections of a graph can be described by its adjacency matrix $A = [a_{ij}] \in \{0, 1\}^{N \times N}$, where $N = \|V\|$ is the number of nodes, and $a_{ij} = 1$ means node $v_i$ and $v_j$ has a connection $e_{ij}$ between them. The node feature matrix of a graph can be denoted as $X \in \mathbb{R}^{N \times F}$, where $F$ is the feature dimension per node. $x_i \in \mathbb{R}^F$ denotes the $i$-th row of $X$ and corresponds to the feature of node $v_i$. In this paper, we focus on the semi-supervised node classification task, which aims to learn a mapping $f : V \rightarrow C$, where $C = \{c_1, c_2, \ldots, c_M\}$ is the label set with $M$ classes, given $A$, $X$ and partially labeled nodes $\{(v_1, y_1),(v_2, y_2), \ldots\}$ with $y_i \in C$.

### 2.2 Message-passing Framework

Currently, most graph neural networks (GNNs) apply message-passing framework [Gilmer et al., 2017] to formulate their workflow. Normally the message-passing framework consists of $L$ layers, and in each layer $l$, it aggregates neighbor and central nodes with the rule of:

$$h_i^{l+1} = U(h_i^l, \text{AGG}(h_j^l : j \in N_i))$$

where $h_i^l$ denotes the embedding of node $v_i$ in layer $l$; $N_i$ is the neighbor set of node $v_i$; $\text{AGG}(\cdot)$ is the neighbor aggregation function; $U(\cdot)$ is the updating function, to renew the central node embedding with aggregation information and original node information.

### 2.3 Homophily Ratio

Here we introduce the concept of homophily ratio [Pei et al., 2019] to estimate the homophily level of a graph.

**Definition 1 (Homophily ratio).** The homophily ratio of a node $v_i$ is the proportion of its neighbors belonging to the same class as it. The homophily ratio of a graph is the mean of homophily ratios of all its nodes:

$$H = \sum_{v_i \in V} \left| \left\{ e_{ij} : e_{ij} \in E \land y_i = y_j \right\} \right| / |N_i| \in [0, 1]$$

A high homophily ratio represents the graph possesses a strong homophily property, and a low homophily ratio indicates a weak homophily property or strong heterophily property.
3 Methodology

3.1 VR-GNN Framework

The core idea of VR-GNN is to introduce relation vectors to describe diverse homophilic and heterophilic connections of the graph, for helping GNN achieve a more effective message passing. Furthermore, we treat such process as an encoder-decoder paradigm, to firstly encode the connection characteristics into relation vectors, then decode the relation vectors through GNN to complete the downstream task, i.e. node classification here.

In this work, we take Variational Auto-Encoder (VAE), a popular probabilistic technique to encode/decode hidden embedding of the data [Kingma and Welling, 2014], as our overall framework. Specifically, we treat the relation vector of graph connections as latent variable \( z \), and the node classification as a prediction process guided by \( z \), hence the process of VR-GNN can be formalized as following:

\[
p_\theta(Y | A, X, Y_{tr}) = \int p_\theta(z | A, X, Y_{tr}) p_\theta(Y | z, A, X, Y_{tr}) \, dz
\]

where \( A \) is adjacency matrix; \( X \) is node feature matrix; \( Y \in \mathbb{R}^{N \times M} \) is label matrix; \( Y_{tr} \) is training label matrix; \( \theta \) denotes learnable parameters.

Since the true posterior \( p_\theta(z | A, X, Y_{tr}) \) is intractable, we adopt variational inference [Mnih and Gregor, 2014] to learn it. We introduce a variational distribution \( q_\phi(z | A, X, Y_{tr}) \), parameterized by \( \phi \), to approximate \( p_\theta(z | A, X, Y_{tr}) \), and we aim to minimize KL divergence between the two distributions:

\[
\min_{\phi} \text{KL} [q_\phi(z | A, X, Y_{tr}) \| p_\theta(z | A, X, Y_{tr})]
\]

then following the standard derivation of variational inference (details in appendix A), we can get the ELBO (Evidence Lower Bound) learning object:

\[
\max_{\theta, \phi} \mathcal{L} = - \text{KL} [q_\phi(z | A, X, Y_{tr}) \| p(z)] + \mathbb{E}_{q_\phi(z | A, X, Y_{tr})} \left[ \log p_\theta(Y_{tr} | z, A, X) \right]
\]

The derived ELBO includes two terms, which respectively correspond to the encoder and decoder training of VR-GNN. The first term is a KL divergence, that the encoder \( \phi \) is trained to generate relation vector \( z \) by observed graph information \( A, X, Y_{tr} \). Meanwhile, \( z \) is controlled by a manually assigned prior distribution \( p(z) \). For the second term, the decoder \( \theta \) is trained to employ generated \( z \), together with \( A \) and \( X \), to predict observed node labels \( Y_{tr} \). We abbreviate the two terms as \( \mathcal{L}_{en} \) and \( \mathcal{L}_{de} \) respectively.

In the inference phase, the learned encoder \( \phi \) can be directly used to generate relation vectors, and the decoder \( \theta \) is used to predict the unknown node labels. Hence we derive the final formulization of VR-GNN:

\[
p_{\theta, \phi}(Y | A, X, Y_{tr}) = \int q_\phi(z | A, X, Y_{tr}) p_\theta(Y | z, A, X, Y_{tr}) \, dz
\]

The framework demonstration can be seen in figure 2.

3.2 Encoder: Relation Vector Generation

We model the relation vector of each connection as independent identically distribution, given \( A, X \) and \( Y_{tr} \), therefore the variational posterior distribution \( q_\phi(z_{ij} | A, X, Y_{tr}) \) and prior distribution \( p(z) \) can be factorized as:

\[
q_\phi(z_{ij} | A, X, Y_{tr}) = \prod_{e_{ij} \in E} q_\phi(z_{ij} | A, X, Y_{tr}) \quad p(z) = \prod_{e_{ij} \in E} p(z_{ij})
\]

and the learning object of encoder can be rewritten as:

\[
\mathcal{L}_{en} = - \sum_{e_{ij} \in E} \text{KL} [q_\phi(z_{ij} | A, X, Y_{tr}) \| p(z_{ij})]
\]

Inspired by the implementation of VAE [Kingma and Welling, 2014], we let the posterior be a multivariate normal distribution, and the prior a standard multivariate normal distribution, which is flexible and could make the computation analytical:

\[
n(\mu_{ij}, \sigma^2_{ij} I) \\
p(z_{ij}) = N(0, I)
\]

where \( \mu_{ij} \) and \( \sigma^2_{ij} \) are distribution parameters to be learned.

Furthermore, the relation vector \( z_{ij} \) expects to encode the comprehensive homophily and heterophily characteristics of a connection. To achieve this goal, we mainly consider three aspects of information to generate \( z_{ij} \): structure, feature and label (corresponding to \( A, X \) and \( Y_{tr} \)), for there have been works showing graph topology, node feature and node labels to serve as important parts for homophily and heterophily modeling [Suresh et al., 2021; Yang et al., 2021; Zhu et al., 2021].

Specifically, we decompose \( z_{ij} \) into three sub-relation vectors to be separately generated from varying aspects, then linearly combined to fuse the information:

\[
z_{ij} = \alpha_s z_{s,ij} + \alpha_f z_{f,ij} + \alpha_l z_{l,ij}
\]

where \( \alpha \) are hyper-parameters for composing weight, \( z_{s,ij}, z_{f,ij} \) and \( z_{l,ij} \) denote structure, feature and label sub-relation vectors, which like \( z \), are set as multivariate normal distribution with mutual independence:

\[
q_\phi(z_{s,ij} | A, X, Y_{tr}) = q_\phi(z_{s,ij}) = N(\mu_{s,ij}, \sigma^2_{s,ij} I) \\
q_\phi(z_{f,ij} | A, X, Y_{tr}) = q_\phi(z_{f,ij} | X) = N(\mu_{f,ij}, \sigma^2_{f,ij} I) \\
q_\phi(z_{l,ij} | A, X, Y_{tr}) = q_\phi(z_{l,ij} | Y_{tr}) = N(\mu_{l,ij}, \sigma^2_{l,ij} I)
\]

hence if we have got each sub-relation’s expectation \( \mu_{-,ij} \) and variance \( \sigma^2_{-,ij} \), we can derive the distribution of \( z_{ij} \) as:

\[
\mu_{ij} = \alpha_s \mu_{s,ij} + \alpha_f \mu_{f,ij} + \alpha_l \mu_{l,ij} \\
\sigma^2_{ij} = \alpha^2_s \sigma^2_{s,ij} + \alpha^2_f \sigma^2_{f,ij} + \alpha^2_l \sigma^2_{l,ij}
\]

and we detail the design of each sub-relation vector below.
Structure Sub-relation Vector For capturing structure aspect information, we assign a randomly initialized expectation and variance embedding for each connection:

$$\mu_{s,ij} \in \mathbb{R}^{|E| \times H}$$
$$\sigma_{s,ij} \in \mathbb{R}^{|E| \times H}$$

(12)

where $H$ denotes hidden dimension. Because there is no guidance for generation, the subsequent learning of sub-relation vector is in fact based on the graph structure. This is inspired by many knowledge graph embedding works [Bordes et al., 2013; Wang et al., 2021], where entity and relation embedding are normally randomly initialized, and could achieve meaningful steady state by learning triplet structure over the graph.

Feature Sub-relation Vector This is motivated by the observation that, the feature of edge endpoints could be regarded as weak label information, and may also serve as an indicator for connection homophily and heterophily [Yang et al., 2021]. Specifically, we employ the Multi-layer Perceptron (MLP) to transform the concatenation of two endpoints feature, and generate expectation and variance as follows:

$$f_{ij} = \text{ReLU} (\text{MLP}([x_i \| x_j]))$$
$$\mu_{f,ij} = \text{MLP}(f_{ij})$$
$$\sigma_{f,ij}^2 = \text{MLP}(f_{ij})$$

(13)

Note that the above MLPs are different modules, for reducing symbols we adopt the same denotation (the same below).

Label Sub-relation Vector The label of two end-nodes can provide direct homophily and heterophily description for a connection, but the usage of label information faces two problems: 1. There are only partially observed node labels; 2. The introduction of label information for in-degree node may lead to label leakage problem, as message passing will bring the “correct answer” to the node. Therefore we only use out-degree node label to generate sub-relation vector. Specifically, for a connection $e_{ij}$, we take node $v_i$’s label $y_i$ as one-hot vector, and feed it into MLP to generate expectation and variance embedding. For unobserved labels, we set the one-hot vector as zero. The process can be formulized as following:

$$\mu_{l,ij} = \text{MLP}(y_i)$$
$$\sigma_{l,ij}^2 = \text{MLP}(y_i)$$

(14)

Relation Vector Generating After getting each sub-relation’s mean and variance embedding, we combine them into the final embedding $\mu_{ij}$ and $\sigma_{ij}^2$ by equation 11. Additionally, instead of directly sampling $z_{ij}$, we apply the re-parameterization trick of VAE [Kingma and Welling, 2014] to make the sampling process derivable:

$$z_{ij} = \mu_{ij} + \sigma_{ij}^2 \epsilon$$

(15)

where $\epsilon \sim \mathcal{N}(0, I)$. After getting each edge’s posterior $z_{ij}$, equation 7 is conducted to calculate the encoder loss.

3.3 Decoder: Message Passing with Relation Vector

The decoder aims to incorporate generated relation vectors into message-passing framework, to complete downstream node classification task. Currently, there existing several relation-based GNN works, like R-GCN [Schlichtkrull et al.,
of TransE [Bordes et al., 2013], a classical knowledge graph model, that the relation both serves as a semantic and numerical translation for connected nodes. Our message-passing function can be formalized as follows:

\[ h_i^{l+1} = U(h_i^l, \text{AGG}(\varphi(h_{ij}^l, z_{ij}) : j \in \mathcal{N}_i)) = W^l h_i^l + z_{ji} \]

where \( h_i^l \) denotes the embedding of node \( v_i \) in layer \( l \); \( z_{ji} \) denotes the relation vector of edge \( e_{ji} \) in layer \( l \), with \( z_{0i} = z_{ji} \). For each neighbor, we apply a matrix transformation and relation translation before aggregating. This can convert neighbors to a more proper feature with the central node, and flexibly model the homophily and heterophily property of each connection when message passing.

After each layer, relation vectors will also go through a matrix transformation, to maintain the layer consistency with node embedding:

\[ z_{ji}^{l+1} = W_{rel}^l z_{ji} \]

Next, we give the overall procedure of the decoder and corresponding implementation details. Firstly, we apply MLP to transform original node feature to higher-level embedding:

\[ h_i^0 = \text{ReLU}(\text{MLP}(x_i)) \]

Secondly, we conduct aggregation function. Considering that attention mechanism can adaptively model the influence of different nodes, we take self-attention [Bahdanau et al., 2015] to aggregate neighbor information:

\[ \overline{h}_i^l = \text{AGG}(\varphi(h_{ij}^l, z_{ij}) : j \in \mathcal{N}_i) = \sum_{j \in \mathcal{N}_i} \beta_{ij}^l(\varphi(h_{ij}^l, z_{ji})) \]

where \( \beta_{ij}^l \) is attention coefficient:

\[ \beta_{ij}^l = \frac{\exp\{h_i^l \varphi(h_{ij}^l, z_{ji})\}}{\sum_{k \in \mathcal{N}_i} \exp\{h_i^l \varphi(h_k^l, z_{ki})\}} \]

Thirdly, we conduct updating function to renew the central node embedding:

\[ h_i^{l+1} = \theta \overline{h}_i^l + (1 - \theta) h_i^0 \]

where \( \theta \) is to balance \( \overline{h}_i^l \) and \( h_i^0 \), that can maintain the computing stability by attaching a residual of initial layer. Then the second and third steps will iterate \( L \) times to get the output node representation:

\[ h_i = h_i^L \]

Finally, we employ an MLP to perform node classification:

\[ y_i^{\text{pred}} = \text{MLP}(h_i) \]

### 3.4 Training and Inference

**Training** After getting the prediction of each node, we can calculate a semi-supervised loss for the decoder, which corresponds to the second term of equation 4:

\[ L_{de} = -\frac{1}{N_{tr}} \sum_{v_i} \text{CE}(y_i^{\text{pred}}, y_i) \]  

where \( N_{tr} \) is the training node number; \( \text{CE}(\cdot) \) denotes the cross entropy function. Then with the encoder loss of equation 7, we could derive the overall loss of the model:

\[ L_{(\theta, \phi)} = \gamma L_{en} + (1 - \gamma) L_{de} \]

Here we add a weighting hyper-parameter \( \gamma \) between the encoder and decoder, which aims to provide training process a more flexible focus.

**Inference** In the inference phase, when generating \( z_{ij} \) by \( q_\phi(z_{ij}|A, X, Y_{tr}) \), we directly use the expectation \( \mu_{ij} \) as the relation vector of edge \( e_{ij} \). We ignore the variance \( \sigma_{ij} \) to reduce the noise for inference, which is similar as [Kipf and Welling, 2016].

### 4 Experiments

#### 4.1 Experiment Setup

**Datasets** We conduct experiments on eight real-world datasets. Among them, Cora, Citeseer and Pubmed are normally regarded as homophilic graphs, and Chameleon, Squirrel, Actor, Cornell and Texas are considered as heterophilic graphs. We use the same dataset partition as [Chien et al., 2020], which randomly splits nodes into train/validation/test set with a ratio of 60%/20%/20%. The details of datasets can be seen in appendix C.

**Baselines** We compare VR-GNN with several state-of-the-art baselines to verify the effectiveness of our method, including: MLP: that only considers node features and ignores graph structure; Homophily-based GNNS: GCN [Kipf and Welling, 2017], GAT [Veličković et al., 2018] and SGC [Wu et al., 2019], which are designed with the homophily assumption; Heterophily-based GNNS: FAGCN [Bo et al., 2021], GPR-GNN [Chien et al., 2020], BernNet [He et al., 2021], ACM-GCN [Luan et al., 2022], that take the approach of passing signed messages, and GeomGCN [Pei et al., 2019], H+GCN [Zhu et al., 2020], HOC-GCN [Wang et al., 2022], BM-GCN [He et al., 2022], GloGNN++ [Li et al., 2022b], that take the approach of mixing high-order neighbors. For all methods, we report the mean accuracy with a 95% confidence interval of 10 runs. Appendix D gives more details of model settings.

#### 4.2 Results of Node classification Task

Table 1 lists the results of VR-GNN and other baselines for node classification task, from which we can observe that: VR-GNN outperforms all the other methods on all five heterophilic datasets. This proves the effectiveness of employing relation vectors to achieve a heterophily-based GNN. Specifically, VR-GNN significantly outperforms traditional GNNS, i.e. GCN, GAT and SGC, relatively by 24.8%,
On homophilic datasets, i.e. Cora, Citeseer and Pubmed, VR-GNN performs better or comparably to the baselines. Specifically, VR-GNN outperforms all the methods on Citeseer and Pubmed dataset. For Cora dataset, VR-GNN also achieves the second best report with only 0.87 difference with GAT. These show that VR-GNN possesses a consistent performance on homophily scenarios, which further proves the adaptive modeling capacity of relation vectors.

### 4.3 Ablation Study of Three Sub-relations

To evaluate the effect of each sub-relation vector part, we do the ablation study of only removing one sub-relation part and simultaneously removing two of them. We take Chameleon, Squirrel, Texas and Citeseer as example datasets. The results are demonstrated in table 2. The subscripts $s$, $f$, $l$ respectively denotes the sub-relation used. We can see that generating relation vectors with absence of some relation cannot provide stable performance across datasets compared to VR-GNN, which verifies the necessity of composing all three parts.

### 4.4 Visualization Analysis

To show the modeling effect of VR-GNN more intuitively, we conduct the node embedding visualization for Squirrel dataset. We extract the node embedding of VR-GNN and five

#### Table 2: Ablation study of three sub-relations.

| Datasets | Chameleon | Squirrel | Texas | Citeseer |
|----------|-----------|----------|-------|----------|
| VR-GNN | 69.89 | 53.37 | 93.18 | 81.02 |
| VR-GNN | 69.54 | 52.74 | 93.51 | 81.16 |
| VR-GNN | 70.00 | 53.03 | 92.79 | 80.96 |
| VR-GNN | 70.22 | 55.12 | 93.71 | 81.36 |
| VR-GNN | 70.69 | 56.78 | 93.71 | 81.20 |
| VR-GNN | 70.30 | 54.38 | 93.51 | 81.88 |

| VR-GNN | 71.21 | 57.50 | 94.86 | 81.95 |

#### Table 1: Results on homophilic and heterophilic datasets with mean accuracy (%) ± 95% confidence interval. The best and second best results are in bold and underlined. OOM means out of memory when reproducing. H$_2$GCN and HOC-GCN report mean accuracy (%)± standard deviation.

| Datasets | Chameleon | Squirrel | Texas | Citeseer |
|----------|-----------|----------|-------|----------|
| VR-GNN | 69.89 | 53.37 | 93.18 | 81.02 |
| VR-GNN | 69.54 | 52.74 | 93.51 | 81.16 |
| VR-GNN | 70.00 | 53.03 | 92.79 | 80.96 |
| VR-GNN | 70.22 | 55.12 | 93.71 | 81.36 |
| VR-GNN | 70.69 | 56.78 | 93.71 | 81.20 |
| VR-GNN | 70.30 | 54.38 | 93.51 | 81.88 |

| VR-GNN | 71.21 | 57.50 | 94.86 | 81.95 |

#### Figure 3: Node embedding visualization for Squirrel dataset. Different colors correspond to different node classes.
Figure 4: Influence of weight parameter γ on Chameleon, Squirrel, Cora and PubMed dataset.

Figure 5: Influence of weight parameter θ on Chameleon, Squirrel, Cora and PubMed dataset.

Figure 6: Analysis of parameters α_s, α_f, α_l.

4.5 Hyper-parameter Analysis

In this section, we investigate the sensitivity of hyper-parameters used in VR-GNN. We take Chameleon, Squirrel, Cora and PubMed as example datasets.

Weight Parameter γ. To investigate the influence of KL divergence loss (encoder loss) for learning effect, we conduct the sensitivity experiment for parameter γ (equation 25). We test the node classification accuracy of VR-GNN with γ ranging from 0.1 to 0.9. The results are reported in figure 4. We can discover that the trends of γ are the same in all datasets, which from a low point slowly rise to a maximum and then gradually decline. This is because KL loss restricts the generated relation vector not to deviating far from the prior distribution, and the small γ may lead to too large or too small embedding, while the large γ will harm the learning of classification task.

Weight Parameter θ. The parameter θ balances the node’s original feature and neighbor aggregation information (equation 21). A larger θ indicates a greater role graph structure plays. We test the node classification accuracy of VR-GNN with θ from 0.1 to 0.9. The results are shown in figure 5. We can observe that VR-GNN has greater θ on Chameleon and Squirrel datasets. This is because in Chameleon and Squirrel graph structure is more important, while in Cora and PubMed node feature is more important. This can also be proven in table 1: VR-GNN improves 49.6% and 81.2% over MLP on Chameleon and Squirrel, while only 13.4% and 4.6% on Cora and PubMed.

Analysis of Parameters α_s, α_f, α_l. Figure 6 shows the best results of α_s, α_f and α_l on four datasets. We can observe that although the parameters of different datasets are not completely consistent, they still show some similarity, which is related to the characteristics of corresponding datasets.

5 Related Work

According to the connection characteristics of the applied graphs, we introduce two families of GNN works: homophily-based GNNs and heterophily-based GNNs.

The homophily-based GNNs are developed mainly for homophilic graphs, which are the earliest proposed and extensively studied. GCN [Kipf and Welling, 2017] proposes an expressive and efficient graph convolution paradigm by simplifying the polynomial convolution kernel; GAT [Veličković et al., 2018] applies the self-attention mechanism to adaptively adjust aggregation weights; SGC [Wu et al., 2019] designs a lightweight GNN by disentangling convolutional filters and weight matrices; GraphSage [Hamilton et al., 2017] proposes an inductive node embedding method with sampling and aggregating features from neighborhood. GIN [Xu et al., 2018] designs a simple yet effective convolution mechanism to explore the upper bound of message-passing based GNNs under homophily.

The poor performance of homophily-based GNNs on heterophily scenarios inspires the study of heterophily-based GNNs. Geom-GCN [Pei et al., 2019] proposes a novel geometric aggregation scheme to acquire more homophilic neighbors; BM-GCN [He et al., 2022] explores block-guided...
neighbors and conducts classified aggregation for both homophilic and heterophilic nodes; GloGNN [Li et al., 2022b] learns a coefficient matrix from graph and utilizes it to aggregate nodes with global homophily; FAGCN [Bo et al., 2021] proposes an adaptive method to capture both low and high-frequency graph signal by passing signed message; GPR-GNN [Chien et al., 2020] learns signed weighting of different orders of graph structure to deal with both homophily and heterophily.

6 Conclusion

In this paper, we propose a new method that utilizes relation vectors to model homophily and heterophily. Then we propose a novel model named Variational Relation Vector Graph Neural Network (VR-GNN). VR-GNN builds the framework based on Variational Auto-Encoder (VAE) and provides an effective end-to-end solution for both relation vector generation and relation fused message-passing. Extensive experiments on eight real-world datasets verify the validity of our method.

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A ELBO Derivation

We start from the KL divergence of equation 3, which can be transformed with following steps:

\[
\begin{align*}
\text{KL} \left[ q_{θ}(z|A, X, Y_{tr}) || p_{θ}(z|A, X, Y_{tr}) \right] \\
= E_{z \sim q_{θ}} \left[ \log q_{θ}(z|A, X, Y_{tr}) - \log p_{θ}(z|A, X, Y_{tr}) \right] \\
= E_{z \sim q_{θ}} \left[ \log q_{θ}(z|A, X, Y_{tr}) - \log \frac{p_{θ}(z, Y_{tr}|A, X)}{p_{θ}(Y_{tr}|A, X)} \right] \\
= E_{z \sim q_{θ}} \left[ \log q_{θ}(z|A, X, Y_{tr}) - \log p_{θ}(z, Y_{tr}|A, X) \right] + \\
E_{z \sim q_{θ}} \left[ p_{θ}(Y_{tr}|A, X) \right] \\
= -L(θ, φ) + p_{θ}(Y_{tr}|A, X) \geq 0
\end{align*}
\]

Therefore, maximizing the log-likelihood \( p_{θ}(Y_{tr}|A, X) \) is equivalent to maximizing its lower bound, i.e. ELBO:

\[
L(θ, φ) = -E_{z \sim q_{θ}} \left[ \log q_{θ}(z|A, X, Y_{tr}) - \log p_{θ}(z, Y_{tr}|A, X) \right] \\
\]

B Algorithm Complexity Analysis

Here we analyse the time complexity of VR-GNN.

The generation of each sub-relation vector costs \( O(|E|) \), hence the time complexity of encoder is \( O(|E|) \). For the decoder, the feature transformation in equation 18 is of \( O(|V|) \) complexity. For each GNN layer, the aggregation function and updating function respectively cost \( O(|E|) \) and \( O(|V|) \) complexity. Finally, the MLP for classification is of \( O(|V|) \) complexity.

Therefore, the overall time complexity of VR-GNN is:

\[
O(L|E| + |L||V|)
\]

where \( L \) is the layer number. This matches the complexity degree of other GNN baselines, like FAGCN [Bo et al., 2021] and GPR-GNN [Chien et al., 2020].

C Dataset Details

In the experiments, we utilize eight real-world datasets with different homophily ratio:

- Cora, Citeseer and Pubmed are three citation networks [Sen et al., 2008; Namata et al., 2012] with high homophily ratio.
- Chameleon and Squirrel [Pei et al., 2019] are page-page networks extracted from Wikipedia of specific topics, with low homophily ratio.
- Actor [Pei et al., 2019] is constructed according to the actor co-occurrence in Wikipedia pages and holds low homophily ratio.
- Cornell and Texas [Pei et al., 2019] are two sub-datasets of WebKB, a webpage database constructed by Carnegie Mellon University, and possess low homophily ratio.

In practice, Cora, Citeseer and Pubmed are regarded as homophilic graphs, and Chameleon, Actor, Cornell and Texas are considered as heterophilic graphs. The statistics of datasets are demonstrated in table 3.

D Model Settings

For fair comparison, we reproduce all the baselines in our environment. For MLP, GCN, GAT and SGC model, we tune them for the optimal parameters. For FAGCN, GPR-GNN, ACM-GCN, BM-GCN and GloGNN++, we rerun the models with the default parameters given by the author. For GeoGNN, H2GCN, BernNet and HOC-GCN, we report the results of published papers.

For our method, we use early stopping strategy with 200 epochs and set an maximum epoch number as 1000. We set the dimension of node embedding and relation vector as 64, and the layer number of GNN as 2. We use Adam optimizer to train the model, and tune learning rate from \{0.01, 0.02, 0.05, 0.001, 0.002, 0.005\}, weight decay from \{0, 1e-4, 5e-4, 1e-5, 5e-5\}. We tune the hyperparameters \( α, β, γ \) from 0 to 1, with 0.1 step size. To mitigate the overfitting problem, we take dropout when training. We implement our method based on PyTorch Geometric (PyG) library [Fey and Lenssen, 2019] and Python 3.9.12. The program is executed on 32GB Tesla V100 GPU.

E Visualization Analysis of Relation Vectors

In this section, we give some intuitive demonstrations of the relation vector and compare it with the signed message method.

For the message passing on edge \( e_{ji} \), we denote the relation vector message as \( m^{rel}_{ji} \) and compute it according to equation 16:

\[
m^{rel}_{ji} = Wh_j + z_{ji}
\]

For the signed message, we directly assign the correct sign for the connection, with +1 for homophily and -1 for heterophily:

\[
m^{sign}_{ji} = \begin{cases} Wh_j, & y_j = y_i \\ -Wh_j, & y_j \neq y_i \end{cases}
\]

where matrix \( W \) is the same in \( m^{rel}_{ji} \) and \( m^{sign}_{ji} \). Then we conduct two aspects of analysis, to compare the effect of two messages for modeling homophily/heterophily connections and helping node classification task.

E.1 Effect for Modeling Homophily/Heterophily

Modeling homophily/heterophily property of a connection means that the message could conduct effective assimilating/dissimilating operation between connected nodes. To evaluate this, we utilize the embedding of VR-GNN in \( L - 1 \) layer and compute the relation vector message \( m^{rel}_{ji} \) and signed message \( m^{sign}_{ji} \) for each edge. Then by adding the messages to \( h_i \), respectively, we can get the new representation of central node \( h_i^{rel} \) and \( h_i^{sign} \). We compare \( h_i^{rel}, h_i^{sign} \).
### Table 3: Dataset Statistics

|            | Cora | CiteSeer | PubMed | Chameleon | Squirrel | Actor | Texas | Cornell |
|------------|------|----------|--------|-----------|----------|-------|-------|---------|
| # Node     | 2708 | 3327     | 19717  | 2277      | 5201     | 7600  | 183   | 183     |
| # Edge     | 10556| 9228     | 88651  | 62742     | 396706   | 53318 | 558   | 554     |
| # Feature  | 1433 | 3703     | 500    | 767       | 2089     | 932   | 1703  | 1703    |
| # Class    | 7    | 6        | 5      | 5         | 5        | 5     | 5     | 5       |
| Homophily Ratio $\mathcal{H}$ | 0.656 | 0.578 | 0.644 | 0.024 | 0.055 | 0.008 | 0.16 | 0.137 |

(E.2) Effect for Helping Node Classification

In addition to accurately describing the connection property, a valid message should also be consistent with the central node class, so as to facilitate the node classification. To show this, we first calculate the mean center for each node class, based on $L$ layer’s node embedding of VR-GNN. Then we compute the message $m_{ji}^{rel}$ and $m_{ji}^{sign}$ of $L−1$ layer. For each edge, we compare $m_{ji}^{rel}$ and $m_{ji}^{sign}$ with the class center of node $v_i$ using cosine similarity. The results are shown in figure 7. We can observe that relation vector messages are more similar with the central node class than signed messages on most edges, which achieves a more center-cohesive node representation for classification and corresponds to the node visualization results in figure 3.

| Encoder | Chameleon | Datasets | Squirrel | Texas | Citeseer |
|---------|-----------|----------|----------|-------|----------|
| GCN     | 69.38     | 52.76    | 91.35    | 80.68 |
| SGC     | 69.93     | 53.75    | 91.08    | 80.78 |
| Ours    | 71.21     | 57.50    | 94.86    | 81.95 |

Table 4: Comparison results with other encoder designs.
Comparison with Other Encoder Designs

Currently, many works use GNN as an encoder to get the hidden embedding of data [Kipf and Welling, 2016; Kipf et al., 2018]. To further verify the efficacy of our encoder design, we compare it with some GNN-based encoders such as GCN and SGC on four datasets. Specifically, we first employ GCN (SGC) to get node embeddings, then concatenate the embeddings of two endpoints of each edge, and use MLP to calculate the mean $\mu$ and variance $\sigma$ of the relation vector. Other structure of VR-GNN remains the same. The results are shown in table 4. We can observe that our encoder outperforms GCN and SGC by 3.1% and 2.5% on average. Our method is designed to explicitly extract three aspects of information for generation, which can make the encoding process more efficient and less noisy. Unlike GCN and SGC, we design to explicitly extracts three aspects of information for generation, which can make the encoding process more efficient and less noisy.