



Multi-feature representation-based graph attention networks for predicting potential supply relationships in a large-scale supply chain network

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ABSTRACT

This study aims to predict potential supply relationships within a large-scale supply chain network. Identifying appropriate suppliers can help companies mitigate disruptions in the supply of materials and finances. Furthermore, it offers the companies potential profits by enabling more effective resource allocation and fostering innovation. While previous studies have adopted machine learning approaches, these methods may not fully capture the complexity of network topology. Graph neural network-based methods have recently gained attention as a promising alternative. However, since graph neural network-based methods mainly rely on fixed aggregation weights, these methods often struggle to capture the complexity of supply relationships between companies. This study proposes multi-feature representation-based graph attention networks, which explore hidden topological relationships between companies by incorporating semantic characteristics such as product and network features. Our findings demonstrate that the proposed method outperforms machine learning-based and state-of-the-art graph neural network-based methods. In addition, ablation studies confirm that the proposed components significantly improve prediction performance.

1. Introduction

Recently, many companies have encountered economic disruptions due to dynamic changes in supply chain environments (Massari & Giannoccaro, 2021), struggling to effectively manage their supply chain networks (Chen et al., 2013; Karmaker et al., 2021; Sawik, 2013). For instance, during the COVID-19 pandemic, several companies faced adverse financial situations due to disruptions in the supply of materials from China (Ivanov, 2020). Clothing companies in Bangladesh lost USD 3.16 billion in profits as a result of order cancellations (Ali et al., 2021).

Previous studies have shown that identifying alternative supplier relationships can help companies recover from disruptive events (Altan et al., 2021) and ensure the smooth flow of resources and finances necessary for effective supply chain management (Ghodspour & O'Brien, 2001). Collaborating with appropriate suppliers enables companies to reduce material costs and expedite the procurement process (Ecer, 2022), subsequently improving their operational performance (Ma et al., 2020). Additionally, it helps mitigate financial risks associated with purchasing relationships and provides economic advantages

by ensuring access to sufficient funds.

Some researchers have adopted flexible and intuitive decision-making approaches, such as analytical hierarchy process (AHP), to effectively identify relevant suppliers within supply chain networks (Lin et al., 2023; Mafakheri et al., 2011). Saputro et al. (2024) utilized a fuzzy AHP to assess suppliers based on multiple criteria and supply risks in the context of a green supply chain. However, as AHP relies on subjective judgments from stakeholders, its reliability may be limited (Sahoo & Goswami, 2023). In addition, prior research has utilized machine learning (ML) approaches, including support vector machine (SVM), random forest, and logistic regression (Guo et al., 2009; Mori et al., 2012; Sasaki & Sakata, 2021), k-NN algorithm-based supplier selection methods (Cavalcante et al., 2019), and neural networks (NNs)-based methods (Lee & Kim, 2022). Despite their potential, these approaches may fall short in identifying relevant suppliers within large-scale supply chain networks due to their limited capability. ML approaches, such as SVM, k-NN, and random forest, generally focus on the dependency between input and output features, neglecting the network topology, which is an essential component for a comprehensive understanding of

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supply chain networks.

A supply chain network can be characterized as a large-scale system encompassing various dimensions, including extensive connections between multiple buyers and suppliers (Joubert & Meintjes, 2015), the flow of substantial resources throughout the network (Galvez & Bornstein, 2023), and complex interaction structure among its members (Scholz-Reiter et al., 2011). Predicting alternative suppliers in such networks is inherently challenging and computationally demanding, as it requires analyzing the likelihood of supplier relationships based on industry and product characteristics (Lee & Kim, 2022). A supply chain network consists of supply relationships between companies, as well as the flow of resources exchanged between them.

Graph attention network (GAT) can capture complex local and global topological features through the use of an attention mechanism (Veličković et al., 2018). Moreover, graph semantic representation approaches have been employed to model the intricated and heterogenous nature of nodes and edges in large-scale networks (Liu & Krishnan, 2021; Mo et al., 2022). Semantic word representation approaches have also been used to encode the meaning of words as semantic vectors (Grave et al., 2018; Mikolov et al., 2013). Previous studies have shown that two semantic representation approaches improve performance in large-scale networks (Kumar et al., 2020; Mallick et al., 2019).

This study proposes a multi-feature representation-based graph attention network, named MFRGAT, to predict potential supplier relationships within large-scale supply chain networks. MFRGAT captures semantic characteristics, such as industrial and network features, through two distinct representation approaches and uncover hidden topological relationships between companies. The main contributions of this study are threefold.

- (1) We propose a multi-feature representation scheme that integrates product and graph representations. The effectiveness of this scheme is validated through comprehensive ablation studies.
- (2) The proposed method identifies both positive and negative relationships using GAT, even when the network structure is modified without re-training.
- (3) We conduct experiments comparing the proposed method with machine learning methods and graph convolutional neural networks on a real-world large-scale supply chain network. The results demonstrate that our method outperforms these baseline methods.

This paper is structured as follows. Section 2 reviews relevant previous studies. Section 3 outlines the details of the proposed framework and method. In Section 4, we present the results from numerical experiments, including sensitive analysis and ablation studies. Finally, conclusions and implications are discussed in Section 5.

2. Literature review

2.1. Machine learning approaches

Many researchers have embraced ML-based methods to resolve the issues in supply chain networks, as ML has proven effective in solving complex problems across diverse domains such as energy prediction (Lee et al., 2023), natural language processing (Vaswani et al., 2017), and recommendation systems (Li et al., 2023). Mori et al. (2012) utilized a SVM and found that reciprocal characteristics between companies enhance supplier selection performance. Cavalcante et al. (2019) introduced a hybrid approach combining linear regression and k-NN to identify resilient suppliers in digital manufacturing based on financial data. Other approaches include Bayesian belief network (Qazi et al., 2018) and artificial neural network (Wong et al., 2024) for credit risk management. Lee and Kim (2022) proposed a deep learning-based business partner recommendation model that leverages company characteristics, such as industry, product property, and transaction volume.

Their findings show that their method outperforms traditional ML-based approaches. Islam et al. (2024) utilized a deep learning technique to forecast product demand for selecting suitable suppliers and allocating orders. Their proposed approach reduced demand prediction errors by 55.42 % and 13.1 % compared to seasonal auto-regressive integrated moving average and Light-GBT models, respectively. Despite these advancements, significant challenges remain in improving performances within supply chain networks, particularly due to the difficulty of incorporating qualitative factors, such as supplier relationships, reputation, and strategic alliance information, into machine learning and deep learning models. Moreover, traditional ML and deep learning models face limitations in addressing the prediction of supply relationships, as they often struggle to capture the topological features of supply chain networks while preserving the unique characteristics of individual nodes.

2.2. Graph neural network approaches for supply chain management

Previous studies have applied Graph Neural Networks (GNNs) to capture topological supply relationships while preserving the structural properties of supply chain networks (Kosasih et al., 2024; Kosasih & Brintrup, 2022; S. Yang et al., 2024). Additional findings indicate that GNNs are effective in predicting alternative suppliers, classifying companies by industry, and managing risks within supply chains (Kosasih et al., 2024; Kosasih & Brintrup, 2022; Wu et al., 2023). Given the high computational demands of GNNs, Kipf and Welling (2017) introduced Graph Convolutional Network (GCN) as a more efficient alternative for handling topological features. GCN primarily focuses on key neighbors, which helps to reduce computation complexity. Prior research has shown the benefits of GCN in addressing challenges within large-scale network, such as credit risk management (Mitra et al., 2024), routing optimization (Duan et al., 2020), and classification (Xie et al., 2020). Tu et al. (2024) applied a GCN with text2vec to select appropriate suppliers in a large-scale supply chain network. They found that the GCN-based method outperforms other GNN-based approaches, such as Light-GCN and neural graph collaborative filtering.

2.3. Graph attention network approaches

Graph Attention Network (GAT) was first introduced by Veličković et al. (2018) and has been widely utilized across various domains due to its ability to model the varying influence levels of nodes and relationships in large-scale networks using an attention mechanism. Previous studies have adopted GAT in various areas, such as multi-behavior recommendation (Jin et al., 2020; Wang et al., 2019), missing links prediction (Gu et al., 2019), traffic prediction (Huang et al., 2021), vehicle routing (Zhang et al., 2023), and outlier detection (Qiu et al., 2022). Drori et al. (2020) proposed a GAT-based reinforcement learning method to address combinatorial optimization problems. Multi-relation graph attention network (MRGAT), proposed by Dai et al. (2022), utilizes self-attention and multi-head attention mechanisms to capture relational connections among neighboring nodes for link prediction problems. While MRGAT considers the importance of relationships, it does not explicitly incorporate the specific characteristics of individual nodes. In contrast, the method proposed in this study introduces a multi-feature representation mechanism that hierarchically captures both topological graph features and semantic industry features of companies. Consequently, the proposed method can analyze relational connections in a large-scale graph by considering node-specific properties, thereby enhancing the prediction of supply relationships.

This study aims to identify supply relationships, similar to the study of Kosasih and Brintrup (2022), by extracting abundant node and topological features within a large-scale supply chain network. We propose a Graph Attention Network (GAT) with multiple semantic representation approaches to hierarchically capture topological supply relationships while incorporating semantic industry characteristics. To

the best of our knowledge, this is the first attempt to utilize multiple semantic representation approaches in conjunction with GAT to identify supply relationships in a real-world supply chain network.

2.4. Feature representation approaches

Feature representation approaches have been applied to various domains, such as text classification (Kurnia et al., 2020), recommendation system (Lee & Kim, 2022), dialogue recognition (Cerisara et al., 2018), and word presentation (Bojanowski et al., 2017; Mikolov et al., 2013; Pennington et al., 2014). These approaches are useful in capturing and representing the underlying semantic meaning within large textual datasets.

To extract semantic network features while preserving the structural properties of graphs, Perozzi et al. (2014) proposed a graph representation approach that leverages local information obtained through random walks. Tang et al. (2015) introduced a large-scale information network embedding technique, with node proximity, to represent large network features in a low-dimensional space. However, these approaches have limitations in capturing the diverse connectivity patterns within networks. Grover and Leskovec (2016) proposed a node2vec approach considering both local and global information within networks based on a skip-gram technique (Mikolov et al., 2013). They found that node2vec outperforms earlier methods, such as DeepWalk and LINE, by producing better representation performance, as well as being effective in classification and link prediction. Table 1 summarizes previous studies that explore various approaches to supply chain management and feature representation.

3. Proposed method

The proposed method, MFRGAT, operates in two phases: training and testing. In the training phase, MFRGAT explores hidden relationships between companies to accurately predict both positive and negative links within the supply chain network. A *positive relationship* indicates the existence of a supply link between two companies, while a *negative relationship* denotes the absence of such a link. Given that the dataset contains both textual data representing industrial features and network data reflecting supply relationships, we employ both product feature representation and graph feature representation approaches. These methods are effective in capturing both the semantic characteristics of companies and the topological structure of the network. This integrated approach enhances prediction accuracy. Specifically, during

Table 1
Summary of previous studies.

Domains	Categories	Approaches	References
Supply chain management	Machine learning	SVM	(Mori et al., 2012)
		Bayesian belief network	(Qazi et al., 2018)
	Deep learning	k-NN	(Cavalcante et al., 2019)
		DNNs	(Lee & Kim, 2022; Islam et al., 2024)
	Graph learning	GNNs	(Kosasih et al., 2024; Kosasih & Brintrup, 2022; S. Yang et al., 2024)
		GCNs	(Tu et al., 2024)
		Multi-relation GAT	(Dai et al., 2022)
Feature representation	Word representation Graph representation	Word2vec	(Mikolov et al., 2013)
		fastText	(Grave et al., 2018)
		DeepWalk	(Perozzi et al., 2014)
		LINE	(Tang et al., 2015)
		Node2vec	(Grover & Leskovec, 2016)

the training phase, we extract company-level attributes and construct a network structure. The graph representation captures the topological features of companies within the network, while the product representation encodes their industrial features. In these two forms of representations, we can observe complex resource flows aligned with industry-specific contexts. Then, a GAT-based decoder integrates these features to predict whether a relationship between two companies is positive or negative. Fig. 1 illustrates the overall framework of MFRGAT.

In the test phase, the trained MFRGAT model is utilized to predict supplier relationships within the network. The model's performance is evaluated using multiple predictive accuracy metrics. To address the effectiveness of MFRGAT, we compared its performance against traditional machine learning and graph neural network-based methods.

3.1. Graph representation in the encoder

The supply chain network considered in this research is defined as a directed graph, denoted as $G = (V, E)$. $V = \{1, 2, \dots, N\}$ is the set of nodes, which represent companies, and $E = \{(i, j) | i, j \in V\}$ is the set of edges, which indicate supply relationships between companies. To extract the topological features within G , we utilize node2vec approach, which is a semi-supervised learning-based graph representation method (Grover & Leskovec, 2016). This approach is known to be effective in capturing local and global network structures through graph learning and improving prediction accuracy when combined with neural network-based approaches (Ha & Park, 2022). Specifically, we adopt the random walk approach suggested by Grover and Leskovec (2016) to observe sequences of nodes that capture the structural and semantic aspects of a graph. For i , the probability of walking to the next node x , $x \in V$, is defined as follows:

$$P(c_i = x | c_{i-1} = i) = \begin{cases} \frac{\pi_{xi}}{z}, & \text{If } (i, x) \in E \\ 0, & \text{Otherwise.} \end{cases} \quad (1)$$

where c_i , z , and π_{xi} is the i^{th} node in the walk, the normalized constant, and the unnormalized transition probability from i to x , respectively. If the previous node of the random walk is j , $\pi_{xi} = \alpha_{uv}(j, x)$, since the weights of edges in the considered network are not included (Grover & Leskovec, 2016). Specifically, $\alpha_{uv}(j, x)$ is formalized as follows:

$$\alpha_{uv}(j, x) = \begin{cases} \frac{1}{u}, & \text{If } d_{jx} = 0 \\ 1, & \text{If } d_{jx} = 1 \\ \frac{1}{v}, & \text{If } d_{jx} = 2 \end{cases} \quad (2)$$

where d_{jx} is the shortest distance between j and x . u is the control parameter for the probability of repeatedly visiting a node that has just been accessed. The higher the value of u , the lower probability of a repeated visit. If the value of v is higher than 1, the random walk tends to visit nodes that are close to j . Otherwise, the random walk tends to access nodes far from j . Finally, skip-gram (Mikolov et al., 2013) is used to learn the graph properties and represent topological features for companies by using the obtained sequence of all nodes in the considered supply chain network. The graph features of i obtained by this approach is defined as T_i .

3.2. Product representation in the encoder

To semantically represent the product properties of each company, we employ a word embedding approach as suggested by the study of Bojanowski et al. (2017). This approach is useful to handle rare words or morphologically rich languages. Moreover, it allows us to maintain consistent dimensions for input vectors while preserving the semantic

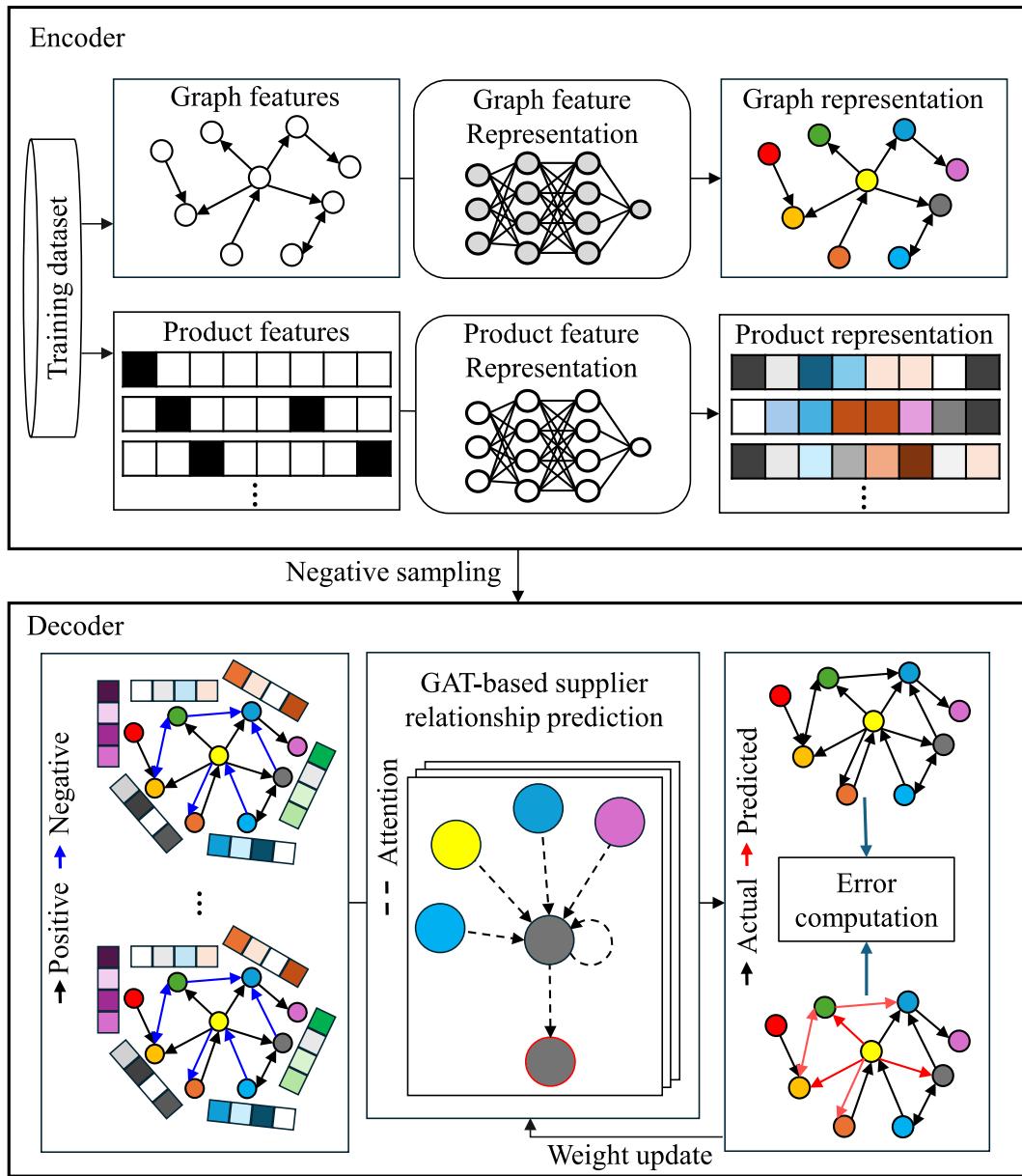


Fig. 1. The proposed framework of MFRGAT.

information of product properties, even when the number of product properties varies between companies.

Specifically, for company i , we define the set of product properties as $Q_i = \{p_1, p_2, \dots, p_n\}$, where p_r is the r^{th} product properties. Before using product representation, p_r is simply represented as a one-hot vector, denoted as \vec{p}_r , with the dimension of $\mathbb{R}^{1 \times l}$, where l is the number of product properties for all companies within the considered supply chain network. Afterward, \vec{p}_r is represented as an embedded vector using the proposed product representation approach, denoted as $\rho(\vec{p}_r)$.

has a dimension of $\mathbb{R}^{1 \times q}$, where q is a learnable parameter for the proposed product representation. Finally, each one-hot vector for all product properties in Q_i is represented as each embedded vector, and these vectors are computed as dot product summation of each other using the proposed product representation to extract the semantic features of i , denoted as S_i with the dimension of $\mathbb{R}^{1 \times q}$.

3.3. GAT-based supplier relationship identification method in the decoder

We utilize GAT in the decoder to identify supplier relationships by learning the importance levels of locations and relationships between companies, incorporating semantic features from the encoder. We consider different levels for nodes in the supply chain network, where the characteristics and number of neighbors vary significantly, using an attention mechanism (Velicković et al., 2018).

We combine the represented features T_i and S_i , along with the industry feature of i , denoted as I_i , to use as input features for the GAT-based supplier relationship identification method, since the product properties vary across the same industry sector. I_i has a dimension of $\mathbb{R}^{1 \times b}$, simply represented as a one-hot vector. GAT takes the combined features denoted as $h_i = \{T_i, S_i, I_i\}$, to learn importance levels of locations and relationships among companies while considering network structure.

Specifically, GAT calculates an attention coefficient between i and j , denoted as e_{ij} , as follows:

$$e_{ij} = a(\text{Concat}[Wh_i, Wh_j]) \quad (3)$$

where $W, W \in \mathbb{R}^{F \times F}$, is a learnable weight parameter applied to every node. e_{ij} represents the significance of \vec{h}_j in relation to i . As suggested in (Vaswani et al., 2017), we utilize a feedforward neural network as attention mechanism, denoted as a , $a \in \mathbb{R}^{2F}$. Afterward, we calculate the graph attention value is denoted as α_{ij} and is represented as follows:

$$\alpha_{ij} = \frac{\exp(\text{LeakyReLU}(a^T \text{Concat}[Wh_i, Wh_j]))}{\sum_{k \in M_i} \exp(\text{LeakyReLU}(a^T \text{Concat}[Wh_i, Wh_k]))} \quad (4)$$

where M_i and $(\bullet)^T$ are the neighbor nodes of i and the transpose

operation, respectively. LeakyReLU is used as an activation function (Veličković et al., 2018).

The computed α_{ij} is employed to calculate a linear combination of the features corresponding to each of neighbor nodes to obtain the topological feature of i representing importance levels in terms of locations and relationships. The topological feature of i produced by GAT is denoted as \vec{h}_i and defined as follows:

$$\vec{h}_i = \text{ELU} \left(\sum_{j \in M_i} \alpha_{ij} h_j W \right) \quad (5)$$

We applied ELU activation function as a non-linear transformation,

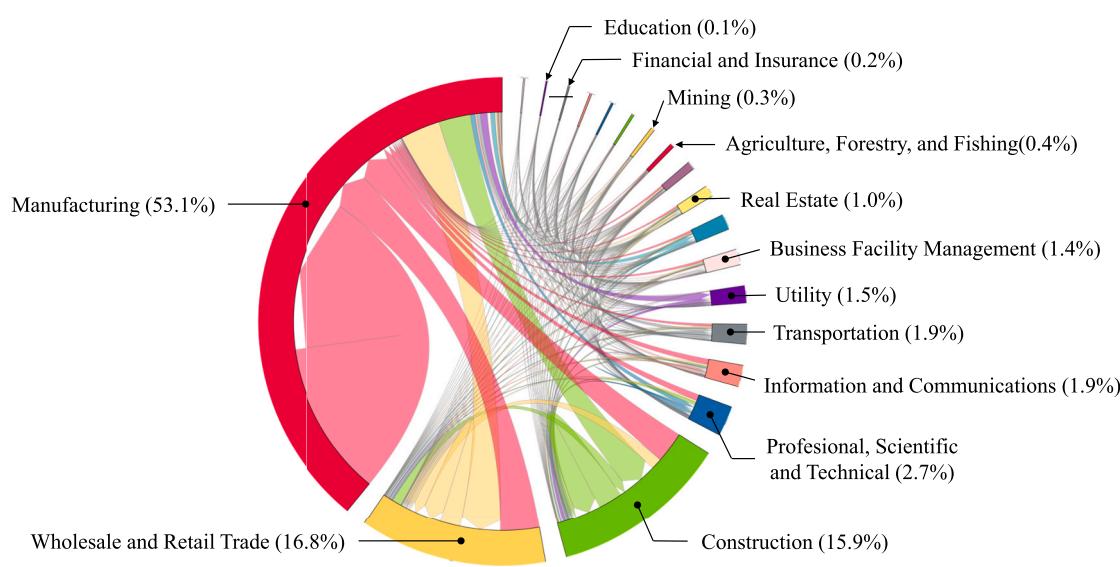
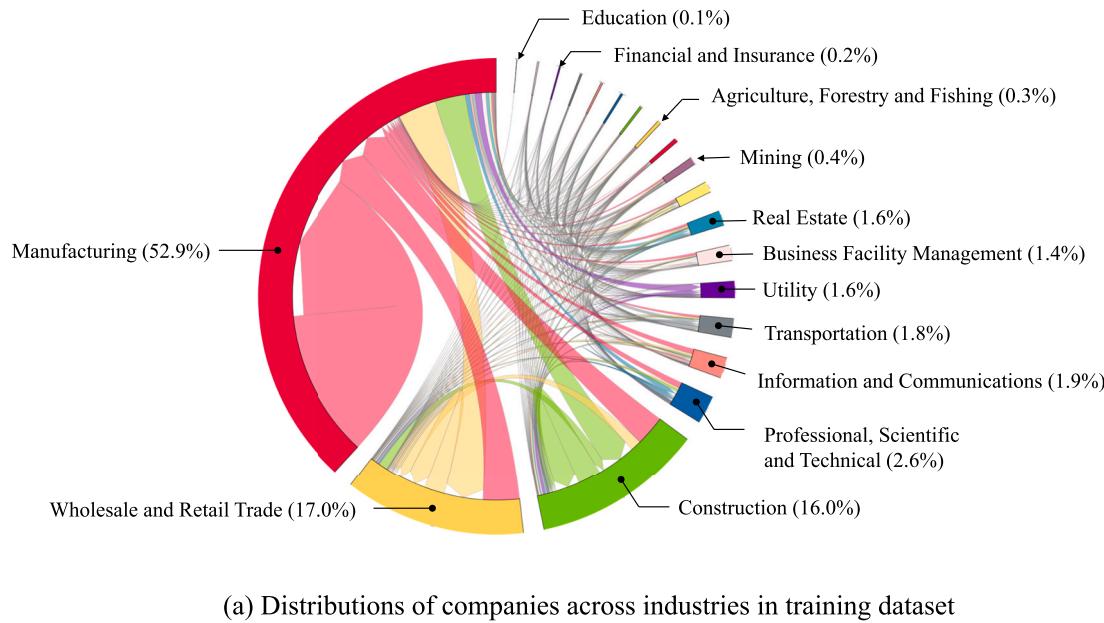


Fig. 2. Chord diagram showing distributions of companies across industries for both the training and test datasets.

following the approach adopted in (Veličković et al., 2018).

After obtaining \vec{h}_i and \vec{h}_j , we compute the probability of the supply relationship between i and j , denoted as P_{ij} , and it is formalized as follows (Gu et al., 2019):

$$P_{ij} = \frac{1}{1 + \exp\left(\left(\vec{h}_i \odot \vec{h}_j\right) \odot \theta\right)} \quad (6)$$

where θ is a g dimensional learnable parameter vector and \odot is dot product operation.

Finally, θ and W are updated by Equation (7), to accurately identify supplier relationships between companies.

$$L = y_{ij} \log(P_{ij}) + (1 - y_{ij}) \log(1 - P_{ij}) \quad (7)$$

where y_{ij} represents actual supplier relationship between i and j . If y_{ij} is 1, it is a positive supplier relationship, otherwise, it is a negative supplier relationship.

4. Experiments

4.1. Dataset

This study utilizes a dataset comprising supply relationships between companies across 20 industries in South Korea. The dataset includes 211,434 companies and 220,971 relationships, represented as nodes and edges, respectively. The dataset is randomly divided into training and test sets at the instance level using a uniform distribution to train the proposed method and validate its performance, ensuring similar industry distribution in both sets. This minimizes the risk of performance evaluation bias caused by uneven industry representation, providing a reliable assessment of the method's effectiveness. Specifically, the instance-level split results in 154,679 training instances (70 % of the total instances) and 66,292 test instances (30 % of the total instances). Both datasets include the same set of nodes, representing 211,434 companies. For the edge-level split, among the 154,679 edges indicating supply relationships in the training dataset, 108,275 edges are used to train the proposed method, while the remaining 46,404 edges are employed to validate the performance of the proposed method during the training. Fig. 2 displays the distribution of companies, expressed as percentage, across industries, in both training and test datasets.

The features utilized in this study are categorized into three groups such as industrial features, product feature, and graph features. These are summarized in Table 2, which highlights their relevance to method selection for modeling supply chain relationships.

Since the datasets contain only positive supply relationships, we

Table 2
Categories of features and their relevance to method selection.

Feature categories	Example variables	Description	Relevance to method selection
Industrial features	Manufacturing, construction, transportation, etc.	Industry classification of companies	Enables the method to consider sector-specific supply chain patterns
Product features	Shredder, scrap, die casting molds, Firefighting etc.	Representation of their product properties based on industry	Enables the method to understand industry-specific product characteristics with respect to supply relationships
Graph features	Link weights, Edge importance level	Representation of the importance level of links within supply chain	Enhances the capability of the method to capture varying levels of importance among supply relationships

perform negative sampling to reduce potential bias in predicting supplier relationships. This is achieved by randomly selecting supply relationships between companies from unknown supply relationships, a method widely utilized in link prediction problems (Gu et al., 2019; He et al., 2020; Trouillon et al., 2016; B. Yang et al., 2014), and performance evaluation (Kosasih & Brintrup, 2022; Tu et al., 2024). Table 3 presents detailed supply chain network information based upon the negative sampling ratios to generate the test dataset. We conduct five independent trials for each negative sampling ratio to reduce potential bias from randomly selected negative samples. These trials allow us to assess the robustness and generalizability of the prediction methods across unseen data under varying supply relationship structures (Bouasria et al., 2023).

4.2. Experiment settings

The parameters u and v used in the graph representation approach are each set to 1. The dimension is set to 128, as referenced in the previous study by Grover and Leskovec (2016), and its effectiveness is validated through repeated experiments in our research. In the product representation approach, we utilize a pre-trained word embedding model (Grave et al., 2018) that embeds a single word into a 300-dimensional vector. This model can be easily implemented using a Python library. Therefore, the dimension of T_i and S_i are 128 and 300, respectively. The dimension of industry vector is 20, resulting in the final input dimension of 448 for the GAT-based supplier identification method. The number of multi-attention heads is set to be 1. Leaky rectified linear unit (Xu, 2015) is employed for all hidden layers as an activation function, but sigmoid function for the output layer is employed as an activation function to identify supplier relationships between companies. Finally, MFRGAT is trained by Adam optimizer (Kingma & Ba, 2015) with a learning rate of 0.01. If the probability yielded by MFRGAT is greater than 0.5, it represents a positive supplier relationship. Otherwise, it indicates a negative relationship. This threshold value is reasonable since it ensures a fair balance between identifying true positives and avoiding false positives, aligning with standard practices in binary classification and commonly used in link prediction tasks (Gu et al., 2019; He et al., 2020; Trouillon et al., 2016). In our evaluation, we varied the negative-to-positive class ratio from 0.3 to 1.5, and the 0.5 threshold consistently yielded balanced classification outcomes across all settings. All experiments are carried out on a PC with an Intel Xeon W-2265 CPU-3.5 GHz, 32 GB of memory, and an RTX 4000 GPU.

To demonstrate the effectiveness and superiority of the proposed method through performance comparison analysis, the baseline methods are implemented as follows.

- (1) SVM: We implemented the SVM-based supplier relationship identification method proposed by Mori et al. (2012), as it represents a machine learning approach often used in supply relationship prediction tasks. This method demonstrated outstanding prediction performance compared to logistic regression in prior studies, justifying its inclusion as a baseline ML model. While this method does not utilize a graph representation for input features,

Table 3
Supply chain network information across negative sample ratios for the test dataset.

Dataset	Negative sample ratios	Positive relationships	Average and standard deviation of the number of negative relationships
D1	0.3	66,292	18,963.6 ± 15.32
D2	0.5	66,292	30,685.4 ± 51.31
D3	1.0	66,292	56,942.4 ± 26.43
D4	1.3	66,292	70,815.8 ± 46.01
D5	1.5	66,292	79,367.0 ± 97.23

- its output features are aligned with those used in the proposed method for consistency in evaluation.
- (2) DBR: We implemented the DNN-based business partner recommendation method proposed by [Lee and Kim \(2022\)](#), as it demonstrated superior performance compared to various ML methods, such as SVM and gradient-boosted trees, as well as a traditional statistical approach. This method serves as a state-of-the-art non-graph deep learning baseline. The input and output features remain consistent with those in the SVM-based method considered in this study.
- (3) IDNS-GCN: We included IDNS-GCN, recently proposed by [Tu et al. \(2024\)](#), for identifying supply relationships. Its network architecture is based on GCN and has demonstrated superior prediction accuracy compared to state-of-the-art GNN-based methods, including neural graph collaborative filtering ([Wang, He, Wang, et al., 2019](#)) and Light-GCN ([He et al., 2020](#)).

Additionally, we adopt *accuracy*, *F1* score, and *specificity* score measures to individually evaluate the supplier identification performance of the proposed methods and baseline methods as they are typically utilized in classification problems ([Altman & Bland, 1994](#); [Xiong et al., 2020](#)). *F1* score is beneficial for balancing between precision and recall by preventing biased performance when considering only one measure. The *specificity* measure evaluates the effectiveness of a method in identifying negative supplier relationships, which significantly affects the flow of resources for companies. *Accuracy* is defined as Equation (8), where *TP* is the number of correctly identified positive supplier relationships, and *FP* is the number of incorrectly identified positive supplier relationships. Conversely, *TN* is the number of correctly identified negative supplier relationships, and *FN* is the number of incorrectly identified negative supplier relationships.

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN} \quad (8)$$

F1 score is computed as the harmonic mean of precision and recall and is defined as follows:

$$F1 = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}} \quad (9)$$

Specificity is defined as Equation (10), where *TN* and *TP* have the same meanings as in Equation (9).

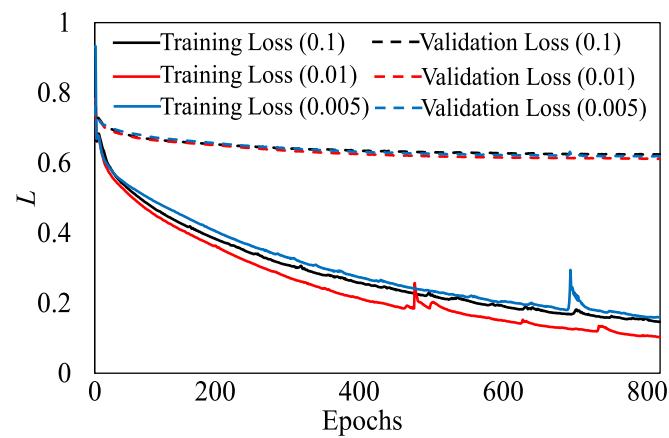
$$\text{Specificity} = \frac{TN}{TN + FP} \quad (10)$$

4.3. Experiment results

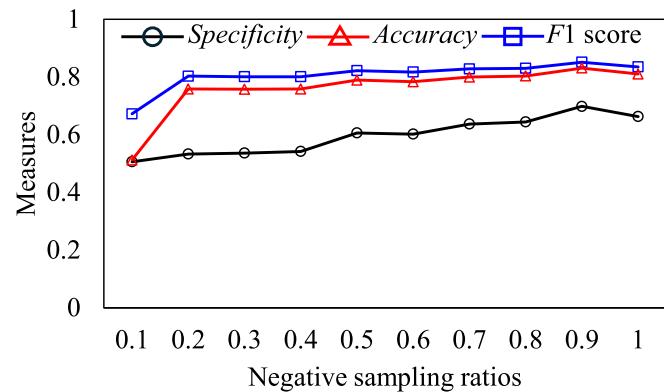
The analysis of training performance with respect to hyperparameters was conducted to investigate sensitivity and assess training performance. [Fig. 3](#) visualizes the training performance of the proposed method across the different learning rates. We observe that a learning rate of 0.01 results in a lower training loss compared to both 0.1 and 0.005, and the validation loss decreases slightly more with a learning rate of 0.01. Based on these results, we found that a learning rate of 0.01 in MFRGAT is effective for identifying supplier relationships.

Furthermore, we analyze the training performance of different negative sampling ratios to determine which ratio yields the best performance. [Fig. 4](#) illustrates the *specificity*, *accuracy*, and *F1* score from the trained MFRGAT with various negative sampling ratios using D3. In [Fig. 4](#), we can see performance differences across negative sampling ratios. It is described that determining an appropriate negative sampling ratio is crucial for achieving improved performance.

[Table 4](#) presents the *accuracy*, *F1* score, and *specificity* of MFRGAT and the baseline methods using the test dataset with different negative sample ratios. Each value in [Table 4](#) represents the means and standard deviations for each measure considered in this study. Moreover, bold



[Fig. 3](#). Training and validation curves across hyperparameters in MFRGAT.



[Fig. 4](#). Training performance comparisons for different negative sampling ratios.

text indicates the best performance among the methods considered in this research. We observe in [Table 4](#) that the standard deviations for all methods are very low. This implies that the performance of all methods might not be sensitive to changes in supply chain network structures. Although IDNS-GCN performs better than the other baselines, MFRGAT surpasses IDNS-GCN in terms of *accuracy* and *F1* score. The results can be attributed to the effectiveness of the proposed graph representation approach and the attention-based neural network architecture, which together enhance the prediction of supplier relationships within large-scale supply chain networks. On the other hand, the improvement in *specificity* is relatively modest compared to the improvements in *accuracy* and *F1* score. This result is likely to be associated with the fact that negative supply relationships are relatively sparse in the training dataset, which may lead to less detailed learning of these relationships. DBR exhibits relatively lower performance, which may be due to the limitations of a learning mechanism that relies on the dependency between input and output values without considering the topological relationships. SVM shows significantly low *specificity* compared to its *F1* score, suggesting that its predictions of supplier relationships might be biased due to a limited ability to capture graph structural information.

Additionally, we perform paired *t*-tests at the 99 % confidence level to validate the performance of MFRGAT compared to the baseline methods. The paired *t*-test is particularly suitable for evaluating the statistical significance of performance differences between two methods based on performance measures and is more appropriate than ANOVA or Wilcoxon test when comparing paired results ([Hodges & Lehmann, 1973](#)). Since the observed performance differences approximately follow a normal distribution, the *t*-test is considered appropriate. Alternative tests, such as McNemar's test, are designed for binary

Table 4

Accuracy, F1 score, and specificity obtained by each method across different negative sample ratios.

Datasets	Measures	Methods			
		SVM	DBR	IDNS-GCN	MFRGAT
D1	Accuracy	0.755 ± 0.001	0.700 ± 0.001	0.881 ± 0.001	0.902 ± 0.001
	F1 score	0.854 ± 0.001	0.789 ± 0.001	0.928 ± 0.001	0.938 ± 0.000
	Specificity	0.168 ± 0.003	0.613 ± 0.002	0.534 ± 0.002	0.699 ± 0.003
D2	Accuracy	0.676 ± 0.001	0.699 ± 0.001	0.835 ± 0.001	0.874 ± 0.001
	F1 score	0.793 ± 0.001	0.758 ± 0.001	0.889 ± 0.001	0.910 ± 0.001
	Specificity	0.167 ± 0.001	0.616 ± 0.003	0.535 ± 0.003	0.694 ± 0.003
D3	Accuracy	0.548 ± 0.002	0.671 ± 0.002	0.760 ± 0.000	0.831 ± 0.000
	F1 score	0.673 ± 0.001	0.689 ± 0.000	0.804 ± 0.001	0.850 ± 0.000
	Specificity	0.166 ± 0.001	0.615 ± 0.001	0.534 ± 0.002	0.697 ± 0.001
D4	Accuracy	0.498 ± 0.000	0.663 ± 0.002	0.730 ± 0.001	0.812 ± 0.001
	F1 score	0.617 ± 0.001	0.652 ± 0.001	0.761 ± 0.000	0.797 ± 0.000
	Specificity	0.165 ± 0.001	0.614 ± 0.002	0.534 ± 0.002	0.696 ± 0.001
D5	Accuracy	0.471 ± 0.000	0.660 ± 0.001	0.714 ± 0.002	0.803 ± 0.000
	F1 score	0.585 ± 0.000	0.631 ± 0.001	0.734 ± 0.000	0.817 ± 0.001
	Specificity	0.165 ± 0.001	0.615 ± 0.001	0.534 ± 0.002	0.696 ± 0.001

outcomes and are therefore not suitable in this context. **Table 5** shows the *p*-value obtained from the paired *t*-tests for each method. The results show that all *p*-values are less than 0.01, indicating the performance of MFRGAT significantly differs from that of the other methods.

We compare the performance of MFRGAT with that of IDNS-GCN across industries using the dataset of D3 to investigate robustness. **Fig. 5** displays the results in terms of *F1* score. Higher values indicate better performance. The white box presents “no test instance” for supply relationships in that category. The *x* and *y* axes represent industry indices, respectively, and the order of the industry index is determined by the dataset distribution in **Fig. 2(b)**. For instance, the industry index of 1 corresponds to “manufacturing,” while the industry index of 2 is “wholesale and retail trade.” As the industry index decreases, it becomes more challenging to identify supply relationships between companies due to the smaller number of training instances for these relationships. Based on the results, MFRGAT achieves *F1* scores exceeding 0.8, while IDNS-GCN exhibits *F1* scores below 0.7 in identifying supply

relationships. Furthermore, **Table 6** presents the predicted probability values of IDNS-GCN and MFRGAT for supply relationships. When the actual label is True, a probability value closer to 1 indicates better performance. Conversely, when the actual label is False, a probability value closer to 0 reflects better prediction performance. These findings suggest that MFRGAT demonstrates higher reliability and accuracy in predicting supply relationships between companies, regardless of whether they belong to the same industry or different industries.

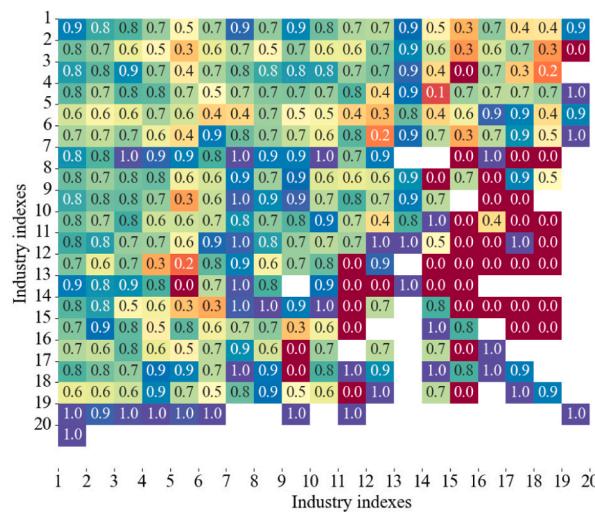
We conduct ablation studies to analyze the importance of the components used in MFRGAT. **Table 7** presents all configurations. GAT is trained solely using industry features, without incorporating features obtained through product or graph representations. On the other hand, PRGAT is trained using both industry and product features extracted through product representation, while GRGAT is trained using industry and graph features embedded through graph representation. Each configuration is trained using the same hyper-parameters, and we evaluate its performance on D1-D5 using the performance measures, as visualized in **Fig. 6(a)–(c)**. Based on the observations, PRGAT underperforms GAT across all datasets, while GRGAT outperforms both GAT and PRGAT on these datasets in terms of performance measures. This finding suggests that the proposed product representation alone may be insufficient to effectively capture the dynamics of supply relationships in a large-scale network. In contrast, leveraging both the structure and features of the network through the proposed graph representation enhances the prediction performance of supply relationships. Our results clearly show that the performance of MFRGAT can be enhanced by incorporating both product representation and graph representation approaches, regardless of imbalanced data distributions. This outcome is likely attributable to the integration of multi-features derived from both the product and graph representation approaches, which provides a more detailed understanding of the dynamics of supply relationships.

Furthermore, paired *t*-tests at the 99 % confidence level are conducted to demonstrate the significance of MFRGAT compared to other configurations. **Table 8** presents the *p*-value obtained from the paired *t*-tests for each method, showing that all *p*-values are less than 0.01. These results indicate that integrating the proposed product and graph representation approaches significantly improves the prediction performance of supply relationships.

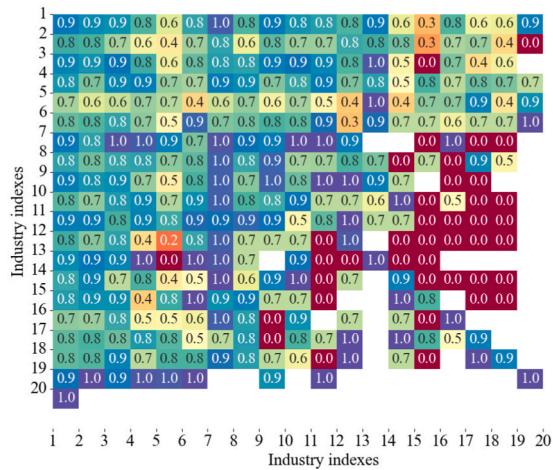
In addition, **Table 9** shows the prediction performance from the top five industries, in terms of their proportion. **Table 10** presents a summary of the method limitations. In **Tables 9 and 10**, MFRGAT outperforms the other configurations in most cases, except for the

Table 5
Paired *t*-test results on MFRGAT with baseline methods.

Datasets	Measures	Methods		
		SVM	DBR	IDNS-GCN
D1	Accuracy	1.08×10^{-15}	2.54×10^{-18}	1.44×10^{-10}
	F1 score	1.03×10^{-10}	1.94×10^{-11}	2.34×10^{-9}
	Specificity	3.45×10^{-16}	3.62×10^{-11}	9.56×10^{-12}
D2	Accuracy	3.91×10^{-15}	2.96×10^{-17}	6.63×10^{-10}
	F1 score	6.19×10^{-18}	7.81×10^{-19}	1.35×10^{-11}
	Specificity	7.38×10^{-15}	1.80×10^{-10}	8.24×10^{-11}
D3	Accuracy	4.08×10^{-19}	1.50×10^{-18}	3.14×10^{-10}
	F1 score	3.81×10^{-20}	1.03×10^{-18}	1.97×10^{-10}
	Specificity	2.84×10^{-19}	7.48×10^{-13}	1.95×10^{-10}
D4	Accuracy	4.40×10^{-18}	8.63×10^{-17}	6.10×10^{-14}
	F1 score	3.25×10^{-15}	4.64×10^{-16}	2.13×10^{-12}
	Specificity	8.81×10^{-17}	1.54×10^{-12}	2.24×10^{-14}
D5	Accuracy	2.89×10^{-18}	5.27×10^{-18}	1.47×10^{-11}
	F1 score	1.19×10^{-19}	8.41×10^{-19}	1.11×10^{-11}
	Specificity	4.91×10^{-20}	1.15×10^{-13}	1.32×10^{-13}



(a) F1 score of IDNS-GCN



(b) F1 score of MFRGAT

Fig. 5. F1 score observed by IDNS-GCN and MFRGAT according to industries across D3.

Information and Communications industry. This suggests that multi-feature representation is effective in capturing complicated relationships within large-scale supply chain networks. Meanwhile, GRAGT

Table 6

Predicted probability values of IDNS-GCN and MFRGAT for the supply relationships.

From company		To company		Actual label	Probability of IDNS-GCN	Probability of MFRGAT
c_i	Industry index	c_j	Industry index			
c_{183}	1	c_{188}	7	True	0.02	0.98
c_{174487}	2	c_{68288}	9	True	0.73	1.00
c_{75653}	3	c_{80942}	10	True	0.24	0.79
c_{2982}	4	c_{143053}	8	True	0.80	1.00
c_{196403}	5	c_{116730}	2	True	0.25	1.00
c_{147}	8	c_{198}	3	True	0.51	0.99
c_{1314}	12	c_{17474}	1	True	0.78	0.97
c_{152389}	1	c_{136659}	16	False	0.59	0.36
c_{179}	2	c_{124}	9	False	0.74	0.01
c_{86}	3	c_{30664}	10	False	0.49	0.11
c_{18575}	5	c_{71124}	5	False	0.99	0.44
c_{32}	6	c_{1610}	1	False	0.67	0.02
c_{16}	6	c_{110}	4	False	0.99	0.24
c_{10}	8	c_{73973}	3	False	0.58	0.70
c_{27096}	9	c_{154263}	4	False	0.41	0.00

shows superior performance compared to PRGAT, indicating that graph features contribute more significantly to prediction accuracy than industrial features. However, GAT exhibits lower prediction accuracy in industries with a large proportion of industrial entities, highlighting its limitation in capturing complex supply chain topologies.

To verify the practical applications of the proposed method, Fig. 7(a) and (b) illustrate the original and extended supply chain networks generated by MFRGAT for a suburban region in South Korea. In Fig. 7, the color and size of each circle represent industry and degree centrality for each company, respectively. From Fig. 7(a) and (b), we observe that MFRGAT effectively extends supply relationships within real-world supply chain networks. This implies that MFRGAT is able to reduce material costs and expedite the purchasing process for companies, thereby enhancing their operational performance by identifying potential supply relationships. Moreover, it promotes economic growth by extending supply relationships across various industries, contributing to the balanced development of industries in the suburban region.

5. Conclusions and implications

This study introduces multi-representation approaches with GAT to predict supplier relationships in a real-world large-scale supply chain network. The proposed method is designed to capture both product features and graph topological characteristics. Our findings demonstrate that the proposed method outperforms existing ML-based and GCN-based approaches. Furthermore, ablation studies confirm that the proposed components significantly enhance prediction performance in a large-scale network. Compared to the previous study (Tu et al., 2024), our findings suggest that the proposed method is more effective in predicting supplier relationships across diverse industries in real-world supply chain settings.

Our examination of multi-feature representation with GAT makes a significant contribution to the existing body of research, advancing the application of machine learning techniques. First, this study is the first to integrate multi-feature representation with GAT for predicting supply relationships in a real-world supply chain network. Incorporating the

Table 7
Methods on different ablation settings.

Methods	Ablation settings	
	Product representation	Graph representation
GAT	✗	✗
PRGAT	✓	✗
GRGAT	✗	✓
MFRGAT	✓	✓

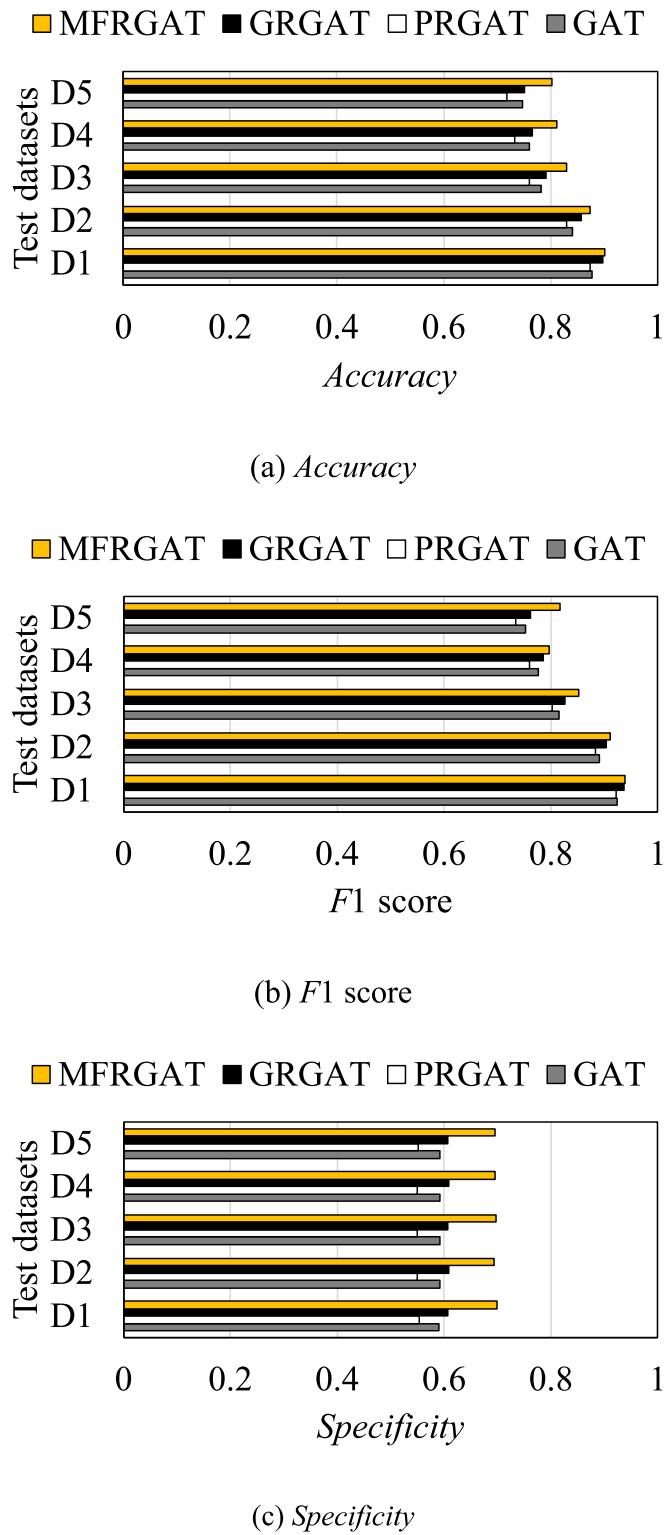


Fig. 6. Ablation results on performance measures considered in this study.

financial features of the companies may offer deeper insights into future research. Second, while most existing studies have focused on individual node attributes, such as industrial sector and product characteristics (Kosasih & Brinstrup, 2022; Lee & Kim, 2022; Tu et al., 2024), our work evaluates the combined benefits of incorporating both node-level features and the topological structure of supply relationship. This approach reveals distinct patterns within supplier networks, laying a strong foundation for further research. Future investigations could explore

Table 8
Paired t-test results comparing MFRGAT with other configurations.

Datasets	Measures	Methods		
		GAT	PRGAT	GRGAT
D1	Accuracy	1.33×10^{-6}	2.31×10^{-12}	2.79×10^{-12}
	F1 score	3.23×10^{-4}	1.06×10^{-11}	1.00×10^{-12}
	Specificity	2.28×10^{-12}	4.83×10^{-13}	8.79×10^{-12}
D2	Accuracy	1.85×10^{-8}	8.30×10^{-13}	1.97×10^{-11}
	F1 score	1.73×10^{-7}	5.02×10^{-13}	5.45×10^{-11}
	Specificity	5.23×10^{-11}	4.13×10^{-13}	5.57×10^{-11}
D3	Accuracy	4.14×10^{-13}	4.42×10^{-15}	2.81×10^{-13}
	F1 score	8.31×10^{-13}	1.47×10^{-14}	5.20×10^{-13}
	Specificity	8.04×10^{-14}	3.48×10^{-15}	2.74×10^{-13}
D4	Accuracy	4.42×10^{-13}	1.31×10^{-14}	5.85×10^{-13}
	F1 score	4.55×10^{-12}	5.67×10^{-14}	1.05×10^{-12}
	Specificity	6.06×10^{-14}	1.16×10^{-14}	6.92×10^{-13}
D5	Accuracy	3.12×10^{-14}	1.27×10^{-16}	3.08×10^{-15}
	F1 score	1.78×10^{-14}	4.40×10^{-16}	2.93×10^{-15}
	Specificity	5.43×10^{-15}	2.51×10^{-16}	4.60×10^{-15}

Table 9
Accuracy of GAT, PRGAT, GRAGT, and MFRGAT from the top five industries.

Industries	Proportion (%)	GAT	PRGAT	GRGAT	MFRGAT
Manufacturing	45.35	0.774	0.792	0.799	0.844
Wholesale and retail trade	19.29	0.729	0.708	0.742	0.798
Construction	16.53	0.836	0.777	0.791	0.848
Information and communications	4.26	0.824	0.662	0.696	0.756
Transportation	2.48	0.828	0.718	0.719	0.832

Table 10
Summary of method limitations.

Methods	Limitations
GAT	Difficulty in capturing complex supply chain topologies
PRGAT	Limited by industrial features alone
GRGAT	Lacks complementary industry semantics without multi-features
MFRGAT	Minor performance degradation in industries such as Information and Communications

these patterns within a more comprehensive network context, considering factors such as dynamic market conditions or long-term contractual relationships.

This study provides valuable implications for supply chain managers. Our findings suggest that companies should carefully consider complex relational properties of both nodes and edges when establishing partnerships with buyers and/or suppliers. As supply chain networks continue to expand and become increasingly interconnected, managing these relationships effectively presents greater challenges. The proposed method can assist managers in capturing semantic characteristics of network structure to identify potential supplier relationships, enabling more strategic and innovative resource allocations. Moreover, it can support the identification of alternative suppliers in the event of disruption, such as production inefficiencies or financial distress, thereby enhancing supply chain resilience. For instance, managers in the automotive industry can leverage MFRGAT to strategically identify suppliers that contribute to product innovation by evaluating key product attributes of potential partners. Similarly, in the pharmaceutical

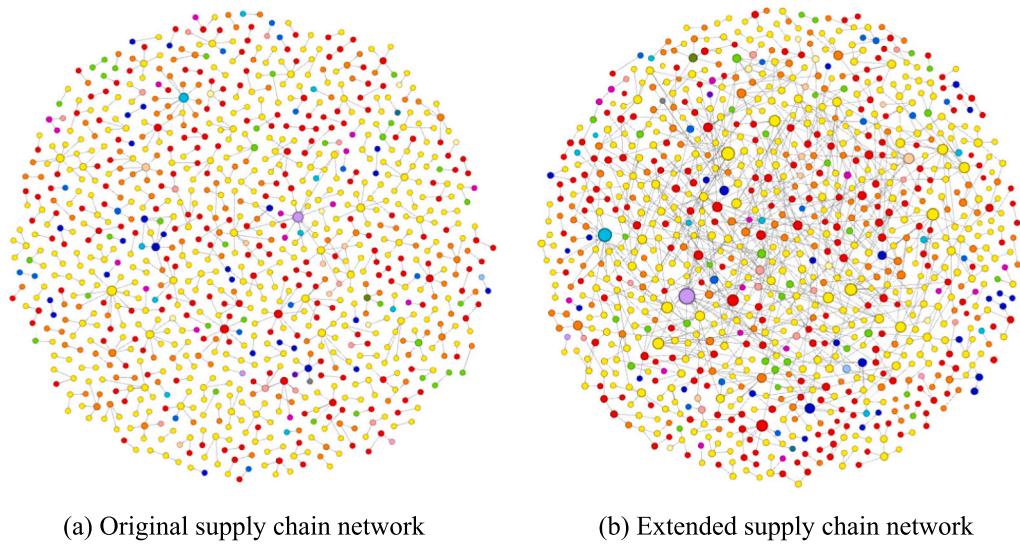


Fig. 7. Visualization of both the original and extended supply chain networks generated by the proposed method for a suburban region in South Korea.

industry, MFRGAT can support the effective selection of suppliers that ensure regulatory compliance and enhance supply chain resilience. These applications are enabled by MFRGAT's ability to accurately capture industrial characteristics and assess compatibility between companies. Moreover, this study opens new avenues for connecting predictive modeling with foundational concepts in network science. For example, the attention-based graph architecture can be extended to identify network motifs or community structures that characterize recurring patterns in supply chain formations. This integration contributes not only to advances in relational machine learning but also to a deeper understanding of structural dynamics in real-world business networks.

This study has several limitations. First, our analysis focuses on a supply chain network in South Korea, which may limit the generalizability of our findings to broader contexts. Future research should incorporate datasets from multiple countries to enable broader validation and extend the applicability of our proposed method to diverse international contexts. Second, the study uses cross-sectional data collected during a specific period, which limits the ability to fully capture the dynamic evolution of supply chain networks. Given that these networks often adapt in response to market fluctuations, technological advancements, and economic conditions, future research should incorporate longitudinal datasets. This approach would provide deeper insights into the temporal dynamics of supply chain relationships and support long-term financial planning. Third, although the proposed method demonstrates strong performance, it is not tested within global supply chain environments. Future research should investigate how our method performs under diverse conditions across the global networks and aim to enhance its effectiveness by integrating of advanced learning algorithms such as graph transformers (Yun et al., 2019), graph transfer learning (Gritsenko et al., 2023), and reinforcement learning (Nie et al., 2023). Incorporating these advanced techniques could significantly enhance adaptability, predictive accuracy, and practical utility, particularly in addressing the complexity and scale of global supply chains.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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