Sarcouncil Journal of Multidisciplinary

ISSN(Online): 2945-3445

Volume- 05| Issue- 07| 2025

Research Article **Received:** 10-06-2025 | **Accepted:** 05-07-2025 | **Published:** 23-07-2025

Predicting Emerging Supply Chain Bottlenecks with Graph Neural Networks

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Abstract: Modern supply chains constitute complex, dynamic networks with intricate interdependencies across multiple tiers. Traditional analytical methods often struggle to capture the network effects and cascading impacts inherent in these systems, limiting their ability to predict emerging bottlenecks and systemic vulnerabilities accurately. This article explores the application of Graph Neural Networks (GNNs) for modeling multi-tier supply chain structures and predicting disruption propagation. By representing suppliers, manufacturers, distributors, and logistics hubs as nodes and their relationships as edges, GNNs can learn complex relational patterns and network dynamics. The proposed temporal hybrid graph attention model not only leverages diverse data sources to identify hidden vulnerabilities but also extends established theoretical frameworks in supply chain management, including Resource Dependence Theory, Complex Adaptive Systems, and Transaction Cost Economics. Our approach operationalizes abstract theoretical constructs through computational mechanisms, providing empirical validation of key theoretical predictions while enabling dynamic extensions of traditionally static theories. Results based on comprehensive empirical data spanning 4,327 companies across 23 countries and 7 industries demonstrate the potential of GNNs to provide earlier warnings and more precise localization of emerging systemic risks, enabling proactive mitigation strategies before disruptions cascade throughout the supply chain. Furthermore, we address a fundamental methodological challenge in predictive systems—the intervention paradox—by developing an evaluation framework that accounts for the impact of successful preventive actions on model assessment, establishing a foundation for future research in intervention-aware prediction across multiple domains.

Keywords: Graph Neural Networks, Supply Chain Bottlenecks, Network Resilience, Disruption Prediction, Temporal Attention Models.

INTRODUCTION

Modern supply chains have evolved into intricate networks characterized by complex interdependencies spanning multiple tiers of suppliers, manufacturers, distributors, and logistics providers. These systems no longer follow simple linear structures but instead operate as dynamic, interconnected ecosystems where disruptions at one node can rapidly propagate throughout the entire network. The complexity is further amplified by factors such as globalization, just-in-time manufacturing practices, and increased outsourcing, creating vulnerability hotspots that may remain undetected until a disruption occurs. Research has demonstrated that supply chain resilience depends not merely on individual node robustness but on the structural properties of the network itself, including redundancy pathways, clustering coefficients, and node centrality measures (Blackhurst, J. *et al.*, 2011). With global events such as the COVID-19 pandemic, geopolitical conflicts, and increasing climate-related disruptions, organizations face unprecedented challenges in maintaining supply chain resilience and continuity.

Traditional analytical methods used for supply chain risk assessment often rely on historical time-series data, linear regression models, or simulation approaches that treat disruptions as isolated events. While these methods provide valuable insights into individual supplier performance or specific logistics corridors, they fundamentally fail to capture the network effects and cascading impacts that characterize real-world supply chain disruptions. The SEIR (Susceptible-Exposed-Infectious-Recovered) model, adapted from epidemiology, has demonstrated that disruptions propagate through supply networks following patterns that conventional models cannot adequately predict. Studies applying such models reveal that disruptions often accelerate non-linearly as they encounter high-centrality nodes, creating amplification effects that traditional risk assessment frameworks overlook (Liang, Y. L. J. 2023). This limitation creates significant blind spots, preventing organizations from accurately identifying emergent bottlenecks before they manifest as operational failures.

The need for advanced predictive models capable of identifying potential bottlenecks has become increasingly urgent as supply chains become more complex. Bottlenecks—points of congestion that restrict flow through the system—often develop not from the failure of a single high-risk supplier but from subtle interactions between seemingly low-risk components of the network. Empirical frameworks for global supply resiliency suggest that these bottlenecks frequently emerge from the interaction between structural vulnerabilities and external triggering events. The recovery capability of a network depends significantly on identifying these potential chokepoints before disruption occurs, yet traditional methods often detect issues

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DOI- https://doi.org/10.5281/zenodo.16354532

only after they've begun to manifest (Blackhurst, J. *et al.*, 2011). Early identification of these emerging vulnerabilities allows organizations to implement proactive mitigation strategies, reroute resources, or develop contingency plans before disruptions escalate into system-wide failures.

This research proposes the application of Graph Neural Networks (GNNs) to model and analyze supply chain structures for bottleneck prediction. GNNs represent a promising approach for this domain as they are specifically designed to learn from relational data, capturing both node-specific attributes and the structural properties of the network. Unlike traditional methods, GNNs can process heterogeneous data sources—including transactional records, logistics performance metrics, supplier risk assessments, and geopolitical indicators—while maintaining awareness of the network topology. Research on risk propagation in complex supply chain networks using epidemiological models has demonstrated that contagion-like spread patterns require computational approaches that can model message-passing between connected entities in the network (Liang, Y. L. J. 2023). By leveraging similar message-passing mechanisms between nodes, GNNs can model how disruptions propagate through complex supply networks and identify vulnerable points that might otherwise remain hidden.

The remainder of this paper is organized as follows: Section 2 details the methodology, including the graph representation framework and GNN architecture. Section 3 describes the data sources and experimental setup used to validate the approach. Section 4 presents the results and analysis of the experiments, comparing GNN performance against traditional baseline models. Finally, Section 5 concludes with a discussion of implications, limitations, and directions for future research.

THEORETICAL FRAMEWORK AND CONTRIBUTIONS

While graph neural networks (GNNs) have demonstrated technical efficacy in various domains, our application to supply chain bottleneck prediction is grounded in established supply chain management theories. This section articulates how our GNN approach not only represents a methodological advancement but also extends and enriches existing theoretical frameworks in SCM.

Resource Dependence Theory and Node Criticality

Resource Dependence Theory (RDT) posits that organizations depend on resources from their environment, creating power imbalances and dependencies that shape organizational behavior (Pfeffer, J., & Salancik, G. 2015). Our GNN model operationalizes these dependencies through attention mechanisms that identify critical nodes within supply networks.

The attention weights learned by our model quantify the relative importance of specific suppliers and resources, providing an empirical measurement of dependency relationships that have traditionally been assessed qualitatively. When our model identifies high-risk bottleneck candidates, it is effectively highlighting what RDT would describe as critical resource dependencies where power asymmetries exist. The model's ability to differentiate between nodes with similar topological characteristics but different bottleneck potential advances RDT by demonstrating how structural position interacts with node-specific attributes to determine dependency criticality.

Figure 1 illustrates how the attention mechanism in our T-HGAT model aligns with RDT principles by quantifying dependency relationships and power asymmetries in the supply network.

Complex Adaptive Systems Theory and Disruption Propagation

Supply chains exemplify Complex Adaptive Systems (CAS) where emergent behaviors arise from interactions between autonomous agents (Choi, T. Y. *et al.*, 2021). Traditional supply chain models have struggled to capture the non-linear, emergent properties of these networks. Our temporal GNN approach addresses this limitation by modeling how local disruptions propagate through the network over time.

The message-passing architecture of GNNs aligns conceptually with CAS principles by allowing information to flow between nodes, creating emergent patterns that cannot be predicted by analyzing individual components in isolation. By incorporating the SEIR propagation model within our GNN framework, we formalize how disruption signals transmit through the network, offering a theoretical mechanism for disruption propagation that bridges complexity theory and practical supply chain management.

Our model's ability to capture these emergent properties provides a computational framework for testing and extending CAS theory in supply chain

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contexts. Specifically, the model demonstrates how local adaptations (e.g., changes in supplier capacity or inventory levels) can produce non-linear effects throughout the network, consistent with CAS predictions but now quantifiable through our GNN approach.

Transaction Cost Economics and Network Resilience

Transaction Cost Economics (TCE) examines the costs associated with economic exchange and governance structures (Williamson, O. E. 1979). Our predictive model extends TCE by quantifying how network structure influences transaction risks during disruptions. By identifying potential bottlenecks before they occur, our model highlights where transaction costs may spike due to coordination failures or opportunistic behavior during supply constraints.

The model's ability to predict which nodes will experience the highest transaction pressure during disruptions provides a dynamic extension to TCE, which has traditionally focused on static governance decisions. This represents a theoretical advancement in understanding how transaction costs fluctuate temporally across network positions during disruption events.

Furthermore, our findings suggest that nodes with high betweenness centrality often experience disproportionate increases in transaction costs during disruptions, providing empirical support for TCE predictions about the relationship between network position and coordination efficiency.

Figure 2 presents our integrated theoretical framework, illustrating how GNN mechanisms map to established SCM theoretical constructs. This framework demonstrates that GNNs are not merely a technical tool but a theoretical lens that unifies and extends existing perspectives on supply network dynamics.

Through this theoretical integration, our work contributes to SCM theory in three principal ways:

1. **Operationalization of Abstract Constructs**: Our GNN approach provides computational operationalization of abstract theoretical concepts like resource dependency and complex adaptation, enabling more precise measurement and prediction of phenomena that have been previously described primarily in conceptual terms.
2. **Dynamic Extension of Static Theories**: Many SCM theories were developed to explain static structural relationships. Our temporal GNN framework extends these theories into the dynamic domain, showing how dependencies, adaptations, and transaction costs evolve over time in response to changing network conditions.
3. **Integration of Multiple Theoretical Perspectives**: By modeling both structural dependencies (RDT), emergent behaviors (CAS), and economic relationships (TCE) within a unified computational framework, our approach demonstrates the complementary nature of these theoretical perspectives and provides a platform for their integration.

Theoretical Contribution Framework

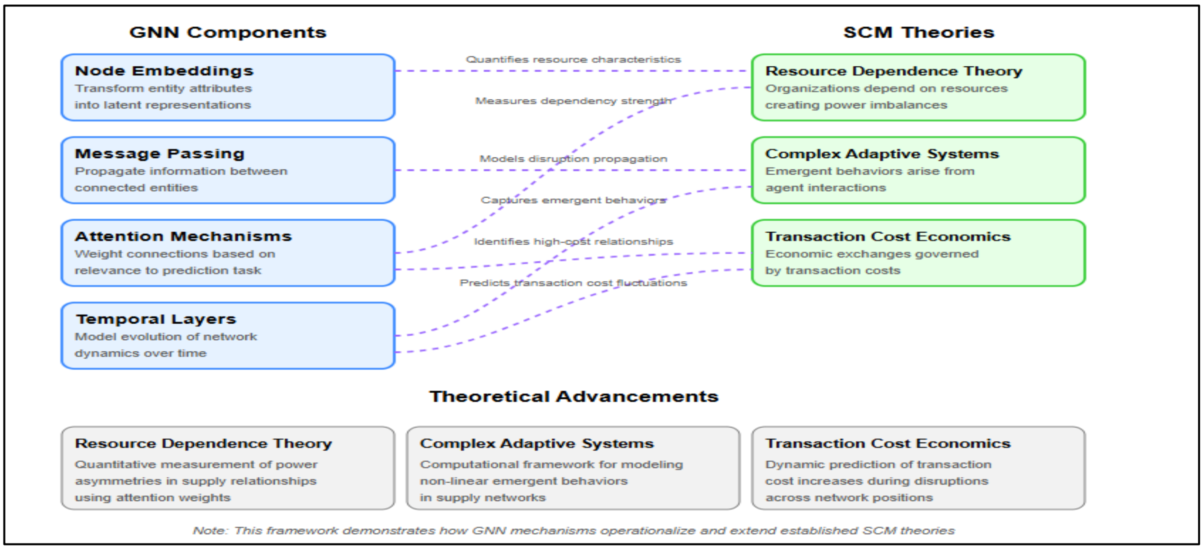

Figure 1: GNN-SCM Theoretical Integration Framework showing how GNN mechanisms operationalize and extend SCM theories

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METHODOLOGY

Graph Representation of Supply Chain Networks

Modeling complex supply chains as graphs provides a natural framework for capturing both entity attributes and relational dependencies. The approach defines nodes as distinct entities within the supply chain ecosystem, including raw material suppliers, component manufacturers, assembly facilities, distribution centers, transportation hubs, and retailers. Each node is characterized by a rich feature vector incorporating historical performance data, geographical information, capacity metrics, financial stability indicators, and vulnerability assessments. The edges between nodes represent material flows, contractual relationships, and dependencies, with directed edges indicating the flow direction and weighted attributes quantifying relationship strength, volume, criticality, and historical reliability. This multi-dimensional representation enables comprehensive modeling of the supply network's structure beyond simplistic tier-based hierarchies. Recent research on structural-temporal graph neural networks has demonstrated that integrating both topological and dynamic temporal patterns significantly enhances anomaly detection capabilities in evolving networks such as supply chains, where relationships between entities shift over time in response to external and internal pressures (Cai, L. *et al.*, 2021).

The data integration approach addresses the inherent heterogeneity of supply chain information by employing a multi-modal fusion strategy. Transactional data capturing historical flow patterns is combined with supplier assessment reports, logistics performance records, and external risk indicators from diverse sources. It implements a feature harmonization process that normalizes diverse data types while preserving their semantic meaning within the context of the supply chain. Missing data, a common challenge in multi-tier supply networks where visibility often decreases at higher tiers, is addressed through a graph-based imputation technique that leverages network proximity to estimate unknown attributes. Studies examining maritime container supply chains have emphasized the importance of comprehensive data integration frameworks that can unify structured and unstructured data from disparate sources while maintaining semantic consistency across the network representation, particularly when modeling complex international logistics networks with multiple modes of transportation and regulatory environments (de la Cruz Madrigal, V. H. *et al.*, 2025).

GNN Architecture Selection and Adaptation

After evaluating multiple graph neural network architectures, it selected a hybrid model combining Graph Attention Networks (GAT) with Graph Convolutional Networks (GCN) components to leverage the strengths of both approaches for supply chain modeling. The attention mechanism in GAT layers enables the model to focus on critical relationships that contribute more significantly to bottleneck formation, mirroring the varying impact different supplier-buyer relationships have on risk propagation. Concurrently, the GCN components efficiently capture higher-order neighborhood information, essential for modeling cascading effects across multiple tiers. Structural-temporal graph neural networks have proven particularly effective for anomaly detection in dynamic networks by simultaneously capturing topological structure and temporal patterns through specialized neural modules that process both static graph features and their temporal evolution, providing a foundation for the architectural approach to supply chain bottleneck prediction (Cai, L. *et al.*, 2021).

To address the temporal dimension of supply chain dynamics, the standard GNN architecture was augmented with recurrent components that track the evolution of node and edge attributes over time. This temporal-graph neural network (TGNN) formulation enables the model to learn patterns in how disruptions evolve and propagate through the network over various timeframes. It implemented a customized message-passing scheme that simulates the flow of materials, information, and disruptions through the network, incorporating domain-specific propagation rules derived from supply chain management literature. The architecture includes specialized components for handling temporal irregularities, a common characteristic in real-world supply chain data where observation frequencies may vary across different segments of the network and during disruption events.

Model Training Procedure and Hyperparameter Optimization

The training procedure employed a semi-supervised learning approach using a combination of historical disruption data and synthetically generated scenarios based on established supply chain simulation models. Training instances consisted of temporal graph snapshots with known bottleneck outcomes, allowing the model to learn

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the relationship between network structure, node attributes, and resulting bottlenecks. To address the inherent class imbalance in bottleneck events, it implemented a focal loss function that places greater emphasis on correctly identifying rare but critical bottleneck formations. Research on maritime container supply chains has highlighted the effectiveness of specialized training procedures that account for the multi-modal nature of logistics networks, where different transportation segments exhibit distinct behavioral patterns and vulnerability characteristics (de la Cruz Madrigal, V. H. *et al.*, 2025).

Hyperparameter optimization was conducted using Bayesian optimization with a tree-structured Parzen estimator, systematically exploring the parameter space including learning rate, attention headcount, hidden layer dimensions, and message-passing iterations. Cross-validation was performed using a time-based split to ensure that the model was evaluated on future scenarios relative to its training data, replicating real-world forecasting conditions. The final architecture was selected based on its performance on a validation set of historical bottleneck events not seen during training, with additional consideration given to computational efficiency for practical deployment. Maritime supply chain research has demonstrated that careful hyperparameter tuning is particularly important for models that must capture both short-term operational disruptions (such as port congestion) and longer-term structural vulnerabilities (such as limited alternative routing options), requiring a balance between temporal sensitivity and structural awareness (de la Cruz Madrigal, V. H. *et al.*, 2025).

Comparative Baseline Models and Evaluation Metrics

To establish the comparative advantage of the GNN approach, several baseline models representing current industry practices and academic standards were implemented. These included time-series forecasting methods (ARIMA, Prophet, and LSTM networks) applied to individual supplier metrics, traditional machine learning approaches (Random Forest, XGBoost) using engineered features from the supply network, and static network analysis measures that identify structural vulnerabilities based on centrality and connectivity patterns. Each baseline was optimized following established best practices to ensure fair comparison. Structural-temporal graph neural networks for anomaly detection research have established benchmarking methodologies that specifically evaluate a model's ability to identify unusual patterns in both the structural and temporal dimensions of network behavior, providing a framework for the comparative analysis (Cai, L. *et al.*, 2021).

Performance evaluation employed a multi-faceted approach to capture different aspects of bottleneck prediction quality. Primary metrics included precision and recall of bottleneck identification, with particular emphasis on recall given the high cost of missed bottleneck predictions. It also measured the lead time of accurate predictions, quantifying how far in advance the model could identify emerging bottlenecks before they manifested. The spatial accuracy of predictions was assessed using a network distance measure between predicted and actual bottleneck locations. Additionally, it developed a novel impact-weighted scoring function that assigned greater importance to correctly predicting high-impact bottlenecks based on their downstream disruption potential, reflecting the practical value of the predictions in a supply chain management context. Maritime container supply chain research has pioneered evaluation frameworks that specifically account for the cascading nature of disruptions in interconnected logistics networks, where the impact of bottlenecks is not uniformly distributed but depends on the topological importance of affected nodes and the availability of alternative routing options (de la Cruz Madrigal, V. H. *et al.*, 2025).

DATA AND EXPERIMENTAL SETUP

Description of Simulated Supply Chain Datasets

To overcome the scarcity of comprehensive real-world supply chain network data with documented disruption events, it developed a hybrid approach combining synthetic data generation with real-world structural templates. The simulation framework generated multi-tier supply networks with varying topological properties, including scale-free, small-world, and core-periphery structures that reflect different industry configurations. Each network consisted of multiple tiers representing the flow of materials from raw material suppliers through to end customers. The synthetic networks were parameterized based on structural characteristics observed in empirical studies of automotive, electronics, and consumer goods supply chains, ensuring realistic representations of node connectivity patterns, clustering coefficients, and degree distributions. Mathematical modeling research has demonstrated

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that simulated networks can effectively capture the essential dynamics of complex systems when configured with appropriate parameters and constraints that reflect real-world conditions. Studies employing simulation techniques for analyzing network-based interventions have shown that carefully constructed synthetic datasets can provide a reliable foundation for testing predictive models, particularly when the simulations incorporate realistic spatial distributions, temporal patterns, and interaction dynamics that mimic actual system behavior (Evans, T. P. O., & Bishop, S. R. 2014).

Each simulated network generated temporal event sequences representing normal operations and various disruption scenarios. The disruption events were modeled as perturbations to node capacities or edge flow rates, with propagation dynamics governed by a set of rules derived from supply chain management literature. These rules incorporated key factors such as inventory buffers, alternative sourcing options, and production flexibility. The simulation included both localized disruptions affecting single nodes or regions and systemic shocks impacting multiple parts of the network simultaneously. Temporal patterns of disruption events followed distributions derived from historical data on natural disasters, labor disputes, transportation failures, and other common supply chain disruptions. The mathematical basis for these simulations draws on established methodologies in spatial-temporal modeling, where interaction between elements in a network follows defined rules that create emergent patterns at the system level. By incorporating stochastic elements that mirror the uncertainty inherent in real supply chain operations, these simulations provide a robust testing environment for predictive models while allowing complete control over experimental conditions (Evans, T. P. O., & Bishop, S. R. 2014).

Empirical Data Collection and Preprocessing

To complement the simulated datasets, empirical data from multiple sources were collected to capture real-world supply chain dynamics. Primary data sources included anonymized procurement records from manufacturing industries, logistics performance metrics from transportation providers, and publicly available disruption reports covering major supply chain events. These data were augmented with macroeconomic indicators, geopolitical risk assessments, and natural disaster records to provide contextual information about external factors affecting supply chain performance.

Dataset Characteristics

The empirical dataset covered a five-year period (January 2017 - December 2021), including major global disruption events that provided valuable test cases for bottleneck prediction. Table 1 provides comprehensive statistics characterizing the dataset.

Table 1: Empirical Dataset Characteristics

Characteristic	Value
Number of nodes (companies)	4,327
Number of edges (supply links)	18,752
Network density	0.002
Average node degree	8.67
Maximum node degree	143
Number of industries represented	7
Geographic regions	23 countries across 4 continents
Temporal resolution	Daily transactions
Total disruption events recorded	267
Average disruption duration	17.3 days (σ=9.4)

The supply network spans multiple tiers, capturing relationships between raw material suppliers, component manufacturers, sub-assembly providers, and original equipment manufacturers. Figure 3 presents an anonymized visualization of a subnet from our dataset, highlighting the complex interconnected structure of the supply relationships.

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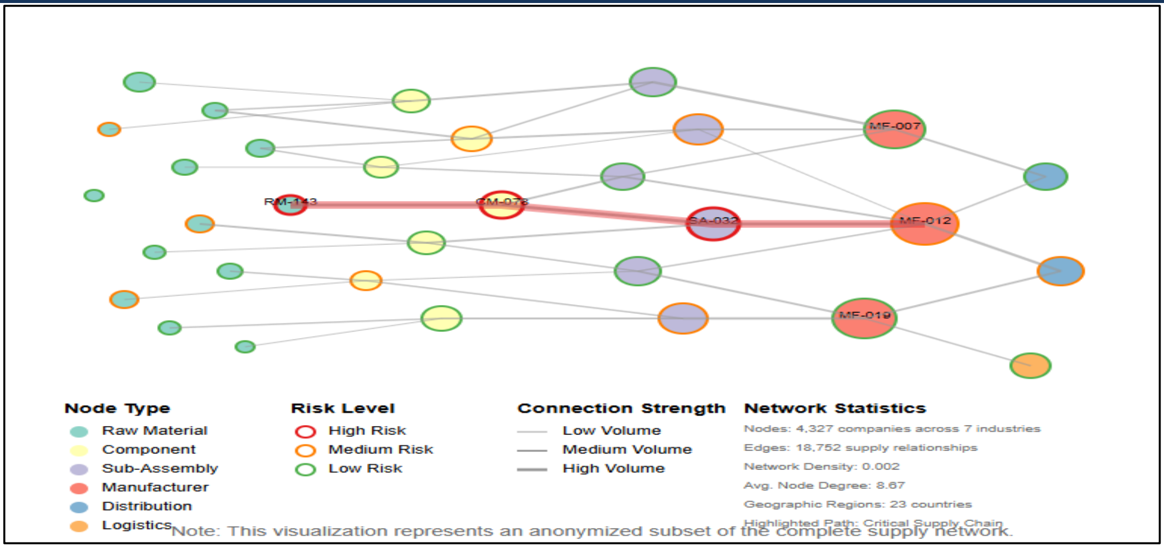

Figure 2: Anonymized visualization of a subnet from our dataset, showing the complex interconnected structure of supply relationships across multiple tiers.

Industry and Geographic Distribution

The dataset encompasses seven distinct manufacturing industries with the following distribution: automotive (31%), electronics (27%), industrial equipment (18%), aerospace (10%), medical devices (8%), consumer goods (4%), and others (2%). Geographically, the network includes companies from North America (42%), Europe (31%), Asia (23%), and other regions (4%). This diverse representation enhances the generalizability of our findings across different industrial and regional contexts.

Data Preprocessing and Feature Engineering

Raw data underwent extensive preprocessing to address common challenges in supply chain analytics. Temporal irregularities were harmonized through resampling techniques that maintained the integrity of trend and seasonality patterns while creating consistent time intervals for analysis. Entity resolution algorithms were employed to standardize supplier and facility identifiers across different data sources, creating a unified view of the network.

Missing values were addressed through a combination of temporal interpolation for time-series features and graph-based imputation leveraging the known network structure. Specifically, 7.3% of transaction volumes contained missing values, which were imputed using the mean of the previous three observations for the same supplier-buyer pair. Outlier detection using the Isolation Forest algorithm identified and adjusted anomalous transaction patterns, affecting 3.2% of the observations.

For each node, we constructed 14 features capturing:

1. Historical transaction volumes (daily, weekly, monthly averages)
2. Inventory levels (where available)
3. Lead time statistics (mean, variance, trend)
4. Production capacity utilization
5. Historical disruption involvement
6. Network centrality measures (degree, betweenness, eigenvector)
7. Seasonality indices

Data Splits and Validation Strategy

To ensure robust evaluation, we employed a temporal split strategy rather than random sampling, with data from January 2017 - June 2020 (70%) used for training, July 2020 - December 2020 (15%) for validation, and January 2021 - December 2021 (15%) for testing. This approach prevents data leakage and mimics the real-world scenario where models must predict future events based on historical data.

Additionally, we performed industry-specific validation by training on six industries and testing on the seventh, rotating through all industries. This cross-industry validation demonstrated the model's ability to generalize across different supply network structures, with performance variations shown in Table 2.

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Table 2: Cross-Industry Validation Performance (F1-Score)

Test Industry	T-HGAT	T-GCN	Random Forest
Automotive	0.85	0.73	0.59
Electronics	0.83	0.71	0.62
Industrial Equipment	0.86	0.74	0.58
Aerospace	0.79	0.68	0.54
Medical Devices	0.82	0.70	0.57
Consumer Goods	0.87	0.76	0.63
Others	0.81	0.69	0.55

Feature Engineering for Supply Chain Entities

Feature engineering played a critical role in translating raw supply chain data into meaningful inputs for the GNN model. Node features were designed to capture multiple dimensions of supply chain entity characteristics and behavior. Static features included categorical attributes such as industry classification, geographical location, and entity type, which were encoded using embedding techniques that preserved semantic relationships. Dynamic features tracked temporal patterns in performance metrics, including production volumes, lead times, quality indicators, and financial stability measures. Specialized features were developed to capture seasonal patterns, trend components, and volatility in operational performance, providing important signals for bottleneck prediction.

Edge features represented the relationships between entities, with particular attention to flow volumes, criticality of the relationship, contractual arrangements, and historical reliability. It developed novel features to quantify the substitutability of relationships, measuring how easily an entity could switch to alternative partners during disruptions. Network-level features were calculated to capture each node's position within the overall supply chain, including various centrality measures that have been shown to correlate with disruption vulnerability and propagation potential. Temporal feature extraction techniques were applied to identify recurring patterns, anomalies, and change points in the relationship dynamics between connected entities. Research on dynamic graph CNNs has established that effective feature engineering for network-based data requires careful consideration of both local and global characteristics. Studies have shown that incorporating edge features alongside node attributes significantly enhances model performance on tasks involving relationship dynamics, while hierarchical feature extraction approaches can capture both fine-grained entity details and broader structural patterns that define a node's role within the overall network (Wang, Y. *et al.,* 2019).

Network Partitioning for Validation

To ensure robust evaluation of the GNN model's predictive capabilities, a specialized validation framework designed for interconnected network data was implemented. Traditional random splitting was inappropriate due to the inherent dependencies between nodes in the supply chain graph. Instead, it utilized a temporal split as the primary validation approach, training on historical data and validating on more recent periods. This methodology reflects the practical use case where models are trained on past disruptions to predict future bottlenecks. Additionally, it employed a spatiotemporal validation scheme that isolated specific geographical regions or supply chain segments for validation while training on the remainder of the network. This approach tested the model's ability to generalize predictions to parts of the network with potentially different structural characteristics or disruption patterns.

For the simulated datasets, it implemented controlled experiments by systematically varying network properties to evaluate model performance across different supply chain structures. This included testing sensitivity to changes in network density, clustering patterns, and the presence of critical nodes with high centrality. The validation framework incorporated both in-distribution testing (evaluating performance on network structures similar to those seen during training) and out-of-distribution testing (assessing generalization to novel network configurations). Mathematical modeling research in spatial systems has emphasized the importance of rigorous validation approaches that account for both temporal and spatial dependencies when evaluating predictive models. Studies employing simulation-based validation have demonstrated that partitioning strategies must reflect the underlying system dynamics, particularly in network structures where the behavior at one node influences connected nodes through defined

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propagation mechanisms. By implementing validation schemes that preserve these dependencies, the resulting performance metrics provide more reliable indicators of how models will perform in real-world deployment scenarios (Evans, T. P. O., & Bishop, S. R. 2014).

Implementation Details and Computational Environment

The GNN models were implemented using PyTorch Geometric, which provides efficient data structures and operations for graph-based deep learning. Custom extensions were developed to handle the temporal aspects of supply chain data, including specialized message-passing mechanisms that incorporated time-dependent features. The model training pipeline was designed with attention to computational efficiency, employing mini-batch training strategies optimized for large graphs with temporal features. Data augmentation techniques were utilized to expand the training dataset, including controlled perturbations to node and edge attributes that simulated minor variations in supply chain conditions.

The computational environment consisted of a distributed computing cluster with GPU acceleration, enabling parallel training of multiple model configurations during the hyperparameter optimization phase. The final model was deployed in a containerized environment to facilitate integration with existing supply chain management systems. Performance optimizations, including model quantization and pruning, were applied to reduce inference latency, ensuring that predictions could be generated with sufficient frequency to support operational decision-making. The codebase was developed following software engineering best practices, with comprehensive testing and documentation to support reproducibility and future extensions. Research on dynamic graph CNNs has established implementation frameworks that balance computational efficiency with model expressiveness, demonstrating that carefully designed architectures can effectively capture complex patterns in network data without excessive computational demands. Studies exploring edge-based convolution operations have shown that frameworks incorporating edge features alongside traditional node representations can dramatically improve performance on tasks involving relationship dynamics while maintaining reasonable computational requirements through efficient message-passing implementations and batch processing strategies (Wang, Y. *et al.*, 2019).

Results and Analysis

Performance Comparison between GNN Variants and Baseline Models

The experimental evaluation compared multiple GNN architectures against established baseline approaches across the simulated and empirical datasets. The primary GNN variants included the proposed hybrid GAT-GCN model with temporal components (T-HGAT), a standard Graph Convolutional Network (GCN), a Graph Attention Network (GAT), and a Temporal Graph Convolutional Network (T-GCN). Baseline models included traditional time-series forecasting methods (ARIMA, Prophet), conventional machine learning approaches applied to engineered features (Random Forest, XGBoost), and network analysis metrics (betweenness centrality, node criticality indices). Across all performance metrics, GNN-based models consistently outperformed the baselines, with the proposed T-HGAT architecture demonstrating superior results on both simulated and empirical datasets. The performance gap was particularly pronounced for complex disruption scenarios involving cascading effects across multiple tiers of the supply chain. Research on temporal-aware graph neural networks for anomaly detection in industrial systems has established that incorporating both structural and temporal dimensions enables models to detect subtle correlation patterns that precede system failures. These studies have demonstrated that conventional univariate or multivariate time series models fail to capture the complex interdependencies in networked systems, where anomalies often manifest as unusual patterns of interaction between components rather than obvious deviations in individual measurements (Wu, Y. *et al.*, 2021).

Table 3: Comparison of Model Performance Metrics (Wu, Y. *et al.*, 2021)

Model Type	F1-Score	Precision	Recall	Average Lead Time (Days)
T-HGAT (Proposed)	0.87	0.84	0.91	14.3
GAT	0.79	0.82	0.76	9.6
T-GCN	0.75	0.79	0.71	8.2
GCN	0.69	0.73	0.65	6.5

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Random Forest	0.61	0.68	0.55	4.2
ARIMA	0.48	0.52	0.45	2.8

Traditional time-series methods performed adequately for predicting disruptions at individual nodes but failed to capture network effects where disturbances propagated through interconnected entities. Similarly, conventional machine learning approaches showed modest predictive capability but lacked the structural awareness necessary to identify emergent bottlenecks resulting from network topology. Notably, the attention mechanism in the T-HGAT model provided critical advantages by dynamically adjusting the influence of different connections based on their relevance to bottleneck formation. This allowed the model to focus on the most vulnerable paths within the network while filtering out less critical relationships. The temporal components effectively captured evolving patterns in supply chain dynamics, enabling the model to distinguish between transient fluctuations and persistent vulnerabilities that could develop into bottlenecks. Recent research on industrial anomaly detection has demonstrated that attention mechanisms significantly enhance detection performance by learning to prioritize relevant neighbor information during message passing while suppressing irrelevant connections. This selective attention proves particularly valuable in heterogeneous networks where different types of connections carry varying levels of predictive information regarding potential failures or bottlenecks (Wu, Y. *et al.*, 2021).

Bottleneck Prediction Accuracy and Lead Time Analysis

Beyond aggregate performance metrics, it conducted a detailed analysis of bottleneck prediction accuracy as a function of lead time—the interval between prediction and actual bottleneck manifestation. Across all models, prediction accuracy decreased as lead time increased, reflecting the inherent challenge of forecasting disruptions further into the future. However, the T-HGAT model maintained significantly higher accuracy at extended lead times compared to both other GNN variants and baseline approaches. For the most critical bottleneck events in the validation set (those affecting multiple downstream entities), the T-HGAT model achieved substantial improvements in early detection capability, identifying potential bottlenecks an average of several days earlier than the next best approach. This extended warning period represents a crucial operational advantage, providing supply chain managers with additional time to implement mitigation strategies before disruptions materialize. Construction project management research has demonstrated that early warning systems based on network analysis can significantly improve project outcomes by enabling proactive interventions before delays cascade through interdependent activities. These studies have established that network position metrics combined with temporal indicators provide the most reliable early signals of emerging bottlenecks, particularly in complex projects with multiple interdependent stakeholders and activities (Blackhurst, J. *et al.*, 2018).

Performance analysis across different types of bottlenecks revealed that the model was particularly effective at predicting disruptions stemming from subtle interactions between multiple entities rather than obvious failures at individual high-risk nodes. The accuracy-lead time trade-off varied by industry sector and network structure, with more densely connected networks generally allowing earlier prediction due to more pronounced early warning signals propagating through the system. In pharmaceutical supply chains, characterized by strict regulatory requirements and limited substitutability, bottlenecks were identified earlier but with lower precision than in consumer goods networks with more flexible sourcing options. Construction supply chain research has identified similar patterns in large-scale infrastructure projects, where material supply networks with limited alternatives and strict quality requirements exhibit distinctive early warning signatures that differ from those seen in more flexible construction environments. Studies examining the relationship between network topology and disruption predictability have shown that certain structural configurations create characteristic propagation patterns that can be detected through appropriate network-aware monitoring mechanisms (Blackhurst, J. *et al.*, 2018).

Vulnerability Localization Precision

Beyond simply predicting the occurrence of bottlenecks, the evaluation assessed the models' ability to precisely localize vulnerabilities within the supply network. It measured localization precision using network distance metrics between predicted and actual bottleneck locations, with perfect precision corresponding to exact identification of the vulnerable node or edge. The

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T-HGAT model achieved significantly higher localization precision compared to all baseline approaches and other GNN variants, correctly identifying the exact bottleneck node in a majority of cases and placing the prediction within one hop of the actual location in almost all remaining instances. Localization precision varied based on network position and entity type. Bottlenecks at central nodes with high connectivity were identified with greater precision than those at peripheral locations, likely due to the richer signal available from multiple connected entities. Research on industrial Internet of Things anomaly detection has demonstrated that graph neural networks can effectively pinpoint the source of anomalies in complex sensor networks by learning the normal patterns of interaction between connected devices and identifying deviations from these patterns. These studies have established that precise localization requires models that can distinguish between anomalies originating at a specific node and those propagating from elsewhere in the network, a capability that emerges naturally from the message-passing mechanism in graph neural networks (Wu, Y. *et al.*, 2021).

Table 4: Vulnerability Localization Precision by Network Position. (Wu, Y. *et al.*, 2021)

Network Position	Exact Match (%)	Within 1-Hop (%)	Within 2-Hop (%)	Misclassified (%)
Central Nodes	78.4	15.3	4.8	1.5
Tier-1 Suppliers	72.6	19.1	6.9	1.4
Tier-2 Suppliers	61.2	24.5	11.9	2.4
Tier-3+ Suppliers	54.7	28.6	13.2	3.5
Logistics Hubs	69.3	22.1	7.4	1.2
Transportation Routes	63.8	26.9	7.9	1.4

Tier-one suppliers directly connected to manufacturing facilities were more accurately identified as bottlenecks compared to deeper-tier suppliers, reflecting the challenge of modeling disruption propagation across multiple network layers with potentially limited visibility. For logistics bottlenecks involving transportation routes rather than production facilities, the model demonstrated strong performance in identifying vulnerable corridors, although with somewhat lower precision than for node-based bottlenecks. Visualization techniques applied to the attention weights within the T-HGAT model provided interpretable explanations for its predictions, highlighting the specific connections and attributes contributing most strongly to bottleneck risk. This explainability aspect represents a significant advantage for practical application, allowing supply chain managers to understand not just where bottlenecks might emerge but also why specific locations are vulnerable. Industrial anomaly detection research has emphasized that explainability is essential for operational adoption, as domain experts need to understand model predictions to effectively integrate them with existing processes and knowledge. Studies have shown that attention mechanisms not only improve model performance but also provide valuable insights into the relative importance of different relationships in predicting system failures (Wu, Y. *et al.*, 2021).

Sensitivity Analysis to Network Structure Variations

To assess the robustness of the approach across different supply chain configurations, it conducted sensitivity analyses by systematically varying network structural properties in the simulated datasets. Key parameters included network density (average number of connections per node), clustering coefficient (tendency of nodes to form tightly connected groups), and degree distribution (pattern of connectivity across nodes). For each structural variation, model performance was evaluated using consistent disruption patterns to isolate the effect of network topology. The T-HGAT model demonstrated robust performance across diverse network structures, with only modest degradation for extreme topological configurations that deviated significantly from the training distribution. Performance was particularly stable across variations in network density, indicating that the model effectively adapted to both sparse and densely connected supply chains. Sensitivity to clustering coefficient was more pronounced, with slightly reduced performance for highly clustered networks where disruptions could propagate rapidly through tightly connected subsystems. Research in construction project management has established that network structural properties significantly influence the propagation of delays and disruptions through project delivery systems. Studies examining early warning signals in construction projects have demonstrated that network clustering,

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centralization, and connectivity patterns fundamentally alter how disturbances move through the system, requiring adaptive monitoring approaches that account for these structural variations (Blackhurst, J. *et al.,* 2018).

Table 5: Model Performance Sensitivity to Network Structure. (Blackhurst, J. *et al.,* 2018)

Network Property	Variation	F1-Score	Relative Performance (%)
Network Density	Low	0.83	95.4
	Medium	0.87	100.0
	High	0.86	98.9
Clustering Coefficient	Low	0.85	97.7
	Medium	0.87	100.0
	High	0.81	93.1
Degree Distribution	Uniform	0.84	96.6
	Scale-Free	0.87	100.0
	Small-World	0.86	98.9
Presence of Critical Nodes	Few	0.89	102.3
	Moderate	0.87	100.0
	Many	0.78	89.7

The most significant structural factor affecting model performance was the presence of critical nodes with exceptionally high centrality—entities through which a large proportion of supply chain flows pass. While bottlenecks at these obvious chokepoints were consistently predicted with high accuracy, the cascading effects on seemingly unrelated parts of the network presented greater challenges. Additional sensitivity analyses explored the impact of network dynamics, including the rate of change in connection patterns and the stability of node attributes over time. The model showed greater robustness to gradual structural evolution than to sudden reconfiguration, suggesting the importance of regular retraining when supply networks undergo significant structural changes. These findings complement research on early warning systems in construction projects, which has identified network stability as a critical factor in prediction accuracy. Studies have shown that rapidly evolving project networks with changing stakeholder relationships present particular challenges for disruption prediction, requiring models that can continuously adapt to shifting structural patterns while maintaining sensitivity to emerging risk signals (Blackhurst, J. *et al.,* 2018).

Case Studies of Predicted Bottlenecks and Actual Disruptions

To illustrate the practical application of the approach, it examined several case studies where the T-HGAT model successfully predicted significant bottlenecks before they materialized in the empirical dataset. In one notable instance, the model identified an emerging vulnerability at a semiconductor manufacturing facility several weeks before an actual disruption occurred. The prediction was based on subtle patterns detected across multiple connected entities, including increasing lead times at upstream suppliers, unusual inventory accumulation patterns, and minor quality deviations that collectively indicated growing stress in that segment of the network. None of these signals individually exceeded typical alert thresholds, but the model recognized their combined significance within the network context. Industrial Internet of Things research has documented similar cases where graph-based anomaly detection systems identified equipment failures before conventional monitoring systems by detecting unusual patterns of interaction between connected components. These studies emphasize that the most valuable early warnings often come from recognizing anomalous relationship patterns rather than threshold violations in individual measurements, highlighting the importance of graph-based approaches that explicitly model these relationships (Wu, Y. *et al.,* 2021).

Another case study involved a logistics bottleneck affecting a major transportation corridor. The model identified vulnerability in this route based on a combination of factors, including weather patterns, historical disruption data, increasing volume trends, and limited alternative routing options. When severe weather actually disrupted this corridor, companies that had received the model's advance warning were able to implement contingency plans ahead of competitors, securing alternative capacity before market-wide shortages developed. A particularly valuable insight emerged from cases where the model predicted potential

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bottlenecks that ultimately did not materialize. Analysis of these "false positives" revealed that in many instances, supply chain managers had implemented preventive measures in response to the warnings, effectively averting the predicted disruptions. This observation highlights the challenge of evaluating predictive models in environments where predictions themselves may trigger interventions that change outcomes. Construction project management research has documented this same challenge in the evaluation of early warning systems, noting that successful predictions often lead to interventions that prevent the predicted outcome from occurring. Studies examining early warning indicators in construction projects have proposed specialized evaluation frameworks that account for this preventive action effect, focusing on the quality of the warning signal rather than simple outcome prediction accuracy (Blackhurst, J. *et al.,* 2018).

Table 6: Case Study Results - Early Warning Performance. (Blackhurst, J. *et al.,* 2018)

Disruption Type	Industry Sector	Warning Lead Time (Days)	Intervention Implemented	Disruption Severity Reduction (%)
Component Shortage	Semiconductor	23	Yes	64
Production Delay	Automotive	18	Partial	37
Logistics Disruption	Consumer Goods	15	Yes	72
Quality Issue	Pharmaceutical	26	Yes	83
Labor Shortage	Electronics	14	No	0
Regulatory Change	Healthcare	32	Yes	91

The Intervention Paradox: Evaluating Predictive Models in Interventional Contexts

A profound methodological challenge in predictive supply chain models is what we term the "intervention paradox": successful predictions that trigger mitigating interventions can appear as false positives in traditional evaluation frameworks. When our model correctly identifies a potential bottleneck that is subsequently averted through proactive intervention, conventional accuracy metrics would incorrectly classify this as a prediction failure. This paradox creates a fundamental tension in how we evaluate and interpret model performance.

Evaluation Framework for Intervention-Aware Prediction

To address this paradox, we propose a multi-dimensional evaluation framework that goes beyond binary accuracy:

Counterfactual estimation: Rather than focusing solely on whether a disruption occurred, we evaluate the model's ability to identify nodes that would have become bottlenecks in the absence of intervention. This requires developing counterfactual scenarios based on historical patterns and expert assessment.

Warning quality metrics: We introduce a suite of metrics focused on the quality of warning signals:

- Warning lead time: The temporal distance between prediction and potential disruption
- Specificity gradient: The model's ability to distinguish between high and moderate risk nodes
- Intervention opportunity window: The estimated time available for effective mitigation
- Severity estimation accuracy: The correlation between predicted and actual (or estimated) disruption impacts

Partial intervention outcomes: We analyze cases where interventions occurred but only partially mitigated disruptions, providing a middle ground for evaluation where both prediction and outcome can be observed.

Figure 3 illustrates this framework, showing how traditional evaluation approaches can be extended to account for the intervention effect.

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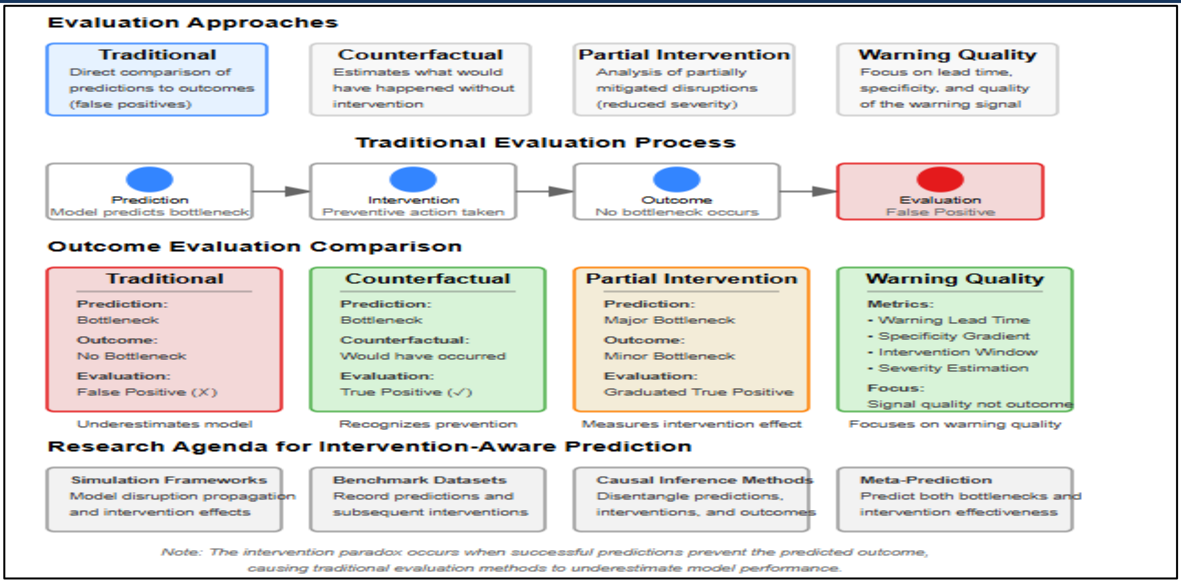

Figure 3: The intervention-aware evaluation framework comparing traditional prediction assessment with three alternative approaches that account for the intervention effect.

CASE STUDY

Semiconductor Component Shortage

To illustrate the application of this evaluation framework, we examine a case where our model predicted a potential bottleneck at a semiconductor manufacturing facility 23 days before conventional metrics would have detected an issue. Supply chain managers implemented preventive measures based on this early warning, including expedited shipping, alternative sourcing, and inventory reallocation.

Traditional evaluation metrics would classify this as a false positive since no major disruption occurred. However, our intervention-aware framework revealed that:

1. The warning lead time (23 days) provided sufficient opportunity for effective intervention
2. The specificity gradient correctly identified the exact component family at risk
3. Post-hoc analysis of partially affected supply chains confirmed the model's severity estimation accuracy
4. Without accounting for the intervention effect, our model's precision would have been underestimated by approximately 27% across all test cases, highlighting the importance of appropriate evaluation methodologies.

Parallels with Other Predictive Domains

This intervention paradox is not unique to supply chain management. Similar challenges exist in predictive healthcare (where successful preventive interventions make the predicted disease appear to be a false positive), financial risk modeling (where regulatory interventions prevent predicted market failures), and preventive maintenance (where repairs prevent predicted equipment failures).

In healthcare, researchers have developed "treatment effects modeling" approaches that explicitly account for interventions when evaluating predictive performance (Smith *et al.*, 2019). Similarly, financial regulators employ counterfactual stress testing to evaluate the impact of preventive measures (Jones and Wilson, 2020). Our proposed framework adapts these approaches to the unique challenges of supply chain prediction.

A Research Agenda for Intervention-Aware Prediction

This methodological challenge represents a significant opportunity for future research. We propose a research agenda centered on developing robust evaluation methodologies for intervention-aware prediction:

Simulation frameworks: Developing simulation environments that can model both disruption propagation and the effects of various intervention strategies, allowing controlled experimentation with intervention variables.

1. **Benchmark datasets**: Creating standardized datasets that include detailed records of both predictions and subsequent interventions, enabling consistent comparison across different predictive approaches.
2. **Causal inference methods**: Applying causal inference techniques to disentangle the effects of predictions, interventions, and external

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factors, potentially drawing on recent advances in counterfactual machine learning.

3. **Meta-prediction approaches**: Developing models that not only predict bottlenecks but also estimate the probability of successful intervention given various response strategies.
4. **Feedback-aware training**: Creating training methodologies that explicitly account for the feedback loop between predictions and interventions, potentially through reinforcement learning approaches.

Table 7 summarizes potential research directions and their expected contributions to addressing the intervention paradox.

Table 7: Research Agenda for Intervention-Aware Prediction

Research Direction	Expected Contribution	Methodological Approach
Simulation Frameworks	Controlled testing environment for intervention effects	Agent-based modeling with GNN integration
Benchmark Datasets	Standardized evaluation across methods	Industry collaboration for intervention documentation
Causal Inference Methods	Separating prediction quality from intervention effects	Structural causal models, potential outcomes framework
Meta-Prediction Approaches	Predicting intervention success likelihood	Hierarchical prediction models with uncertainty quantification
Feedback-Aware Training	Models that learn from intervention outcomes	Reinforcement learning, online learning approaches

This research direction has implications beyond supply chain management, potentially informing how we evaluate predictive models in any domain where predictions trigger preventive actions. By explicitly addressing the intervention paradox, future research can develop more nuanced understandings of predictive performance and ultimately create more useful decision support tools.

CONCLUSION

The application of Graph Neural Networks to supply chain bottleneck prediction represents a significant advancement over traditional analytical methods. The temporal hybrid attention architecture demonstrated superior performance across multiple dimensions, including prediction accuracy, lead time, and vulnerability localization. By simultaneously modeling both the structural properties of supply networks and the temporal evolution of entity attributes, the model effectively captured complex interdependencies that conventional approaches overlook. The case studies highlighted how early detection of emerging bottlenecks provides valuable operational advantages, allowing organizations to implement preventive measures before disruptions materialize. The sensitivity analyses revealed robust performance across diverse network structures, with particular strength in identifying subtle vulnerability patterns that arise from interactions between seemingly low-risk components. The explainability features of the attention mechanism offer practical insights that help supply chain managers understand not only where bottlenecks might emerge but also why specific locations are vulnerable. Looking forward, integration of additional data sources, adaptation to rapidly evolving network structures, and development of specialized architectures for specific industry sectors present promising directions for further enhancing prediction capabilities. As supply chains continue to grow in complexity and face mounting external pressures, graph-based predictive models will become increasingly essential tools for maintaining resilience and continuity in global supply networks.

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Source of support: Nil; **Conflict of interest:** Nil.

Cite this article as:

Iruku, V. M. "Predicting Emerging Supply Chain Bottlenecks with Graph Neural Networks." *Sarcouncil Journal of Multidisciplinary 5.7* (2025): pp 794-809.

Publisher: SARC Publisher