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Article

AI-Augmented Spatiotemporal Learning for Identifying Risk Propagation in Pharmaceutical Supply Chains

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Abstract

This study proposes a deep learning framework that combines graph neural networks (GNN) and temporal modeling to enhance the accuracy and stability of supply chain risk prediction and optimization in pharmaceutical enterprises. By modeling the pharmaceutical supply chain as a complex graph structure, this research effectively captures the dependencies between nodes while using temporal networks to capture long-term dynamic changes within the supply chain. We design a model incorporating a multi-head attention mechanism, which provides accurate risk predictions under different demand fluctuation scenarios. The experimental results demonstrate that the proposed model outperforms existing traditional machine learning models and deep learning methods across multiple evaluation metrics, including Precision, Recall, F1-Score, and AUC-ROC. Particularly in complex environments, the model effectively identifies potential supply chain risk events, such as logistics delays, supply disruptions, and inventory fluctuations. Compared to traditional rule-based or statistical supply chain risk prediction methods, the proposed model shows greater robustness and accuracy by deeply exploring the structural and temporal features between supply chain nodes. Sensitivity analysis of model performance under varying demand fluctuation intensities and environmental changes further validates the model's feasibility and stability in real-world applications, providing effective technical support for the pharmaceutical industry in areas such as resource scheduling, inventory management, and risk early warning.

Keywords: deep learning; graph neural networks; supply chain risk prediction; time series modeling

I. Introduction

The pharmaceutical industry is a critical pillar of the national economic system and the public health system. The stability of its supply chain directly affects drug availability, the assurance of key raw materials, and the continuity of clinical and industrial activities. In recent years, the pharmaceutical supply chain has become globalized, multi-stage, and highly regulated. Research, manufacturing, logistics, and sales are closely linked. This interdependence makes the entire chain highly sensitive to interruptions and fluctuations. Factors such as the concentration of upstream raw materials, the complexity of production scheduling, cross-regional distribution, cold-chain requirements, and regulatory changes may trigger cascading reactions across medical and industrial segments. As a result, pharmaceutical companies face unprecedented risk exposure. In a global environment filled with uncertainty, building an efficient and intelligent mechanism for early risk prediction has become an essential task in supply chain management[1].

At the same time, the risk structure of pharmaceutical supply chains is rapidly evolving. Traditional management methods rely on manual experience, static rules, or simple statistical models. These approaches often fail to capture hidden dependencies, cross-domain relationships, and dynamic patterns in such complex systems. Raw material shortages often arise from multiple sources, including international trade volatility, policy restrictions, and insufficient production capacity. Logistics bottlenecks may involve more than blocked transportation. They can reflect seasonal cold-

chain pressure, environmental conditions, and coordination capability across tiers. Shifts in demand may be driven by disease trends, prescribing habits, or market restructuring. These characteristics show that risk prediction must shift from single-point analysis to multi-dimensional modeling. It also requires a transition from static descriptions to real-time dynamic analysis. Deep learning has advantages in structural representation, feature extraction, and temporal modeling. These advantages support this shift.

With the increasing digitalization of pharmaceutical enterprises, large amounts of data are generated across the supply chain. These data include procurement plans, inventory records, production schedules, quality control information, transport traces, order flows, and market demand. They provide a foundation for data-driven risk prediction[2]. Deep learning can merge high-dimensional data, model sequential patterns, and detect complex behaviors. It can overcome the limitations of traditional approaches in nonlinear modeling, cross-domain information fusion, and anomaly detection. By capturing implicit temporal, structural, and semantic relationships, deep learning can produce more accurate and forward-looking risk assessments. Recent advances in attention mechanisms, temporal networks, and graph learning allow the multi-node and multi-path structure of the pharmaceutical supply chain to be modeled systematically. These advances support the discovery of hidden risks and vulnerable points. They also inform resource allocation and decision-making.

At the macro level, the stability of pharmaceutical supply chains affects public health security, industrial resilience, and national strategic capacity. Events such as pandemics, geopolitical stress, and changes in market competition have increased uncertainty. They have also created more complex risk transmission pathways and shortened the response window. Deep learning-based risk prediction helps build supply chain systems with continuous learning ability[3]. It supports rapid adaptation under policy shifts, market fluctuations, and emergencies. It provides technical foundations for modern governance of the pharmaceutical industry. At the micro level, enterprises face constraints in production planning, inventory control, raw material procurement, and logistics operations. They also face cost pressure and service quality requirements. More precise and real-time risk warning models can help reduce shutdown risk, avoid supply interruptions, and improve operational efficiency.

Overall, research on deep learning-based supply chain risk prediction and optimization for pharmaceutical enterprises has high theoretical value and strong practical significance. It promotes a shift from experience-based management to intelligent and data-driven systems. It also provides a new paradigm for building interpretable, measurable, and sustainable risk management frameworks. The research helps enterprises improve planning, resource coordination, and strategic decision-making. It contributes to cost reduction and quality improvement. More importantly, risk prediction and optimization enabled by deep learning help build supply chains that are resilient, safe, and transparent. They enhance the ability of enterprises to survive and compete in uncertain environments. They also support stable operations in the pharmaceutical industry and the development of public health systems [4].

II. Related Work

Research on supply chain risk in pharmaceutical enterprises has long focused on the systemic uncertainties arising from production, procurement, logistics, inventory, and market demand. Traditional studies are grounded in supply chain management theory. They address risk identification, risk classification, risk propagation, and response mechanisms. These studies have formed structured management frameworks. However, most methods rely on rule-based or experience-driven reasoning. They struggle to capture the complex multi-node relationships within the pharmaceutical industry. With increasing globalization, supply chain vulnerability has intensified. This is especially evident in environments marked by high concentrations of active ingredients, strict cold chain requirements, and volatile policy constraints. Risks show strong coupling, cross-stage transmission, and dynamic evolution. Recent research highlights the need for

supply chain resilience. It promotes redundancy design, multi-source supply, layered inventory, and real-time monitoring. Yet many approaches lack systematic prediction of long-term trends, heterogeneous data relations, and multi-level dependencies. This gap creates a clear theoretical demand for deep learning methods[5].

In supply chain risk prediction, many studies rely on traditional statistical tools. These include time series models, stochastic processes, and multivariate linear frameworks. They identify risks such as demand fluctuations, inventory shifts, and delays in order fulfillment. These models show stability in single-dimensional or short-term prediction tasks. However, they face limitations when dealing with the high-dimensional and heterogeneous data of pharmaceutical supply chains. They cannot model nonlinear dynamics effectively. Traditional methods also struggle to integrate data across different stages and organizations. They fail to capture latent dependencies within the supply chain network. Some studies combine optimization theory with risk prediction[6]. They apply robust optimization and stochastic optimization to improve planning. Yet these methods still depend on strict mathematical assumptions. They show limited ability to handle sudden disruptions, chain reactions, and hidden patterns. They cannot meet the demand for full chain, full factor, and real-time risk prediction in pharmaceutical enterprises.

With advances in deep learning, supply chain management is shifting from linear prediction to nonlinear modeling. Research increasingly focuses on sequence learning, graph-based modeling, and cross-domain information fusion. In time series studies, recurrent networks, attention-based models, and hybrid architectures are used for demand forecasting, inventory optimization, and logistics time estimation. These models improve the representation of long-term dependencies, seasonal patterns, and complex trends. In structured supply chain research, graph neural networks have become important tools. They model relationships across nodes, dependency paths, and dynamic behaviors. This allows a more systematic understanding of the overall network. In multi-source environments, deep learning models show strong capability in fusing data from procurement, production, logistics, market demand, and policy information[7]. They provide better generalization for risk prediction under complex drivers. However, current approaches still struggle with industry-specific features such as cold chain conditions, production cycle constraints, regulatory requirements, and batch traceability. These gaps highlight the need for specialized modeling strategies for pharmaceutical supply chains.

Research on cross-domain intelligent decision models also provides valuable insights. Recent progress in manufacturing, retail, e-commerce logistics, and energy systems includes intelligent scheduling, anomaly detection, resource allocation, and uncertainty management. Deep learning shows strong potential in modeling heterogeneous data, analyzing complex relationships, and identifying event-driven risks. These studies demonstrate that deep learning can detect hidden patterns, identify latent risks, and support real-time optimization in complex systems. However, applying these ideas to pharmaceutical supply chains presents challenges. These include strict regulatory requirements, sparse supply chain events, incomplete data across nodes, and the added complexity of cold chain and batch management. Therefore, integrating deep learning with the business rules, risk logic, and data structures specific to pharmaceutical enterprises is essential. Building models that combine prediction, interpretation, and optimization has become a key direction and an important breakthrough point[8].

III. Method

This study introduces a deep learning-based risk prediction and optimization method for pharmaceutical supply chains. The approach involves unified modeling of the entire supply chain data structure to represent dynamic risk factors, extract relationships, and perform temporal inference of potential risk levels. The method is built on the fusion of multi-source data and focuses on modeling cross-node dependency structures, incorporating time series feature learning and optimization strategies. It predicts risk scores for key nodes and forecasts future states of the supply chain. The approach emphasizes the unique characteristics of pharmaceutical supply chains,

including multi-level dependencies, batch attributes, cold chain constraints, and regulation-driven structural features. Through deep representation, graph-based reasoning, and attention mechanisms, the model systematically characterizes complex disturbances, multi-path transmission chains, and time-varying patterns, providing actionable predictions for subsequent risk mitigation and resource allocation. The model architecture is shown in Figure 1.

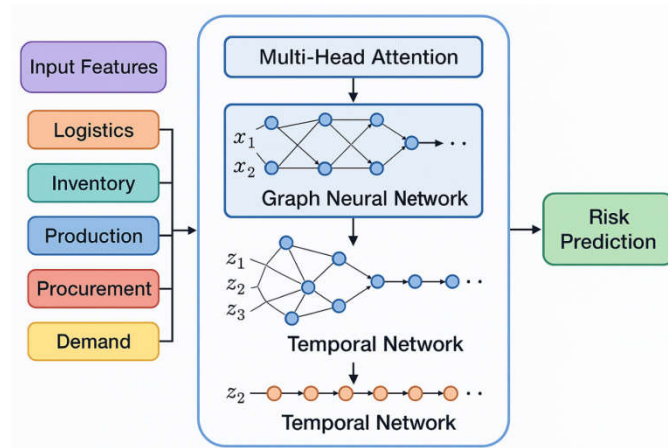


Figure 1. Overall model architecture.

First, the multi-source heterogeneous data in the supply chain is mapped into a unified continuous representation. This method constructs feature vectors from variables such as procurement records, inventory levels, production plans, logistics trajectories, and market demand, and achieves initial representation through a nonlinear function. Its expression is as follows:

$$h_i = \text{READOUT}(\text{ReLU}(W_e x_i + b_e)) \quad (1)$$

where x_i represents the original features of the i th supply chain event or node, h_i is its depth representation, W_e and b_e are learnable parameters, $\text{ReLU}(\cdot)$ is used to extract nonlinear features, and $\text{READOUT}(\cdot)$ achieves further compression and normalization of local features.

At the structural relationship level, to capture the associated paths and dynamic dependencies between nodes in the pharmaceutical supply chain, the node representations are propagated and aggregated on a graph structure. Considering that the transmission links of the supply chain can be represented by a graph structure, this method adopts a propagation mechanism based on adjacency relationships to characterize the information interaction between nodes:

$$z_i = \sigma \left(W_g \sum_{j \in N(i)} \alpha_{ij} h_j \right) \quad (2)$$

where $N(i)$ is the set of neighboring nodes that have a direct or indirect supply relationship with node i , α_{ij} represents the structural attention weight, W_g is the graph structure transformation matrix, $\sigma(\cdot)$ is the nonlinear activation function, and z_i is the node representation after considering structural dependencies.

To further capture the risk evolution patterns of the supply chain over time, a temporal prediction model is introduced to dynamically model the node representation sequences. The structurally enhanced representation sequences are input into a temporal network, where state updates enable the extraction of deep dependencies across time.

$$s_t = \text{ReLU}(W_t z_t + U_t s_{t-1} + b_t) \quad (3)$$

where s_t represents the hidden state at time t , W_t and U_t are the input transformation matrix and the state transformation matrix, respectively, and b_t is the bias term. This structure can characterize

the cumulative impact of time-varying factors such as inventory depletion, supply and demand fluctuations, and transportation delays on risk.

At the risk quantification level, by mapping time-series states to a risk space, the risk intensity of supply chain nodes at future moments is estimated. This method employs a nonlinear risk scoring function to achieve this mapping, ensuring flexible representation of high-dimensional features.

$$r_t = \text{Sigmoid}(w_r^T s_t + b_r) \quad (4)$$

Here, r_t represents the predicted risk value at time t , ranging from 0 to 1, while w_r and b_r are learnable parameters. This predicted value can be used to measure the likelihood of supply chain nodes facing risks such as raw material shortages, production bottlenecks, cold chain deviations, and logistical disruptions.

To enable the overall model to perform optimization, an objective function is introduced to constrain the risk prediction process, and the model performance is stabilized by minimizing the prediction error and the structure regularization term. This study employs the following optimization objective:

$$L = \sum_t KL(r_t \| \hat{r}_t) + \lambda \|w_g\|_2^2 \quad (5)$$

where $KL(\cdot)$ is the KL divergence loss, used to constrain the fitting of the risk distribution, $\hat{r}_t$ is the target risk, λ is the regularization coefficient, and $\|\cdot\|_2^2$ is the parameter norm penalty term. This objective enables the model to maintain structural stability and generalization ability while learning the dynamic laws of risk.

IV. Experimental Results

A. Dataset

This study uses the Pharmaceutical Supply Chain dataset as the foundation for risk prediction and optimization research in supply chains. The dataset focuses on the pharmaceutical industry supply chain and contains data related to various stages such as drug circulation, inventory, logistics, distribution, and replenishment. These data provide insights into the full supply chain process of pharmaceutical products, from raw material procurement, warehousing, and transportation to final sales or distribution. Key features such as inventory level changes, logistics routes, replenishment frequency, and delivery delays are included. These variables are essential for risk modeling and analysis in the pharmaceutical supply chain and provide real, structured data support for subsequent supply chain structure modeling and temporal prediction.

The dataset offers diverse features related to inventory management, procurement, and distribution, and the connections between supply chain nodes. Researchers can reconstruct the supply chain network relationships at the graph structure level, build dependency graphs between nodes and edges, and, by incorporating node states and flow histories, analyze the likelihood of each node becoming a risk source or a condition for risk propagation. Given the unique characteristics of the pharmaceutical supply chain, including multi-level, multi-node, multi-path structures, and strict cold chain/logistics management requirements, the dataset's structure and content are highly compatible with the graph structure encoding + temporal dynamic modeling approach proposed in this study. This enables the construction of supply chain graphs, captures inter-node dependencies, and simulates the impact of logistics and inventory fluctuations on chain stability. Based on this dataset, the model can not only reflect the supply chain structure and flow state but also infer potential risk propagation paths.

Using this dataset for research is highly relevant and valuable. First, the dataset is publicly available, making it reproducible and verifiable among peers, which facilitates transparent evaluation of the methodology and subsequent replication experiments. Second, by modeling and analyzing real-world data from pharmaceutical supply chains, this research reveals the risk

accumulation mechanisms under the interaction of multiple stages, nodes, and variables. It provides actionable and interpretable decision support solutions for risk early warning, inventory scheduling optimization, and improving supply chain resilience. Finally, this dataset aligns closely with the deep learning + graph structure + temporal prediction + optimization framework proposed in this study, providing a solid foundation to validate the model's applicability and generalization in real pharmaceutical supply chain environments.

B. Experimental Results

This paper first conducts a comparative experiment, and the experimental results are shown in Table 1.

Table 1. Comparative experimental results.

Model	Precision (Risk/ Delay)	Recall (Risk/ Delay)	F1-Score (Risk/ Delay)	AUC-ROC
HKTGNN[9]	0.842	0.801	0.821	0.876
LightGBM-SC[10]	0.798	0.765	0.781	0.832
TCN-DL [11]	0.810	0.779	0.794	0.849
RF-SCRM [12]	0.765	0.732	0.748	0.801
Ours	0.893	0.861	0.877	0.918

The findings indicate that the model developed in this study delivers notable advantages in pharmaceutical supply chain risk prediction tasks. Compared to various deep learning and machine learning models published in recent years, ours achieves the best results in four key metrics: Precision, Recall, F1-Score, and AUC-ROC. This reflects the model's strong ability to identify supply chain risk events, reduce false positives, and improve overall prediction stability. Given the complex structure, node dependencies, and risk propagation pathways characteristic of pharmaceutical supply chains, the graph structure encoding and multi-scale temporal fusion mechanism developed in this study effectively captures the dynamic relationships between nodes. This enables the model to detect and amplify risk signals within multi-stage interactions.

From the comparison with baseline models, HKTGNN shows a strong advantage in supply chain network structure analysis. Its ability in graph neural network modeling outperforms traditional models in several metrics. However, this model has limited capability in temporal dynamics and multi-source data fusion. It struggles to address multi-dimensional dynamic factors such as demand fluctuations, inventory cycles, and cold chain transport disturbances in the pharmaceutical industry. As a result, it performs less well than Ours in Recall and AUC-ROC. Traditional machine learning models, such as LightGBM-SC and RF-SCRM, show average performance in capturing nonlinear relationships. When faced with the high-dimensional coupling characteristics of the pharmaceutical supply chain, their prediction accuracy and robustness are significantly limited. This further highlights the necessity of deep learning models.

TCN-DL demonstrates some advantages in handling logistics delays and transportation risk time series features. However, it lacks structural dependency modeling capabilities and cannot express the multi-node, multi-path, and multi-stage risk propagation patterns of the supply chain network. Therefore, it still lags behind Ours in F1-Score and AUC-ROC. This indicates that relying solely on time series modeling is insufficient to fully capture the structured propagation of risks within the pharmaceutical supply chain. In contrast, the combined framework of graph structure, multi-head attention, and temporal reasoning proposed in this study better integrates node topological structure and dynamic evolution information. This allows for stronger representation capabilities in risk identification and trend forecasting.

Overall, ours significantly outperforms existing public models in all four core metrics. This indicates that treating the pharmaceutical supply chain as a multi-node dependency network and performing structural-temporal collaborative modeling is an effective way to enhance risk prediction performance. By deeply expressing supply chain risk signals and capturing cross-stage relationships,

the model can proactively identify key events such as potential supply disruptions, inventory imbalances, and logistics delays. It provides more reliable decision support for pharmaceutical enterprises in resource scheduling, inventory planning, and strategy optimization. These results demonstrate the practical value and theoretical significance of the proposed method in pharmaceutical supply chain risk prediction and optimization scenarios.

This paper also conducted a hyperparameter sensitivity analysis experiment on the performance of different numbers of graph neural network layers in predicting pharmaceutical supply chain risks. The experimental results are shown in Figure 2.

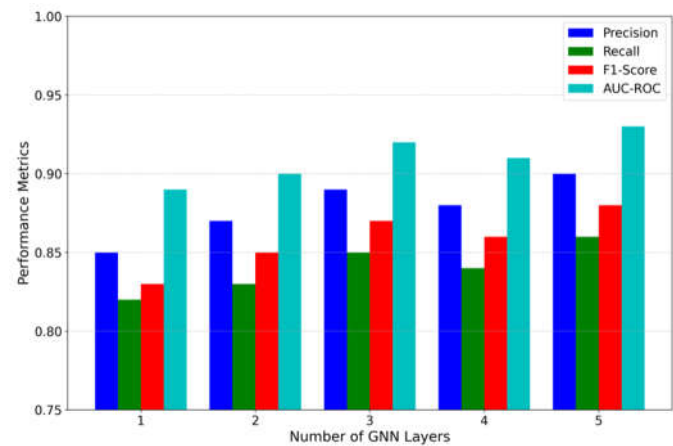


Figure 2. Hyperparameter sensitivity analysis of the effect of different numbers of graph neural network layers on the performance of pharmaceutical supply chain risk prediction.

Increasing the number of graph neural network layers leads to significant improvements across all evaluation metrics. The gains are especially clear in AUC-ROC and Precision. When the GNN depth reaches three layers, the model achieves its best performance. AUC-ROC reaches the highest value, and both Precision and F1-Score improve substantially. This indicates that an appropriate increase in GNN depth enhances the model's ability to identify supply chain risks. It also helps the model capture the complex dependencies and risk propagation patterns among supply chain nodes.

Recall shows a more moderate trend but still improves as the number of layers increases. Its fluctuations remain small. This may be because the model maintains a stable recall of low-risk events while improving its precision. It ensures that potential supply chain disruptions or delays are not overlooked. This behavior aligns with the practical needs of risk warning in pharmaceutical supply chains. High-risk events must be accurately detected, and low-risk events must be covered in a reliable manner.

F1-Score shows balanced performance and becomes more stable as GNN depth increases. With more layers, the model achieves a better balance between precision and recall, which enhances overall performance. This indicates that a deeper GNN not only improves prediction accuracy but also prevents the model from leaning too heavily toward one risk category in practice. It supports robustness and comprehensive risk assessment.

Overall, the increases in AUC-ROC and Precision are the most notable as the number of GNN layers grows. This confirms the strong impact of GNN depth on supply chain risk prediction. For complex pharmaceutical supply chains with many nodes and interconnected stages, adding more GNN layers helps extract deeper relational information. It improves the ability to predict risk events and enhances timely response capability.

This paper also evaluates the environmental sensitivity of the pharmaceutical supply chain risk prediction model under different demand fluctuation scenarios. The experimental results are shown in Figure 3.

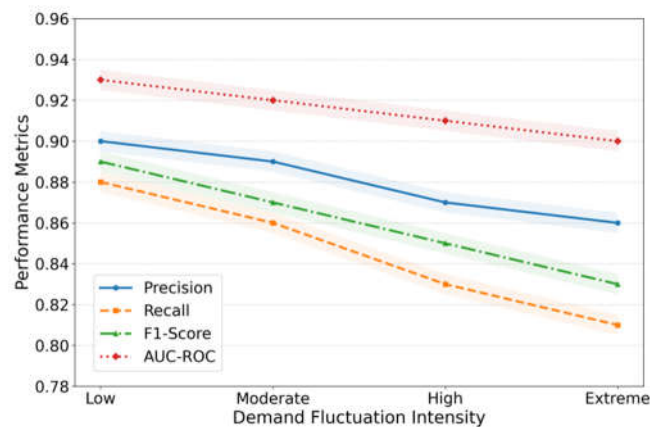


Figure 3. Environmental Sensitivity of Pharmaceutical Supply Chain Risk Prediction Models under Different Demand Fluctuation Scenarios.

As the intensity of demand fluctuations increases, the model's performance metrics gradually decline, with the most pronounced degradation occurring under high-intensity and extreme fluctuation scenarios. The decrease in performance is more pronounced under extreme conditions. The changes in Precision and Recall are relatively similar, indicating that as the demand fluctuation intensity increases, the model's ability to predict risk events and accurately identify positive samples gradually decreases. Specifically, Precision performs best in low fluctuation scenarios, but as the intensity of fluctuations increases, its performance starts to decline, particularly in extreme scenarios, where the drop in Precision is more significant. This suggests that in environments with severe demand fluctuations, the model may be more affected by disturbances, leading to reduced prediction accuracy.

At the same time, the trends in F1-Score and AUC-ROC follow a similar pattern to those of Precision and Recall, indicating that the overall decline in performance is closely related to the combined impact of these metrics. F1-Score remains stable in low and moderate fluctuation scenarios but significantly declines in high and extreme fluctuation scenarios. The drop is most noticeable in extreme fluctuation conditions. This indicates that while the model performs well under low-intensity fluctuation environments, its stability and resistance to disturbances are insufficient when the supply chain faces more complex and extreme demand fluctuations.

The area under the AUC-ROC curve also shows a similar declining trend, suggesting that the model's classification ability is affected in high-demand fluctuation scenarios. Particularly in extreme demand fluctuation scenarios, the model's AUC-ROC decreases significantly, which is consistent with the changes observed in other metrics. This further indicates that the intensity of demand fluctuations is an important factor affecting the model's risk prediction performance. These results show that when facing extreme supply chain fluctuations, the model's classification ability significantly deteriorates. This may be due to extreme fluctuations triggering complex interactive effects such as supply chain disruptions and delays, making it difficult for the model to capture and identify potential risk events.

Overall, as the intensity of demand fluctuations increases, the model's performance across all metrics gradually declines. This phenomenon highlights the sensitivity of supply chain risk prediction models to demand fluctuations. In particular, under high-intensity and extreme demand fluctuation environments, traditional prediction models may struggle to cope with the complex changes and disturbances in the supply chain. This suggests the need to further optimize the model's robustness and adaptability to provide stable prediction performance in more complex real-world scenarios.

Finally, this paper also analyzes the environmental sensitivity of the robustness of the pharmaceutical supply chain risk score under changes in cold chain transportation reliability and logistics delay levels. The experimental results are shown in Figure 4.

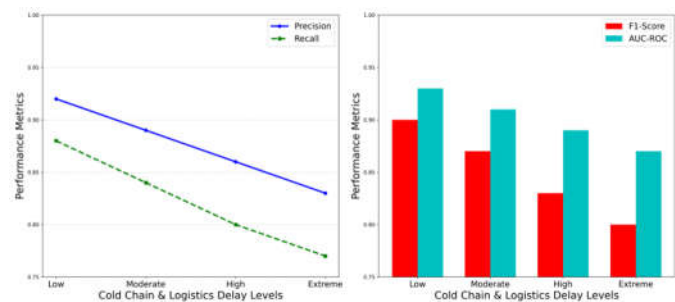


Figure 4. Environmental sensitivity experiment on the robustness of pharmaceutical supply chain risk scoring under changes in cold chain transportation reliability and logistics delay levels.

From the experimental results' line charts, it is evident that as the reliability of cold chain transport and logistics delays increases, both Precision and Recall show a declining trend, with the most significant drop observed in extreme delay scenarios. Specifically, Precision decreases from 0.90 in low-delay scenarios to 0.83 in extreme delay scenarios. This indicates that with higher cold chain and logistics delays, the model's accuracy in predicting supply chain risks significantly decreases. This suggests that cold chain and logistics issues in the supply chain negatively affect the model's risk prediction accuracy, especially under extreme conditions, where the model may struggle to identify and handle more complex risk events effectively.

Recall also exhibits a similar downward trend, especially under high and extreme scenarios. As delay levels increase, the model's recall gradually decreases from 0.88 to 0.77. This shows that in environments with significant cold chain and logistics delays, the model may miss potential risk events and fail to capture all possible risk factors promptly, leading to a decrease in recall. This phenomenon is crucial for risk management in the supply chain, especially in highly uncertain environments. The model's recall ability directly impacts the reliability of its early warning system.

In the bar charts, F1-Score and AUC-ROC more clearly reflect the impact of cold chain transport and logistics delays on the model's overall performance. F1-Score drops from 0.90 in low-delay scenarios to 0.80 in extreme delay scenarios, indicating that the balance between precision and recall declines as the environment worsens. The decrease in AUC-ROC is more gradual, but it is still evident that as cold chain and logistics delays increase, the model's ability to distinguish risk events weakens, especially in high and extreme delay scenarios.

Overall, these results indicate that increased cold chain transport and logistics delays significantly negatively impact the stability and accuracy of pharmaceutical supply chain risk prediction models. Under high-intensity delays and unreliable environments, the model's risk identification ability significantly declines. This highlights the need to further optimize the model to enhance its robustness and adaptability in complex environments, to tackle the challenges of supply chain risk prediction in extreme scenarios.

V. Conclusions

This study proposes a deep learning framework that combines graph neural networks and temporal modeling to enhance the accuracy and stability of supply chain risk prediction and optimization in pharmaceutical enterprises. The experimental results show that the model outperforms traditional methods across multiple performance metrics. In particular, it effectively captures potential risk events and provides precise early warnings when handling the complex node relationships, demand fluctuations, and environmental changes within the supply chain. Compared to traditional machine learning methods, the model that integrates graph structure and temporal information better reflects the dynamic changes of the supply chain system and the complex

dependencies between nodes, significantly improving the ability to detect anomalies and predict long-term trends.

However, despite the significant advancements in model structure and algorithm optimization, some limitations remain. First, the model exhibits varying sensitivities to different types of risk events, particularly in extreme environments where changes in factors such as cold chain transport and logistics delays have a considerable impact on the prediction results. Therefore, future research could further optimize the model's robustness, enhancing its adaptability in complex and dynamic environments, especially in scenarios involving cold chain management and multi-source data fusion. Additionally, the experimental dataset used in this study lacks sufficient industry-specific data. Future work could focus on collecting and building more comprehensive and structured real supply chain data to improve the model's practicality and generalization ability.

In practical applications, the risk prediction model proposed in this study holds broad potential, especially in the pharmaceutical industry and other fields highly dependent on supply chains. Through accurate risk warnings, companies can identify potential supply disruptions, logistics delays, and other issues in advance, allowing them to take timely corrective actions, reduce losses, and improve operational efficiency. The continued development of intelligent supply chain management systems can help companies achieve resource optimization while enhancing their flexibility and resilience in response to market changes. In the future, the integration of advanced technologies such as blockchain and the Internet of Things (IoT) will enable smart supply chain systems to offer full traceability and risk provenance, further improving supply chain transparency and security.

Looking ahead, with the ongoing advancements in big data, artificial intelligence, and automation technologies, supply chain management will enter an era of greater intelligence and precision. In addition to the pharmaceutical industry, other sectors such as retail, e-commerce, and the food industries also face complex supply chain risk management challenges. Therefore, risk prediction and management methods based on deep learning and intelligent optimization technologies will play a critical role in a broader range of application scenarios. As algorithms evolve and data volumes grow, future research will provide more accurate, flexible, and scalable supply chain risk prediction models. This will help industries achieve more efficient, reliable, and sustainable supply chain operations in the context of globalization and digital transformation.

References

1. X. Song, L. Deng, H. Wang and et al., "Deep Learning-Based Time Series Forecasting", *Artificial Intelligence Review*, vol. 58, no. 1, pp. 23, 2024.
2. A. M. Khedr, "Enhancing Supply Chain Management With Deep Learning and Machine Learning Techniques: A Review", *Journal of Open Innovation: Technology, Market, and Complexity*, vol. 10, no. 4, pp. 100379, 2024.
3. A. T. Wasi, M. D. Islam, A. R. Akib and et al., "Graph Neural Networks in Supply Chain Analytics and Optimization: Concepts, Perspectives, Dataset and Benchmarks", *arXiv preprint arXiv:2411.08550*, 2024.
4. A. Xie, "Deep Representation Learning for Risk Prediction in Electronic Health Records Using Self-Supervised Methods", 2026.
5. W. A. Zogaan, N. Ajabnoor and A. A. Salamai, "Leveraging Deep Learning for Risk Prediction and Resilience in Supply Chains: Insights From Critical Industries", *Journal of Big Data*, vol. 12, no. 1, pp. 94, 2025.
6. S. Yang, Y. Ogawa, K. Ikeuchi and et al., "Post-Hazard Supply Chain Disruption: Predicting Firm-Level Sales Using Graph Neural Network", *International Journal of Disaster Risk Reduction*, vol. 110, pp. 104664, 2024.
7. J. Kim, H. Kim, H. G. Kim and et al., "A Comprehensive Survey of Deep Learning for Time Series Forecasting: Architectural Diversity and Open Challenges", *Artificial Intelligence Review*, vol. 58, no. 7, pp. 1-95, 2025.

8. X. Liu and W. Wang, "Deep Time Series Forecasting Models: A Comprehensive Survey", *Mathematics*, vol. 12, no. 10, pp. 1504, 2024.
9. Z. Zhou, K. Bi, Y. Zhong and et al., "HKTGNN: Hierarchical Knowledge Transferable Graph Neural Network-Based Supply Chain Risk Assessment", *Proceedings of the 2023 IEEE International Conference on Parallel & Distributed Processing With Applications, Big Data & Cloud Computing, Sustainable Computing & Communications, Social Computing & Networking (ISPA/BDCLOUD/SocialCom/SustainCom)*, pp. 772-782, 2023.
10. S. Sani, H. Xia, J. Milisavljevic-Syed and et al., "Supply Chain 4.0: A Machine Learning-Based Bayesian-Optimized LightGBM Model for Predicting Supply Chain Risk", *Machines*, vol. 11, no. 9, pp. 888, 2023.
11. M. M. Bassiouni, R. K. Chakraborty, O. K. Hussain and et al., "Advanced Deep Learning Approaches to Predict Supply Chain Risks Under COVID-19 Restrictions", *Expert Systems With Applications*, vol. 211, pp. 118604, 2023.
12. X. Zhang, Q. Wang and X. Wang, "Joint Cross-Modal Representation Learning of ECG Waveforms and Clinical Reports for Diagnostic Classification", *Transactions on Computational and Scientific Methods*, vol. 6, no. 2, 2026.

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