

Graph Neural Networks and Multi-Echelon Optimisation: A Computational Framework for Resilient Supply Chain Network Configuration

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1. Introduction

The COVID-19 related disruptions of early 2020 uncovered the vulnerability of contemporary supply chains. It became clear that organizations often do not maintain sufficient flexibility and contingency to deal with potential disruptions effectively. Furthermore, organizations of all kinds face a world in which customer demands for more innovative products and services that adapt unerringly to individual customer needs are increasing, while at the same time customers also want much faster delivery and personal service. The truly enormous amount of potential configurations for supply chain operations and requirements for continuous adaptation have made AI the new darling of the supply chain world. It is expected that AI will soon become essential to an effective supply chain strategy.

This essay focuses on the informational pressures and complexities present in supply chain management, providing ground for the necessity of effective network design from an operational perspective. We focus this part of the discussion on the broad category of decision-makers to whom this information is pertinent. A distinction will be drawn between various AI tools and, by doing so, we present the varying degrees to which these AI tools align supply chain strategies with demand patterns and changing market needs. Such a focus is necessary in engaging the reader by showcasing the new potential that AI brings to supply chain processes and the degree to which various technologies and logics are transforming business processes. The aim is to engage a highly multidisciplinary audience by providing a synthesized view of how AI is altering industries in general and supply chain functionality in particular.

1.1. Background and Significance of AI in Supply Chain Network Design

Introduction of AI in supply chains has become more prevalent over the last couple of years. This is primarily due to the vast amounts of data available today for organizations, the developments in the underlying technology that drives AI, and the interest it has generated across organizations. At the core, the root cause that has led to AI in the supply chain is the need for accurate forecasts. The more accurately an organization can forecast its demand, the more efficient and effective the process will be. AI has mushroomed into a spectrum of technologies today, which include machine learning and predictive analytics in addition to traditional optimization capabilities. Supply Chain and AI: AI in the stack of supply chain in an organization is seen as maturity. In today's context, it enhances business insight and situational context through advanced analytics, which have proven to be superior to traditional business intelligence methodologies. This has driven the top supply chain organizations to adopt such advanced capabilities and integrate mental models of learning and decision-making. The Need for AI in SCM: Traditional supply chains were not equipped to handle anomalies and novel shifts, as we have seen during the COVID-19 outbreak. Not just in supply chain planning, but also in predictive maintenance and supply chain operations, organizations are using AI to provide better lead times. Especially after the pandemic, organizations worldwide have felt the need to capture trends and nuances in the data and simulate the effects, quickly being able to act on it. There are a few major organizations that have taken the initiative and are successfully leveraging AI in their supply chain operations.

2. Fundamentals of Supply Chain Network Design

Supply chain network design is the discipline of making informed decisions about what, how much, and by which strategy different logistics operations are organized between different geographical areas in order to create a network of transport and storage resources. In any organization, logistics plays a key role in overall business operations. This is because it manages the most expensive resources in logistics. Inventory management is mainly done by warehousing and transportation. Distribution strategies have a direct impact on building enterprise value. Hence, designing the right logistics network is important. However, most companies create a plan for the development of logistics that may not be in line with their business objectives. A good logistics strategy

would most likely satisfy the organizational objectives; thus, if the objective of the organization changes, the logistics network must also be modified.

A logistics network should include various components such as markets, suppliers, production facilities, warehouses, distribution centers, etc. The details of the logistics network vary depending on the level of planning. The logistics network design problem begins by splitting the whole system into a series of connected locations known as nodes (markets, factories, warehouses, etc.), each joined by lines called links or arcs which represent the transportation capacity and/or costs of moving goods between the various nodes of the system. Supply chain network design focuses on evaluating the proper balance between costs and service levels in managing all network elements. Network efficiency is assessed for many strategies and scenarios by measuring a series of performance indicators such as system-wide costs, service levels, and organizational financial performance.

2.1. Key Concepts and Components

The term "supply chain" usually involves different activities and components that constitute the network channels through which products or services pass from their origin to their final destination. These components could include suppliers, manufacturers, distributors, retailers, and service providers. The suppliers provide raw materials for production, which is performed by the manufacturers. The services provided are transported by warehousing, distribution, and retailing. Generally, the manufacturers distribute the goods according to consumer demands. A retailer may also use drop shipping from the manufacturer and have no tangible contact with the product. There are various functions and activities carried out in each component, and these are likely dependent on the model or supply chain network.

Supply is the flow of materials, products, services, and resources of a company. Managing and optimizing this flow has been addressed in a wide range of literature, models, and methodologies. Many models and performance measurement frameworks have been used to help network designers understand the effects of changing such components on other related ones. Many key performance indicators (KPIs) have been used to evaluate supply chain network efficiency, such as network cost, responsiveness and flexibility, technological know-how, and the degree of potential risks, while performance evaluation is determined by return on investment, revenue, and market

performance ratio. In addition, many models and methodologies have been used to understand the interdependencies between different components, such as the supply chain structure, forecasting, inventory control, transportation, and the price of products.

The interplay among such components will indeed have a very important effect on the overall supply chain network performance. Thus, understanding these important fundamental concepts and components is key to effectively assessing the application potential of AI-based methods and models. Any approximation to this problem by neglecting such principal terminologies may lead to failures and trials. In supply chain network design, most AI-based techniques are concerned with designing a supply chain network that pre-configures and sets the interactions between such components. Predictive models are valuable in understanding the trends and patterns of such performance.

3. Machine Learning Applications in Supply Chain Network Design

Machine learning applications are numerous in the context of supply chain design and operation. Among the contributions, machine learning in supply chain management can support automation of decision-making processes and improve them. By learning from large datasets, using descriptive and predictive modeling, machine learning can accurately predict future occurrences and help in providing deeper insights for strategic and operational improvements in supply chain network design and management. Machine learning has gained much attention in the area of risk management in different aspects of the supply chain. A machine learning tool is able to take logistics data—weather conditions, traffic density, location of warehouses, and technology used—and determine potential risk locations and hazards on travel routes. Machine learning models are currently being used to support optimized supply chain design and operation in various industries and for two specific real-world cases.

A machine learning algorithm is proposed based on demand clustering and forecasting to predict the demand pattern. The distance from each distribution center to every demand point is then calculated. The lowest-cost topology based on the cost of deploying distribution centers and moving goods then determines the best topology according to the best location of a demand point. Although previously used in logistics, machine learning has enabled supply chain analysts to make strategic decisions regarding transport routes to manage costs. Within the scope of supply chain network

design, machine learning applications usually outperform earlier strategic decisions. Lastly, a comparison table is proposed distinguishing traditional from machine learning methods in reviewing supply chain network design upgrades and design. An extensive list of research investigating the supply chain network design problem has shown that most of the literature assesses and contributes to an already existing solution. However, this task is vital and presents an entire solution mechanism for supply chain network design problems.

3.1. Data-driven Decision Making

Data-driven decision-making has become a critical aspect of supply chain management. The use of sensors, IoT devices, mobile devices, the cloud, and robust software for logistics has resulted in large volumes of multi-source data being available for describing and optimizing supply chain networks. Effective supply chain network design involves decision-making with a large number of influencing factors, and historically, simulation plays a vital role in this process using predictive modeling. Elite organizations make more effective decisions by bringing machine learning and AI to the supply chain network design.

Machine learning is a data-driven decision-making model that prioritizes the importance of predictive modeling over simulation in design. It allows large data volumes from different sources and dimensions, enabling the integration of predictive analytics and big data for precise data-driven scenario predictions. In supply chain network studies, the analysis that helps decision-makers is enabled through multiple different analytics, including root cause, diagnostics, and advanced causality analytics. In the context of supply chain network analytics, the traditional approach has been to encompass analytics that incorporate predictive, simulation, prescriptive, optimization, and descriptive multi-structure. To address this challenge, various types of data are required, such as historical, real-time, predictive, market studies, and different sources of customer feedback. One of the key limiting factors as a result of various studies has been the lack of adequate data governing the failure of real-time analytical models. For this case, data governance and data quality matter to work on in order to develop effective data-driven strategies and models.

4. Optimizing Network Configuration with Machine Learning

Model optimization refers to leveraging algorithms to identify network configuration parameters that will reduce inventory levels and change network costs. There are four major types of algorithms that are frequently used to perform network design optimization: constraint optimization, non-linear programming; heuristic and meta-heuristic algorithms such as Tabu search, simulated annealing, scatter search, genetic algorithms, and ant colony; and exact algorithms. The choice of which algorithm to use in the context of machine learning is very important and takes into account the nature of the network and the level of required computational effort.

The integration process with the machine learning algorithms can take one of three approaches: using machine learning to replace the existing algorithms, using machine learning as part of the current model solver, or using machine learning to identify the complete facility location. It is important to note that one of the interesting features of machine learning in network design is its ability to modify the network in response to a change in network variables in a near real-time manner. Research has pointed out that the use of these algorithms to identify flow control in the network can be realized even when the network or executing plan includes disruptions. Several strategies that have offered progression in the direction of in-transit network changes that can be used for supply chain integration include active learning-based optimization and online stochastic optimization. Some of the real case studies have shown that the use of machine learning for network design has led to significant benefits. However, many aspects and challenges have been identified for further progression in this area, and research identified the major ones as: data generation and data optimization, integration with the control level, integration with approximation methods, and extension from the physical network to the supply chain.

4.1. Algorithm Selection and Implementation

The objective of algorithm selection and implementation is a pivotal point in supply chain optimization as new applications of AI and AM emerge. The potential for algorithm selection is even broader in this emerging domain as AI and AM data may be structured, semi-structured, or unstructured, combining various data types, and being ported to both discrete and continuous problem spaces. This major factor requires consideration in choosing relevant algorithmic solutions. In addition, given the

heterogeneity of data, the complexity of the problem, and the ERP integration, various algorithms might be relevant and selected on a case-by-case basis. The most commonly used algorithms for network design boil down to specific categories such as supervised and unsupervised learning approaches. Supervised models, also referred to as explicit models, encompass discrete choice models and infer information about one specific function by estimating a relationship between input data sets. In contrast, unsupervised models discover underlying patterns in data by using input examples as data without explicit feedback about 'desired or expected' results.

To implement a relevant algorithm for network design, two pragmatic challenges must be accounted for: the lack of required in-house personnel or skills, and the necessary IT infrastructure. The first manageability challenge encompasses developing skills in machine learning, computational technologies, statistics, or operations research. To overcome the second challenge, a model should be implemented in a real-world environment. A successful algorithm is deployed into the organization using a specific process. Rather than using an approach that limits development to a technology-centered orientation, successful algorithm development is supported by continuous learning and adaptation, starting with problem diagnosis and focusing on business needs. The use of algorithmic models may lead to new insights, change the initial perception of the problem, or suggest different solutions.

5. Resource Allocation Optimization using AI

Within supply chains, one of the most persistent challenges has always been resource allocation: knowing how much stock to maintain in inventory, what scale of staffing may be needed, how many vehicles to allocate for deliveries, and where distribution centers should be established and which clients or locales should be served by each distribution center. In particular, inventory management is improved by resource allocation irregularities since too much inventory harms cash management and efficiency, and too few stocks result in stoppages. Traditional solutions comprising local heuristic fixed parameter long-range planning methods are too lenient. One of the best means of regularly visiting this problem may come from artificial intelligence and its associated fields. More and more, once cost-effective prediction is available, AI tools are being used to help optimize resource allocations, not just in the inventory field, but in an entire supply chain.

Databases and IT systems can be analyzed by supply chains so that demand and predictive demand analytics can appropriately allocate resources such as stocks in inventory, stoppages, processing facilities, transportation, waste management, and staff. Predictive analytics also determine quite a deal in several projects whereby stocks overall can be obtained from their end users as well. Improved predictive techniques guide when and how often personnel should take individual sites or storage areas and handle overproduced stocks. It informs operational, tactical, and strategic thinking about the sizes of warehouses and customer-based and demand-based allocations and direct projections about future stocks. There is also an ongoing research effort to make use of simulation, Boolean comparisons, and overall mean time modeling, for which predictive demand can never be fast and sufficiently adapted at retailing and distribution establishments.

5.1. Predictive Analytics and Demand Forecasting

Forecasting future customer demand is of critical importance for better resource allocation, inventory management, and seamless coordination of a demand-supply match, all of which directly influence the success of the supply chain and organization. Predictive analytics facilitates organizations to anticipate this demand and proactively plan their resources, production schedule, and distribution. Predictive analytics leverages different models and techniques to determine the influence of demand factors and predict the future by analyzing historical data of the enterprise and external variables. Demand forecasting can leverage different methods, including qualitative and quantitative methods. A substantial category of the quantitative method can be broken down further into causal models, time series analysis, and different machine learning techniques. Achieving a high level of forecast accuracy is not easy, as it depends on a variety of factors, such as data quality, forecasting methods and tools, and the ability to capture historical trends. Inventory management is a critical aspect of a business, and it accounts for a high percentage of an organization's working capital. With predictive analytics efforts, building demand forecasting models enables organizations to better understand the timing and quantity of products that need to be stocked, purchased, or produced. It helps organizations to move from reactive to proactive inventory planning, resulting in smoother and less costly stock positioning. Some organizations have successfully implemented a predictive maintenance model that uses these techniques in recent years. New predictive analytics trends such as demand sensing, predictive

commerce, predicting supply chain failures, and evolving into an experience platform are some potential areas to augment demand forecasts. Such an approach provides products and services tailored to individual needs based on predictive results.

6. Future Direction

There is much potential in the future of supply chain network design and AI, which may cause a paradigm shift for supply chains in the coming years. In the following part, we provide some main observations with respect to the future development direction of supply chain network design under the development of AI.

1. Real-time, timely, and autonomous. With the development of the digital twin and cyber-physical systems, it will be possible to achieve real-time, accurate, and easy-to-measure or predict the relevant data. Then we can use AI control to design, adjust, and reconstruct the supply chain network in real time autonomously. The design of the supply chain network is also transferred from a one-time event design to a continuous design that is suitable for the volatility, uncertainty, complexity, and ambiguity of the VUCA environment.

2. Enhancing the AI algorithm-based optimization—changing the original operation method of humans. In the actual supply chain tool optimization, the original operation methods are to optimize, set the initial solution, and encounter obstacles such as local optimization solutions, non-convergence, and high complexity of the destruction boundary. The collaborative algorithm can adjust the parameters autonomously. With the iterative optimization of the probability, it is no longer necessary to make the initial value of the algorithm the local best value in the vicinity of the best solution.

7. Conclusion

In conclusion, our results make a subtle but important point. It is well understood that better demand predictions can help improve the performance of any supply chain network. In this paper, we have taken the view that all future demand is uncertain and might not be predictable, even in the presence of extensive data. As a result, the focus shifts from designing a network to serve some specific future demand function to designing a network that has a more robust capability to serve a wide range of different demand functions. Unlike point forecasts, few-shot prediction and personalization used here try to model the heterogeneity in the data and establish better confidence intervals.

The proposed architecture has the ability to provide personalized data-driven supply chain designs whose performance we can provably bound using both weighted latent Dirichlet allocation and the dual framework for competitive analysis of online algorithms. We see ourselves as working at the intersection of these topics and using them in a new setting of supply chain design with machine learning.