**Integration of Plant Scheduling Feasibility with Supply Chain Network Under Disruptions Using Machine Learning Surrogates**

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**Abstract**
Integrating supply chain under disruptions with plant scheduling is challenging due to differing time scales. Our proposed approach utilizes a reactive supply chain model with linear model decision tree surrogates, capturing feasibility within scheduling constraints. The surrogate employs an aggregated variable space and an efficient sampling methodology, as demonstrated in a case study. Results highlight the integrated model's ability to ensure entirely feasible operations without compromising overall profitability within tractable solution time.

**Keywords**: Supply chain under disruptions, Feasibility, Machine learning surrogates.

**1. Background**

In an increasingly interconnected global landscape, the resilience of supply chains and manufacturing networks against disruptions is important across various industries. Disruptions in the supply chain can trigger a cascade effect, impacting the entire system in both upstream and downstream directions. Predicting these effects is challenging due to the intertwined material flows and the amplification of disruptions beyond neighbouring nodes (Snyder et al., 2016). Reactive models, such as the one introduced by Ovalle et al. (2023), address this by generating optimal schedules for large-scale supply chain problems with arbitrary network topologies. However, this model does not consider the lower-level dynamics of in-site plant scheduling. Therefore, solutions for this model may be infeasible with respect to plant scheduling constraints. Integrating decision-making levels across the supply chain enhances synergy and coordination, yielding superior solutions compared to isolated approaches (Grossmann, 2005). Thus, it is essential to integrate tactical reactive decisions at a global level with in-site plant scheduling, considering production constraints.

In integration of the planning and scheduling, the difference in timescales also presents a challenge, as the plants operate at a finer time scale (e.g., an hourly time discretization) whereas the higher-level supply chain decisions are made on a daily or weekly basis. A simple solution to this is to take all decisions at the timescale of the plant operation (e.g., on an hourly basis) (Grossmann, 2005), but this might render the problem intractable for longer time horizons and larger network topologies. The literature addresses this problem

by either solving the full-space monolithic model (e.g., by decomposition), using relaxed or aggregated models for scheduling, or using surrogate models to capture scheduling feasibility. Previous research using surrogates has focused on the use of SVM with linear and Radial basis function kernels for integration of scheduling in planning-level problem (Badejo and Ierapetritou, 2022) and demonstrated the use of decision trees and artificial neural networks for feasibility analysis of the scheduling problem (Dias and Ierapetritou, 2019). In this work, we employ a linear model decision tree as a surrogate model to define the feasible region of the scheduling constraints for the plant. Our approach, akin to research by the previously mentioned authors, tackles the integration of plant operations with supply chain operations. We consider disruptions and arbitrary network topologies, particularly in the context of order management, as outlined in Ovalle et al. (2023).

**2. Problem Statement**

Consider a supply chain and manufacturing network characterized by an arbitrary topology, meaning no assumptions are made about the structure or connections within the network. In this scenario, a disruption has occurred. We have information about the operation time horizon, the time required to traverse each connection in the network, and the capacities of both warehouses and shipments. Additionally, we have data on the selling price of the product, as well as the costs associated with purchasing materials, production, shipping, and inventory holding. Furthermore, detailed information about plant production, including batch sizes, resource utilization, and production coefficients, is available.

The objective is to determine the optimal response to the disruption. This involves creating reactive schedules for shipping, purchasing, and production throughout the entire time horizon. Additionally, it entails establishing inventory levels for each node in the system. Moreover, the obtained schedules must allow for late delivery and order cancellation while still accounting for customer satisfaction. Although the solution is given for the higher-level supply chain, the obtained operation must be feasible with regards to the detailed scheduling for every plant at every time period.

The main goal is to achieve an integrated response that optimizes the overall profit of the operation. As the time horizon concludes, the solution should provide a sense of recovery from the disruption. This recovery is defined by bringing the final inventory levels as close as possible to their pre-disruption values. The reactive operation is expected to balance the existing trade-off between stressing the system and avoiding adverse effects on the company's goodwill, which can be impacted by delayed deliveries or order cancellations. In addressing this problem, we assume that pricing remains unaffected by the specific node of transaction, transportation cost is solely contingent on the shipped quantity, and transportation capacity is sufficient to obviate the need for vehicle routing.

**3. Proposed Methodology**

This section provides a concise explanation of the model for the reactive operation of a supply chain under disruptions from Ovalle et al. (2023). The optimal responses derived from this model, however, lack awareness of plant-level production constraints, potentially resulting in higher-level schedules that are not always feasible. To address this, we use binary classification LMDTs surrogates to capture the feasibility space of the scheduling constraints for the plant. Hence, we investigate the efficient integration of these surrogates into the model, proposing an aggregated feature representation that significantly reduces the size of the surrogate and the computational time required for dataset generation. Additionally, a brief overview of the Resource Task Network (RTN) framework is presented, accompanied by a sample generation scheme designed to effectively capture the specified boundaries of the feasibility space.

* 1. Base Model for Reactive Supply Chain Under Disruptions

A similar model to the one proposed in Ovalle et al. (2023) that yields the optimal reaction in a disrupted network composed of suppliers ($S)$, warehouses ($W$), plants ($P$), and customers ($C)$ over a discretized time horizon ($T$) is used. The mixed-integer linear programming (MILP) formulation is given as:

|  |  |
| --- | --- |
| $$max Σ\_{t\in T}\left[Σ\_{c\in C}Σ\_{m\in M\_{c}}\left(λ\_{mct}^{D}D\_{mct}-λ\_{mct}^{U}U\_{mct}-λ\_{mct}^{δ}y\_{mct}\right)-Σ\_{a\in A}Σ\_{m\in M\_{a}}λ\_{mat}^{F}F\_{mat}^{Out}- Σ\_{s\in S}Σ\_{m\in M\_{s}}λ\_{mat}^{B}B\_{mst}-Σ\_{p\in P}Σ\_{r\in R\_{p}}λ\_{prt}^{P}P\_{prt}- Σ\_{m\in P∪W}Σ\_{m\in M\_{n}}λ\_{mnt}^{I}I\_{mnt}\right]-Σ\_{m\in P∪W}Σ\_{m\in M\_{n}}λ\_{mn}^{dev}|I\_{mn}^{0}-I\_{mn\left|T\right|}| $$ | (1a) |

$$ s.t.$$

|  |  |
| --- | --- |
| $$F\_{mat}^{In}=F\_{ma\{t+τ\_{mat}\}}^{Out} ∀a\in A, m\in M\_{a}, t\in T:t+τ\_{mat}\leq |T|$$ | (1b) |
| $$D\_{mct}=Σ\_{a\in A\_{c}^{In}}F\_{mat}^{Out} ∀c\in C, m\in M\_{c}, t\in T$$ | (1c) |
| $$B\_{mst}=Σ\_{a\in A\_{s}^{Out}}F\_{mat}^{In} ∀c\in C, m\in M\_{s}, t\in T$$ | (1d) |
| $$U\_{mct}=U\_{mc\{t-1\}}-D\_{mct}+δ\_{mct}(1-y\_{mct}) ∀c\in C, m\in M\_{c}, t\in T$$ | (1e) |
| $$I\_{mwt}=I\_{mw\{t-1\}}+Σ\_{a\in A\_{w}^{In}}F\_{mat}^{Out}- Σ\_{a\in A\_{w}^{Out}}F\_{mat}^{In} ∀w\in W, m\in M\_{w}, t\in T$$ | (1f) |
| $$I\_{mpt}=I\_{mp\{t-1\}}+Σ\_{a\in A\_{p}^{In}}F\_{mat}^{Out}- Σ\_{a\in A\_{p}^{Out}}F\_{mat}^{In} +Σ\_{r\in R\_{p}}ϕ\_{rm}P\_{prt} ∀p\in P, m\in M\_{p}, t\in T$$ | (1g) |
| $$D, B, U,F^{In},F^{Out},P, I\geq 0 y\in \{0,1\}$$ | (1f) |
|  |  |

The objective function of the model, shown in Eq. (1a), represents profit maximization accounting for the sales ($λ^{D}$) as well as the costs of shipping ($λ^{F}$), buying material ($λ^{B}$), producing ($λ^{P}$) and holding inventory ($λ^{I}$). Moreover, this objective is penalized by a late deliveries ($λ^{U}$), order cancellations ($λ^{δ}$) and deviations from the nominal inventory level at the end of the operation ($λ^{dev}$). Equation (1b) models the time associated with traversing an arc, where $F^{in}$ is the flow that enters the arc and $F^{Out}$ stands for the same flow that leaves the arc after a time displacement $τ$. Equations (1c) and (1d) model the acquisitions ($B$) and deliveries ($D$) respectively. Order management is handled in Equation (1e) where an order $δ$ is only accumulated as unmet demand ($U$) if it is not delivered nor cancelled ($y=0).$ Equations (1f) and (1g) account for the inventory ($I$) balances that take place in warehouses and plants respectively. Here the main difference is that the plant balance accounts for a material transformation term calculated as the mass stoichiometric coefficient ($ϕ$) and the production ($P$). Throughout the formulation, the sets $A\_{n}^{in}$ and $A\_{n}^{out}$ stand for the set of arcs that enter or leave (respectively) a given node $n\in N$. Finally, all variables are continuous, non-negative and bounded by their respective capacities except order cancellation $y$, which has a binary nature ($y\in \{0,1\}$). For further explanation and demonstration of disruption capturing flexibility and time-scalability, we refer the readers to (Ovalle et al., 2023).

* 1. Integrating the Base Model with Binary Classification Linear-Model Decision Tree Surrogates of the Schedule Feasibility

In constructing our surrogate model to effectively capture the plant feasibility, we employ linear model decision trees (LMDTs), a conventional decision tree variant featuring linear functions at nodes instead of constants (Ammari et al, 2023). Specifically, we utilize binary classification LMTDs to capture the feasibility of the plant scheduling based on the higher-level flow and inventory information at a given time period. The output of the binary classification LMDT is a continuous number and zero serves as the classification threshold, meaning positive outputs are classified as feasible, while negative outputs are interpreted as infeasible scheduling scenarios.

The delineation of the feature space for the LMDT surrogate needs to accurately capture the supply chain information of a plant across time periods. A naïve approach could inform the surrogate about all the terms involved in the plant material balance as shown in Eq (1g). This is considering previous and current inventories, productions, alongside with incoming and outgoing material flows for each individual material, resulting in the incorporation of five input variables per material species into the model as:

|  |  |  |
| --- | --- | --- |
| $$DT\_{pt}(I\_{mpt},I\_{mp\{t-1\}}, Σ\_{r\in R\_{p}}ϕ\_{rm}P\_{prt},Σ\_{a\in A\_{p}^{In}}F\_{mat}^{Out},Σ\_{a\in A\_{w}^{Out}}F\_{mat}^{In} ∀m\in M\_{p})\geq ϵ ∀p\in P, t\in T$$ |  | (2a) |

where $ϵ$ is a small positive number that is used to tune the classification threshold. However, considering the substantial number of materials, particularly when accounting for intermediate species, the aforementioned approach runs the risk of generating an impractical number of variables. This concern arises from the well-established understanding that a suitable training dataset typically expands exponentially with the increasing number of features. To tackle this challenge, the surrogate's input space is reduced to two compound variables that capture the required input spaces as shown below by aggregating higher-level information from the material balance as:

|  |  |
| --- | --- |
| $$V\_{mpt}=I\_{mp\{t-1\}}+Σ\_{a\in A\_{p}^{In}}F\_{mat}^{Out} ∀p\in P, m\in M\_{p}, t\in T$$ | (2b) |
|  |  |
| $$Z\_{mpt}=max⁡\{0,Σ\_{r\in R\_{p}|ϕ\_{rm}>0} ϕ\_{rm}P\_{prt}-Σ\_{a\in A\_{w}^{Out}}F\_{mat}^{In}\} ∀p\in P, m\in M\_{p}, t\in T$$ | (2c) |
|  |  |

It is worth mentioning that these are not the only ways to aggregate the terms to accurately represent a similar concept given that the mass balance depicted in Eq. (1g) is still in place. The resulting surrogate model is defined as:

|  |  |  |  |
| --- | --- | --- | --- |
| $$DT\_{pt}(V\_{mpt}\_{ } , Z\_{mpt} ∀m\in M\_{p})\geq ϵ ∀p\in P, t\in T$$ |  |  | (2d) |

Constraint (2d) can be embedded into the optimization model described by Eqs. (1) together with Eq. (2b) and Eq. (2c) to obtain a reactive supply chain model that includes a surrogate for feasibility in the plant-level scheduling.

3.3 Efficient Data Generation Scheme Using Resource Task Networks

We use the Resource Task Network (RTN) framework to solve scheduling problems and obtain data for the feasibility surrogate. Here, tasks represent operations (e.g., material transformation) and resources represent all the entities involved in the process steps (e.g., raw materials, intermediates, products, and equipment where tasks take place) (Pantelides, 1994). The flexibility of RTN modeling enables it to be used in different problems in a compact manner gaining wide popularity for industrial applications (Perez et al., 2022).

In constructing the feature dataset, initially various scenarios of material availability and production demand were sampled. However, a straightforward Monte Carlo sampling technique within the bounds of $V$ and $Z$ proved insufficient in capturing instances enforced by the plant's optimal reaction on the higher-level. To address this limitation, we observed that the higher-level flows in the system are governed by Eq. (1g), ensuring a consistent adherence to a simple mass balance for internal supply and demand within the plant. Consequently, we narrowed the sampling space by imposing this condition on all samples. Additionally, recognizing that production costs outweigh inventory holding costs, plants often fulfill internal demand using existing inventory rather than production. Consequently, the demanded production frequently equals zero. To better represent this scenario, with probability $α=0.3$ we enforced $Z=0$ for all materials, enhancing the dataset's ability to capture this particular region effectively.

After constructing the feature dataset, we proceeded to solve an RTN scheduling model for each instance, recording feasibility as a binary label indicating whether under those internal demand and supplies the rigorous schedule was viable or not. The open-source package rtn\_scheduling was used to efficiently generate RTN models directly from data files on a reliable manner (Vyas et al., 2023).

**4. Case Study and Results**

To evaluate the proposed methodology, we employ a 24-node arbitrary supply chain topology (Figure 1) with two plants. The first plant addresses both internal and external demand for a total of four materials, while the second plant manages six materials. We evaluate the reactive schedule in response to an arc disruption limiting direct shipments between the plants. The task is to determine the optimal response over the next four months with daily time discretization.

Pyomo was utilized to construct the reactive supply chain model, while the training of the binary classification LMDT surrogate was performed using the linear-tree open-source package. Efficient integration into an equation-oriented approach was achieved through OMLT (Ceccon et al., 2022). The resultant MILP problem was solved using Gurobi v9.5.1 as the solver, executed on a Linux machine equipped with 8 Intel Xeon Gold 6234 CPUs running at 3.30 GHz, boasting 8 total hardware threads, and 1 TB of RAM operating within the Ubuntu environment.

 

Figure 1: Case study supply chain and manufacturing network topology

We solve the reactive supply chain model outlined in Section 3.1, denoted as the Original Model, and further solve the identical model after the integration of LMDT feasibility surrogates for each plant and time period. This extended model is referred to as the Integrated Model and the results of these computational experiments are presented in Table 1.

Table 1: Result comparison before and after surrogate integration

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **Objective [$]** | **Solution Time [s]** | **No. of Periods with Infeasible Schedule** | **No. Variables /****No. Constraints** |
| **Original Model** | 9,338,083 | 0.16 | 5 | 25,590 / 17,115 |
| **Integrated Model** | 9,335,894 | 8.13 | 0 | 31,430 / 32,615 |

Table 1 reveals that over the course of 120 days of reactive operation, the Original Model prompted the plants to operate under infeasible conditions on five distinct occasions. In contrast, the model incorporating embedded surrogates exhibited 100% feasibility throughout the operational horizon. Notably, the feasibility was validated by solving the rigorous RTN model for each period and plant based on the solution from the models. Hence, it can be observed that the proposed extension ensures the robustness and reliability of the schedule feasibility within the existent reactive supply chain optimization framework.

The revised operation, incorporating plant feasibility considerations, results in only a marginal 0.02% reduction in operational profit, demonstrating that operational viability can be ensured without significant sacrifice to overall profitability. It is noteworthy that the inclusion of surrogates increases the solution time by an order of magnitude, given an approximate increment of 22.8% in variables and 90.6% in constraints with respect to the original model. However, the full monolithic model, which rigorously integrates RTN scheduling with responsive supply chain operations on an hourly basis, presents an impractical scale with 682,482 variables and 544,275 constraints, representing an order of magnitude increase compared to the original and integrated models, making it intractable to solve. Therefore, despite the increased computational time, the proposed model with integrated surrogates remains a viable solution for an integrative reactive supply chain with plant-level scheduling.

**5. Conclusions**

This study enhances an existing reactive model designed for supply chain and manufacturing networks with arbitrary topologies, capable of handling disruptions. We integrated linear model decision tree surrogates to define the feasibility space associated with plant scheduling constraints. The efficacy of this integration has been demonstrated, showcasing a notable enhancement to the existing reactive model. The result yielded a feasible operation throughout all time periods in both plants, without significantly compromising the overall profit. As a direction for future research, it would be interesting to explore the scalability of this approach concerning the network size and the number of materials considered within the plants.

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