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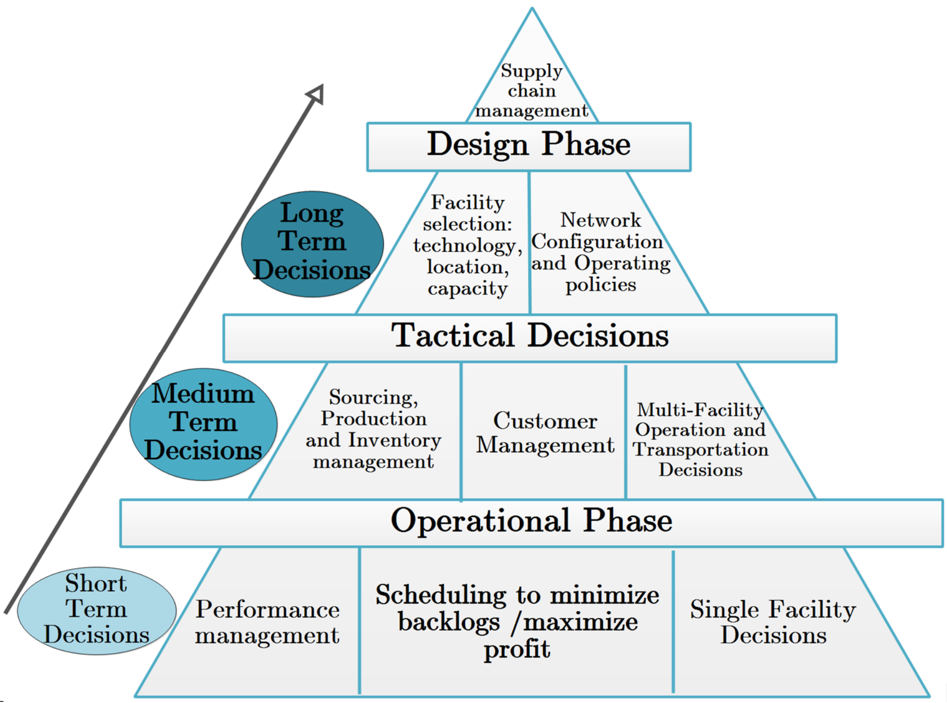
Supply chain management
Design Phase
Facility selection: technology, location, capacity
Network Configuration and Operating policies
Long Term Decisions
Tactical Decisions
Sourcing, Production and Inventory management
Customer Management
Multi-Facility Operation and Transportation Decisions
Medium Term Decisions
Operational Phase
Short Term Decisions
Performance management
Scheduling to minimize backlogs /maximize profit
Single Facility Decisions

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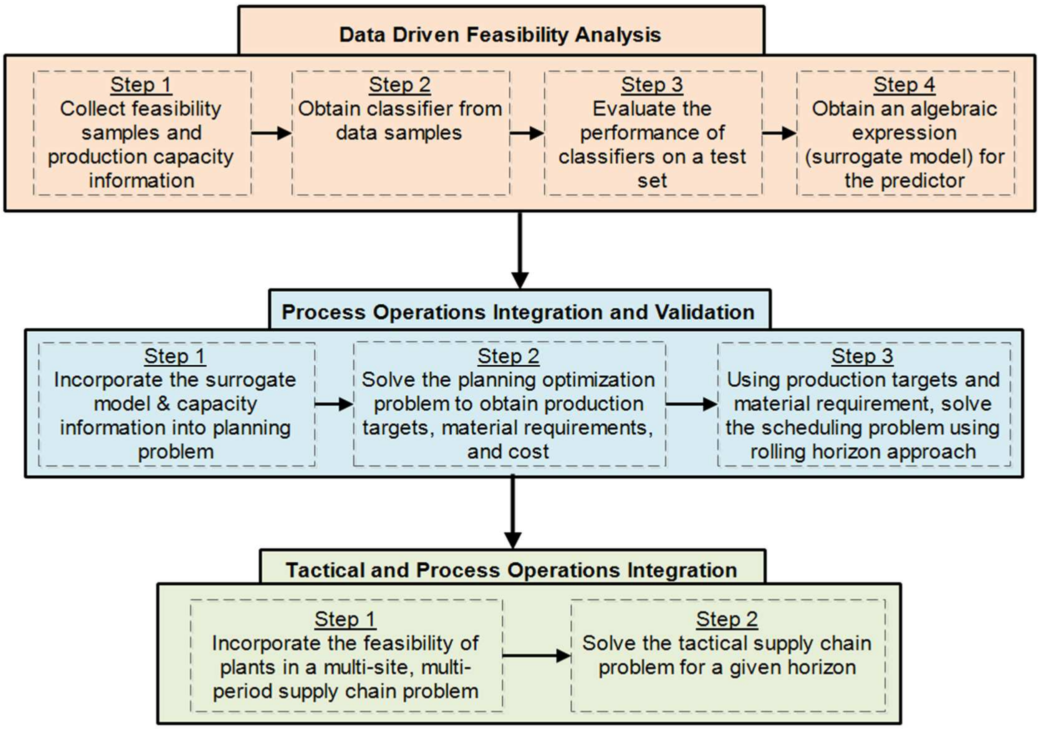

Data Driven Feasibility Analysis
Step 1
Collect feasibility samples and production capacity information
Step 2
Obtain classifier from data samples
Step 3
Evaluate the performance of classifiers on a test set
Step 4
Obtain an algebraic expression (surrogate model) for the predictor
Process Operations Integration and Validation
Step 1
Incorporate the surrogate model & capacity information into planning problem
Step 2
Solve the planning optimization problem to obtain production targets, material requirements, and cost
Step 3
Using production targets and material requirement, solve the scheduling problem using rolling horizon approach
Tactical and Process Operations Integration
Step 1
Incorporate the feasibility of plants in a multi-site, multi-period supply chain problem
Step 2
Solve the tactical supply chain problem for a given horizon

variable d, a control variable z, and uncertain parameter θ, a feasibility measure ψ, defined given by equation (1), is used to determine if the process is feasible. A detailed explanation of the mathematical approach can be found in Grossman et al.(2014). The approach above always assumes that the feasibility function is known. Another approach is to use the black-box surrogate-based feasibility analysis, where a surrogate is used to represent the feasibility function given a set of input parameters and the black-box simulation output for the feasibility function. Thus, $\psi(d,\theta) > 0$ implies one or more constraints are violated, $\psi(d,\theta) = 0$, implies boundary of the feasible region, and $\psi(d,\theta) < 0$ implies feasibility. A good review of this approach can be found in (Banerjee et al., 2010; Boukouvala and Ierapetritou, 2012; Wang and Ierapetritou, 2017).

$$\psi(d,\theta) = \min_{z} \max_{j \in J} \{f_j(d,z,\theta)\} \tag{1}$$

This work hinges on the latter approach interpreting the feasibility of the scheduling problem as a classification problem, in this case, the design variables, d, are production facility data (e.g., unit capacities and network connectivity), production recipe (mixing and splitting rules, processing time, and the change over time) and the scheduling horizon. For the scheduling problem, the design variables are fixed. Control variables, z, are the integers that determine the feasible sequencing and allocation. The uncertain parameters θ are the available resources and production targets, and the feasibility function f_j is the scheduling model constraints. Table *1* delineates the procedure to obtain the feasibility dataset.

Table 1: Procedure to obtain feasibility dataset.

- Obtain the bound of the uncertain parameters by using the state maximization objective
- Using the bounds create a sampling strategy to obtain N sample points.
- For every instance i in the $\mathcal{N}$ sample points, solve the feasibility problem to obtain the corresponding class $y_i \in \{-1, 1\}$. After $|\mathcal{N}|$ instances, we have the dataset $\mathcal{D} = \{(\boldsymbol{x_i}\, y_i)\}_{i=1}^{\mathcal{N}}$ which is a set of input-output pair. Where $x_i \in \mathbb{R}^k$ with k being the sum of number of products and raw materials. $\mathcal{D} \in \mathbb{R}^{(k+1)\times N}$

It is worth noting that the uncertain parameters in a scheduling problem are the states of the system (products and the raw materials required). Furthermore, the method proposed by Dias and Ierapetritou (2020) has been modified to include the raw material as additional features. This modification improves feasibility accuracy and ensures an accurate estimation of the required raw material.

Once the dataset is obtained, the next phase generates a surrogate model which takes as an input the set of novel predictors $\boldsymbol{x}$ and predicts the response y. It should be noted that the responses obtained are discrete entity and we can easily divide the input space into a collection of regions labeled according to the classes. Problems like this can be cast as a classification problem. Generally, the choice of the surrogate model determines the structure of the integration problem. In this work, three methodologies were used to generate the surrogate model. These are discussed individually.

Support Vectors Machines

Support vector machines classifiers combines kernel trick (to define similarity between points) with a modified loss function and attempts to find an optimal hyperplane that separates all data points of one class from those of the other class. The general expression is given as

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(3) and (4) can be applied to the new expanded data. However, because the features are expanded, the Lasso algorithm is used for regularization to ensure selection of the features from the expanded feature set. In this work the model generated by a combination of the expanded feature method and the machine learning procedure is referred to as Linear Expanded Model (LEM).

Feasibility Accuracy Quantification

In this work, the feasibility metrics proposed by Wang and Ierapetritou(2017) were used to analyze the classifier performance of the surrogate models. In the metrics, the whole uncertain space is divided into four regions: Correct feasible region (CF); Correct Infeasible region (CIF); Incorrect feasible region (ICF); and Incorrect Infeasible region ($ICIF$). These regions are used to define the metrics as follows.

$$
\begin{aligned}
CorFeas &= \frac{CF}{CF + ICIF} \times 100 \\
CorInfeas &= \frac{CIF}{CIF + ICF} \times 100 \\
OvEst &= \frac{ICF}{ICF + CF} \times 100 \\
Total\ Error &= \frac{ICF + ICIF}{CF + CIF + ICF + ICIF} \times 100
\end{aligned}
\tag{12}
$$

where $CorFeas$ and the $CorInfeas$ indicate the percentage of feasible region in the correctly captured feasible regions and the percentage of correctly captured infeasible region. These metrics denotes how the uncertain parameter space has been correctly explored and classified with respect to feasibility. Furthermore, $OvEst$ indicates the percentage of feasible region which has been overestimated by the surrogate model. It gives an estimate of the conservativeness of the feasible region predicted by the surrogate model. Finally, $Total\ Error$ measures the percentage of points that are misclassified. Based on these metrics, a surrogate classifier will approximate the feasible region if the $CorFeas$ and $CorInfeas$ are close to 100% and the $OvEst$ and $Total\ Error$ are close to 0% on unseen datasets.

3.2 Process Operations Integration

Process integration procedure is required to validate the effectiveness of the integrated model and compare the solution obtained with the Full Space (FS) method for a given facility. The FS method is formulated by incorporating all subproblems and considering all constraints. Such a model leads to a large scale and becomes intractable with increase in problem size. It should be noted that the data-driven feasibility obtained in section 3.1 is done for a single facility. Thus, for a multiple facilities, the operational feasibility must be done for each. Once the feasibility analysis is completed, a single facility problem is solved to validate the surrogate's efficacy. The procedure involves two steps, and these include:

- Formulate and solve the planning model using the surrogate model to represent the feasible space of the scheduling problem: the solution to the model gives the production target and the raw material requirement for a single facility.
- Using the production target and raw material requirement from the operational planning problem, the scheduling problem is solved by rolling horizon to meet the production target subject to the available raw material. The inputs to the rolling horizon are the states of products and raw material as well as the initial configuration of the equipment. This way, the right scheduling can be obtained. Finally, the cost is compared with the Full Space approach.

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1. [illegible]
2. [illegible]
3. [illegible]
4. [illegible]
5. [illegible]

[illegible]

1. [illegible]
2. [illegible]
3. [illegible]

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Constraints

The mathematical formulation follows the same framework in Dias and Ierapetritou (2019). These consists of four major constrains. Equations 13(a) – (c) ensure allocation of task, feasible sequence while considering sequence changeover. The mass balances are enforced by equation (13d) and equation (13e) determines that the production targets for product states should be achieved at the end of the scheduling horizon and that the difference between the material consumed and material available should be non-negative. Constraints (13f) ensure that the batches stay within restricted limits and (13g) keep the variables within their feasible domain.

Equipment Utilization

$$\sum_{i\in \boldsymbol{I}_j}\sum_{k'=k-\tau_{ij}+1}^{k} X_{ijk'} \leq 1 \quad \forall\, j \in \boldsymbol{J}, k \in \boldsymbol{K} \tag{13a}$$

$$X_{ijk} = 0 \qquad \forall j \in \boldsymbol{J}\,, i \in \boldsymbol{I}_j, k > SH - \tau_{ij} \tag{13b}$$

$$X_{ijk} + X_{i'jk'} \leq 1 \qquad \forall i, j' \neq 1, j, k, k - \tau_{i'j} - \sigma_{i'ij} < k' < k - \tau_{i'j} \tag{13c}$$

Inventory Balance

$$W_{sk} = W_{s,k-1} + \sum_{i\in \boldsymbol{I}_s^+}\sum_{j\in \boldsymbol{J}_i} \rho_{is} B_{i,j,k-\tau_{ij}} + \sum_{i\in \boldsymbol{I}_s^-}\sum_{j\in \boldsymbol{J}_i} \rho_{is} B_{ijk} \leq \sigma_s \qquad \forall s \in \boldsymbol{S}\,, k \in \boldsymbol{K} \tag{13d}$$

$$W_{sk} = P_{st} \qquad \forall s \in S_{fp}, k = SH$$

$$R_{st} - \sum_{k}\sum_{i\in \boldsymbol{I}_s^-}\sum_{j\in \boldsymbol{J}_i} \rho_{is} B_{ijk} \geq 0 \qquad \forall\, s \in S_r \tag{13e}$$

Batch Size Constraint:

$$X_{ijk}\beta_{ij}^{min} \leq B_{ijk} \leq X_{ijk}\beta_{ij}^{max} \qquad \forall j \in \boldsymbol{J}\,, i \in \boldsymbol{I}_j, k \in \boldsymbol{K} \tag{13f}$$

Domain restriction constraint:

$$X_{ijk} \in \{0,1\}; B_{ijk} \geq 0\,; W_{sk} \geq 0 \qquad \forall\, i\,, j\,, s, k \tag{13g}$$

Objective Function:

Although, solution to the scheduling problem determines the order in which tasks use the equipment and resources, different performance criteria lead to different solution. In this article, three performance measures are used as follows:

- Total Operating cost minimization: This determines the best allocation and sequence that minimizes the cost of operation.

$$\text{Min} \sum_{s}\sum_{k} W_{s,k} \times \pi_s \tag{13e}$$

- State maximization: To retrieve the production capacity information from a scheduling model, state maximization can be used. This is done by setting the objective as maximizing certain product state while the other product states are left as free non-negative variables (Li and

Ierapetritou, 2009b). Equation (1f) shows for a given product state; this is done for all product state to retrieve the capacity information.

$$\text{Max } W_{s=i,k=SH} \tag{13f}$$

- Feasibility Equation: This give a boundary between the production combinations that are feasible and infeasible. The objective determines if the scheduling is feasible for a given production target, raw material, initial equipment state, and scheduling horizon. A feasible schedule implies that there is no constraint violation. Hence, it helps to approximate the behavior of the scheduling model in entirety. As discussed in section 3.0, this allows capturing the behavior with a surrogate model.

Based on the scheduling formulation, three variables can be used to describe the possibility of the scheduling operation: production targets for different products (P_{st}) , available raw materials (R_{st}) and the initial configuration of the equipment which is determined by the last task it performed (X_{ijk}). Further this point, the scheduling model would be described as $SC(P_{st}, R_{st}, X_{ijk})$. Also, at the start of the scheduling problem, there are no tasks performed in the equipment a priori, thus X_{ijk} should be zero.

4.2 Planning Model Formulation:

This section covers the equations used at the planning level and describes a general planning problem for both tactical and process operations. While that tactical model considers multi-facility and network distribution optimization, the operational level is restricted to one facility.

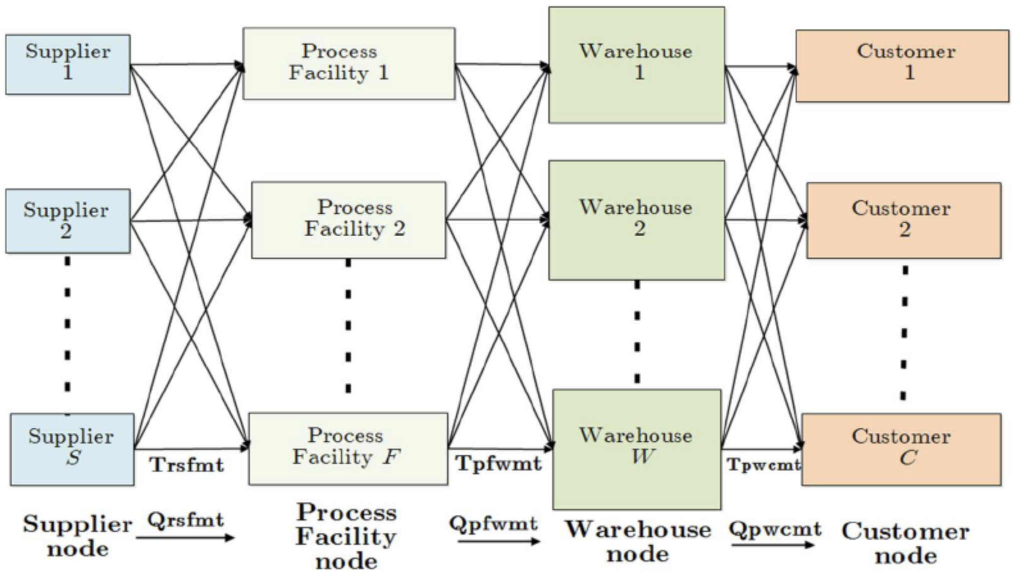


Figure 3: Generic Four-Tier Supply Chain Topology

The supply chain topology is a four-tier supply chain, as shown in Figure 3, consisting of $|\mathcal{S}|$ potential suppliers, $|\mathcal{F}|$ production facilities, $|\mathcal{W}|$ warehouses, and $|\mathcal{C}|$ customers. The network is considered to be connected by the flow of material through interconnected arcs. Each connecting arc embeds $|\mathcal{M}|$ transportation modes and transports commodity which could either be raw material r, or product p. Furthermore, the model abstraction consists of a time-expanded model, and the description follows next.

Objective Functions:

To make a decision that is both responsive and efficient, three objectives are simultaneously considered: economic objective, service level, and customer satisfaction.

- Economic Objective Function: This minimizes cost of the entire supply chain network, and it is given as:

$$\min \text{Cost}$$

$$\text{Cost} = \text{Cost of Raw Materials} + \text{Cost of Production} + \text{Cost of Inventory} + \text{Cost of Transportation} + \text{Cost of Backorders.}$$

$$\text{Cost of Raw Material} = \sum_{t\in T}\sum_{r\in \mathcal{R}}\sum_{s\in \mathcal{S}}\sum_{m\in \mathcal{M}}\sum_{f\in \mathcal{F}} C_r \times Q_{rsfmt}$$

$$\text{Cost of Production} = \sum_{t\in T}\sum_{p\in \mathcal{P}}\sum_{f\in \mathcal{F}}\sum_{m\in \mathcal{M}}\sum_{w\in \mathcal{W}} C_{pf} \times Q_{pfwmt}$$

$$\text{Cost of Inventory} = \sum_{t\in T}\sum_{w\in \mathcal{W}}\sum_{p\in \mathcal{P}} C_{\mathcal{I}} \times I_{pwt} \tag{14a}$$

$$\text{Cost of Transportation} = \sum_{t\in T}\sum_{r\in \mathcal{R}}\sum_{s\in \mathcal{S}}\sum_{m\in \mathcal{M}}\sum_{f\in \mathcal{F}} T_{rsfmt} \times Q_{rsfmt} + \sum_{t\in T}\sum_{p\in \mathcal{P}}\sum_{f\in \mathcal{F}}\sum_{m\in \mathcal{M}}\sum_{w} T_{pfwmt} \times Q_{pfwmt} + \sum_{t\in T}\sum_{p\in \mathcal{P}}\sum_{w\in \mathcal{W}}\sum_{m\in \mathcal{M}}\sum_{c\in \mathcal{C}} T_{pwcmt} \times Q_{pwcmt}$$

$$\text{Cost of Backorder} = \sum_{t\in T}\sum_{c\in \mathcal{C}}\sum_{p\in \mathcal{P}} C_{\mathcal{B}} \times \mathcal{B}_{cpt}$$

- Sales Target: defined as the fraction of customer demands met, maximizing this ensures that we operate at a level in which the amount of product produced is maximized, ensuring solutions robustness. The sales target is represented as:

$$SL = 1 - \frac{\sum_t \sum_p \sum_c B_{cpt}}{\sum_t \sum_p \sum_c \delta_{cpt}} \tag{14b}$$

- Delivery Time: This objective captures the delivery of customer products in due time. For this purpose, the delivery is defined by transportation reliability , a measure of time required to deliver the products. An expensive transportation mode is expected to have a high reliability/responsiveness. This in essence defines the supply chain's responsiveness.

$$CS = \sum_{t\in T}\sum_{f\in \mathcal{F}}\sum_{w\in \mathcal{W}}\sum_{m\in \mathcal{M}} RL_{fwm} \times Q_{pfwmt} + \sum_{t\in T}\sum_{w\in \mathcal{W}}\sum_{c\in \mathcal{C}}\sum_{m\in \mathcal{M}} RL_{wcm} \times Q_{pwcmt} \tag{14c}$$

Constraints:

These are set of equations that must be obeyed while optimizing the objectives.

- Mass Balances between nodes: The mass balances ensure continuity of flow, and must be considered between interconnected nodes, the governing mass balance equations for each nodes are discussed next:
    - Supplier- production facility mass balance: this captures the raw material transformation, and ensures that the amount of raw materials that is entering each facility must be at least equals the amount of products that leaves each facility

$$\sum_{r\in\mathcal{R}}\sum_{s\in\mathcal{S}}\sum_{m\in\mathcal{M}} Q_{rsfmt} - \sum_{p\in\mathcal{P}}\sum_{w\in\mathcal{W}}\sum_{m\in\mathcal{M}} Q_{pfwmt} \geq 0 \qquad \forall f, t \qquad \text{(14d)}$$

- Production facility- Warehouse balance: this is the Inventory balance at a given warehouse node. It ensures that the amount of available inventory satisfies the continuity equation, and it is kept below a given threshold

$$I_{pwt} = I_{p,w,t-1} + \sum_{f\in\mathcal{F}}\sum_{m\in\mathcal{M}} Q_{pfwmt} - \sum_{c\in\mathcal{C}}\sum_{m\in\mathcal{M}} Q_{pwcmt} \qquad \forall p, w, t \qquad \text{(14e)}$$

- Mass balance between the warehouse and customers, calculates the amount of unmet demands. This states that the difference between what is delivered and what is demanded is the backorder

$$\delta_{pct} - \sum_{w\in\mathcal{W}}\sum_{m\in\mathcal{M}} Q_{pwcmt} = \mathcal{B}_{cpt} \qquad \forall p, c, t \qquad \text{(14f)}$$

- Capacity Limitations for each node: this ensures that we cannot go above the capacity of each element of the supply chain. The capacity limitation is considered for supplier, production facility and the warehouses respectively as shown below:

$$\sum_{s\in\mathcal{S}}\sum_{f\in\mathcal{F}}\sum_{m\in\mathcal{M}} Q_{rsfmt} \leq \mathcal{C}_s \qquad \forall s, t \qquad \text{(14g)}$$

$$\sum_{w\in\mathcal{W}}\sum_{m\in\mathcal{M}} Q_{pfwmt} \leq \mathcal{C}_{p,f} \qquad \forall p, f, t \qquad \text{(14h)}$$

$$\sum_{p\in\mathcal{P}} I_{pwt} \leq \mathcal{C}_w \qquad \forall w, t \qquad \text{(14i)}$$

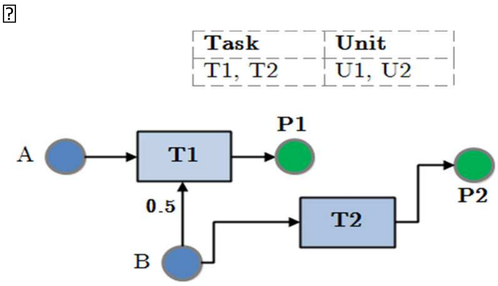
- Feasibility of production for each facility: production targets for each production facility must be feasible at the scheduling level. This is determined by two variables from the planning level: the amount of product itself, Q_{pfwmt} , and the available raw materials Q_{rsfmt}.
First the predictor vector is formed:

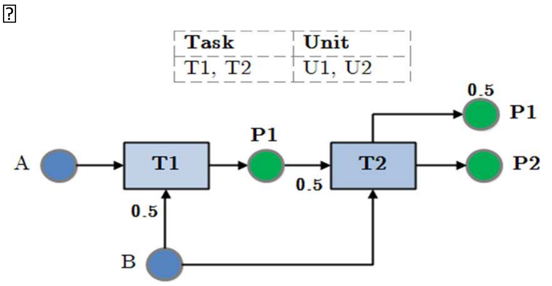
$$x_{feas} = \left[\sum_{s\in\mathcal{S}}\sum_{m\in\mathcal{M}} Q_{rsfmt}, \sum_{w\in\mathcal{W}}\sum_{m\in\mathcal{M}} Q_{pwcmt}\right] \qquad \forall f, t \qquad \text{(14j)}$$

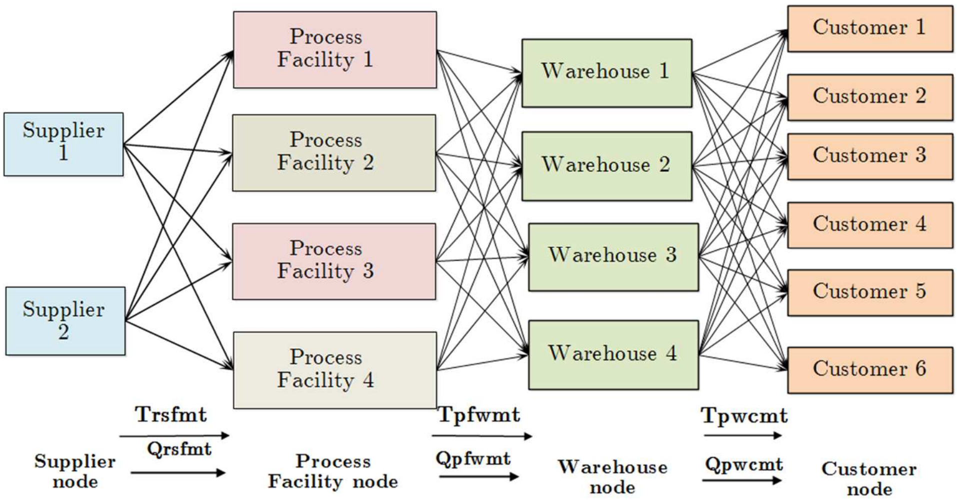
Then the vector is used to determine if the operation is feasible at the scheduling level:

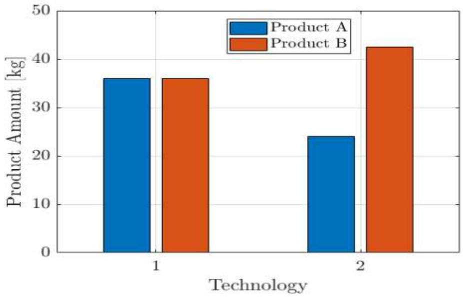
$$Feas(x_{feas}) \leq 0 \qquad \forall f, t \qquad \text{(14k)}$$

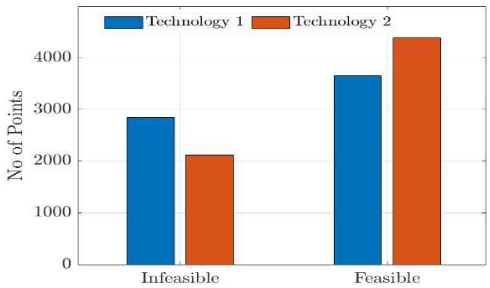
It should be noted that feasibility of production facility implies that the scheduling is possible for the product target and the raw material required. Consequently, while determining the feasibility of the production target, the raw material required to ensure feasibility is also determined during the process. Also, each facility's production state is the same as its production target because it is assumed that once products are produced, they are shipped to the warehouse.

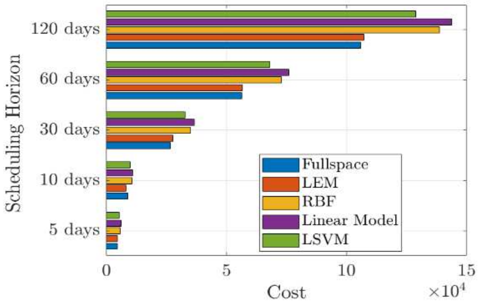

Task
Unit
T1, T2
U1, U2
A
T1
P1
0.5
T2
P2
B

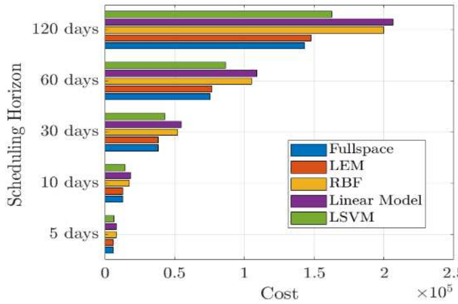

Task
Unit
T1, T2
U1, U2
0.5
P1
A
T1
P1
T2
P2
0.5
0.5
B

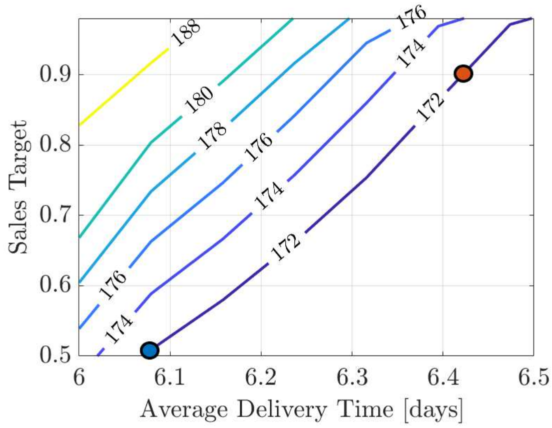

Supplier 1
Supplier 2
Process Facility 1
Process Facility 2
Process Facility 3
Process Facility 4
Warehouse 1
Warehouse 2
Warehouse 3
Warehouse 4
Customer 1
Customer 2
Customer 3
Customer 4
Customer 5
Customer 6
Trsfmt
Qrsfmt
Tpfwmt
Qpfwmt
Tpwcmt
Qpwcmt
Supplier node
Process Facility node
Warehouse node
Customer node


Product A
Product B
Product Amount [kg]
Technology
0
10
20
30
40
50
1
2

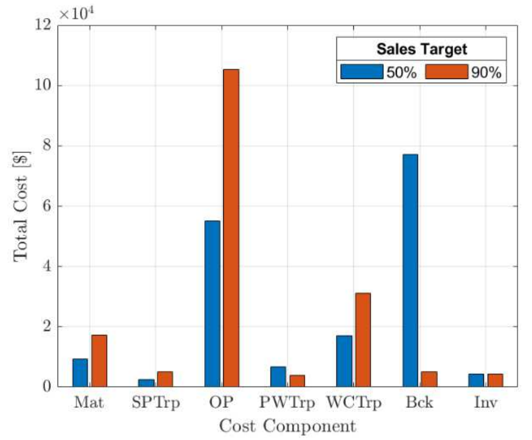

Technology 1
Technology 2
No of Points
0
1000
2000
3000
4000
Infeasible
Feasible


Scheduling Horizon
120 days
60 days
30 days
10 days
5 days
Cost
×10^4
0
5
10
15
Fullspace
LEM
RBF
Linear Model
LSVM

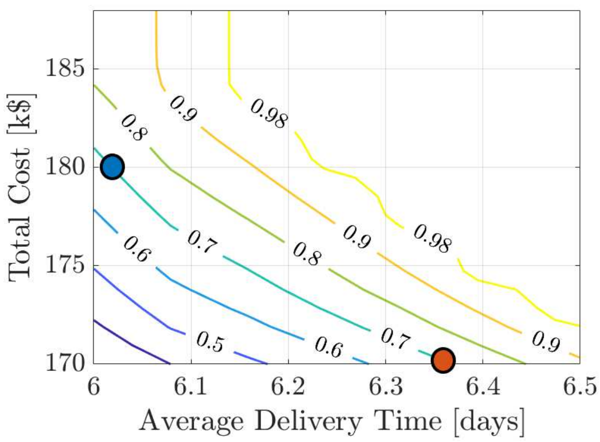

Scheduling Horizon
120 days
60 days
30 days
10 days
5 days
Cost
×10^5
0
0.5
1
1.5
2
2.5
Fullspace
LEM
RBF
Linear Model
LSVM



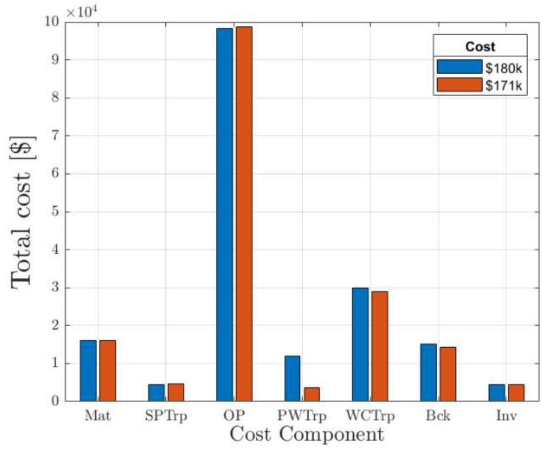
Sales Target
Average Delivery Time [days]
188
180
178
176
174
172



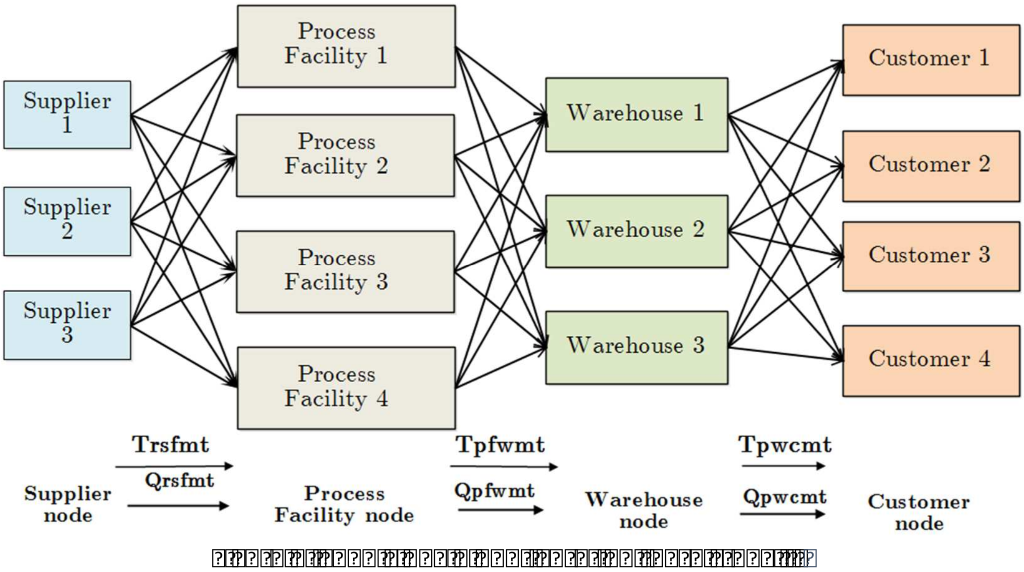
Sales Target
50%
90%
Total Cost [$]
$\times 10^4$
Mat
SPTrp
OP
PWTrp
WCTrp
Bck
Inv
Cost Component

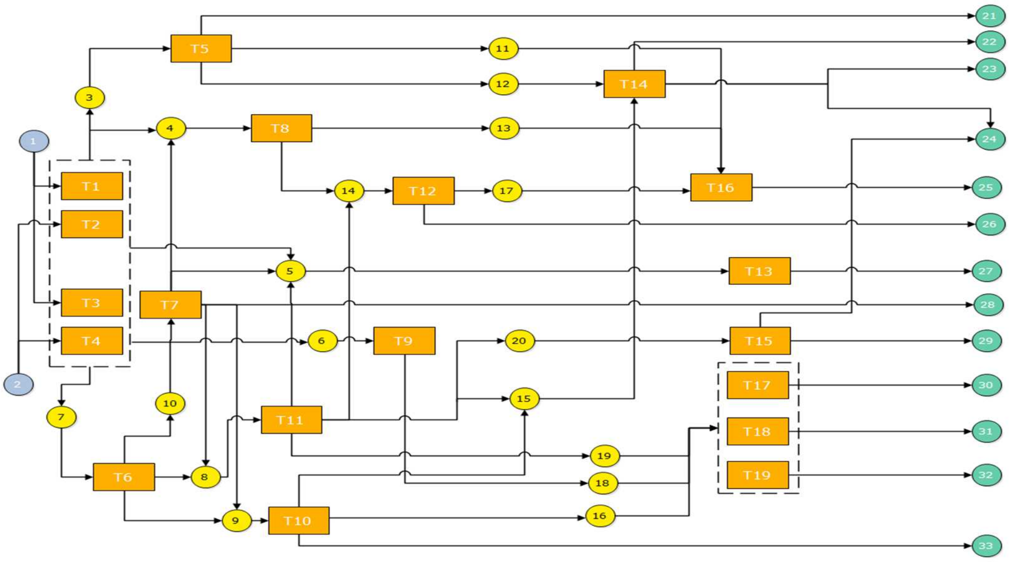


Total Cost [k$]
Average Delivery Time [days]
0.98
0.9
0.8
0.7
0.6
0.5



Cost
$180k
$171k
Total cost [$]
$\times 10^4$
Mat
SPTrp
OP
PWTrp
WCTrp
Bck
Inv
Cost Component


Process Facility 1
Process Facility 2
Process Facility 3
Process Facility 4
Supplier 1
Supplier 2
Supplier 3
Warehouse 1
Warehouse 2
Warehouse 3
Customer 1
Customer 2
Customer 3
Customer 4
Trsfmt
Qrsfmt
Supplier node
Process Facility node
Tpfwmt
Qpfwmt
Warehouse node
Tpwcmt
Qpwcmt
Customer node



T1
T2
T3
T4
T5
T6
T7
T8
T9
T10
T11
T12
T13
T14
T15
T16
T17
T18
T19
1
2
3
4
5
6
7
8
9
10
11
12
13
14
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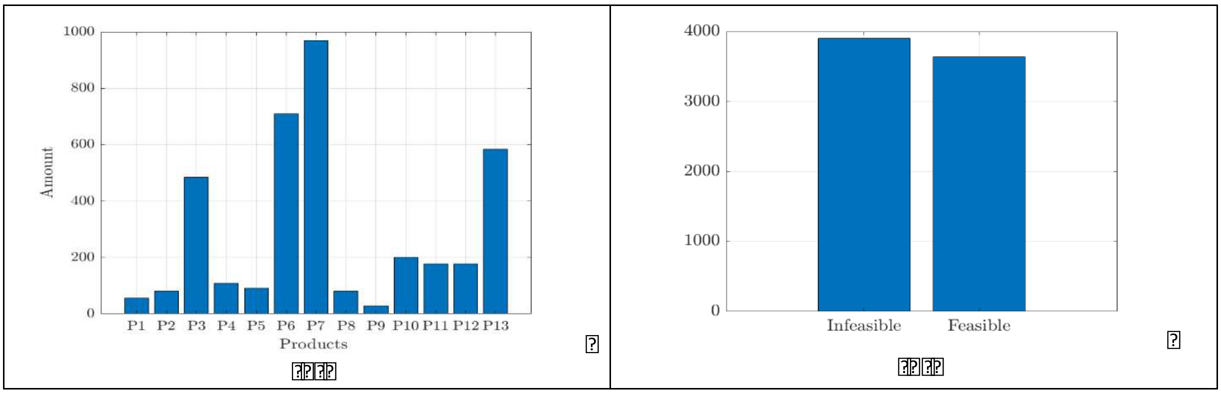
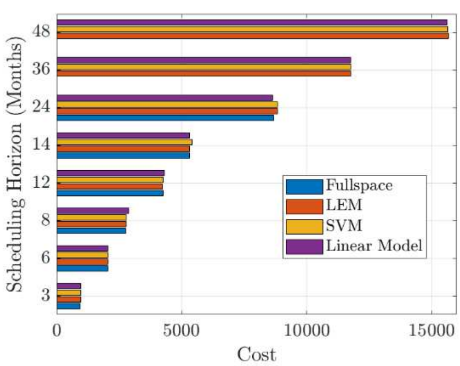
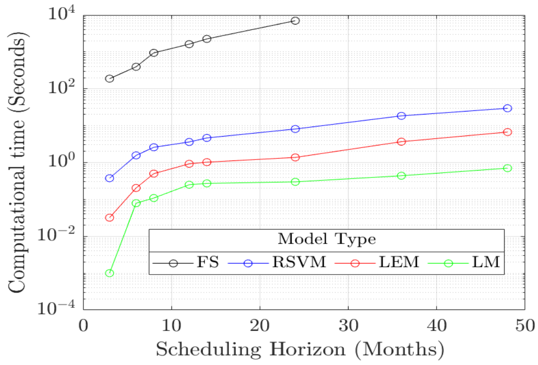
31
32
33

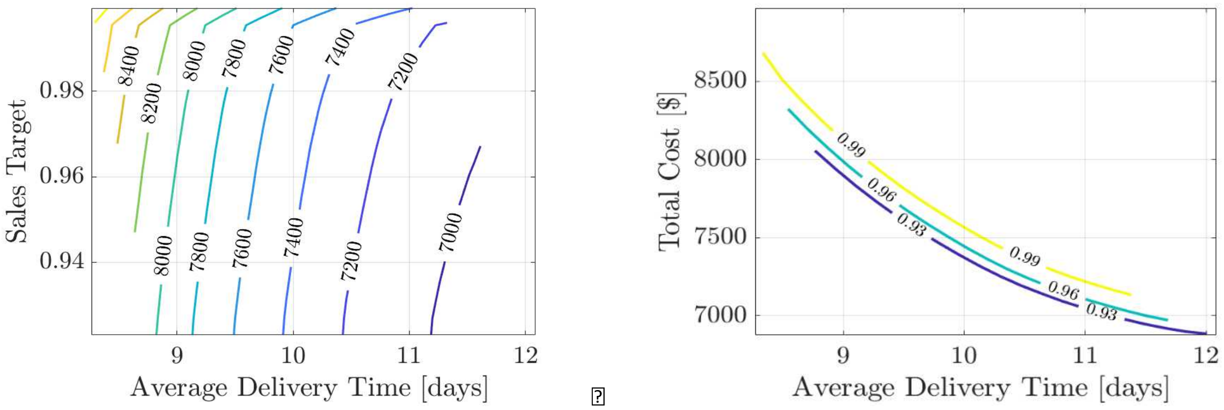

1000
800
600
400
200
0
Amount
P1 P2 P3 P4 P5 P6 P7 P8 P9 P10 P11 P12 P13
Products
4000
3000
2000
1000
0
Infeasible
Feasible



Scheduling Horizon (Months)
48
36
24
14
12
8
6
3
0
5000
10000
15000
Cost
Fullspace
LEM
SVM
Linear Model



Computational time (Seconds)
10^4
10^2
10^0
10^{-2}
10^{-4}
0
10
20
30
40
50
Scheduling Horizon (Months)
Model Type
FS
RSVM
LEM
LM



8400
8200
8000
7800
7600
7400
7200
7000
Sales Target
0.98
0.96
0.94
9
10
11
12
Average Delivery Time [days]
Total Cost [$]
8500
8000
7500
7000
0.99
0.96
0.93
Average Delivery Time [days]

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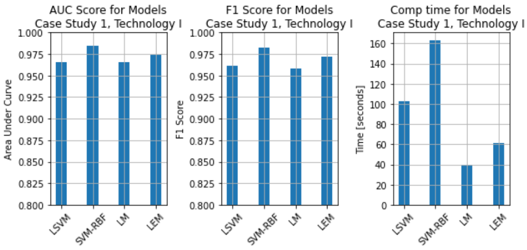
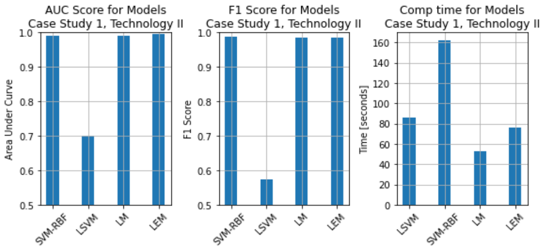
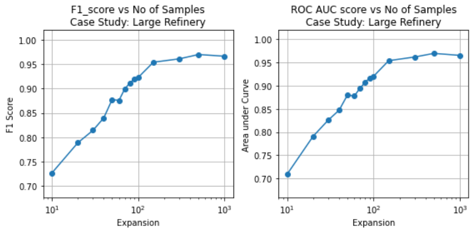
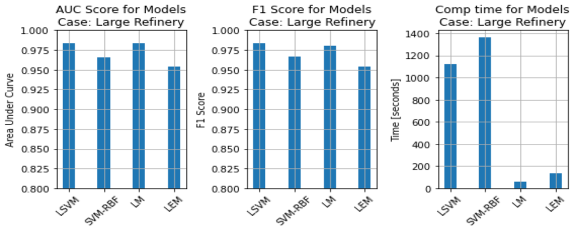

AUC Score for Models
Case Study 1, Technology I
Area Under Curve
F1 Score for Models
Case Study 1, Technology I
F1 Score
Comp time for Models
Case Study 1, Technology I
Time [seconds]
LSVM
SVM-RBF
LM
LEM


AUC Score for Models
Case Study 1, Technology II
Area Under Curve
F1 Score for Models
Case Study 1, Technology II
F1 Score
Comp time for Models
Case Study 1, Technology II
Time [seconds]
SVM-RBF
LSVM
LM
LEM


F1_score vs No of Samples
Case Study: Large Refinery
F1 Score
Expansion
ROC AUC score vs No of Samples
Case Study: Large Refinery
Area under Curve
Expansion


AUC Score for Models
Case: Large Refinery
Area Under Curve
F1 Score for Models
Case: Large Refinery
F1 Score
Comp time for Models
Case: Large Refinery
Time [seconds]
LSVM
SVM-RBF
LM
LEM

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