RESEARCH ARTICLE

Rolling horizon product quality estimation and online optimization for supply chain management of perishable inventory

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ABSTRACT
We introduce new methods inspired from dynamical systems and control theory for estimating the quality of perishable products in inventory in a supply chain based on measurable data. A state-space representation of the supply chain with perishable inventory is constructed from which controllability and observability properties are established to derive inventory management and quality estimation strategies with guaranteed performance. Rolling horizon state estimation is formulated to estimate the quality of inventory at locations where measurements are not available. Observability and controllability properties then allow us to formulate an online optimization framework inspired by model predictive control, that defines an implicit supply chain management policy. Numerical experiments demonstrate the performance of the proposed state estimation and online optimization approach, as well as its benefits for supply chain optimization ($\sim 40\%$ improvement in the cost objective relative to the baseline model).

KEYWORDS
Supply chain management ; Perishable products ; Quality estimation ; Rolling horizon estimation ; Rolling horizon control ; Observability

SDG 2: Zero hunger

1. Introduction

The effective handling of perishable goods is a pivotal challenge for businesses across various sectors. Perishable inventories, characterized by their limited shelf life and susceptibility to spoilage, require meticulous planning and strategic management to minimize losses and ensure optimal utilization. While the concept of perishable inventory management applies broadly, one of its most critical and ubiquitous applications lies within the realm of food products. Recent data reveal that about one-third of the food produced globally each year is lost or wasted, at a cost of nearly US $1 trillion (World Food Programme (WFP) 2024). Food loss pertains to a decline in the quality or quantity of food resulting from decisions made in the food supply chain, excluding retailers and consumers, whereas food waste refers to the losses caused by

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retailers, food service providers, and consumers (Food and Agriculture Organization of the United Nations (FAO) 2024). Europe, North America, and Oceania together lose or waste approximately 30% of fruits and vegetables produced (Food and Agriculture Organization of the United Nations (FAO) 2011). In the United States, food loss amounted to 133 billion pounds and $161 billion worth of food in 2010 (United States Food and Drug Administration 2023). Food Loss and Waste (FLW) arise from various inefficiencies, including overproduction, harvesting and transportation losses, inadequate storage conditions, contamination during processing, flawed allocation strategies, product spoilage due to negligence, and consumer-level waste (Zhu et al. 2023). FLW significantly strain already scarce natural resources, particularly freshwater, cropland, and fertilizers. Freshwater scarcity poses a major global challenge. Agriculture is the leading consumer of freshwater, highlighting the critical link between FLW and water management (Kummu et al. 2012). Substantial greenhouse gas (GHG) emissions are attributable to the food system (around 25 to 33% of the worldwide anthropogenic total)(Crippa et al. 2021). Employing effective supply chain management (SCM) strategies for such perishable products can enhance food security without incurring additional environmental burden, thus underlining its significance in global food systems.

A large fraction of these losses is directly related to the highly perishable nature of many food products. De Ketelaere et al. (2004); Jackman, Marangoni, and Stanley (1990); Lana, Tijskens, and Van Kooten (2006) have shown that such products can degrade significantly over time spans comparable to the time required for the product to transit through the supply chain, and that there is significant uncertainty in the degradation rates. This makes it imperative for supply chain management (SCM) strategies to account explicitly for the time evolution and degradation of product quality (often represented in terms of consumer-perceived attributes such as color and firmness). SCM must guide the optimal production, distribution and storage of inventory, as well as the optimal regulation of environmental conditions (such as temperature and humidity) during storage and shipment (Rong, Akkerman, and Grunow 2011).

Previous work (Sarimveis et al. 2008; Lejarza and Baldea 2020a,b, 2022; Lejarza, Kelley, and Baldea 2022) has shown that online optimization is a computationally efficient and robust approach for handling uncertainties in supply chain operations (i.e., random disturbances such as uncertain customer demand and random product spoilage), thereby reducing costs, energy consumption, and inventory waste. Online optimization relies on *feedback*, i.e., a mechanism for periodically and repeatedly updating supply chain decisions (e.g., orders and shipments) over a rolling time horizon once uncertainties are revealed/realized or new information (regarding orders, product inventories, spoilage, etc.) becomes available.

Implementing such feedback strategies requires comprehensive real-time information pertaining to the inventory and quality of the products in all echelons of the supply chain. However, measuring product quality often involves costly technology and skilled personnel and, in reality, measurements may only be available from a limited number of points in the supply chain. The purpose of this paper is to demonstrate that, under certain conditions, it is possible to accurately estimate the quality of perishable products at the remaining supply chain locations, and do so based on data that can be measured cost-effectively in practice.

The present work relies on translating concepts from dynamical systems and control theory to supply chain management of perishable inventories, and makes the following contributions:

(1) A representation of the perishables supply chain as a dynamical system. A linear state space model is used, and the model is defined such that the output variables are quantities that can be measured in practice.
(2) A novel rolling horizon[1] state estimation scheme that allows for reconstructing the values of inventory quality based on a limited set of measured outputs.
(3) A rolling horizon algorithm for online optimal SCM, focusing on production and distribution planning for supply chains of perishable products.
(4) Extensive numerical experiments are carried out, demonstrating improved supply chain transparency (in terms of the estimated product quality distribution) for echelons of the supply chain where product quality is not directly measured, as well as improved supply chain management performance for the resulting production and distribution decisions.

The paper is organized as follows: the relevant literature is surveyed in the next section. The production and distribution planning problem formulation is introduced in Section 3, followed by the corresponding state-space representation in Section 4. Our results on rolling horizon state estimation and SCM control are presented in Sections 5 and 6, respectively. Numerical experiments are described in Section 7, followed by conclusions in Section 8.

2. Literature review

2.1. *Control theoretic approaches to supply chain management*

Supply chains are dynamical systems (i.e., systems whose state, inputs and outputs change over time). Control theory provides a natural analysis framework for such systems (Ivanov et al. 2018), and control theoretic approaches have helped elucidate phenomena such as the bullwhip and ripple effects caused by, respectively, high-frequency and low-frequency disturbances (Udenio et al. 2017; Ouyang and Li 2010; Ivanov and Dolgui 2021; Llaguno, Mula, and Campuzano-Bolarin 2022; Brusset et al. 2023; Brusset, Jebali, and La Torre 2023).

Optimal control theory has found application in scheduling problems. Optimal control approaches are well suited to these problems owing to their ability to handle complex constraints, incorporate non-stationary job execution dynamics, and represent intricate relationships between process execution, capacity evolution, and physical system configuration (processing parameters, machine setups) (Subramanian, Rawlings, and Maravelias 2014; Dolgui et al. 2019). Optimal control has also been used to support the integration of manufacturing process design and operations (Ivanov, Dolgui, and Sokolov 2012).

Underpinning the use of control theoretic concepts for the analysis, design and operation of supply chains is a mathematical model that represents the supply chain dynamics. Based on the physical structure of supply chains, these models are structured in an input/state/output form. The states comprise the minimum number of differential variables required to represent the evolution of the system in time (inventories at each node are examples of state variables). Inputs include variables that can be altered by the operator (e.g., shipments and production rates), as well as exogenous disturbances, not all of which are known or measured. From a control perspective, the values of the output variables are a function of the states and inputs, and can be regarded as the information that is available regarding the operation of the system.

[1] In the control literature, the term “moving horizon” is also used.

The set of output variables could be the same as the set of state variables (i.e., all state variables can be measured), a subset of the state variables, or a linear or nonlinear function thereof. Control theory is built around standardized representations of the system dynamics, and the state-space representation that will be used here and discussed in depth in Section 4 has been widely used for modeling and analyzing linear systems.

At this juncture, it is important to point out that, in practice, it may not be possible to measure all the system state variables; on the other hand, knowledge of all the states is frequently needed for applying the control theoretical concepts outlined above. In this context, *state estimation* becomes essential.

Broadly speaking, *state estimation* is the process of determining the state (i.e., the values of time varying/differential variables) of a dynamical system by fusing information from (noisy) measurements of (a function of) a subset of the system states, and a mathematical model of the system. It aims to provide the best estimate of the system state variables by accounting for uncertainties in both the model and the measurements. The Kalman filter (KF) (Kalman 1960) and its variants, the extended Kalman filter (EKF) and the unscented Kalman filter (UKF) (Pei et al. 2019), are among the most widespread state estimation approaches. The Kalman filter is based on a linear state-space model, and it is assumed that both the system and measurement noise variables (i.e., the uncertainties or disturbances) are Gaussian. The EKF and UKF are extensions to the KF that allow for state estimation of nonlinear systems when certain assumptions are met. For many physical systems that are highly nonlinear and constrained (such as supply chains, where inventory levels and backorder values must be nonnegative and where there are storage and shipment capacity bounds), Kalman filtering may no longer be applicable. Rolling horizon estimation, also known as moving horizon estimation (MHE) (Rawlings and Mayne 2019), conversely, is a more flexible approach, that relaxes some of the core assumption of KF-based estimators (e.g., noise variables being normally distributed, the dynamics being approximately linear). The MHE algorithm involves using the (nonlinear) system model and solving an optimization problem over a finite time window of measurements to determine the values of the unmeasured system state variables that best fit the measured data.

In the context of supply chains with non-perishable inventory, state and parameter estimation have been applied to forecasting demand, as well as to estimating replenishment lead times (including production and shipment delays). Here, we recall the work of Aviv (2003), who modeled inventory systems with uncertain demand with linear state-space models, using a KF to compute minimum mean squared error forecasts of future demands for all the locations in the network. Hayya et al. (2006) proposed the use of simulation and estimation techniques based on smoothing and autoregressive models to compute the expected lead time demand (i.e., the sum of variable demands over a variable replenishment lead time). In the context of online optimization, Wang, Rivera, and Kempf (2005) and Wang and Rivera (2008) used a KF to perform state estimation under measured demand forecasting errors, and demonstrated superior performance of the integrated optimization and estimation approach for a semiconductor manufacturing case study. Villegas and Pedregal (2018) introduced a KF-based approach to circumvent the limitations and inaccuracies of aggregated forecasting, by reflecting demand hierarchy across geographical dimensions in a state-space model and thereby performing demand estimation with superior accuracy.

The same methods can be applied directly to estimate demand and lead times for supply chains of perishable products (Mor et al. 2019). However, to our knowledge, *estimating the quality of perishable products* has not yet been covered in the literature.

This is a key result of this work and will be covered in depth in Section 5.

2.2. *Supply chain management for perishable products*

The past decades have witnessed a paradigm shift towards an enhanced coordination between the echelons of the perishables supply chain, that yields significant economic advantages (Wilson 1996). A substantial body of research underscores the critical role of food supply chain management in optimizing efficiency (Bakker, Riezebos, and Teunter 2012). A key challenge lies in maintaining consistent product temperature throughout the supply chain, particularly during loading and unloading procedures outside of controlled environments (Bogataj, Bogataj, and Vodopivec 2005). Even brief deviations beyond the optimal temperature range can negatively impact product quality. Studies such as that of Newsome et al. (2014) have shown that current practices of open dating for tracking the expiration date of a perishable product may perform poorly. Products that are still viable may be discarded and, conversely, non-viable products may still be considered sellable, resulting in food safety hazards (Ketzenberg, Bloemhof, and Gaukler 2015; Ketzenberg, Gaukler, and Salin 2018). This occurs due to the fact that perishable goods inherently experience unpredictable and fluctuating conditions, including fluctuating time-temperature profiles, throughout their supply chain journey, which impact their viability.

There is thus a growing interest in improving cold chain traceability by predicting the quality of perishable products as they progress through the supply chain. Supply chain models for perishable products, such as those proposed by Rong, Akkerman, and Grunow (2011), Amorim, Günther, and Almada-Lobo (2012), and Lejarza and Baldea (2022) can account for inventories with heterogeneous quality and variable shelf-life (which depends on time as well as the chosen environmental conditions for each transportation route and facility). These models have then been leveraged to devise SCM strategies for perishable products considering different decision variables, applications, solution heuristics (see e.g., Soto-Silva et al. (2016); Sarimveis et al. (2008), and for strategies inspired by Model Predictive Control, Lejarza and Baldea (2020a,b, 2022); Lejarza, Kelley, and Baldea (2022)).

Most of the aforementioned models and SCM strategies are deterministic. Product quality degradation is represented as a (set of) chemical reaction(s) using kinetic expressions that account for the impact of temperature (and possibly other variables, such as humidity. The reader is referred to Van Boekel (2008) for a detailed review on kinetic modeling of food quality.) The parameters of these expressions (rate constant, activation energy) are assumed to be known with certainty. In practice, these parameters are in fact uncertain: fresh foods such as vegetables, meats and dairy products, which are of natural origin and exhibit inherent variability in initial quality and degradation rates. This *endogenous* uncertainty in the rate of degradation was recognized by, e.g., Ketzenberg, Gaukler, and Salin (2018), who derived order quantities and expiration dates for perishable inventory with random lifetime under periodic review. The results balance the outcomes of selling perished products (but before their expiration date) or discarding viable products (but past the expiration date). In a related work, Amorim, Alem, and Almada-Lobo (2013) introduced a risk-aware supply chain management framework under uncertain degradation rate considering well-defined degradation scenarios (low, medium and high) and solved the SCM problem using scenario-based stochastic optimization.

However, product quality degradation is also subject to *exogenous* uncertainties (i.e., outside disturbances). For example, product spoilage may be accelerated by improper temperature settings in storage facilities, or by events such as loading/unloading and transferring goods between facilities and trucks or shipping containers. Taking corrective action (e.g., adjusting storage temperatures) to deal with these disturbances requires up-to-date information on the state of the supply chain at every relevant echelon. Extensive recent work has been carried out on hardware and software solutions to monitor environmental conditions. Sensors (e.g., RFID tags (Grunow and Piramuthu 2013; Piramuthu, Farahani, and Grunow 2013)) are available to measure environmental factors like temperature, humidity, and pressure in real-time, and internet of things (IoT) technology (e.g., Tsang et al. (2018); Manavalan and Jayakrishna (2019)), facilitates the connection of such devices to the internet, enabling real-time data collection and transmission. As of yet, direct measurements of product quality remain difficult, with some attributes (e.g., firmness, moisture content) requiring destructive testing on individual items (e.g., a single fruit/vegetable), and others (e.g., color) often requiring that the product be removed from packaging. This is acceptable at, e.g., producer facilities or packing houses, where product is generally presented in bulk, but may not be feasible at, e.g., warehouses or ripening facilities.

As such, establishing model-based mechanisms for estimating product quality at all echelons of the supply chain on the basis of measured variables is of elevated interest. Control theory, and in particular state estimation, represent an ideal paradigm to this end. The focus of the present paper is thus to establish observability and controllability properties for supply chains of perishable products, and develop state estimation mechanisms for product quality as degradation driven by endogenous and exogenous factors occurs. As mentioned above, to the best of our knowledge, such mechanisms do not currently exist and their development - uniting supply chain modeling and estimation theory concepts - is the key contribution of this work. Table S5 in the Supporting Information provides a summary of the literature referenced in this section in comparison and contrast to the results presented in this paper, emphasizing the novelty of our contribution.

3. Production and distribution planning problem formulation

We consider a supply chain network consisting of a set of producers $\mathcal{P}$, a set of distribution centers or warehouses $\mathcal{D}$, and a set of retailers $\mathcal{R}$. The set of routes between facilities is known and denoted by $\mathcal{A}$ such that if $(i, j) \in \mathcal{A}$ a route between facility i and facility j exists. The sets $n(i)$ and $v(i)$ denote respectively the set of all successor and predecessor facilities to facility i. We consider production lead time denoted with τ_i^p for facility $i \in \mathcal{P}$, and shipment lead time denoted with $\tau_{i,j}$ for route $(i, j) \in \mathcal{A}$. All facilities can hold inventory in storage by incurring a holding cost, and it is assumed that producers have no predecessors and that retailers have no successors. We consider a discrete time model (typically using days as the time unit), and a planning or control horizon length N such that $t \in \{0, \ldots, N\}$.

3.1. *Product quality and degradation modeling*

The evolution of the quality of perishable products is assumed to be known and represented by a rate of change expression of the form:

$$\frac{dq(t)}{dt} = f(q(t), \kappa(t)) \tag{1}$$

where $q(t) \in \mathbb{R}$ is the time-varying quality attribute, $\kappa(t) \in \mathbb{R}$ is the time-varying (manipulated) environmental conditions, and $f(\cdot) : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ reflects the product quality dynamics.

Further, it is assumed that $f(q(t), \kappa(t)) \leq 0$, which implies that product quality is non-increasing in time. For example, it has been found that a model that follows a first-order Arrhenius-type reaction kinetics (i.e., $f(q(t), \kappa(t)) = -ae^{-bT}q(t)$, with $a, b \in \mathbb{R}^+$, can capture the degradation rate of many quality attributes of fresh produce such as avocados, tomatoes De Ketelaere et al. (2004), avocados Maftoonazad and Ramaswamy (2008), strawberries Hosseinifarahi et al. (2020), etc. More details on deriving these quality models and their parameters can be found in Newsome et al. (2014).

As quality typically decays in time such that $\lim_{t\to\infty} q(t) = q_\infty$ for some $q_\infty \in \mathbb{R}$, the minimum product quality requirement is defined as $q_{\min} \in \mathbb{R}$, such that $q_{\min} \geq q_\infty$, and if $q(t) < q_{\min}$, the product is considered spoiled and must be discarded at a cost. From a practical perspective, q_∞ reflects the quality at which the product is completely spoiled and potentially unsafe for consumption, while $q_{\min}$ is the lower quality bound for which the product is deemed "sellable" and has some remaining economic value. Products with quality lower than $q_{\min}$ cannot be used to fulfill demand. The value of these parameters is strictly dependent on the specific product and market considered.

The environmental conditions ($\kappa(t)$) available to control product quality are determined by the specific features of the supply chain equipment technology (e.g., temperature control or atmospheric composition control). These conditions have a direct impact on the rate of product quality degradation as per the dynamics in (1) (e.g., higher temperature accelerates the biochemical reactions responsible for changes in color, texture and firmness of food products (Newsome et al. 2014)). However, because of the discrete-time nature of production and distribution decision-making (e.g., decisions are made on a hourly, daily, weekly basis) the quality variables are re-scaled and discretized as in Lejarza and Baldea (2022): given a countable set of a total of S environmental condition settings such that $\kappa(t) \in \{\tilde{\kappa}_k | k = \{1, \ldots, S\}\}$, the model output is a set of discrete quality levels Q and discrete degradation values (or quality losses) corresponding to a single time period (e.g., one day) given by $\Delta q_k \ \forall q \in Q, k \in \{1, 2, \ldots, S-1, S\}$. The resulting discretization thus provides an approximation of the (nonlinear) model shown in (1) to an arbitrary accuracy. The reader is referred to Lejarza and Baldea (2022, Section 3) for an extensive theoretical and practical discussion on the implementation of the aforementioned discretization algorithms.

Remark 1. For the sake of simplicity this work considers a single time-varying product quality attribute (i.e., $q(t) \in \mathbb{R}$), an approach that has been largely adopted in the literature (Rong, Akkerman, and Grunow 2011). This attribute typically corresponds to the quality attribute with the fastest degradation rate (Lejarza and Baldea 2021b, Section 3). We also note that more recent work considered production and distribution planning for multi-attribute quality dynamics (i.e., $q(t) \in \mathbb{R}^m$ for $m > 1$)

(Lejarza and Baldea 2022). Further, more sophisticated models capture degradation rates that may be dependent on the quality level and expressed as $\Delta q_{q,k}$, e.g., for the case of first-order degradation dynamics. For notation simplicity we use Δq_k to denote degradation rates, and the reader is referred to Lejarza and Baldea (2022, Sections 3 & 4) for further details on higher-order product quality degradation dynamics.

Remark 2. Previous works discussed the use of environmental conditions (e.g., adaptive temperature control in Lejarza, Pistikopoulos, and Baldea (2021)) to reduce the rate of product degradation. In this contribution, to preserve the clarity of discussion and exposition, it is assumed that optimal values for these variables have been a priori established (e.g., by solving the nominal problem production planning problem without estimation as done previously in Lejarza and Baldea (2020a); Lejarza, Pistikopoulos, and Baldea (2021)), and they are not re-computed. Under this assumption, the degradation rate Δq is a normalized stochastic quantity, and its distribution is independent of environmental conditions (which holds true in some practical settings, e.g. for supply chains that do not have advanced, real-time temperature control and for which the temperature in refrigerated trucks is set at a specific value). An integrated framework for adapting environmental conditions based on the estimated values of quality is a subject of ongoing work. It is hypothesized that the economic advantages resulting from state estimation will be significant, as state estimates might, for example, suggest reducing temperature when high quality degradation occurs.

3.2. *Inventory and backorder balances*

The inventory and backorder balances form the core component of the dynamic model of supply chains. At the basic level, the inventory balance captures inventory inflows and outflows at a given facility.

$$I_{i,t+1} = I_{i,t} + \sum_{j \in \mathcal{U}_i^{\text{in}}} u_{j,i,t-\tau_{j,i}}^{\text{in}} + \sum_{j \in \mathcal{U}_i^{\text{out}}} u_{i,j,t}^{\text{out}} \tag{2}$$

where $I_{i,t}$ denotes the amount of inventory in storage at facility i at time period t. The variables u^{in} and u^{out} denote respectively inflow and outflow of inventory, $t - \tau_{j,i}$ corresponds to the time of arrival of the inventory inflow with some time delay $\tau_{j,i}$. The sets $\mathcal{U}_i^{\text{in}}$ and $\mathcal{U}_i^{\text{out}}$ respectively denote the available sources and sinks of inventory (e.g., shipments from upstream and to downstream facilities). While the form of equation (2) is valid for all facility types (manufacturers, distribution centers, and retailers), it should be noted that each facility might have different kinds of inventory inflows and outflows.

The inventory balance in (2) assumes that the inventory is of a single quality level, which does not change over time. This can be augmented to reflect the presence of inventory of different quality levels and quality degradation over time as follows (Rong, Akkerman, and Grunow 2011; Lejarza and Baldea 2020a, 2022; Lejarza, Pistikopoulos, and Baldea 2021):

$$I_{i,q,t+1} = I_{i,q+\Delta q,t} + \sum_{j \in \mathcal{U}_i^{\text{in}}} u_{j,i,q+\Delta q_{j,i},t-\tau_{j,i}}^{\text{in}} + \sum_{j \in \mathcal{U}_i^{\text{out}}} u_{i,j,q,t}^{\text{out}} \tag{3}$$

where $I_{i,q,t}$ now denotes the amount of inventory in storage at facility i, of quality q, at time period t. The parameter Δq reflects the number of discrete product quality units that are lost due to degradation for a single time period. $\Delta q_{j,i}$ denotes the (discrete) number of quality levels lost during the $\tau_{j,i}$ time delay (e.g., when shipping inventory).

The inventory balance in (4) accounts for product quality dynamics so that inventory at time $t+1$ is of lower quality q and comprised of different sources: (1) inventory that was in storage at the previous time period and was of higher quality $q + \Delta q > q$, and (2) inventory that arrived from upstream facilities which was initially shipped at higher quality $q + \Delta q_{j,i} > q$. The reader is referred to Rong, Akkerman, and Grunow (2011, Section 3) and Lejarza and Baldea (2020a, Section 4) for further details on the derivation of the inventory balance equations.

The model in (3) assumes a deterministic quality degradation process of known rate (as described in Section 3.1). In practice, these degradation rates are in fact not deterministic and are subject to some level of uncertainty due, among others, to inherent variations in the evolution of natural products, as well as to unforeseen and unmeasured changes in environmental factors (e.g., temperature, concentrations of gases such as ethylene that promote ripening) that impact the degradation rate. To our knowledge, this uncertainty has not been considered in the literature on SCM of perishables, where most reports discuss uncertainty with respect to customer demand at the retail facilities.

We propose to describe this uncertainty in degradation rates as random but bounded disturbances in the stored inventory at different quality levels. To this end, we augment the model in (3) as follows:

$$I_{i,q,t+1} = I_{i,q+\Delta q,t} + \sum_{j \in \mathcal{U}_i^{\text{in}}} u^{\text{in}}_{j,i,q+\Delta q_{j,i},t-\tau_{j,i}} + \sum_{j \in \mathcal{U}_i^{\text{out}}} u^{\text{out}}_{i,j,q,t} + \epsilon^i_{q,q-1,t} + \epsilon^i_{q,q+1,t} \tag{4}$$

Here, $\epsilon^i_{q,\bar{q},t}$ for $\bar{q} \in \{q-1, q+1\}$ are discrete random variables with arbitrary probability mass functions, that reflect the aforementioned disturbances. Conceptually, including these variables provides a correction to the predictions of the deterministic model: a portion of the inventory $I_{i,q,t}$ of product of quality q (as predicted by the deterministic model), may in fact be of higher quality $q+1$ or of lower quality, $q-1$. We assume for simplicity that actual inventory is either a single quality level better (or worse) than predicted by the deterministic model, but the idea can be readily expanded to assume that broader variations in quality level are possible.

The conservation of inventory must still be satisfied, and we assume that the randomness in degradation rates does not impact the *total* inventory at node i. Thus, the variables ϵ must satisfy the inventory conservation property:

$$\sum_{\{q \neq \bar{q}\} \in Q} \epsilon^i_{q,\bar{q},t} = 0 \tag{5}$$

where $\mathcal{Q}$ is the discrete set of all quality levels such that $\mathcal{Q} = \{1, \ldots, q_{\max}\}$ for some positive integer $q_{\max}$. In turn, this requires that the following properties hold:

$$\begin{aligned} &\epsilon^i_{q,q-1,t} = -\epsilon^i_{q-1,q,t}, \quad \epsilon^i_{q,q+1,t} = -\epsilon^i_{q+1,q,t} \\ &\epsilon^i_{q,q-1,t} \in [-I_{i,q,t}, I_{i,q-1,t}], \quad \epsilon^i_{q,q+1,t} \in [-(I_{i,q,t} + \epsilon^i_{q,q-1,t}), I_{i,q+1,t}] \end{aligned} \tag{6}$$

Based on these definitions and under the assumptions stated above, the presence of uncertainty in the degradation rate does not cause a *net* change in the total inventory in storage at any node in the supply chain at a given time. However, the disturbance may cause inventory to drop to the a lower quality than $q_{i,\min}$ for a given facility, thus resulting in waste being generated.

Remark 3. From a mass conservation perspective of inventory of quality q at node i, readers may view the model in (4) as representing a transfer of inventory of quality q to a lower quality level $q-1$ or to a higher quality level $q+1$. The transfer of inventory to a higher quality level as introduced above does not imply that the quality of the product improves over time. Rather, it simply means that the degradation rate is lower than the nominal value.

With the above, the inventory balances at producer facilities can be written as:

$$I_{i,q,t+1} = I_{i,q+\Delta q,t} - \sum_{j \in \mathcal{J}(i)} s_{i,j,q,t} + p_{i,q,t-\tau_i^p} + \varepsilon_{q,t}^i \tag{7}$$

for all $i \in \mathcal{P}, q \in \{Q \mid q_{i,\min} \leq q \leq q_{\max}\}, t \in \{0, \dots, N\}$, where $\mathcal{J}(i) \in \{j \in n(i) \mid q \geq q_{i,\min} + \Delta q_{i,j}\}$, and for compact notation we represent the disturbance in (6) as follows:

$$\varepsilon_{q,t}^i = \epsilon_{q,q-1,t}^i + \epsilon_{q,q+1,t}^i \tag{8}$$

which is by definition also a discrete random variable. The decision variables $s_{i,j,q,t}$ correspond to the amount of inventory shipped through route $(i,j) \in \mathcal{A}$, of quality $q \in \mathcal{Q}$, at time period t, and decision variables $p_{i,q,t}$ correspond to the amount of inventory produced at facility $i \in \mathcal{P}$, of quality $q \in \mathcal{Q}$, at time period t. In practice, manufacturers might not have (complete) control of production quality, but rather the quality produced can be modeled as a random variable. From a modeling perspective, this can be accomplished by sampling one or several quality levels $\tilde{Q} \subseteq Q$ from a certain distribution, and setting $p_{i,q,t} = 0 \ \forall \ q \in \tilde{Q}$. This will be discussed in more detail when describing the numerical experiments in Section 6.

For distribution centers, the inventory balances are:

$$I_{i,q,t+1} = I_{i,q+\Delta q,t} - \sum_{j \in \mathcal{J}(i)} s_{i,j,q,t} + \sum_{j \in v(i)} s_{j,i,q+\Delta q_{j,i},t-\tau_{j,i}} + \varepsilon_{q,t}^i \tag{9}$$

for all $i \in \mathcal{D}, q \in \{Q \mid q_{i,\min} \leq q \leq q_{\max}\}, t \in \{0, \dots, N\}$, where $\mathcal{J}(i) \in \{j \in n(i) \mid q \geq \mathcal{Q}_{i,j,k}\}$. Similarly, the inventory balances for the retailers are:

$$I_{i,q,t+1} = I_{i,q+\Delta q,t} + \sum_{j \in v(i)} s_{j,i,q+\Delta q_{j,i},t-\tau_{j,i}} - r_{i,q,t} + \varepsilon_{q,t}^i \tag{10}$$

for all $i \in \mathcal{R}, q \in \{Q \mid q_{i,\min} \leq q \leq q_{\max}\}, t \in \{0, \dots, N\}$.

Lastly, we also account for backorder dynamics which reflect accumulation of unmet demand:

$$BO_{i,t+1} = BO_{i,t} - \sum_{q \in Q} r_{i,q,t} + d_{i,t} \tag{11}$$

for all $i \in \mathcal{R}, t \in \{0, \dots, N\}$, where $BO_{i,t}$ denotes backorder at retailer $i \in \mathcal{R}$, and

$d_{i,t}$ is a random variable corresponding to the customer demand. We recognize that while backlogging demand for some perishable products might be possible (e.g., for pharmaceuticals), it might not be realistic in the context of food products at the retail level. In the latter case, we note that accounting for backorder corresponds to a more general case than when unmet demand is transferred to e.g. missed sales. In the case of the latter, missed sales ($MS_{i,t}$) can be expressed without any dynamics as follows:

$$MS_{i,t} = d_{i,t} - \sum_{q \in Q} r_{i,q,t} \tag{12}$$

where the variable $MS_{i,t}$ simply serves for tracking the cost of unfulfilled demand but has no explicit dynamics.

3.3. *Cost function and additional system constraints*

The production and distribution planning problem consists of minimizing the operating costs of the supply chain, for which we consider a cost function very similar to the one introduced in Lejarza and Baldea (2022). In brief, the objective is a linear function of the decision variables and reflects variable costs per unit associated with production, shipment, inventory holding, backorder, and inventory disposal once spoiled. We additionally consider a fixed cost associated with shipment to reflect the discrete expense incurred for shipping any amount of inventory from one facility to another (e.g., personnel wages and equipment expenses). To highlight the advantages of having more accurate information about the distribution of product quality (obtained by implementing state estimation), we consider an addition to the operating costs to reflect the quality preferences at the retailers. That is, in addition to the minimum quality requirements, the following cost component is included in the objective function:

$$\sum_{i \in \mathcal{R}} \sum_{q \in Q} \rho_{i,q} r_{i,q,t} \tag{13}$$

where $\rho_{i,q} < 0$ captures the value of quality at retailer facilities. The determination of these cost parameters can involve various factors, such as assessing the additional profit margins from selling fresher produce, which can be priced higher at the retail level. However, these parameters are often influenced by market elasticity, encompassing considerations of price, quality, and demand (Giri and Masanta 2020), an aspect of inventory management that is beyond the scope of the present study. These cost considerations, as accounted for in (13), play a significant role in supplier selection at the retail level. Retailers may opt to pay a premium for products from suppliers offering higher quality or shorter lead times, thereby enhancing the quality of their inventory. Conversely, retailers less concerned with product quality, as reflected in (13), may choose to source inventory from less expensive suppliers located further away, reducing operating costs without compromising revenue derived from sales.

The system constraints are based on a previous model (Lejarza and Baldea 2022; Lejarza, Pistikopoulos, and Baldea 2021), and include: (1) inventory that falls below $q_{i,\min}$ is accounted for as waste $\Omega_{i,t}$, (2) the amount of sales must not exceed the observed demand plus back order, and available inventory must be greater than outbound shipments and sales, and (3) capacity constraints are in place for daily production amounts, shipments for each route, and inventory in storage. A detailed description of the model and the corresponding equations are provided in the Supporting Information.

4. State-space representation of system dynamics

The structure of the proposed state-space model is introduced using a prototype supply chain comprising three nodes: a producer (P_1), a distribution center (D_1) and a retailer (R_1), as shown in Figure C1. A discrete representation of time is used as in Lejarza and Baldea (2022); Lejarza, Pistikopoulos, and Baldea (2021). For simplicity the degradation rate is normalized to be equal to one at the given temperature, i.e., the product degrades from one quality level (grade) to the next lower grade in one time interval/sample time. Note that this normalization is a linear transformation of the quality variables and does not affect the model's generalization to other perishable supply chain instances. The inverse transformation can easily be applied to recover the original, non-normalized values (more details are available in Lejarza and Baldea (2022)). Also for simplicity and illustration purposes, a perishable product with three possible quality levels (q_1, q_2, q_3, with q_3 being the highest quality and q_1 the lowest quality) is considered. The supply chain structure and variable definitions are illustrated in Figure C1.

Definition 4.1. The **state** of the system, denoted by $\boldsymbol{x}$, is defined as the level of product inventory for each quality level at each facility. The state vector at sampling time t is defined as:

$$\boldsymbol{x} = \left[I_{P_1,q_1} \ \dots \ I_{P_1,q_3} \ I_{D_1,q_1} \ \dots \ I_{D_1,q_3} \ I_{R_1,q_1} \ \dots \ I_{R_1,q_3} \ BO_{R_1} \right]^T \tag{14}$$

The successor state at the next sampling time $t+1$ is then defined as:

$$\boldsymbol{x}^+ = \left[I_{P_1,q_1-\Delta q} \ \dots \ I_{P_1,q_3-\Delta q} \ I_{D_1,q_1-\Delta q} \ \dots \ I_{D_1,q_3-\Delta q} \ I_{R_1,q_1-\Delta q} \ \dots \ I_{R_1,q_3-\Delta q} \ BO_{R_1} \right]^T \tag{15}$$

Clearly, the successor state $\boldsymbol{x}^+$ can be expressed as an affine function of $\boldsymbol{x}$ for some $\Delta q \in \mathbb{R}$. Further, it should be noted that the dimension of the state space scales linearly with the number of quality levels chosen in the discretization, which ultimately affects the complexity (in terms of number of variables) of the optimization problem. This presents an inherent trade-off between the fidelity of the model (i.e., the accuracy of the approximation of product quality dynamics) versus the computational effort required to solve the optimization problem. Guidance regarding how to determine the minimum number of quality levels can be found in Lejarza and Baldea (2021b), and a more in depth discussion on how the production and distribution planning problem scales with respect to the supply chain network parameters (including the product quality discretization) can be found in Lejarza and Baldea (2020a).

Definition 4.2. The vector of **system inputs**, denoted by $\boldsymbol{u}$, is defined as:

$$\boldsymbol{u} = \left[p_{P_1,q_1} \cdots \ p_{P_1,q_3} \ s_{P_1,D_1,q_1} \cdots s_{P_1,D_1,q_3} \ s_{D_1,R_1,q_1} \ \cdots \ s_{D_1,R_1,q_3} \ r_{R_1,q_1} \ \cdots \ r_{R_1,q_3} \right]^T \tag{16}$$

The system inputs (which become decision variables in SCM optimization problems) defined at each sample time correspond to the production amounts for each product quality level, shipment amounts for each possible route and each possible quality level, and the retail sales at each quality level.

Definition 4.3. We also define the **system disturbances** $\boldsymbol{w}$ as the uncertainties in product quality and customer demand at the retail facilities, both of which are additive with respect to the state variables, as was introduced with the inventory and backorder balances previously in (4) and (11), respectively.

Based on these definitions of the state, the successor state, the input, and the disturbance vectors, the supply chain network dynamics with product quality degradation can be represented in a linear state-space form,

$$\boldsymbol{x}^{+} = A\boldsymbol{x} + B\boldsymbol{u} + \boldsymbol{w} \tag{17}$$

The structure of this model is illustrated graphically in Figure C2 for the example introduced earlier in Figure C1. While the supply chain dynamics can be represented with the above linear model, it should be noted that the embedded discretized quality degradation model captures the nonlinear relationship of the continuous dynamics in (1). Furthermore, constraints discussed previously (i.e., the inventory balance of the general form in equation (4), and additional constraints introduced in Section 3.3) can be represented in compact notation as:

$$(\boldsymbol{x},\boldsymbol{u}) \in \mathbb{Z} \subseteq \mathbb{X} \times \mathbb{U} \tag{18}$$

where the set $\mathbb{Z}$ denotes coupled state and input constraints, and $\mathbb{X}$, $\mathbb{U}$ denote independent constraints imposed respectively on the states and inputs, which define a set of linear inequalities reflecting e.g., production, shipment and inventory holding capacity. In the illustrative example shown in Figure (C2), the input vector indicates a degradation of $\Delta q = 1$ quality levels during shipment e.g., a shipment from P_1 to D_1 at quality level q_3 (i.e., s_{P_1,D_1,q_3}) is accounted for as inventory in D_1 at quality level q_2 (i.e., I_{D_1,q_2}). Matrix B can be easily modified to reflect greater degradation rates, and the state and input vectors can be easily redefined to account for greater production or shipment lead times (e.g., as shown in Subramanian, Rawlings, and Maravelias (2014)). For this example, the inherent assumption is that the lead time between facilities corresponds to the same amount of time (typically one day depending on the time discretization of choice) over which a loss of Δq quality levels occurs. That is, following the definition of the inventory balances in (4), for this example we have that $\Delta q = \Delta q_{j,i} \forall (i,j) \in \mathcal{A}$. We note that this representation is relaxed for the numerical experiments included in Section 7 which consider different lead times.

4.1. *Measurements and output model*

One of the main contributions of this work is establishing a means for reconstructing state variables (i.e., inventory quality) from available measurements.

Definition 4.4. The vector of **outputs**, denoted by $\boldsymbol{y}$, is defined as the set of variables corresponding to measured quantities of the system at every sampling time.

Assumption 4.5 (State measurements)**.** *We assume that the following three measurements of the states are available through the supply chain over time:*

(1) The total amount of inventory at each facility is measured. That is, for all facilities $i \in \mathcal{N}$ and all time periods t, $\sum_q I_{i,q,t}$ is measured.
(2) The quality distribution of inventory is only measured at manufacturing facilities. That is, $I_{i,q,t}$ is measured for all producers $i \in \mathcal{P}$ and time period t, for all quality levels $q \in \mathcal{Q}$. This assumption is justified by the fact that some initial sorting occurs at manufacturing facilities after e.g., harvesting produce products and before shipping to downstream nodes.
(3) Backorder is measured to illustrate the advantages of state estimation for predicting inventory quality. However, in practice we might only observe sales and any unmet demand (i.e., for lack of inventory or because of products being of inferior quality) is accounted for as missed sales that might not be measured or quantified.

This set of measurements of the outputs $\mathbf{y}$ *is denoted by* $\hat{\mathbf{y}}$.

Based on these definitions, the output variables can be expressed as a function of the states by a linear model of the form $\mathbf{y} = C\mathbf{x} + \mathbf{v}$, which also reflects the possibility that noise $\mathbf{v}$ may arise from the measurement procedure (e.g., sensor noise).

Assumption 4.6 (Input measurements)**.** *The estimation problem is posed with* ***partial*** *information regarding the decision variables. Specifically, it is assumes that two additional quantities are measured corresponding to the system inputs:*

(4) The total amount of inventory shipped across each route is measured. That is, for all routes $i, j \in \mathcal{A}$ and all time periods t, $\sum_q s_{i,j,q,t}$ is measured, but inventory at individual quality levels is not measured.
(5) The quality distribution of inventory sold at retail facilities is measured. That is for retailers $i \in \mathcal{R}$ and time periods t, for all quality levels $q \in \mathcal{Q}$, $r_{i,q,t}$ is measured. This assumption is justified by the fact that some final sorting occurs at retailers (e.g., supermarkets) when they display their inventory for customers to purchase.

This set of measured input values is denoted by $\hat{\mathbf{u}}$.

Remark 4. It is reasonable to assume that the product quality distribution of shipments made is not measured/measurable. As mentioned earlier, products may be shipped in packaged form, which makes it practically impossible to efficiently apply quality sampling/measurement techniques for every inventory item.

Remark 5. There are other potential challenges related to measurements, including the presence of biases and measurement delays. Here we assume that measurements are unbiased (albeit noisy) and available without time delays. Further work is required to address these additional challenges.

4.2. *Controllability and observability properties of the supply chain network model*

Before introducing the proposed estimation strategy, it is important to understand how the structural properties of the supply chain (as reflected by the proposed state-space model) respectively affect controllability and observability.

4.2.1. Controllability

A linear state space system of the form (17), defined by the pair of matrices (A, B) is guaranteed be controllable (that is, if for any pair of states $\mathbf{x}_1, \mathbf{x}_2$ in the state-space, $\mathbf{x}_2$ can be reached from $\mathbf{x}_1$ in a finite amount of time) if and only if rank$(\mathcal{C}) = n_x$, where $\mathbf{x}_1, \mathbf{x}_2 \in \mathbb{R}^{n_x}$ and $\mathcal{C}$ is the controllability matrix is given by:

$$\mathcal{C} = \begin{bmatrix} B & AB & \dots & A^{n_x-1}B \end{bmatrix} \tag{19}$$

A useful result for checking controllability of linear systems is provided by the following:

Lemma 4.7 (Hautus lemma for controllability (Hautus 1972))**.** *A system is controllable if and only if*

$$\text{rank}\begin{bmatrix} \lambda I - A & B \end{bmatrix} = n_x \quad \forall \lambda \in \mathbb{C} \tag{20}$$

where $\mathbb{C}$ is the set of complex numbers.

On this basis, we make the following claim:

Claim 1. *The state-space representation of the supply chain dynamics is a controllable system if each facility in the network has available: (1) at least one unique control input corresponding to inventory inflow for all product quality levels, and (2) at least one unique control input corresponding to inventory outflow for all product quality levels.*

Proof. The proof is provided in Appendix A. □

Remark 6. Because of the monotonic nature of product quality degradation, facilities located downstream in the supply chain network (e.g., retailers) are less likely to possess control inputs associated with inflow of high-quality inventory. This is an inherent property of supply chains with product quality degradation and can be seen in the illustration in Figure C2, where facility P_1 has access to inventory of quality q_3, q_2, q_1, facility D_1 only has access to inventory of quality q_2, q_1, and facility R_1 only has access to inventory of quality q_1. Therefore, high quality inventory states are inherently uncontrollable and unreachable downstream the supply chain network. Equivalently, there is an inherent upper bound on the quality of the inventory that may be available at retail facilities, which is naturally lower than the highest quality grade available from a producer. In general, the upper bound of the inventory quality that can reach downstream facilities is determined by the maximum quality available at producers minus the degradation that occurs over the minimum total lead time to reach retailers.

Since some of the supply chain states might be uncontrollable as per Remark 6, it is important to understand the behaviour of these uncontrollable states. In this context, a system is said to be stabilizable if all uncontrollable states are stable, which means that when a state is subject to some perturbation it returns to its associated equilibrium point, or in the bounded-input, bounded-output (BIBO) sense, a bounded perturbation results in a bounded response of the state (or any outputs computed based on it). We adapt previous results (Lejarza and Baldea 2020b) to demonstrate the stability of the supply chain system.

Claim 2. *The supply chain network with product quality degradation is a stabilizable dynamical system.*

Proof. The proof is provided in Appendix B. □

Remark 7. While the supply chain is a stabilizable and partially controllable dynamical system, the presence of system constraints of the form of $\boldsymbol{x} \in \mathbb{X}$ and $\boldsymbol{u} \in \mathbb{U}$ weakens the above controllability result, meaning that not all states might be reachable from a given initial state when e.g., there are constraints on the control inputs (such as production, shipment or storage capacity bounds). Therefore, for decreasing supply chain capacities, high inventory states become unreachable. Reachability in this sense can be established by (theoretically or computationally) proving the feasibility of the optimal control formulation of the SCM strategy, which will be introduced in Section 6.

The sparsity pattern of the controllability matrix for the state-space model in Figure C2 is shown in Figure C10. For this simple prototype system, it is easy to verify (computationally and visually from Figure C10) that the controllability condition $\text{rank}(\mathcal{C}) = n_x$, for $n_x = 10$ in this example, holds and the system appears controllable. As discussed in Remarks 6 and 7, while not all states might be reachable (due to the presence of e.g. non-negativity constraints on the control inputs), the stabilizability of the system is guaranteed based on the monotonic nature of the product quality degradation.

4.2.2. Observability

Observability implies that two non-identical states $\mathbf{x}_1$ and $\mathbf{x}_2$ can be distinguished by applying some input and observing the two corresponding system outputs over a finite amount of time (Sontag 2013). The observability matrix (whose rank is n_x for observable systems) is given by:

$$\mathcal{O} = \begin{bmatrix} C & CA & \dots & CA^{n_x-1} \end{bmatrix}^T \tag{21}$$

Necessary conditions for observability can derived similarly to Lemma 4.7, and the following can used for checking observability of linear systems:

Lemma 4.8 (Hautus lemma for observability (Hautus 1972))**.** *A system is observable if and only if*

$$\text{rank} \begin{bmatrix} \lambda I - A \\ C \end{bmatrix} = n_x \ \ \forall \lambda \in \mathbb{C} \tag{22}$$

in which $\mathbb{C}$ *is the set of complex numbers.*

Claim 3. *The supply chain states are observable if the net inventory amounts (that is,* $\sum_{q \in Q} I_{i,q,t}$ *and backorder (that is* $BO_{i,t}$*) at each facility are measured, per Assumption 4.5.*

Proof. A detailed proof can be found in Appendix C. □

The sparsity pattern of the observability matrix for the state-space model in Figure C2 is shown in Figure C11. For this simple prototype system, it is easy to verify (computationally and visually from Figure C11) that the observability condition $\text{rank}(\mathcal{O}) = n_x$, for $n_x = 10$ in this example, holds and the system is observable.

5. Rolling horizon state estimation

In this section, we develop a rolling horizon state estimation strategy which, as argued in Section 2, provides greater flexibility and robustness compared to e.g., traditional estimators based on the KF. In this sense, approaches based on MHE allow for considering the constraints of the supply chain model and arbitrary distributions of the disturbance (e.g., the structure of the product quality disturbances $\epsilon_{q,\bar{q}}$ presented in (6)). MHE is a real-time, optimization-based state estimation technique that employs past measurements of output variables and decisions/control inputs (i.e., from time periods $k \in [1-\tilde{N}, -1]$). The *estimator* computes a sequence of state estimates over a finite horizon, in a moving-window/rolling horizon fashion, by solving the following quadratic program at each sampling time:

$$\begin{aligned}
\min_{\tilde{\mathbf{x}},\tilde{\mathbf{y}},\tilde{\mathbf{u}},\tilde{\mathbf{w}},\tilde{\mathbf{v}}} \quad & \sum_{k=1-\tilde{N}}^{-1} ||\tilde{\mathbf{y}}_k - \hat{\mathbf{y}}_k||_W^2 + ||\tilde{\mathbf{w}}_k||_{Q^{-1}}^2 + ||\tilde{\mathbf{v}}_k||_{R^{-1}}^2 + ||\tilde{\mathbf{x}}_k - \tilde{\mathbf{x}}_k^{\text{pre}}||_{W_{\text{pre}}}^2 \\
\text{s.t.} \quad & \tilde{\mathbf{x}}_{k+1} = A\tilde{\mathbf{x}}_k + B\tilde{\mathbf{u}}_k + \tilde{\mathbf{w}}_k \qquad \forall k \in \mathbb{I}_{-\tilde{N}+1:-1} \\
& \tilde{\mathbf{y}}_k = C\tilde{\mathbf{x}}_k + D\tilde{\mathbf{u}}_k + \tilde{\mathbf{w}}_k \qquad \forall k \in \mathbb{I}_{-\tilde{N}+1:-1} \\
& \tilde{\mathbf{u}}_k = E\hat{\mathbf{u}}_k \qquad \forall k \in \mathbb{I}_{-\tilde{N}+1:-1} \\
& (\tilde{\mathbf{x}}_k, \tilde{\mathbf{u}}_k) \in \mathbb{Z} \qquad \forall k \in \mathbb{I}_{-\tilde{N}+1:-1} \\
& \tilde{\mathbf{y}}_k \in \mathbb{Y} \qquad \forall k \in \mathbb{I}_{-\tilde{N}+1:-1}
\end{aligned} \tag{23}$$

where the objective function has four components:

- A penalty on the difference between the predicted outputs $\tilde{\mathbf{y}}$ and the current measurements $\hat{\mathbf{y}}$. Penalizing this difference drives the estimation algorithm to approximate the observed data (i.e., the inventory measurements described in Assumption 4.5) thereby improving the accuracy of the estimates.
- A penalty on the difference between current estimates $\tilde{\mathbf{x}}$ and previous estimates $\tilde{\mathbf{x}}^{\text{pre}}$ weighted using matrix W_{pre}. This penalty promotes temporal consistency in the estimation process to produce estimates that evolve smoothly over time, and such that there are no abrupt changes in the inventory quality estimated from one iteration to the next.
- Penalties on process noise estimate weighted by the inverse of the process noise covariance Q, and on measurement noise estimate weighted by the inverse of the measurement noise covariance R. These penalties help prevent overfitting and improve the generalization ability of the estimation algorithm, as well as promote interpretability by encoding distributional information about the noise variables.

The reader is directed to the works of Muske, Rawlings, and Lee (1993); Robertson, Lee, and Rawlings (1996) and Ge and Kerrigan (2017) for more information on choosing the matrices W, W_{pre}, Q, R.

The estimation horizon is denoted by $\tilde{N}$, and the constraints imposed on the output variable predictions are denoted by $\mathbb{Y}$. In this case the computed state estimate $\tilde{\mathbf{x}}_0$

corresponds to the initial state value used for solving the supply chain management problem that will be discussed in Section 6. The constraint $(\tilde{\mathbf{x}}_k, \tilde{\mathbf{u}}_k) \in \mathbb{Z}$ ensures that the resulting estimates satisfy all the supply chain constraints (e.g., inventory capacities, minimum quality requirements at retailers, and all other constraints covered in the Supporting Information). Similarly, the formulation in (23) can accommodate a wider range of objective functions and non-Gaussian distributions for $\mathbf{w}$ and $\mathbf{v}$ hence being more suited for the supply chain estimation problem than KF-based approaches.

Initially, before there are sufficient data perform estimation (that is, when $t < \tilde{N}$), (23) is solved for a shorter estimation horizon length, which is increased by one at each sampling time until $\tilde{N} \geq t$. Previous estimates used are denoted as $\tilde{\mathbf{x}}_k^{\text{pre}}$ which is initially set as some initial guess for the mean of the states, similarly to other estimation approaches (Kalman 1960). The resulting optimization problem is a quadratic program that can be solved efficiently with off-the-shelf optimization software assuming that $\tilde{N}$ is not exceedingly large. In this case, since we do not measure inventory at all quality levels separately (these measurements are only available for producers), we cannot assume that the exact values of the control inputs are known (e.g., we do not exactly know how much inventory of which quality was shipped through a given route). Therefore, shipment variables are included in (23) as decision variables $\tilde{\mathbf{u}}$, and are related to the available input measurements via matrix E.

6. SCM based on rolling horizon control

Model predictive control (MPC) (Rawlings and Mayne 2019), sometimes referred to as rolling horizon control, has been discussed as a SCM approach for non-perishable (Subramanian et al. 2013; Subramanian, Rawlings, and Maravelias 2014) and perishable (Lejarza and Baldea 2020a,b) inventories. The *controller* uses demand forecasts and state estimates (i.e., the amount of inventory at each quality level at each facility) to compute the optimal production and shipment decisions by solving an optimization problem of the form:

$$\begin{aligned}
\min_{\mathbf{u}} \; & \sum_{k=0}^{N-1} \ell(\mathbf{x}_k, \mathbf{u}_k) + V_f(\mathbf{x}_N) \\
\text{s.t.} \; & \mathbf{x}_{k+1} = A\mathbf{x}_k + B\mathbf{u}_k + \mathbf{w}_s \quad \forall k \in \mathbb{I}_{0:N-1} \\
& (\mathbf{x}_k, \mathbf{u}_k) \in \mathbb{Z} \quad \forall k \in \mathbb{I}_{0:N-1} \\
& \mathbf{x}_0 = \tilde{\mathbf{x}}_0 \\
& \mathbf{x}_N \in \mathbb{X}_f
\end{aligned} \tag{24}$$

where $\mathbf{u} = \{\mathbf{u}_0, \ldots \mathbf{u}_{N-1}\}$ is the set of control input vectors over the control horizon N (i.e., $\mathbf{u}_k$ corresponds to the control input, that is production, shipment and sales decisions to be implemented at sampling time $t + k$). The cost function is denoted by $\ell : \mathbb{X} \times \mathbb{U} \to \mathbb{R}$, reflecting a trajectory tracking objective or an economic performance metric as discussed previously in Section 3. The terminal costs $V_f(\cdot)$ and terminal constraints $\mathbb{X}_f$ are used to guarantee the stability of the nominal closed-loop system, resulting from repeated rolling horizon optimization as will be discussed subsequently. These terminal components ensure that the optimal production and shipment decisions from the solution of (24) always steer for the supply chain inventory towards some desirable state (e.g., this could be a steady state or some a priori determined safety stock level). For further details on the properties and the design of these terminal conditions the reader is referred to Amrit, Rawlings, and Angeli (2011); Angeli, Amrit, and Rawlings (2011); Amrit, Rawlings, and Biegler (2013).

The optimization problem (24) is based on the production and distribution planning model presented in Section 3, with the addition of the terminal components. The vector $\mathbf{w}_s$ denotes the nominal disturbance, and is used to incorporate demand forecasts for each retail facility in the supply chain network (see Figure C2, and note that in the nominal case, $\varepsilon_q^i = 0$ for all facilities i and all quality levels q, and that demand represents the disturbance for the backorder state).

Problem (24) is solved at each sampling time t, and the first element of the optimal sequence of control inputs, denoted by $\mathbf{u}_0^*$, is implemented in the supply chain. After implementing $\mathbf{u}_0^*$, a measurement of the system outputs $\hat{\mathbf{y}}$ is made, and a new initial state estimate is computed by solving (23). This procedure is repeated in real-time, and defines an implicit supply chain management policy (or control law) $\mathbf{u} = \kappa_N(\mathbf{x})$ that maps estimates of the supply chain inventories (for both quantity and quality) to production, shipment, and sales decisions. The rolling horizon nature of the proposed estimation and control algorithms is illustrated in Figure C4. Figure C4 also illustrates the concept of "move blocking" which is a technique that limits the frequency of control input changes (i.e., the same value of the control input is used for multiple consecutive time steps) to reduce computational complexity and improve real-time performance.

Figure C5 summarizes the proposed integrated state estimation and control approach for closed-loop supply chain management, highlighting the correspondence between the supply chain variables and the systems notation used to define the estimation and control optimization problems in (23) and (24) respectively. The model-based controller uses information regarding demand forecasts and state estimates corresponding to inventory (that is, the amount of inventory at each quality level at each facility) to compute the optimal production and shipment decisions, which are implemented in the supply chain. More specifically, the approach uses the estimate at the current sampling time ($\tilde{\mathbf{x}}_0$) to initialize the supply chain model embedded in the optimization problem in (24). The time overlap between the estimates and decision variables for the estimation and control problems in illustrated graphically in Figure C4. Once new measurements are received, the estimation and control horizons are shifted forward in time by one sample time and the procedure is repeated.

6.1. *Implementable policy computation*

A challenge with implementing the proposed simultaneous estimation and control framework is that the decisions obtained by solving (24) are based on the state estimate. The resulting decisions may not be feasible when considering the true state of the supply chain. For example, consider the case where the computed control decision corresponds to shipping a total of $s_{i,j,q}^*$ product units from facility i to facility j with quality q, but the true system has inventory $I_{i,q} < s_{i,j,q}^*$. Then, implementing the control is not possible (i.e., the computed decision is infeasible in practice).

To circumvent this issue, a systematic approach is required for translating the computed control input into an implementable decision for the true state of the supply chain. The resulting policy is intuitively expected to be suboptimal relative to the control input computed with perfect state feedback, as was described in previous works (Lejarza and Baldea 2020a,b; Lejarza, Pistikopoulos, and Baldea 2021). However, we posit that the implementable version of the policy computed using state estimation has superior (cost) performance in practice than the policy computed merely based on the nominal state of the system (i.e., by setting $\epsilon_{q,\bar{q}} = 0$).

We propose to determine the closest (in a norm sense) possible *implementable* value of the optimal control input (focusing on shipments, since production rates cannot be infeasible based on the inventory of the true system) by solving the following optimization problem at each sampling time t:

$$
\begin{aligned}
\min_{s_{i,q,t}} \sum_{(i,j)\in\mathcal{A}} & \Big[\sum_{q\in\mathcal{Q}} \sum_{\bar{q}\in\mathcal{Q}} \lambda_{q,\bar{q}} \left(s_{i,j,q,t} - s^*_{i,j,\bar{q},t}\right)^2 \Big] + \psi_{i,j}\gamma_{i,j}^2 \\
\text{s.t.} \quad & I_{i,q+\Delta q,t} \geq \sum_{j\in n(i)} s_{i,j,q,t} && \forall q \in \mathcal{Q} \\
& \sum_{q\in\mathcal{Q}} s_{i,j,q,t} = \sum_{q\in\mathcal{Q}} s^*_{i,j,q,t} - \gamma_{i,j} && \forall (i,j) \in \mathcal{A} \\
& \gamma_{i,j} \geq 0 \quad \forall (i,j) \in \mathcal{A}
\end{aligned}
\tag{25}
$$

where $s^*_{i,j,q,t}$ denotes the shipments computed by solving (24) based on the state estimate, and $s_{i,j,q,t}$ denotes the approximation of these shipment decisions based on the true inventory available in the supply chain denoted by $I_{i,q,t}$. In the above quadratic program, the first constraint enforces feasibility by ensuring that the actual shipments do not exceed the current amount of inventory available to ship. The second constraint enforces that the same net shipments from the SCM policy are preserved. An auxiliary variable $\gamma_{i,j}$ is added to soften the constraint in case that shipping the exact net amount as indicated by the SCM policy defined by solving the control problem is not feasible. The cost coefficient $\psi_{i,j}$ should be set to a sufficiently large value to ensure that the net shipments match between the SCM policy value, $s^*_{i,j,q,t}$ and its feasible approximation $s_{i,j,q,t}$. Otherwise, for small values of $\psi_{i,j}$ the optimization problem in (25) may allow for large values of $\gamma_{i,j}$ such that the resulting implementable policy may differ considerably form the proposed estimation and control SCM policy.

Furthermore, we introduce a coefficient $\lambda_{q,\bar{q}}$ to penalize differences in the quality shipped, such that for all $q, \bar{q} \in \mathcal{Q}$: $\lambda_{q,\bar{q}} = 1$ if $q = \bar{q}$, else $(q - \bar{q})^2 + 1$ if $q \neq \bar{q}$. The underlying idea for this choice of coefficient $\lambda_{q,\bar{q}}$ is to have a penalty that increases proportionally to the absolute difference between the estimated shipment and the implemented shipment decisions (e.g., there should be a greater penalty for a difference of ten quality levels than for a difference of one quality level between estimated and implemented shipment). This penalty in (25) is also proportional to the difference in the amount shipped, so that the implementable policy is as close as possible (in terms of product quality, and inventory amounts) to the policy resulting from the proposed SCM approach.

Remark 8. In practice, when the true state of the system is not known, robust control approaches may be required to ensure that the computed control inputs are feasible under some assumption regarding the distribution of the state estimation error. Robust control is beyond the scope of the present work, and details regarding its design and implementation can be found elsewhere (Lejarza and Baldea 2021a; Mayne 2016; Rawlings and Mayne 2019).

7. Numerical experiments

We consider a supply chain network structure based on our previous work (Lejarza and Baldea 2020a,b; Lejarza, Pistikopoulos, and Baldea 2021)) as shown in Figure S1 of the Supporting Information, consisting of two producers, one distribution center, and four retailers. Table S.1 summarizes the network model parameters used to perform the numerical experiments. All simulations were carried out on a computer featuring a Apple M2 processor and 24 GB of RAM. All resulting linear programs were formulated in Python using Pyomo (Hart, Watson, and Woodruff 2011) and solved with CPLEX 12.10.0.0 (IBM Corporation 2019) (using a 1% absolute optimality gap and all other default settings of the solver).

We perform experiments considering three specific instances of the problem:

(1) *Full-state feedback* where the states (i.e., inventory at all quality levels and in every facility of the system) are assumed to be measured perfectly (this corresponds to the closed-loop management strategies discussed in earlier publications (Lejarza and Baldea 2020a,b; Lejarza, Pistikopoulos, and Baldea 2021)).
(2) *Nominal quality degradation plus feedback control* where the states are predicted by the supply chain model and setting $\epsilon_{q,\bar{q}} = 0$, i.e., no disturbances are detected and no state estimation is performed. The predicted values are then used to solve (24).
(3) *State estimation plus feedback control* where (23) is solved to compute a state estimate based on the available measurements at each sampling time. The resulting estimate is then used to solve (24).

The nominal quality degradation plus feedback, and estimation plus feedback policies (Instances 2 and 3) are implemented by computing the closest implementable policy to the one predicted by the controller by solving (25). For illustration purposes, Instances 2 and 3 use the true state of the system as the initial value. We consider disturbances that are sampled from a discrete set of values in $\epsilon_{q,\bar{q}} \in [-I_{i,q}, I_{i,\bar{q}}]$ with probabilities approximated from a normal distribution centered around zero, so that nominally the system has zero product quality disturbances. The Supporting Information provides a detailed description of the supply chain instance considered. We use the root mean squared error to measure the accuracy of a state estimate with respect to the true value. That is, for a facility i and time period t:

$$\text{RMSE}_{i,t} = \frac{1}{|\mathcal{Q}|}\sqrt{\sum_{q\in\mathcal{Q}}(I_{i,q,t} - \tilde{I}_{i,q,t})^2} \tag{26}$$

for a true inventory state I and the respective estimate $\tilde{I}$.

Since measurements are collected for inventory quality at manufacturing facilities, we focus on estimation of product quality at distribution centers and retailers. Note that although measurements are made with respect to the quality of products sold at each sampling time t, sales information is available after the quality of inventory at retailers is estimated, so we posit that the state estimate will not exactly align with the true state of the system. That is, we consider the estimation performance at points in the supply chain between the two sources of data (i.e.., manufacturing and customer sales) used to perform state estimation. The results in Figure C6 show the performance of the estimator (Instance 3) in comparison to the state tracked nominally (Instance 2). Figure C6 (left) shows the RMSE of the two instances as a function of time with respect to the true inventory quality at D_1. Evidently, the closed-loop system with estimation (Instance 3) performs better at predicting the distribution of product quality than the nominal system (Instance 2). Performing a t-test confirms that the RMSE of Instance 3 is statistically significantly lower than that of Instance 2 for the runs considered, with a p-value < 0.01 (more details about the test can be found in the Supporting Information). The improved performance of the estimator (Instance 3) is more clearly seen in Figure C6 (right), in which the ratio of the RMSE of the estimator (Instance 3) to that of the nominal system (Instance 2) is evidently less than one.

To gain further quantitative insight in the improved SCM performance afforded by the estimator (Instance 3), Figure C7 shows the cumulative distribution of product quality at the distribution center at different points in time of the closed-loop simulation. Initially, the quality tracked by the nominal system (Instance 2) aligns closely with that tracked by the estimator (Instance 3) and that of the true system (Instance 1). Over time, however, we see that the nominal system (Instance 2) fails to account for inventories of low and high quality relative to the other two instances. This is expected to result in economic advantages for the controller leveraging the improved estimate of the state (Instance 3) in comparison to the nominal controller (Instance 2). For facilities further downstream in the supply chain (that is, $R_1, \ldots, R_4$) which are subject to disturbances that accumulate over time, the ability of the nominal system to track product quality worsens considerably. In contrast, Figure C7 indicates that the system in (Instance 3) continues to accurately track the quality distribution over time even for downstream facilities in the supply chain.

Having discussed the (superior) performance of the closed-loop system with estimator (Instance 3) in predicting the distribution of product quality, we focus on investigating its implications on the resulting supply chain management strategy. Figure C8 (right) shows the daily operating cost over time for each of the three instances considered. Intuitively, the state feedback instance (Instance 1), which has perfect information about the system state, exhibits the lowest costs. Nevertheless, it is noticeable that performing state estimation (Instance 3) results in lower operating costs (by about 40% on average over all demand instances) of the supply chain compared to the nominal instance (Instance 2). T-tests confirm that: (1) operating costs with state estimation (Instance 3) are statistically significantly lower than those of the nominal instance (Instance 2) (p-value < 0.01), and (2) as expected, perfect feedback (Instance 1) leads to statistically significantly lower costs compared to state estimation (p-value < 0.01). Further details on the statistical tests are provided in the Supporting Information.

In this case, the lower costs associated with state estimation (Instance 3) stem from the ability of the proposed rolling horizon SCM strategy to deliver the appropriate product quality to retailers with different product quality preferences, significantly reducing backorder and (to a lesser extent) inventory waste, while increasing revenue derived from sales as shown in Figure C8 (left). Additional results, shown in Figure S4 in the Supporting Information, indicate that the relative performance of the three control instances considered in Figure C8 holds for decreasing demand redundancy (that is, increasing the nominal demand while keeping production, shipment, and inventory capacity constant).

Furthermore, if the supply chain were to be operated at the lower limit of product quality, delivering the minimum quality required at the retail nodes to e.g., minimize quality dependent production costs, it is expected that the observed advantages of state estimation-based operation would translate to more considerable waste reduction than the one shown in Figure C8 (right). Inventory waste in this case would be minimized by shipping inventory of lower (estimated) quality to facilities downstream having the shortest lead time to prevent products from arriving below the required quality threshold for facilities with long lead times.

Table C1 offers further insights into the contribution of the different cost components for each instance considered. These results suggest that state feedback has a greater share of core operating costs (that is, production, shipment and inventory holding which are necessary to fulfill demand), while the other two strategies that do not rely on perfect product quality information operate less efficiently as they have a greater share of backorder and waste costs. It should be noted that the aforementioned cost contributions are, to a large extent, dependent on the choice of cost parameters, which in this case were determined similarly to previous studies Lejarza and Baldea (2020a, 2021b); Lejarza, Pistikopoulos, and Baldea (2021); the reader is directed to these works for further information.

Previous studies Lejarza and Baldea (2020a, 2021b) have demonstrated the resilience of feedback-based SCM strategies. Here, we conducted additional numerical simulations to test our approach under extreme production capacity disruptions. Specifically, we considered a scenario where production capacity is lost (i.e., the capacity of both producers drops to zero between $t = 20$ and $t = 30$). The results in are discussed in detail in the Supporting Information.

Lastly, in Figure C9 we evaluate the computational performance of the proposed rolling horizon optimization and estimation approach for supply chain networks with increasing number of facilities. The results in Figure C9 correspond to the average of ten demand realizations for ten iterations (i.e., producing ten executable actions) of the proposed rolling horizon approach. We note that the CPU time for all instances considered is well under one day (i.e., the frequency with which supply chain decisions are updated in this study), suggesting that computational complexity would not hinder implementation in real-world settings.

8. Conclusions and directions of future research

This work demonstrates the importance of state estimation for managing supply chains with perishable inventory. Methodologically, we introduced a state-space representation of supply chain dynamics to derive conditions for controllability and observability. Based on these results, we proposed a framework for product quality (state) estimation and online optimization to compute optimal production and distribution planning decisions on a rolling horizon. Numerical experiments demonstrated that employing state estimation improves the accuracy of predicting product quality distribution at distribution centers and retailers compared to using nominal quality degradation models. These enhanced estimates lead to better supply chain management (SCM) policies, resulting in reduced operating costs through improved inventory allocation tailored to retailers' quality preferences. Additionally, state estimation helps reduce waste by efficiently allocating lower-quality products to facilities with shorter lead times or lower quality preferences, thereby preventing products from falling below required quality thresholds at facilities with longer lead times or higher quality preferences. In summary, our results support the following **managerial insights**:

- Product quality measurements throughout the supply chain are important and necessary to guarantee the quality of perishable products delivered to end consumers. While it is impractical and costly to measure product quality at every stage of the supply chain, this work introduces a computationally efficient and scalable approach for estimating product quality from sparse measurements in the presence of random product degradation.

- A systems theoretic analysis of the perishables supply chain provides insights regarding uncontrollable and unobservable states, which can support identifying supply chain vulnerabilities and risks, and improve resilience and enhance decision-making.
- Inventory management policies based on more accurate product quality estimates result in improved operational efficiency by reducing costs associated with backorder, missed sales, and waste due to product spoilage.

Incorporating state estimation into SCM strategies offers significant economic and environmental benefits. With supply chains under increasing pressure from uncertain customer demand and stricter product quality standards, state estimation techniques can greatly enhance network efficiency and sustainability. Future research should explore adaptive or learning-based approaches, such as reinforcement learning, to develop supply chain policies that adapt to temporal variations in uncertainties. Additionally, applying the proposed framework to specific instances of perishables supply chains would further validate its effectiveness.

Data availability statement

All the code and data that support the findings of this study are openly available in `https://github.com/Baldea-Group/perishables_SCM_estimation`

Disclosure statement

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Nomenclature/Notation

See Table S1 in the Supporting Information.

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Appendix A. Proof of Claim 1

Proof. The proof consists of showing that the pair (A, B) of the supply chain state-space satisfies the Hautus controllability criteria in Lemma 4.7. The two conditions in Claim 1, imply that matrix B has at least a bidiagonal structure, where each state variable is associated with two distinct control inputs. The resulting bidiagonal structure implies that there are distinct control inputs for increasing and decreasing inventory at each facility and quality level. Intuitively, in the bidiagonal case, the column rank of matrix B satisfies $\text{rank}(B) = n_x$, hence $\text{rank}\begin{bmatrix}\lambda I - A & B\end{bmatrix} = n_x \; \forall \; \lambda \in \mathbb{C}$ and the system is controllable irrespective of the structure of matrix A. Similarly, by the definition of the controllability matrix in (19), $\text{rank}(B) = n_x$ implies that controllability matrix in (19) satisfies $\text{rank}(\mathcal{C}) = n_x$, meaning that the supply chain network is controllable. □

Appendix B. Proof of Claim 2

Proof. By definition, the quality variables are bounded from above and below so that $q_\infty \leq q(t+1) \leq q(t) \leq q_0$. This follows from the monotonicity assumption which establishes that $dq(t)/dt < 0$, and implies that eventually the product spoils such that $\lim_{t\to\infty} q(t) = q_\infty \leq q_{i,\min}$ and inventory losses occur. Clearly, q_∞ is an asymptotically stable equilibrium for product quality, which implies that $\lim_{t\to\infty} \mathbf{x} = 0$, and the origin is an asymptotically stable equilibrium point for the states. Physically, this means that eventually all inventory that is not shipped downstream or sold at a given facility will spoil and will be discarded.

Furthermore, stability defined in the BIBO sense is guaranteed by the fact inventory will always be non-negative, will not exceed storage capacity for all time periods, and can always be discarded to preserve stability (i.e., each state variable corresponding to inventory amount and quality has an additional associated control input corresponding to inventory disposal not depicted in Figure C2). Similarly, the input will always be bounded considering that production and shipment capacity is finite, reflected by the constraints in (18). □

Appendix C. Proof of Claim 3

Proof. Intuitively, if backorder is measured there is no need to demonstrate observability for these state variables (i.e., observability is guaranteed since the output model for these state variables corresponds to the identity matrix so that the local observability matrix is of rank equal to the number of bacorkder variables, which corresponds to the number of retailer facilities).

For inventory variables we begin by considering a single facility i having a number of states corresponding to the number of quality levels $|Q|$. The state and output matrices are given by:

$$A_i = \underbrace{\begin{bmatrix} 0 & 1 & 0 & 0 & \dots & 0 \\ 0 & 0 & 1 & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 1 \\ 0 & 0 & 0 & 0 & \dots & 0 \end{bmatrix}}_{q_1 \quad q_2 \quad q_3 \quad q_4 \quad \cdots \quad q_{|Q|}} \in \mathbb{R}^{|Q|\times|Q|}, \quad C_i = \underbrace{\begin{bmatrix} 1 & 1 & \dots & 1 & 1 \end{bmatrix}}_{q_1 \quad q_2 \quad \cdots \quad q_{|Q|}} \in \mathbb{R}^{1\times|Q|} \tag{C1}$$

where output matrix C_i implies that inventory is measured in aggregate, without distinguishing the amount of inventory at each quality level in the measurement.

From the structure of A_i all information regarding the lowest quality inventory is lost in the subsequent state reflecting the fact that low quality inventory goes to waste. In contrast, for all higher quality levels, A_i reflects quality degradation of inventory form one quality level to the next based on its off-diagonal structure. Therefore, if inventory of quality q_1 is accounted for in the measurement (whether it is measured individually, or measured in aggregate with the rest of the quality levels), it straightforwardly follows that

$$\text{rank}(\mathcal{O}_i) = |Q| \tag{C2}$$

rendering the states for single facility i observable.

For a supply chain comprised of multiple facilities given by set $\mathcal{N}$, we have that the state and output matrices have the following block-diagonal structure:

$$A = \begin{bmatrix} A_1 & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & A_2 & \ddots & \mathbf{0} \\ \vdots & \ddots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \dots & A_{|\mathcal{N}|} \end{bmatrix} \in \mathbb{R}^{(|\mathcal{N}||Q|)\times(|\mathcal{N}||Q|)}, \quad C = \begin{bmatrix} C_1 & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & C_2 & \ddots & \mathbf{0} \\ \vdots & \ddots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \dots & C_{|\mathcal{N}|} \end{bmatrix} \in \mathbb{R}^{|\mathcal{N}|\times(|\mathcal{N}||Q|)} \tag{C3}$$

where $\mathbf{0}$ is a matrix of zeros of appropriate dimensions. The observability matrix has a similar block diagonal structure:

$$\mathcal{O} = \begin{bmatrix} \begin{bmatrix} C_1 & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & C_2 & \ddots & \mathbf{0} \\ \vdots & \ddots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \dots & C_{|\mathcal{N}|} \end{bmatrix} \\ \begin{bmatrix} C_1 A_1 & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & C_2 A_2 & \ddots & \mathbf{0} \\ \vdots & \ddots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \dots & C_{|\mathcal{N}|} A_{|\mathcal{N}|} \end{bmatrix} \\ \vdots \\ \begin{bmatrix} C_1 A_1^{|Q|-1} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & C_2 A_2^{|Q|-1} & \ddots & \mathbf{0} \\ \vdots & \ddots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \dots & C_{|\mathcal{N}|} A_{|\mathcal{N}|}^{|Q|-1} \end{bmatrix} \end{bmatrix}^T \tag{C4}$$

Because each of the columns of the matrix in (C4) corresponds to a verticall matrix of of rank $|Q|$ (based on the observability property of each facility), and since each column clearly has a different range, then it follows that $\text{rank}(\mathcal{O}) = |Q||\mathcal{N}|$ and the system is observable. □

List of Figures

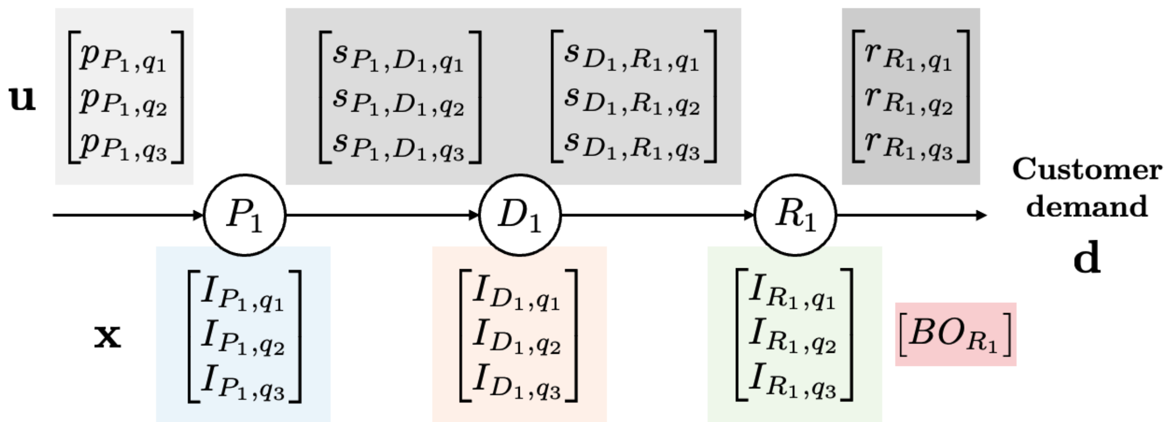

Figure C1. Caption: Structure and variable definition for supply chain networks with product quality dynamics for an illustrative example. All control inputs and state variables are respectively outlined at the top and bottom of the supply chain network diagram.

Figure C1 Alt-text: A supply chain structure with three entities: a producer, a distribution center and a retailer. The nomenclature of the inventory variables for each entity is shown, along with the production rate and product demand

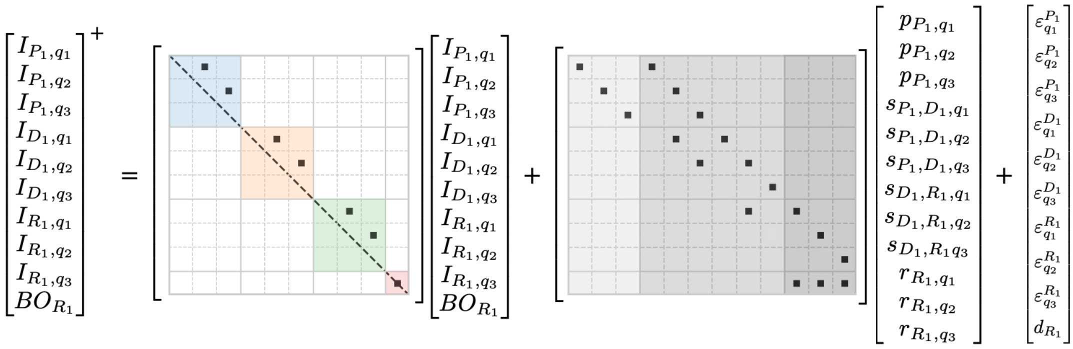

Figure C2. Caption: Illustration of state-space formulation ($\mathbf{x}^+ = A\mathbf{x} + B\mathbf{u} + \mathbf{w}$) for supply chain network with product quality dynamics for the illustrative example in Figure C1. The illustration highlights the sparsity pattern (i.e., non-zero entries) of matrices A and B, and uses the same color coding as in Figure C1 to highlight the control inputs and state variables of the supply chain example. Demand represents the disturbance for the backorder state.

Figure C2 Alt-text: A matrix equation showing the evolution of the state $\mathbf{x}$ of a state-space system. The state at the next sample time, $\mathbf{x}^+$ is computed by summing the product of the system matrix A with the current state vector $\mathbf{x}$, with the product of the input matrix B with the current input vector $\mathbf{u}$, and with the disturbance vector. Matrices are represented as a grid. The blocks of matrices A and B that correspond to the three entities in Figure C1 are highlighted. The non-zero elements of the matrices are shown using black dots, and the zero elements are blank.

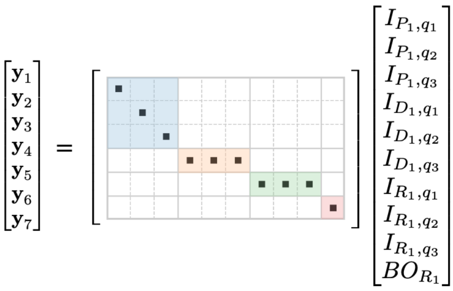

Figure C3. Caption: Linear model $\mathbf{y} = C\mathbf{x}$ for computing the output variables for a supply chain network with product quality dynamics for an illustrative example.

Figure C3 Alt-text: A matrix equation showing the calculation of the output $\mathbf{y}$ of a state-space dynamical system. The output is computed as the product of the output matrix C with the current state vector $\mathbf{x}$. The matrix is represented as a grid. The blocks that correspond to the three entities in Figure C1 are highlighted. The non-zero elements of the matrix are shown using black dots, and the zero elements are blank.

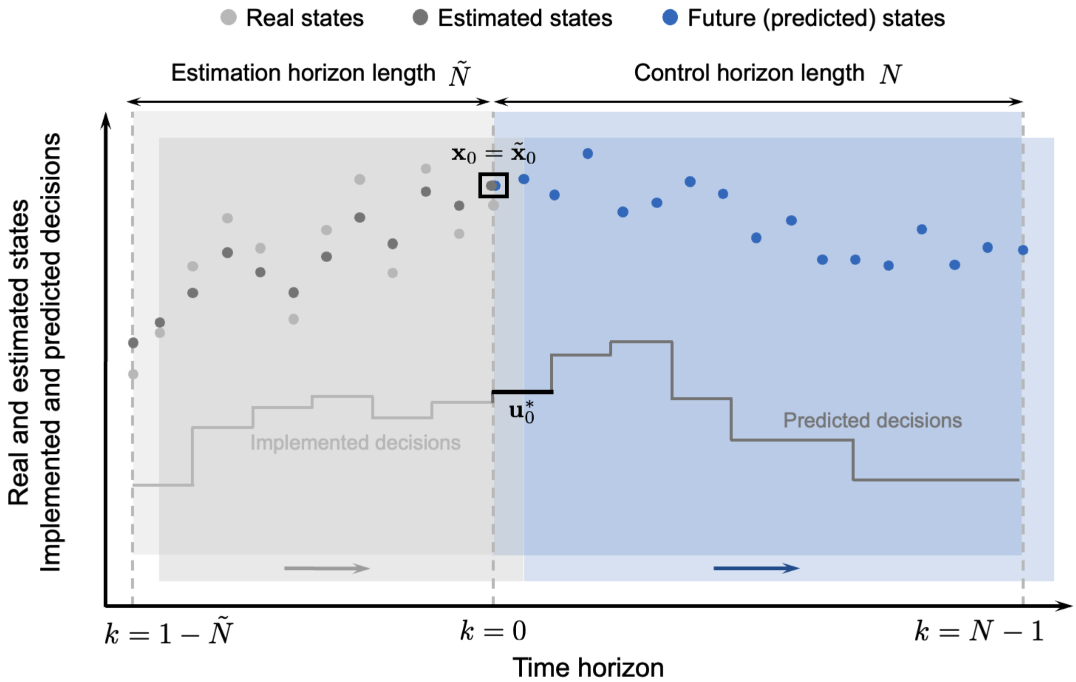

Figure C4. Caption: Illustration of rolling horizon concept for simultaneous state estimation and control for supply chain management of perishable inventory.

Figure C4 Alt-text: The combination of rolling horizon estimation and rolling horizon control for supply chain management of perishable products is illustrated. With reference to the current sample time $k = 0$, rolling horizon estimation utilizes state and output data from the past $\tilde{N}$ sample times as well as measured outputs from the current sample time to estimate all the system states at the current time. Rolling horizon estimation overlaps at the current sample time with rolling horizon control. Rolling horizon control computes the optimal system inputs for N future sample times based on the estimated current state and predicted future system states. The first element of the optimal system inputs is implemented in the supply chain, and the estimation and control time horizons are shifted to the right (into the next sample time), then the estimation and control process are repeated.

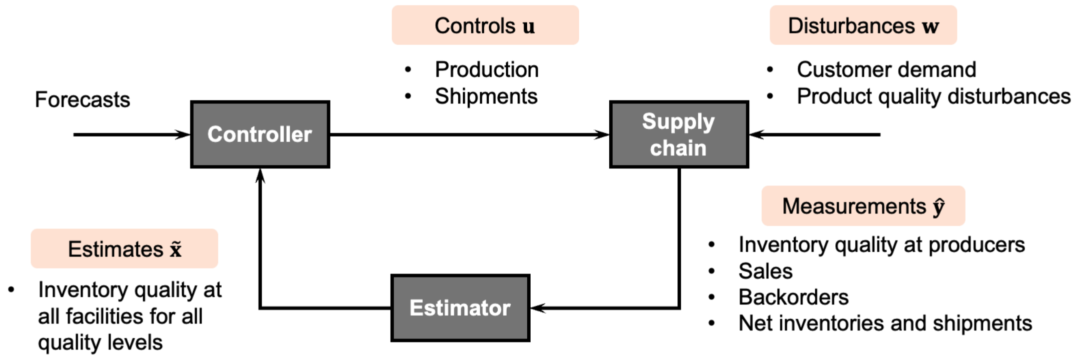

Figure C5. Caption: Simultaneous state estimation and control for supply chain management of perishable inventory.

Figure C5 Alt-text: The connections and information exchange between state estimation, control, and the supply chain are shown. The information exchange proceeds in a cycle. The state estimator receives information regarding inventory quality at producer nodes, net inventories and shipments at and between all nodes, and sales. It produces an estimate of inventory at all quality levels at all nodes of the supply chain, which is transmitted to the controller. The controller receives this information along with demand forecasts, and utilizes these data to compute production quantities for producers and shipment quantities between all entities. These decisions are transmitted to and implemented in the supply chain. The supply chain is subject to disturbances such as changes in customer demand and product quality. New measurements are transmitted from the supply chain to the estimator and the cycle repeats.

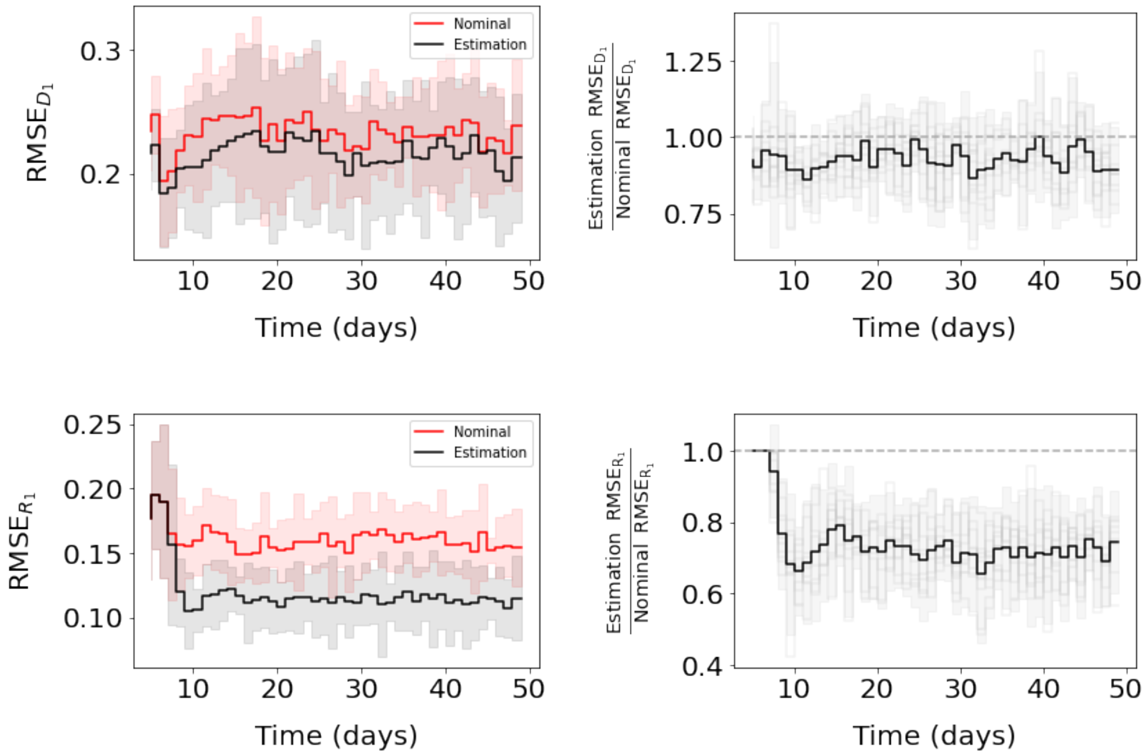

Figure C6. Caption: Estimation performance resulting from rolling horizon and by tracking the nominal state (that is, assuming that no product quality disturbances occur and $\epsilon_{q,\bar{q}} = 0$ in equation (4)). (Left) Shows the RMSE between the nominal and estimated states with respect to the true state of the system. Solid lines denote the mean of ten random simulations (for both demand and quality disturbances) and shaded region shows the 95% confidence interval around the mean. (Right) Shows the ratio of the RMSE values shown on the left for the estimated states over the nominal states. Grey lines correspond to the values for all ten random instances evaluated.

Figure C6 Alt-text: There are four figures grouped in two columns of two figures each. The figures show the results of ten random simulations of the supply chain example. The two figures in the first column show the evolution in time of the root mean square error (RMSE) computed as the difference between the predicted supply chain state (material inventories at all quality levels) and the actual supply chain state for the distribution center node and for one of the retailer nodes. The sample time is one day and the abscissa is marked in days. The case where the proposed state estimation approach is used is compared to a nominal case where it is assumed that no product quality disturbances occur. The figures show that the RMSE is lower for the case where the proposed state estimation approach is used. The two figures in the second column represent plots of the evolution in time of the ratio of the RMSE computed for the two cases. The ratio is less or equal to one for the distribution center and for the retail node at all sample times, illustrating the point that the state predictions produced by the proposed approach are more accurate than when considering the nominal case.

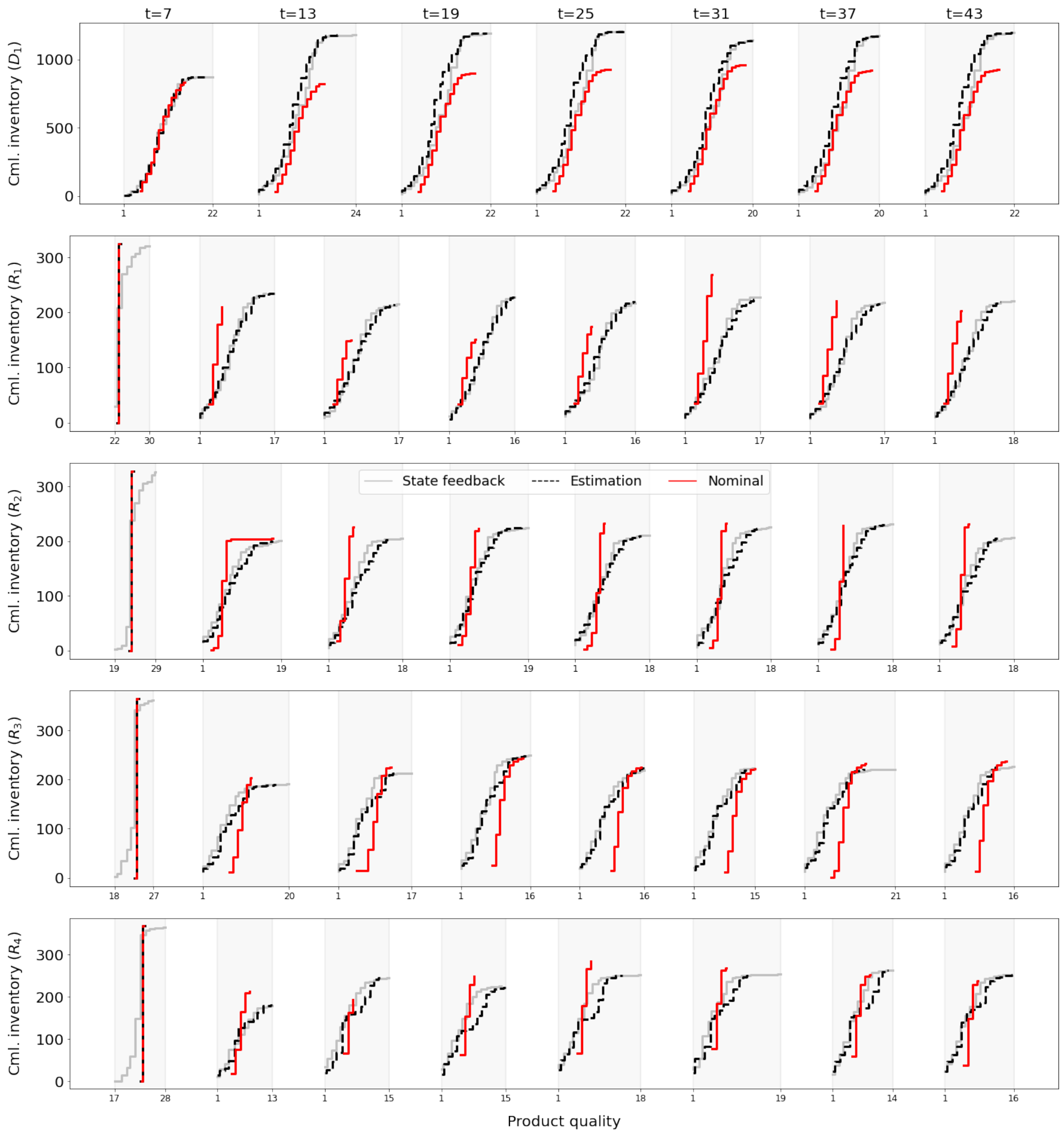

Figure C7. Caption: Distribution of inventory quality over time corresponding to the case of perfect state feedback, feedback with the nominal state, and for feedback using state estimation. Shaded vertical regions correspond to a period of time, and for brevity only a few time periods are shown. From top to bottom, the figures correspond to cumulative (cml.) inventory at the distribution center (D_1), and at the four retailers ($R_1, \ldots, R_4$). Recall that $\mathcal{Q} = \{1, \ldots, 30\}$ quality levels are considered, with $\Delta q = 1$.

Figure C7 Alt-text: Three inventory control strategies are compared: perfect state feedback, feedback with the nominal state, and feedback with the state computed using the proposed state estimation strategy. The figure shows snapshots of the inventory quality distribution at the distribution center node and the four retailer nodes as a function of time. There are five rows of snapshots, one for each of the five nodes. Snapshots are shown at seven sample times that are seven days apart, starting from day 7. It is shown that in the case where feedback control decisions are made based on the nominal state, the quality of the inventory degrades more significantly over time than in the case where decisions are based using the state estimated with the proposed approach, and that the results with the proposed state estimator align closely to those corresponding to decisions made using the true state of the system. The discrepancies between inventory distribution obtained using the nominal state and the other two cases become more stark in the case of the retailer nodes, which are further away from the producer node than the distribution center.

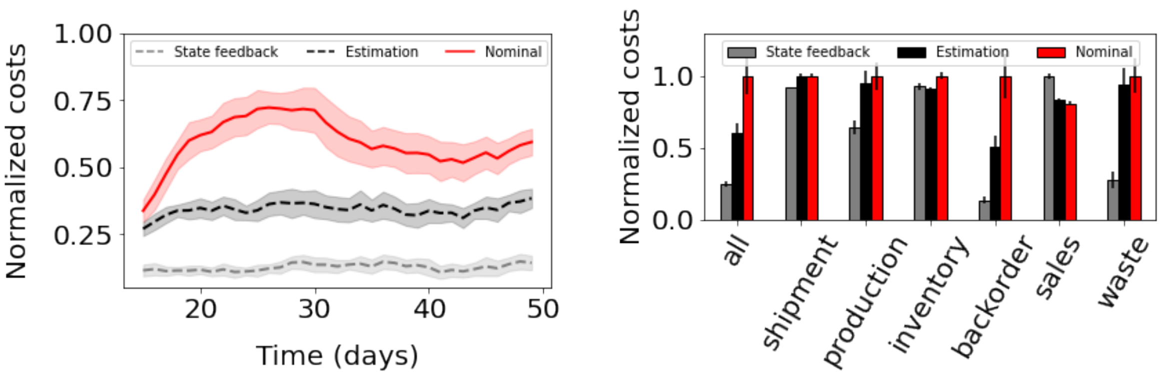

Figure C8. Caption: Comparison of daily operating costs corresponding to the case of perfect state feedback, feedback with the nominal state, and for feedback using state estimation. (Left) Aggregated total costs over time. (Right) Breakdown of cost function components aggregated over time. Solid lines and bars denote the mean cost for ten random simulations (for both demand and quality disturbances), and shaded region and error bars show the 95% confidence interval around the mean.

Figure C8 Alt-text: The daily operating costs corresponding to the case of perfect state feedback, feedback with the nominal state, and for feedback using state estimation, are compared. There are two plots. In the left plot, the daily cost for the three strategies (averaged for ten random simulations) is plotted as a function of time. Perfect state feedback yields the lowest cost, feedback using nominal state has the highest cost, while feedback control using the estimated state has higher cost than the perfect state feedback case, but its cost is considerably lower (by about 40%) than in the case of feedback with the nominal state. 95% confidence intervals are shown for each data set. In the right plot, normalized costs for the six components of the objective function (shipment, production, inventory, backorder, sales and waste) are compared for the three feedback control cases.

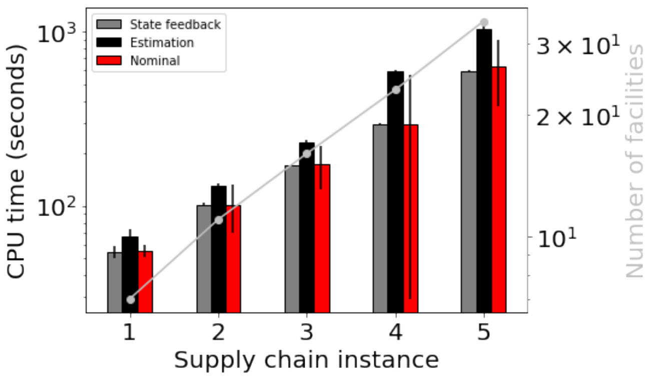

Figure C9. Caption: Computational performance of different cases (perfect state feedback, feedback with the nominal state, and for feedback using state estimation) for five supply chain network instances with increasing number of facilities, each solved for ten random demand realizations.

Figure C9 Alt-text: The average CPU time of ten demand realizations for ten iterations (i.e., producing ten executable actions) of the proposed rolling horizon control approach are shown for supply chains with increasing numbers of facilities (10, 20 and 30). 95% confidence intervals are provided. The CPU time for the largest supply instance is less than 20 minutes. This observation holds true for the three cases considered (perfect state feedback, feedback with the nominal state, and for feedback using state estimation).

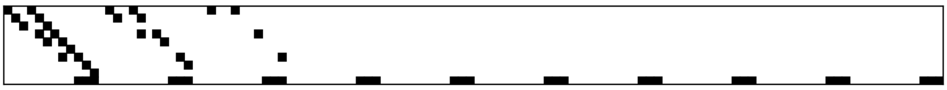

Figure C10. Caption: Sparsity pattern of controllability matrix $\mathcal{C}$ corresponding to the state-space model in Figure C2.

Figure C10 Alt-text: The controllability matrix for an example system with ten states and 12 inputs is visualized. The matrix has ten rows and 120 columns. The non-zero entries are shown as black squares and the zero entries of the matrix are blank. There are at least ten columns with unique non-zero entry patterns, showing that the rank of the matrix is ten (full row rank) and therefore the system in this example is controllable.

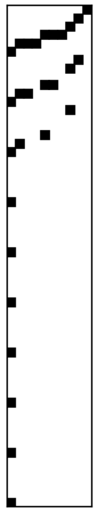

Figure C11. Caption: Sparsity pattern of observability matrix $\mathcal{O}$ corresponding to the output model in Figure C3.

Figure C11 Alt-text: The observability matrix for an example system with ten states and seven outputs is visualized. The matrix has 70 rows and ten columns. The non-zero entries are shown as black squares and the zero entries of the matrix are blank. There are at least ten rows with unique non-zero entry patterns, showing that the rank of the matrix is ten (full column rank) and therefore the system in this example is observable.

List of Tables

Table C1. Contribution of cost components to total operating costs for the case of perfect state feedback (Instance 1), feedback with the nominal state (Instance 2), and feedback using state estimation (Instance 3) for the results in Figure C8. Total costs correspond to the 50 day time window considered in Figure C8 (Left). Costs are in arbitrary units (a.u.)

	State Feedback (%)	**Estimation (%)**	**Nominal (%)**
Shipment	17.3%	8.4%	5.1%
Production	1.9%	1.2%	0.8%
Inventory	35.1%	15.2%	10.3%
Backorder	37.1%	62.4%	75.4%
Waste	8.6%	12.9%	8.4%
Total cost (a.u.)	1.59×10^5	3.88×10^5	6.44×10^5

Table C2. Nomenclature for indices, sets, parameters, and decision variables used to formulate the production and distribution planning optimization problem.

Notation	Description
Indices	
i	facility index, $i \in \mathcal{N}$
i, j	index pair for route between facilities i and j, $(i, j) \in \mathcal{A}$
q	quality index, $q \in \mathcal{Q}$
t	time index
Sets	
$\mathcal{P}$	Set of all producers
$\mathcal{D}$	Set of all distribution centers
$\mathcal{R}$	Set of all retailers
$\mathcal{N}$	Set of all facilities, $\mathcal{N} = \mathcal{P} \cup \mathcal{D} \cup \mathcal{R}$
$\mathcal{A}$	Set of all routes
$\mathcal{Q}$	Set of discrete quality levels
$v(i)$	Set of successors to facility $i \in \mathcal{N}$
Parameters	
c_i^p	Per unit production costs at facility $i \in \mathcal{P}$
$c_{i,j}^s$	Per unit shipment costs for route $i, j \in \mathcal{A}$
c_i^h	Per unit inventory holding costs for facility $i \in \mathcal{N}$
c_i^w	Per unit waste/disposal costs for facility $i \in \mathcal{N}$
c_i^b	Per unit backorder costs for facility $i \in \mathcal{R}$
$\rho_{i,q}$	Per unit quality-dependent sales revenue $i \in \mathcal{R}, q \in \mathcal{Q}$
τ_i^p	Production lead time for facility $i \in \mathcal{P}$
$\tau_{i,j}$	Shipment lead time for route $i, j \in \mathcal{A}$
Δq	Quality degradation for inventory in storage over one time period
$\Delta q_{i,j}$	Quality degradation for inventory in transit over the $\tau_{i,j}$
$q_{i,\min}$	Minimum quality requirement for facility $i \in \mathcal{N}$
p_i^{UB}	Production capacity over a single time period for facility $i \in \mathcal{P}$
$s_{i,j}^{UB}$	Shipment capacity over a single time period for route $i, j \in \mathcal{A}$
I_i^{UB}	Inventory capacity over a single time period for facility $i \in \mathcal{N}$
I_i^s, BO_i^s	Steady-state inventory and backorder terminal conditions for $i \in \mathcal{R}$
Decision variables	
$I_{i,q,t}$	Inventory at facility $i \in \mathcal{N}$, of quality $q \in \mathcal{Q}$, at time t
$BO_{i,t}$	Backorder at facility $i \in \mathcal{R}$, at time t
$p_{i,q,t}$	Amount produced at facility $i \in \mathcal{P}$, of quality $q \in \mathcal{Q}$, at time t
$s_{i,j,q,t}$	Amount shipped on route $i, j \in \mathcal{A}$, of quality $q \in \mathcal{Q}$, at time t
$r_{i,q,t}$	Amount sold at facility $i \in \mathcal{R}$, of quality $q \in \mathcal{Q}$, at time t
$\Omega_{i,t}$	Amount wasted at facility $i \in \mathcal{P}$, at time t

Supporting Information: Integrated product quality estimation and online optimization for supply chain management of perishable inventory

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Complete production and distribution planning optimization problem

Table S1 summarizes the nomenclature used to denote indices, sets, parameters and decision variables in the model. The objective corresponds to minimizing the operating costs of the supply chain as follows:

$$\min \sum_{t=0}^{N} PC_t + SC_t + IC_t + WC_t + BC_t + SR_t$$

where PC_t are production costs, SC_t are shipment costs, IC_t are inventory holding costs, WC_t are waste costs, BC_t are backorder costs, and SR_t are sales revenue (such that $SR_t \leq 0$). These cost components are defined as:

$$PC_t = \sum_{i\in\mathcal{P}} \sum_{q\in\mathcal{Q}} c_i^p p_{i,q,t}$$

$$SC_t = \sum_{i,j\in\mathcal{A}} \sum_{q\in\mathcal{Q}} c_{i,j}^s s_{i,j,q,t}$$

$$IC_t = \sum_{i\in\mathcal{N}} \sum_{q\in\mathcal{Q}} c_i^h I_{i,q,t}$$

$$WC_t = \sum_{i\in\mathcal{N}} c_i^w \Omega_{i,t}$$

$$BC_t = \sum_{i\in\mathcal{R}} c_i^b BO_{i,t}$$

$$SR_t = \sum_{i\in\mathcal{R}} \sum_{q\in\mathcal{Q}} \rho_{i,q} r_{i,q,t}$$

The system constraints correspond to inventory balances for producers, distribution centers and retailers, given by:

$$I_{i,q,t+1} = I_{i,q+\Delta q,t} - \sum_{j\in\mathcal{J}(i)} s_{i,j,q,t} + p_{i,q,t-\tau_i^p} + \varepsilon_{q,t}^i \quad \forall i \in \mathcal{P}, q \in \mathcal{Q}, t \in \{0, N-1\}$$

$$I_{i,q,t+1} = I_{i,q,t} - \sum_{j\in\mathcal{J}(i)} s_{i,j,q,t} + \sum_{j\in v(i)} s_{j,i,q+\Delta q_{j,i},t-\tau_{j,i}} + \varepsilon_{q,t}^i \quad \forall i \in \mathcal{D}, q \in \mathcal{Q}, t \in \{0, N-1\}$$

$$I_{i,q,t+1} = I_{i,q,t} + \sum_{j\in v(i)} s_{j,i,q+\Delta q_{j,i},t-\tau_{j,i}} - r_{i,q,t} + \varepsilon_{q,t}^i \quad \forall i \in \mathcal{R}, q \in \mathcal{Q}, t \in \{0, \ldots, N-1\}$$

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The backorder balances for retail facilities are give by:

$$BO_{i,t+1} = BO_{i,t} - \sum_{q \in Q} r_{i,q,t} + d_{i,t} \quad \forall i \in \mathcal{R}, t \in \{0, \ldots, N-1\}$$

The following additional constraints are introduced to reflect the following:

- Inventory that falls below the minimum quality requirement at a given facility is accounted for as waste:

$$\Omega_{i,t} = \sum_{q=q_{i,\min}}^{q_{i,\min}+\Delta q-1} I_{i,q,t} + \sum_{j \in v(i)} \sum_{q=q_{i,\min}}^{q_{i,\min}+\Delta q_{i,j}-1} s_{j,i,q+\Delta q_{j,i},t-\tau_{j,i}} \quad \forall i \in \mathcal{N}, t \in \{0, \ldots, N-1\}$$

- Sales must not exceed demand plus backorder:

$$\sum_{q \in \{\mathcal{Q} | q \geq q_{i,\min}\}} r_{i,q,t} \leq BO_{i,t} + d_{i,t} \quad \forall i \in \mathcal{R}, t \in \{0, \ldots, N-1\}$$

- Inventory must exceed sales from a given retail facility:

$$r_{i,q,t} \leq I_{i,q+\Delta q,t} \quad \forall i \in \mathcal{R}, q \in \mathcal{Q}, t \in \{0, \ldots, N-1\}$$

- Inventory must exceed outgoing shipments from a given facility:

$$\sum_{j \in v(i)} s_{i,j,q,t} \leq I_{i,q+\Delta q,t} \quad \forall i \in \mathcal{N}, q \in \mathcal{Q}, t \in \{0, \ldots, N-1\}$$

- Production must not be exceeded capacity:

$$\sum_{q \in \{\mathcal{Q} | q \geq q_{i,\min}\}} p_{i,q,t} \leq p_{i,t}^{UB} \quad \forall i \in \mathcal{P}, t \in \{0, \ldots, N-1\}$$

- Shipment must not be exceeded capacity:

$$\sum_{q \in \{\mathcal{Q} | q \geq q_{i,\min}\}} s_{i,j,q,t} \leq s_{i,j,t}^{UB} \quad \forall i, j \in \mathcal{A}, t \in \{0, \ldots, N-1\}$$

- Inventory must not be exceeded capacity:

$$\sum_{q \in \{\mathcal{Q} | q \geq q_{i,\min}\}} I_{i,q,t} \leq I_{i,t}^{UB} \quad \forall i \in \mathcal{N}, t \in \{0, \ldots, N-1\}$$

- Terminal constrains at the end of the time horizon:

$$\sum_{q \in \mathcal{Q}} I_{i,q,N} = I_i^s \quad \forall i \in \mathcal{N}$$
$$BO_{i,N} = BO_i^s$$

Table S1: Nomenclature for indices, sets, parameters, and decision variables used to formulate the production and distribution planning optimization problem.

Notation	Description
Indices	
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c_i^h	Per unit inventory holding costs for facility $i \in \mathcal{N}$
c_i^w	Per unit waste/disposal costs for facility $i \in \mathcal{N}$
c_i^b	Per unit backorder costs for facility $i \in \mathcal{R}$
$\rho_{i,q}$	Per unit quality-dependent sales revenue $i \in \mathcal{R}, q \in \mathcal{Q}$
τ_i^p	Production lead time for facility $i \in \mathcal{P}$
$\tau_{i,j}$	Shipment lead time for route $i, j \in \mathcal{A}$
Δq	Quality degradation for inventory in storage over one time period
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$p_{i,q,t}$	Amount produced at facility $i \in \mathcal{P}$, of quality $q \in \mathcal{Q}$, at time t
$s_{i,j,q,t}$	Amount shipped on route $i, j \in \mathcal{A}$, of quality $q \in \mathcal{Q}$, at time t
$r_{i,q,t}$	Amount sold at facility $i \in \mathcal{R}$, of quality $q \in \mathcal{Q}$, at time t
$\Omega_{i,t}$	Amount wasted at facility $i \in \mathcal{P}$, at time t

Details for numerical experiments

We consider the following quality preference value functions for each retailer:

$$\rho_{i,q} = \begin{cases} -\sqrt{q} & \text{if } i = R_1 \\ -q & \text{if } i = R_2 \\ -q^3 & \text{if } i = R_3 \\ -q^2 & \text{if } i = R_4 \end{cases} \tag{S1}$$

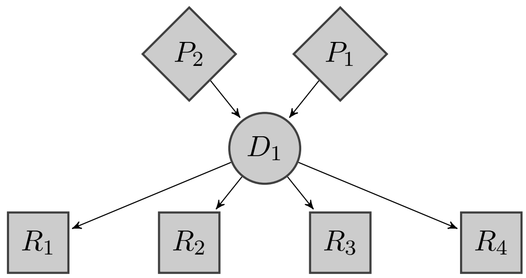

Figure S1: Supply chain network structure used for numerical experiments.

Table S2: Values and configurations of numerical experiments

Parameter	**Value**
Horizon length N	20 days
Quality levels	$\mathcal{Q} = \{1, \ldots, 30\}$ with $\Delta q = 1$
Initial inventories	$I_{i,q,0} = 350 \forall i \in \mathcal{R}, q = 30$, else $I_{i,q,0} = 0$
Initial backorders	$BO_{i,0} = 0 \forall i \in \mathcal{R}$
Production capacity	$p_i^{UB} = 400,000 \forall i \in \mathcal{P}$ units per day
Shipment capacity	$s_{i,j}^{UB} = 500,000 \forall i, j \in \mathcal{A}$ units per day
Inventory capacity	$I_i^{UB} = 50,000 \forall i \in \mathcal{N}$ units per day
Production costs	$c_{P_1}^p = 0.1, c_{P_2}^p = 4$
Shipment costs	$c_{i,j}^s = 2 \forall i, j \in \mathcal{A}$
Holding costs	$c_{P_1}^h = 3, c_{P_2}^h = 3, c_{D_1}^h = .5, c_{R_1}^h = 2, c_{R_2}^h = 2, c_{R_3}^h = 2, c_{R_4}^h = 2$
Backorder costs	$c_{R_1}^{BO} = 50, c_{R_2}^{BO} = 54, c_{R_3}^{BO} = 58, c_{R_4}^{BO} = 82$
Waste costs	$c_i^w = 25 \forall i \in \mathcal{N}$
Prod. lead time	$\tau_i^p = 0 \forall i \in \mathcal{P}$
Ship. lead time	$\tau_{P_1,D_1} = 5, \tau_{P_2,D_1} = 2, \tau_{D_1,R_1} = 1, \tau_{D_1,R_2} = 2, \tau_{D_1,R_3} = 3, \tau_{D_1,R_4} = 4$
Nominal demand	$d_i = 40 \forall i \in \mathcal{R}$

Customer demand disturbance

The nominal demand is time invariant and has a value of 40 units per day for all retailers as indicated in Table S2. At each sampling time t, after computing control input $\mathbf{u}_t$ based on the value of the state estimate $\tilde{\mathbf{x}}$. The realized demand is simulated as follows:

$$d_{i,t} = d_{i,t}^s + \delta_t^i \tag{S2}$$

where δ_t^i is sampled from a normal distribution given by:

$$\boldsymbol{\delta}_t \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \tag{S3}$$

where $\boldsymbol{\delta}_t = [\delta_t^{R_1}, \ldots, \delta_t^{R_4}]$ and $\boldsymbol{\mu}$ is the mean demand vectors, and Σ is the covariance matrix. For performing numerical experiments, the following mean vector and covariance matrix were used:

$$\boldsymbol{\mu} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \boldsymbol{\Sigma} = \begin{bmatrix} 20 & 0 & 0 & 0 \\ 0 & 20 & 0 & 0 \\ 0 & 0 & 20 & 0 \\ 0 & 0 & 0 & 20 \end{bmatrix} \tag{S4}$$

Production quality disturbance

Disturbances for production quality are simulated by sampling values of random variable $\alpha_{i,q} \in \mathbb{R}$ at each sampling time t, and enforcing the following constraints on the production rate:

$$\begin{aligned} &\alpha_{i,q} \sum_{q \in \mathcal{Q}} p_{i,q,t} \leq p_{i,q,t} && \forall i \in \mathcal{P}, q \in \mathcal{Q} \\ &\alpha_{i,q} \sim \frac{1}{\beta_i} \mathcal{N}(\mu_{i,q}^p, \sigma_{i,q}^p) && \forall i \in \mathcal{P}, q \in \mathcal{Q} \\ &\beta_i = \sum_{q \in \mathcal{Q}} \alpha_{i,q} && \forall i \in \mathcal{P} \end{aligned} \tag{S5}$$

The equations in (S5) imply that the fraction of inventory produced at a given quality is random, reflecting the fact that manufacturing of perishable products (e.g., fresh produce) often results in heterogeneous and uncontrollable quality. In this case, β_i is used as a normalization constant to ensure that the sum of $\alpha_{i,q}$ for all quality levels is equal to one. The following values were used for the distribution of α:

$$(\mu_{i,q}^p, \sigma_{i,q}^p) = \begin{cases} (0.05, 0.025) & \text{if } q \in \{13, 19\} \\ (0.09, 0.045) & \text{if } q \in \{14, 18\} \\ (0.19, 0.095) & \text{if } q \in \{15, 17\} \\ (0.29, 0.145) & \text{if } q = 16 \\ (0, 0) & \text{otherwise} \end{cases} \quad \forall i \in \mathcal{P} \tag{S6}$$

Inventory quality disturbance

We consider disturbances to the quality of inventory in storage as described by equation (7) of the main paper. Because of the discrete nature of inventory, $\epsilon_{q,\bar{q},t}^i$ must be a discrete random variable. To simulate this disturbance, we draw from a multinomial distribution where the probabilities are calculated from a normal distribution. We begin by defining a range of possible values of the disturbance:

$$\gamma = [-I_{i,q,t}, -I_{i,q,t} + 1, \ldots, I_{i,\bar{q},t} - 1, I_{i,\bar{q},t}] \tag{S7}$$

we then compute upper and lower bounds as:

$$\gamma^U = \gamma + 0.5, \quad \gamma^L = \gamma - 0.5 \tag{S8}$$

The probability of each value of γ, denoted by $\mathbb{P}(\gamma)$, is approximated using the normal cumulative density function $f_\sigma(x)$, with zero mean and standard deviation σ:

$$\mathbb{P}(\gamma) = f(\gamma^U, \sigma) - f(\gamma^L, \sigma) \tag{S9}$$

which are then normalized so that the probabilities sum to one:

$$\mathbb{P}(\gamma) = \frac{1}{\sum \mathbb{P}(\gamma)} \mathbb{P}(\gamma) \tag{S10}$$

Lastly, $\epsilon^i_{q,\bar{q},t}$ is sampled from the resulting non-uniform discrete distribution of γ. Figure S2 illustrates the discrete probability distribution of $\epsilon^i_{q,\bar{q},t}$ for increasing values of the standard deviation.

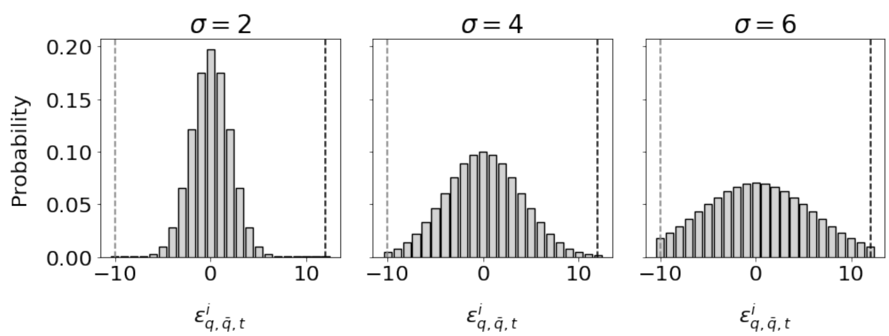

Figure S2: Example probability distribution for inventory quality disturbance $\epsilon^i_{q,\bar{q},t}$ for different standard deviation values for $I_{i,q,t} = 10$ (shown in vertical dashed grey line), and $I_{i,\bar{q},t} = 12$ (shown in vertical dashed black line).

Statistical validation

The supply chain optimization problem was solved for each of the three instances (state feedback, estimation, and nominal) for 40 random simulations for the demand and disturbance. The resulting data was used to perform t-tests to establish statistical significance around the claims of the estimator performance. All data and code used to perform the statistical validation can be found online in our GitHub repository (`https://github.com/Baldea-Group/perishables_SCM_estimation`). The table below summarizes the hypotheses tested and the test results:

Table S3: Summary of statistical validation tests for 40 random samples for each optimization instance.

Hypothesis	**Comparison**	**Mean**		**t-statistic**	**p-value**	**Significant**
		Test	**Control**			
H1: State estimation provides more accurate states than the nominal case	RMSE estimation (test) < RMSE nominal (control)	0.222	0.241	7.31	1.1×10^{-10}	Y
H1: State estimation results in lower operating costs than we using the nominal states	Costs estimation (test) < Costs nominal (control)	26,100	13,200	16.0	3.5×10^{-23}	Y
H1: Perfect feedback results in lower operating costs than we using state estimation	Costs perfect feedback (test) < Costs estimation (control)	3,680	26,100	23.6	2.0×10^{-31}	Y

Extreme disruptions and decreasing capacity redundancy scenarios

This section includes details regarding the extreme scenario disruption simulations to assess the resilience of the proposed supply chain management method. While demand and product quality disturbances are present at every time period, we now consider the case where there are unforecasted production disruptions for an extended period of time. More specifically, we simulate the scenario in which there is no production capacity, i.e. inventory cannot be sourced from producers P_1 and P_2, from $t = 20$ to $t = 30$, and the duration of the outage is unforecasted and unknown. That is, at every time period we assume that production capacity is restored, but orders placed to producers are not getting fulfilled. As a result, retailers deplete all their inventory (Figure S3 top left), and retailer backorder builds up (Figure S3 top right), which also causes operating costs to increase due to rising unfulfilled demand (Figure S3 bottom right). When production at P_1 and P_2 is back online, we see that the system states (inventory and backorder) and operating costs rapidly return to their previous operating levels for both solution approaches (State feedback, and state estimation). Table S4 shows the integral error (IE) comparison for inventory and state variables for all instances considered, confirming that both state feedback and estimation approaches cope with extreme disruptions comparably well. The integral absolute error is given by:

$$IE = \int_{t_0}^{t_f} |x(t) - x_{ss}| \, dt \tag{S11}$$

where $x(t)$ corresponds to the system states and and x_{ss} corresponds to the steady state. For simplicity, we compute the intgeral error over the aggregated states, corresponding to the total retailer inventory and backorder, given by:

$$\sum_{i \in \mathcal{R}} \sum_{q \in \mathcal{Q}} I_{i,q,t}, \quad \sum_{i \in \mathcal{R}} BO_{i,t} \tag{S12}$$

The integral error is estimated numerically using the trapezoidal rule and the inventory and backorder trajectories shown in Figure S3. The steady state value is intended to be a meaningful reference in this case, and is compute as the average for the inventory and backorder states of the undisturbed system after the system stabilizes (based on empirical observation, this was considered to happen at $t > 20$).

Table S4: Integral absolute error for state feedback (Instance 1) and estimation (Instance 3) for the nominal and production disruption scenarios.

Instance	**Inventory IE**	**Backorder IE**
State feedback	643.5	994.5
State feedback (disrupted)	2565.5	6240.3
Estimation	626.0	868.1
Estimation (disrupted)	2553.5	6186.2

We also performed numerical experiments for increasing demand values at the same production, shipment and inventory capacities to evaluate if our managerial claims hold for decreasing system redundancy. The results for these numerical experiments are shown in Figure S4, which indicate that increasing demand loads (that is lower supply chain redundancy) do not change the performance of the proposed estimation technique relative to when perfect information (i.e. state feedback) is implemented.

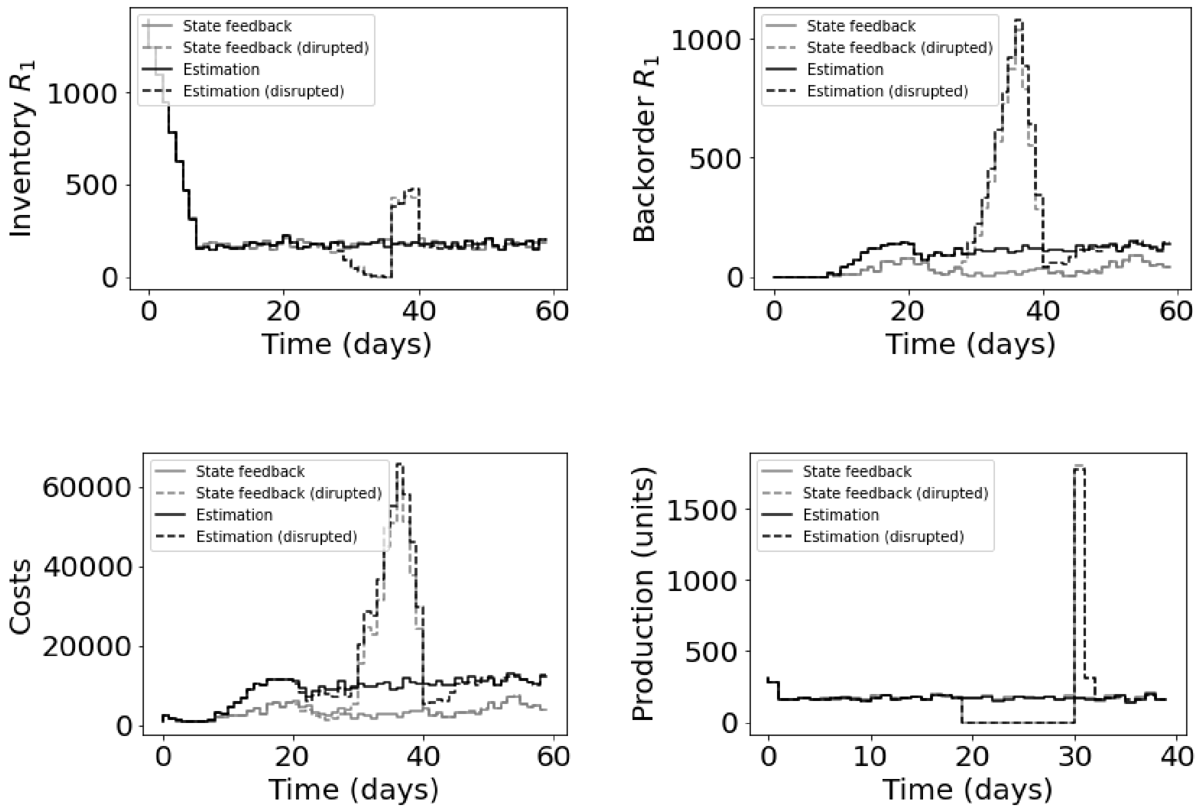

Figure S3: Inventory (top left), backorder (top right), operating costs (bottom left) and production (bottom right) trajectories comparing the proposed receding horizon strategy using perfect feedback (Instance 1) and state estimation (Instance 3) for the undisrupted and production disruption scenarios.

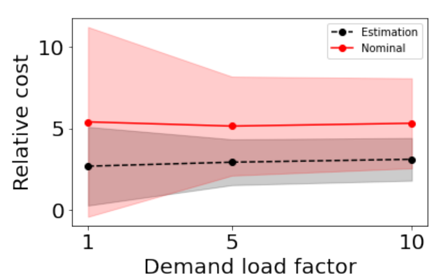

Figure S4: Costs for Estimation and Nominal instances relative to State Feedback for increasing demand loads. The demand load corresponds to factor used to scale the nominal demand in Table S2 to simulate a supply chain operated with lower redundancy.

Practical Implementation Guidelines for Online Estimation of Perishable Inventory in Supply Chains

Step 1. ***Gather Required Data and Supply Chain Parameters***

The following information is required in order to set up the proposed model:

- **Number of Facilities (n):** Total number of nodes in the supply chain, including producers, distribution centers, and retailers.
- **Capacities (C_i):** Maximum capacity of each facility, such as production capacity for producers (p_i^{UB}), shipment capacity for routes ($s_{i,j}^{UB}$), and inventory capacity for distribution centers (I_i^{UB}).
- **Distances ($d_{i,j}$):** Distance between nodes i and j, such as between producers and distribution centers, and between distribution centers and retailers.
- **Demand (D_i):** Demand at each retailer i for perishable products, considering product shelf life and consumer demand patterns.
- **Production Costs (c_i^p):** Per unit production costs at facility i for producers.
- **Shipment Costs ($c_{i,j}^s$):** Costs associated with moving perishable products from node i to node j.
- **Inventory Holding Costs (c_i^h):** Per unit inventory holding costs at facility i.
- **Waste/Disposal Costs (c_i^w):** Per unit waste or disposal costs for facility i.
- **Backorder Costs (c_i^b):** Per unit backorder costs at retailer i.
- **Quality-Dependent Sales Revenue ($\rho_{i,q}$):** Per unit quality-dependent sales revenue at retailer i, for quality q.
- **Lead Times (τ_i^P, $\tau_{i,j}$):** Production lead time (τ_i^P) at facility i and shipment lead time ($\tau_{i,j}$) for route i to j.
- **Degradation Rate Model:** $f(q(t), k(t))$**:** A model of how a particular perishable good degrades over time t, potentially influenced by transportation conditions, storage conditions, and handling (Equation (1)). This will be utilized as described in Step Step 2.
- **Minimum Quality Requirement ($q_i^{\mathbf{min}}$):** Minimum quality requirement for facility i.
- **Steady-State Inventory and Backorder (I_i, BO_i):** Steady-state inventory and backorder terminal conditions for facility i.
- **Transportation Costs ($c_{i,j}$):** Costs associated with moving perishable products from producers to distribution centers and from distribution centers to retailers, including costs related to maintaining product quality during transit (e.g., refrigerated transport).
- **Fixed Costs (f_i):** Fixed costs associated with operating each node in the supply chain, such as production costs for producers, storage costs for distribution centers, and operational costs for retailers.

- **Planning Horizon (T):** The period over which the supply chain decisions with the given network parameters are planned. While shorter horizons enable more frequent replenishment cycles thus reducing the risk of spoilage, longer horizons may be necessary for seasonal planning or capacity decisions.

- **Prediction and Control Horizons (N):** The time span that represents how far ahead the controller forecasts the system's state and outputs to make decisions.

Step 2. ***Build Discretized Version of the Product Quality Degradation Model***

- Following *Algorithm 1* of Lejarza and Baldea (2021b), determine the minimum number of quality levels for the perishable product under consideration. This makes use of the known product quality degradation dynamics as provided by Equation (1) in the paper. The algorithm will provide the number of discrete quality levels, $|Q|$ ($q \in \{1, 2, \ldots, |Q|\}$), as well as Δq, $\Delta q_{i,j}$, which represent the quality degradation over one time period during storage (Δq), or in transit ($\Delta q_{i,j}$) over shipment time ($\tau_{i,j}$).

- Per *Assumptions 4.5 and 4.6*, normalize quality levels such that the quality degradation rate becomes unity. Therefore, $|Q| = ceil(|Q|/\Delta q)$ and $\Delta q' = 1$.

Step 3. ***Build Linear State-Space Model of the Supply Chain Network and Determine Observability and Controllability Properties***

- Build a State-Space representation of the system dynamics by including inventory and backorder balances as outlined in Section 4 of the paper. Construct the state-space matrices **A, B, C, D** followed by the observability and controllability matrices.

- If the system is not observable (Matrix **O** in Equation 19 does not meet the rank condition in *Lemma 4.8*), the MHE algorithm's estimates may be unreliable or even infeasible. In this case, the observability analysis can inform decisions on implementing additional measurements to make the system observable.

- The primary challenge in practice arises from partial/inadequate sensing. This implies that if *Assumption 4.5* is not met (e.g., when the net inventory/shipment measurements are either unavailable at certain instants or are received with time delays), the approach will not be effective.

Step 4. ***Set up the Moving Horizon Estimation (MHE) Framework***

Set up the MHE framework with known initial system states (inventories/backorders) and an initial guess for the process noise covariance matrix **Q** (Equation 23 in the paper). In principle, for a fully observable system, **Q** can be estimated using approaches such as the Expectation Maximization (EM) algorithm with the difference between the estimated states from successive iterations serving as a proxy for residuals. Since all measurements concerning net inventory levels in storage and transit are assumed to be perfect, measurement noise is absent in the MHE objective function (and constraint equations).

Choosing an appropriate horizon length $\tilde{N}$ for MHE involves several considerations, and some trial and error may be involved:

- System dynamics:

– In faster systems, shorter time horizons are typically adequate, whereas slower systems may require longer horizons to effectively capture significant dynamics. The selected horizon length should be sufficiently long to encompass the slowest dynamics of the systems, including delays associated with shipments. One strategy could involve determining the longest duration of shipping delays and degradation times, then adding a few additional time steps.

– Theoretically, MHE remains stable as long as the horizon length exceeds the system's order or observability index. Another practical guideline is to set the horizon length to twice the system's order [10].

- Computational resources: Available processing power and memory constrain the maximum practical horizon length.

- Estimation accuracy: Longer horizons typically improve estimation accuracy but with diminishing returns beyond a certain length.

Step 5. ***Compute Implementable Policy and Transfer to Supply Chain***

- Compute implementable policy as described in Section 6.1. In practical scenarios where the true state of the system is unknown, robust control/chance-constrained optimization approaches may be necessary to guarantee that the computed control inputs remain feasible under certain assumptions about the distribution of state estimation errors.

Computational Aspects

- To optimize computational efficiency without sacrificing accuracy, careful consideration of the control horizon length, as outlined previously, is essential. Additionally, heuristics for quality level discretization and reducing the overall MPC problem size, as detailed in Lejarza, Pistikopoulos, and Baldea [8] and Lejarza and Baldea [7], can further enhance computational performance.

- For representing MHE problems, specialized modeling languages and libraries can greatly simplify implementation by providing high-level abstractions for defining dynamic optimization problems. Our implementation leveraged Pyomo in conjunction with other Python libraries. The solver selection depends on the problem structure, size, and real-time requirements and we have chosen CPLEX as the solver given its compatibility with the linear constraints and quadratic objective functions in our problem. All the code and data that support the findings of this study are openly available in `https://github.com/Baldea-Group/perishables_SCM_estimation`, and can be used as a basis for practical implementation.

Table S5: Summary of relevant literature and comparison to the present work.

Reference	Topic	Modeling Approach	Perishable Inventory	Uertainty source	Information Availability	Control/Estimation
Rong, Akkerman, and Grunow [11]	Production planning in food supply chains	Deterministic production planning using MILP	Yes	None	Complete (all inventories and shipments at all quality levels in all supply chain entities)	No / No
Grunow and Piramuthu [3]	Role of RFID in reducing wastage of perishable food items	Economic order quantities under various conditions with RFID availability	Yes	Demand, product quality	Complete (when RFID technology is implemented)	Yes / No
Amorim, Alem, and Almada-Lobo [2]	Risk-averse production planning in food supply chains	Risk-averse production planning using MILP models, comparing CVaR and UPM	Yes	Stochastic demand and product degradation	Discrete scenarios for demand and degradation	No / No
Amorim, Günther, and Almada-Lobo [1]	Production scheduling and distribution planning in food supply chains	Deterministic, multi-objective MINLP models	Yes	None	Complete (all inventories and shipments along with deterministic known consumer demands)	No / No
Subramanian, Rawlings, and Maravelias [12]	Production and distribution planning with integration of scheduling and control	Model predictive control with multi-objective cost function reflecting economic costs and risks	No	Demand	Complete (perfect inventory measurement and feedback)	Yes / No
Wang and Rivera [14]	Supply chain management in semiconductor manufacturing	Model predictive control with state estimation via Kalman Filtering	No	Demand, throughput times, and yield	Partial (inventory measurements at certain nodes and forecasted demand information)	Yes / Yes
Villegas and Pedregal [13]	Time series forecasting for supply chain decision support	Hierarchical time series forecasting using state space models and Kalman filter	No	Demand	Partial (aggregated demand, e.g., at regional level)	No / Yes
Mor et al. [9]	Time series forecasting for supply chain decision support	Time series forecasting models, including moving averages, multiple regressions, and Holt–Winters	Yes	Demand	Complete (historical data available)	No / Yes
Lejarza and Baldea [6]	Production and distribution planning for supply chains of perishable inventory	Model predictive control with MILP for production and distribution planning	Yes	Demand and degradation rate	Complete (perfect inventory measurement and feedback)	Yes / No
Lejarza, Pistikopoulos, and Baldea [8]	Production and distribution for large-scale supply chains of fresh produce	Model predictive control with efficient strategies for MILP production and distribution planning	Yes	Demand	Complete (perfect inventory measurement and feedback)	Yes / No
Lejarza and Baldea [7]	Production and distribution planning for supply chains of perishable inventory	Deterministic production planning using MILP, solved with efficient strategies	Yes	None	Complete (all inventories and shipments at all quality levels for all attributes in all supply chain entities)	No / No
Ketzenberg, Bloemhof, and Gaukler [4]	Time and temperature information for managing perishables	Markov Decision Processes comparing informed vs. uninformed inventory policies	Yes	Demand and product degradation	Partial (demand and product quality distributions available)	Yes / No
Ketzenberg, Gaukler, and Salin [5]	Perishable inventory control and expiration date setting	Retailer replenishment policies via Markov Decision Process (MDP)	Yes	Demand and product degradation	Partial (demand and product quality distributions available)	Yes / No
Present Paper	Product quality estimation and production and distribution planning for supply chains of perishable inventory	Moving horizon estimation and control with MILP for production and distribution planning	Yes	Demand and product degradation	Partial (aggregated inventory levels available only for certain facilities)	Yes / Yes

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