Data-driven optimization of processes with degrading equipment

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Abstract

In chemical and manufacturing processes, unit failures due to equipment degradation can lead to process downtime and significant costs. In this context, finding an optimal maintenance strategy to ensure good unit health while avoiding excessive expensive maintenance activities is highly relevant. We propose a practical approach for the integrated optimization of production and maintenance capable of incorporating uncertain sensor data regarding equipment degradation. To this end, we integrate data-driven stochastic degradation models from Condition-based Maintenance into a process level mixed-integer optimization problem using Robust Optimization. We reduce computational expense by utilizing both analytical and data-based approximations and optimize the Robust Optimization parameters using Bayesian Optimization. We apply our framework to five instances of the State-Task-Network and demonstrate that it can efficiently compromise between equipment availability and cost of maintenance.

1 Introduction

Most technical processes contain equipment which degrades over time due to its usage. Degradation may lead to serious equipment failures, unless preventive maintenance actions are scheduled regularly to restore equipment conditions. While frequent preventive maintenance can keep equipment availability high, it also incurs significant cost. At the same time, unexpected equipment failures can lead to loss of production and high corrective maintenance costs. Finding the optimal balance between preventive and corrective maintenance is difficult, because degradation
tends to be at least partially random and the health state of equipment can often only be estimated from data subject to uncertainty. To make things worse, scheduling maintenance activities is not independent from production planning and scheduling. A unit undergoing maintenance might, for example, be unavailable for production. Furthermore, the state of equipment health tends to depend not only on the selected maintenance strategy, but also on the process operating strategy. Operating a process with a high throughput might enable higher production volumes and more sales, but could also cause more equipment degradation and therefore a higher maintenance cost. These interactions between process conditions, maintenance strategy, and the equipment’s uncertain state of health make finding optimal and compatible maintenance and operating strategies a very challenging data-driven optimization problem under uncertainty.

One way of reducing the equipment maintenance cost is to determine maintenance schedules based on information regarding the equipment’s state of health collected through condition monitoring\(^1\). This is the Condition-based maintenance (CBM) paradigm\(^1\). Due to the increased availability of cheap sensors and thereby large quantities of system health data, CBM is becoming more attractive\(^5\). While much attention has been paid to data collection & processing and prognostic modeling, the objective is usually to minimize the cost of maintaining a single unit\(^4\). This means that interaction between maintenance strategies for each piece of equipment and the operating strategy of the entire process has largely been neglected.

However, these interactions have been considered by multiple authors in the context of integrated maintenance scheduling and process optimization. Early approaches in this field which explicitly model degradation assume constant, known reliability or decay curves\(^6\)\(^10\). Dedopoulos and Shah\(^6\)\(^7\) combine short-term stochastic scheduling with long-term maintenance scheduling in a two-step procedure, while Vassiliadis and Pistikopoulos\(^9\) determine optimal availability thresholds at which maintenance should be performed. Georgiadis et al.\(^11\) optimize the cleaning and energy management of heat exchanger networks subject to fouling, which is assumed to follow a known profile. Liu et al.\(^12\) consider scheduling of maintenance and biopharmaceutical batch production with a deterministic performance decay. Xenos et al.\(^13\) optimize maintenance and production scheduling of a compressor network. The power consumed by the compressors is assumed to increase linearly with operating time (since maintenance was performed) due to fouling. Zulkafi and Kopanos\(^14\)\(^15\) develop an optimization framework for simultaneous operational planning and maintenance scheduling of production and utility systems. They consider extra energy costs caused by performance degradation. The degradation is assumed to depend on operating time and the production rate. Aguirre and Papageorgiou\(^16\) consider
integrated planning, scheduling and maintenance under schedule-dependent, deterministic performance decay. Rajagopalan et al.\textsuperscript{17} analyze turnaround rescheduling and apply stochastic programming to manage unplanned outages. Biondi et al.\textsuperscript{18} extend the State Task Network (STN), originally proposed by Kondili et al.\textsuperscript{19}, to account for degrading equipment and different operating modes. They assume that each unit, after maintenance, has a given maximum residual lifetime and that each task performed on a unit in a certain operating mode reduces this residual lifetime by a given amount. Noticeably, none of these authors make use of the wealth of knowledge regarding degradation modeling and inference from data available from the CBM literature. Furthermore, degradation is assumed to be deterministic which may not be the case in practice.

Recent works have started to incorporate degradation models from CBM into process level Mixed-Integer Linear Programming (MILP) problems. Yildirim et al.\textsuperscript{20,21} formulate an optimization model for generator maintenance and production scheduling. The cost of maintenance is calculated beforehand using a data-driven degradation model:

$$c_t = c_{\text{prev}} \left(1 - p_f^t\right) + c_{\text{corr}} p_f^t \int_0^t p_f^\tau d\tau,$$

where $c_t$ is the predicted cost of performing maintenance at time $t$ given the cost of preventive ($c_{\text{prev}}$) and corrective ($c_{\text{corr}}$) maintenance. The failure probability $p_f^t = P(\text{unit fails before } t)$ is calculated from the degradation model. The authors later applied the same approach to maintenance and operation of wind farms and extended it to include opportunistic maintenance\textsuperscript{22}. While this approach starts to incorporate information from more sophisticated degradation models into process level optimization problems, degradation is still considered to be deterministic in the MILP optimization. Başçiftci et al.\textsuperscript{23} extend this to consider sudden failures by using stochastic programming and generating scenarios from the underlying degradation model. To the best of our knowledge Başçiftci et al.’s\textsuperscript{23} approach is the only work combining stochastic optimization with information from degradation models.

Unfortunately, the aforementioned approach cannot capture effects of the selected operating strategy on degradation. Since maintenance cost is calculated based on the degradation model before the optimization problem is solved, the degradation is assumed to be independent of the operating strategy. In practice this will often not be the case.

This paper argues for a tighter integration between the sophisticated degradation models used in CBM and process level maintenance scheduling and process optimization. To this end we make multiple contributions:
• We show how Lévy type models, a class of stochastic processes commonly used in Degradation Modeling, can be incorporated into an integrated maintenance and process MILP model. Lévy type models include the Wiener and Gamma processes – two very popular models in CBM. By making the Lévy models parameters depend on a set of operating modes, equipment degradation too depends on the operating strategy.

• We show how uncertainty and randomness in the equipment’s degradation characteristics can be incorporated using adjustable robust optimization. We use results from the CBM literature to efficiently determine the robustness of the obtained solution.

• We prove that, in certain cases, feasible solutions to the adjustable robust optimization problem can be found by solving a deterministic approximation with worst case values for the uncertain parameters.

• Realizing that process planning and scheduling can be computationally expensive yet highly repetitive, we develop a computationally efficient, data-driven way of a-priori estimating equipment failure probabilities. To this end, we generate data using a short-term scheduling model repeatedly. Using this data, we propose two methods based on Logistic Regression capable of cheaply generating a large number of long-term schedules which can be used to estimate failure probabilities.

• We propose Bayesian optimization for efficiently optimizing the uncertainty set. The uncertainty set size depends on a small number of parameters, but solving the robust MILP integrated maintenance and process optimization problem can be computationally expensive. Bayesian optimization is ideal for this kind of low dimensional problem with expensive function evaluations.

As a challenging case study, we apply the proposed method to an extension of the state-task-network (STN)\textsuperscript{18,19}. This model combines both planning and scheduling of production and maintenance with operating mode dependent equipment degradation. We test our method on a number of STN instances\textsuperscript{18,23,27}. 

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2 Combining degradation modeling and robust optimization

Following Vassiliadis and Pistikopoulos, we assume an integrated production and maintenance scheduling problem of the form

\[
\begin{align*}
\min_{x, m} & \quad \text{cost}(x, m) \\
\text{s.t.} & \quad \text{process model}(x, m), \\
& \quad \text{maintenance model}(x, m),
\end{align*}
\]

(1)

where \(x\) are the process variables (continuous and discrete) and \(m\) are the maintenance related variables. The process model includes, e.g., material balances, energy balances, unit constraints, and the maintenance model includes, e.g., maintenance crew constraints or constraints regarding different types of maintenance. Note that cost minimization could easily be replaced by profit maximization.

A health model added to Problem 1 accounts for equipment degradation:

\[
\begin{align*}
\min_{x, m, h} & \quad \text{cost}(x, m, h) \\
\text{s.t.} & \quad \text{process model}(x, m, h), \\
& \quad \text{maintenance model}(x, m, h), \\
& \quad \text{health model}(x, m, h),
\end{align*}
\]

(2)

where \(h\) are health related variables and the health model includes all equipment health or degradation related constraints. Our first contribution is developing a generic health model based on the assumption that the equipments’ state of health can be described by Lévy type processes, a class of stochastic processes commonly used for modeling degradation in CBM.

2.1 Degradation Modeling

The premise in Degradation Modeling is that a degradation signal \(s_{\text{meas}}(t)\) describes the state of degradation of a unit over time. Signal \(s_{\text{meas}}(t)\) can either be measured directly or obtained indirectly from measurements. Two common assumptions adopted in this paper are that:

\((\text{SMAX})\) The unit fails and requires corrective maintenance when \(s_{\text{meas}}(t)\) crosses a threshold \(s_{\text{max}}^{\text{28}}\).
The degradation signal \( s(t) \) is often modeled by stochastic processes\(^4\). One class of stochastic processes are Lévy type processes:

**Definition 1. Lévy type process\(^{30}\).** A stochastic process \( S(t) = \{S_t : t \in T\} \), where \( S_t \) is a random variable, with

1. independent increments: \( S_{t_2} - S_{t_1}, \ldots, S_{t_n} - S_{t_{n-1}} \) are independent for any \( 0 < t_1 < t_2 < \ldots < t_n < \infty \),
2. stationary increments: \( S_t - S_s \) and \( S_{t-s} - S_0 \) have the same distribution for any \( s < t \),
3. continuity in probability: \( \lim_{h \to 0} P(\lvert S_{t+h} - S_t \rvert > \epsilon) = 0 \) for any \( \epsilon > 0, \ t \geq 0 \).

Lévy type processes include both the Wiener and Gamma processes, which are the most commonly used stochastic processes in the Degradation Modeling literature\(^4,31–33\). Due to their independence and stationarity, Lévy type process increments can be described by

\[
S_t - S_{t-\Delta t} = D(\Delta t), \quad D(\Delta t) \sim \mathcal{D}(\theta, \Delta t), \quad \forall t, \tag{3}
\]

where \( D(\Delta t) \) is a random variable that follows a given distribution \( \mathcal{D}(\theta, \Delta t) \) with parameters \( \theta \). A difficulty, however, arises when \( D \) is also dependent on some of the operational variables \( x \):

\[
D(\Delta t) \sim \mathcal{D}(\theta(x), \Delta t). \tag{4}
\]

This dependence has been addressed by assuming that the operational variables \( x \) are piecewise constant, i.e., the process can only operate in a number of discrete operating modes \( k \in K \)\(^{34,35}\). Under this assumption Eqns. 3 and 4 simplify to

\[
S_t - S_{t-\Delta t} = \sum_{k \in K} x_{k,t} \cdot D_k(\Delta t), \quad D_k(\Delta t) \sim \mathcal{D}(\theta_k, \Delta t), \tag{5}
\]

where \( x_{k,t} \) is 1 if the process operates in mode \( k \) at time \( t \) and 0 otherwise. Note that this approach is very similar to regime-switching Lévy models used extensively in finance\(^36\). Biondi et al.\(^{18}\) use a similar approach in their STN extension.

Much of the Degradation Modeling literature focuses on estimating \( \theta \) and using, e.g., Bayesian approaches to update it regularly based on new available data\(^{37,38}\). A major advantage of Bayesian approaches is that \( \theta \) can be estimated based on a population of units first and then individually adjusted to a particular unit\(^{39}\).
2.2 Constructing a health model

We summarize the assumptions on which health model 2c hereafter is based: For each process unit \( j \), a degradation signal \( s_{j,\text{meas}}(t) \) can be obtained from measurements which is modeled well by a Lévy process \( S_j(t) \), i.e., increments follow Eqn. 5. The unit fails when \( S_j(t) \) reaches a maximum threshold \( s_{j,\text{max}} \) (SMAX) \( (T^{\text{fail}} = \inf\{t \in T|S_{j,t} > s_{j,\text{max}}\}) \) and \( S_j(t) \) resets to an initial value \( s_j^0 \) after maintenance (AGAN). Based on these assumptions and assuming a discrete time formulation, the following health model replaces Eqn. 2c:

\[
S_{j,t} \leq s_{j,\text{max}} \quad \forall t, j \in J
\]

\[
S_{j,t} = \begin{cases} 
S_{j,t-1} + \sum_{k \in K} x_{j,k,t} \cdot D_{j,k}, & \text{if } m_{j,t} = 0 \\
0, & \text{otherwise}
\end{cases} \quad \forall t, j \in J, \quad (6)
\]

where \( J \) is the set of process units and \( m_{j,t} \) is 1 if a maintenance action starts on unit \( j \) at time \( t \) and 0 otherwise. To address the random nature of degradation, the random variables \( D_{j,k} \) and \( S_{j,t} \) can be approximated by an uncertain parameter \( \bar{d}_{j,k} \) and a deterministic variable \( s_{j,t} \) respectively. Assuming that \( \bar{d}_{j,k} \) is bounded by a compact uncertainty set \( U \), Problem 2 can be robustified by requiring that all constraints hold for any \( \bar{d}_{j,k} \in U \):

\[
s_{j,t} \leq s_{j,\text{max}} \quad \forall t, j \in J
\]

\[
s_{j,t} = \begin{cases} 
s_{j,t-1} + \sum_{k \in K} x_{j,k,t} \cdot \bar{d}_{j,k}, & \text{if } m_{j,t} = 0 \\
0, & \text{otherwise}
\end{cases} \quad \forall \bar{d}_{j,k} \in U, t, j \in J. \quad (7)
\]

This model explicitly considers preventive maintenance. Corrective maintenance becomes necessary only when realizations of \( \bar{d}_{j,k} \) lie outside the uncertainty set \( U \) and constraint \( s_{j,t} \leq s_{j,\text{max}} \) is violated.

Notice that it is generally not possible to choose \( s_{j,t} \) such that the equality constraint in Problem 7 holds for all values of \( \bar{d}_{j,k} \) in \( U \), except for the trivial solution \( x_{j,k,t} = 0, \forall j, k, t \). This is because the degradation signal \( s_{j,t} \) is an analytical variable, not a decision variable. Interpreting the degradation signal instead as a second stage variable \( s_{j,t}(\bar{d}_{j,k}) \) turns Problem 7 into an adjustable robust optimization problem and a linear decision rule can be used to express \( s_{j,t} \) as a function of \( \bar{d}_{j,k} \):

\[
s_{j,t}(\bar{d}_{j,k}) = [s_{j,t}]_0 + \sum_k [s_{j,t}]_k \bar{d}_{j,k}, \quad (8)
\]

where \([s_{j,t}]_0\) and \([s_{j,t}]_k\) are coefficients which become variables in the adjustable robust problem. Technically, \( \bar{d}_{j,k} \) should also be indexed by \( t \) as every time period constitutes
an independent realization of $D_{j,k}$. Time-indexed uncertain parameters have been previously explored\textsuperscript{21}, but they can lead to a large increase in variables, especially for discrete time formulations. We therefore make the simplifying assumption that uncertainty is only revealed once after all variables except $s_{j,t}$ have been selected.

The health model\textsuperscript{7} can be reformulated to remove the conditional equality constraint, resulting in the final formulation:

$$\begin{align*}
\min_{x,m} \ & \text{cost}(x = [x_{j,k,t}, \ldots]^\top, m = [m_{j,t}, \ldots]^\top, h = [s_{j,t}(\tilde{d}_{j,k})]^\top) \\
\text{s.t} \ & \text{process model}(x, m, h) \\
& \quad \text{maintenance model}(x, m, h) \\
& \quad \text{maintenance model}(x, m, h) \\
& \quad \text{maintenance model}(x, m, h) \\
\end{align*}$$

By replacing $s_{j,t}(\tilde{d}_{j,k})$ with Eqn. 8 in each constraint and using standard robust optimization reformulation techniques, the health model can be transformed into a deterministic robust counterpart (see Appendix A).

Consider a deterministic version of Problem 9 in which cost, process model, and maintenance model are not functions of $s_{j,t}(\tilde{d}_{j,k})$ and $\tilde{d}_{j,k}$ has been replaced by $d_{j,k}^{\max} = \max_{\tilde{d}_{j,k}} \tilde{d}_{j,k}$:

$$\begin{align*}
\min_{x,m} \ & \text{cost}(x, m) \\
\text{s.t} \ & \text{process model}(x, m) \\
& \quad \text{maintenance model}(x, m) \\
& \quad \text{maintenance model}(x, m) \\
& \quad \text{maintenance model}(x, m) \\
& \quad \text{maintenance model}(x, m) \\
\end{align*}$$

where $s_{j,t}$ is not a second stage variable anymore since there are no more semi-infinite constraints. Under certain circumstances, feasible solutions to robust Problem 9 can be found by solving deterministic Problem 10.
Theorem 1. Given that cost, process model, and maintenance model are not functions of $\tilde{d}_{j,k}$ and that $s_j^0 \leq s_j^{\text{init}} = s_{j,t=t_0} \leq s_j^{\text{max}}$ and $\tilde{d}_{j,k} \geq 0, \forall \tilde{d}_{j,k} \in U$, then a feasible solution $(x = [x_{k,t}, \ldots], m = [m_t, \ldots], h = [s_t])$ to Problem 10 forms a feasible solution $(x = [x_{k,t}, \ldots], m = [m_t, \ldots], h = [s_t])$ to Problem 9 with

$$[s_t]_0 = \begin{cases} s^{\text{init}} & t < m,0 \\ s^0 & t \geq m,0 \end{cases}$$

(11a)

$$[s_t]_k = \sum_{t'=m,t} x_{k,t},$$

(11b)

where $s^{\text{init}} = s(t = 0)$, $m,0$ is the first point in time at which maintenance is performed, and $m,t$ is the most recent point in time at which maintenance was performed.

Proof. See Appendix [B].

Theorem 1 only guarantees solution feasibility, not optimality. How well Problem 10 approximates Problem 9 also depends on the selected uncertainty set.

2.3 The uncertainty set

A major decision in robust optimization is the uncertainty set choice. This paper uses a simple box uncertainty set

$$U = \{\tilde{d}_{j,k} | \tilde{d}_{j,k}(1 - \epsilon_{j,k}) \leq \tilde{d}_{j,k} \leq \tilde{d}_{j,k}(1 + \epsilon_{j,k})\},$$

where $\tilde{d}_{j,k}$ is the nominal value of $\tilde{d}_{j,k}$ and $\epsilon_{j,k}$ is a parameter determining the uncertainty set size. Note that this choice assumes that the random increments $D_{j,k}$ are independent, as a box uncertainty set cannot capture correlation between uncertain parameters. This assumption could be relaxed with a more complicated uncertainty set, e.g., a polyhedral set. Since Degradation Modeling assumes that the distribution of $D_{j,k}$ is known, $\epsilon_{j,k}$ can be determined using the inverse cumulative distribution function $F^{-1}$:

$$\epsilon_{j,k} = 1 - F^{-1}(\alpha)/\tilde{d}_{j,k},$$

where $\alpha = P(D_{j,k} \leq \tilde{d}_{j,k}(1 - \epsilon_{j,k}))$. If the distribution of $D_{j,k}$ is unknown, data-driven non-parametric methods such as Kernel Density Estimation can be used to estimate it.

By using $F^{-1}$, the uncertainty set size depends on a single parameter $\alpha \in [0, 0.5]$. For $\alpha = 0$, the uncertainty set includes all possible realizations of $D_{j,k}$ and for $\alpha = 0.5$...
the uncertainty set is a singleton and the robust optimization problem is equivalent to the deterministic problem using the nominal values $\tilde{d}_{j,k}$. While box uncertainty sets are often more conservative than most of the many other available uncertainty set types, the solution robustness/conservatism in this formulation can be varied by adjusting $\alpha$.

2.4 Evaluating robustness

Assume $x_j^k = [k_1, k_2, \ldots, k_T]$, where $k_t = k \iff x_{j,k,t} = 1$, is the sequence of operating modes given by a solution to Problem 9. Its robustness can be measured by the probability $p_j$ that unit $j$ does not fail in the time horizon $T$

$$p_j = P(S_{j,t} \leq S_{j,\text{max}}, \forall t < T|x_j^k),$$

or equivalently its probability of failure

$$p_f^j = 1 - p_j = P(\exists t < T \text{ such that } S_{j,t} > S_{j,\text{max}}|x_j^k).$$

Assuming the parameters $\theta_{j,k}$ of the distributions $D_{j,k}$ are estimated from data, $p_f^j$ can be calculated through Monte-Carlo simulation by randomly generating $N$ realizations $s_{j,t}^n = [s_{j,0}^n, s_{j,\Delta t}^n, \ldots, s_{j,T}^n]$ of $S_j(t, x_j^k)$ with $D_{j,k}(\theta_{j,k}, \Delta t)$ distributed increments and checking how many violate $s_{j,t}^n \leq s_{j,\text{max}}$:

$$p_f^j = \frac{\sum_{n=1}^{N} 1(\exists t < T \text{ such that } s_{j,t}^n > s_{j,\text{max}})}{N}, \quad (12)$$

where $1$ is the indicator function. This is illustrated in Fig. 1 for $N = 3$.

In the special case where $D_{j,k}$ is normal distributed $D_{j,k} \sim N(\mu_{j,k} \Delta t, \sigma_{j,k}^2 \Delta t)$, i.e., the Wiener process model is used, $p_f^j$ can be efficiently calculated using analytical results for the crossing probability of a Brownian motion on a piecewise linear boundary. Instead of sampling from $D_{j,k}$ at regular time intervals $\Delta t$, this approach only randomly samples at operating mode transitions ($k_t \neq k_{t+1}$). It requires far less Monte-Carlo samples and is therefore faster than the general method outlined above. A detailed description of this approach is given in the Appendix D.

2.5 Estimating failure probabilities

Evaluating the probability of failure $p_f^j$, e.g., using Eqn. 12 requires the exact sequence of operating modes $x_j^k$ and maintenance actions to be known over the evaluation horizon $T$. Since maintenance tends to be infrequent, $T$ has to be sufficiently
Figure 1: Example for calculating the failure probability $p_{j}^{f}$ using Eqn. [12] and Monte-Carlo simulation. The operating mode schedule is $x^{k} = [1, 2, \text{Maint.}]$.

Figure 2: Frequency approach: Estimating $p_{j}^{f}$ from historical data using Algorithm 1.
long to obtain meaningful failure probabilities. Solving Problem 9 over a long time horizon may be computationally challenging. Instead, it may be possible to use existing data of past schedules to estimate $p_j^f$. If no historical data is available, it can be generated by solving Problem 9 over a shorter horizon. This section outlines two methods by which an upper estimate of $p_j^f$ can be obtained from data.

2.5.1 Frequency approach

Assuming time discretization, a conceptually easy way to obtain an upper bound $\bar{p}_j^f$ on $p_j^f$ is to generate the set $\mathcal{X}$ of all possible permutations of operating mode sequences $x^k_j = [k_{j,1}, k_{j,2}, \ldots, k_{j,T}]$ and find the maximum probability of failure

$$\bar{p}_j^f = \max_{x \in \mathcal{X}} p_j^f(x^k_j).$$

For any realistic problem $\mathcal{X}$ will be very large, but there are two ways to reduce its size: First, the operating mode sequences can be generated without considering maintenance. Maintenance actions can then be inserted consecutively at the latest point in time $t_{m,l}$ which satisfies

$$\max_{d_{j,k} \in \mathcal{U}} \sum_{t' = t_{m,l} - 1}^{t_{m,l}} \sum_k x_{j,k,t'} d_{j,k} < s_{j,max}^T - s_{j,0}^T,$$

where $t_{m,l-1}$ is the previous maintenance activity and $t_{m,0} = 0$. $\bar{p}_j^f$ remains an upper bound, because maintenance at a later point in time always causes a larger probability of failure. Secondly, it may be possible to estimate the frequency of occurrence $n_{j,k} = \sum_t x_{j,k,t}$ of each operating mode $k$ from data. If these frequencies are modeled as random variables $N_{j,k}$, a smaller $\mathcal{X}$ can be obtained by only generating sequences which obey frequencies drawn from the distributions of $N_{j,k}$. This suggests the following algorithm for obtaining an estimate of $\bar{p}_j^f$ which is also visualized in Fig. 2:

If $N$ is large enough and the estimated distribution of $N_{j,k}$ is accurate, $\bar{p}_j^f$ should be a good upper bound on $p_j^f$.

2.5.2 Markov chain approach

The second approach for estimating $p_j^f$ is inspired by the use of Markov chains in regime-switching models in finance and to some extent also in the CBM literature for modeling different environment or operating regimes of a process. The
Algorithm 1 Frequency approach [illustrated in Fig. 2]

1: procedure estimate $\bar{p}_j^f$
2: $\eta_{n,j,k} = P(N_{j,k} = n_{j,k}) \leftarrow$ estimate from historical data $\forall n_k$
3: $l \leftarrow 1$
4: while $l \leq N$ do
5:   $n_{j,k,l} \leftarrow$ draw random sample from $P(N_{j,k} = n_{j,k})$ for each $k$
6:   $x_{j,l}^{k} \leftarrow$ arrange $n_{j,l} = \sum_k n_{j,k,l} \text{ op. modes in random order } [k_1, k_2, \ldots, k_{n_{j,l}}]$
7:   $p_{j,l}^f \leftarrow p_{j}^f(x_{j,l}^{k}) \quad \triangleright \text{ Eqn. 12}$
8: end while
9: $\bar{p}_j^f \leftarrow \max_{l \leq N} p_{j,l}^f$
10: end procedure

The key idea is to treat the occurrence of operating modes $k$ over time as a Markov chain. Modeling the sequence of operating modes $x_j^k$ on a unit by a memoryless Markov chain $X_j^k(t) = \{X_j^k \mid t \leq T\}$, the probability $\pi_{k,k^*}$ of transitioning from one operating mode $k$ to another $k^*$ is given by

$$\pi_{k,k^*} = P(X_{j,t}^k = k^* \mid X_{j,t-1}^k = k).$$

The transition probabilities $\pi_{k,k^*}$ can be estimated from data.

From this Markov chain random sequences of operating modes $x_{j,l}^k$ can be generated. Maintenance can again be inserted at the latest possible point in time according to Eqn. 13. $x_{j,l}^k$ may not be a feasible solution to Problem 9, but it can be used to estimate $\bar{p}_j^f$. The approach is summarized in Algorithm 2.

2.5.3 Logistic regression

The optimal sequence of operating modes $x_j^{k,*}$ depends not only on the structure of the process and the size of the uncertainty set $\mathcal{U}(\alpha)$, but also on parameters $\psi(t)$ such as product demands or environmental variables. The distributions of $N_k$ and $\pi_{k,k^*}$ are therefore not necessarily stationary:

$$\eta_{n,j,k}(\psi(t)) = P(N_{j,k} = n_{j,k} \mid \psi)$$

$$\pi_{k,k^*}(\psi(t)) = P(X_{j,t}^k = k^* \mid X_{j,t-1}^k = k, \psi),$$

where $\eta_{n,j,k}(\psi)$ is the probability that operating mode $k$ occurs $n_{j,k}$ times in time period $\Delta t$. 

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Algorithm 2 Markov chain approach

1: procedure estimate $\tilde{p}_j^f$
2: \[ \pi_{k,k^*} = P(X_{j,t}^k = k^* | X_{j,t-1}^k = k) \leftarrow \text{estimate from historical data } \forall (k, k^* ) \]
3: \[ l \leftarrow 1 \]
4: \[ \textbf{while } l \leq N \textbf{ do} \]
5: \[ x_{j,t}^k \leftarrow \text{draw random operating mode sequence from Markov chain } \pi_{k,k^*} \]
6: \[ x_{j,t}^k \leftarrow \text{insert maintenance at last possible points in time } \triangleq \text{Eqn. 13} \]
7: \[ p_{j,t}^f \leftarrow p_{j,t}^f(x_{j,t}^k) \triangleq \text{Eqn. 12} \]
8: \[ \textbf{end while} \]
9: \[ \tilde{p}_j^f \leftarrow \max_{l \leq N} p_{j,t}^f \]
10: \[ \textbf{end procedure} \]

Figure 3: Frequency $n_{j,k}$ of operating mode $k$ occurring on unit $j$ for a scheduling problem with two product demands $\psi = [\delta_{1,t}, \delta_{2,t}]^\top$. Points are training data generated by solving the scheduling model and shaded areas are predictions by logistic regression.
Covariate dependency of Markov chain transition probabilities has previously been modeled by using logistic regression. We model both $\eta_{n,j,k}$ and $\pi_{k,k^*}$ using multinomial logistic regression in order to capture the influence of product demands:

$$
\eta_{n,j,k}(\psi(t)) = \frac{\exp(\beta^T_{n,j,k} \psi)}{\sum_{n_k'} \exp(\beta^T_{n',j,k} \psi)} 
$$

(15a)

$$
\pi_{k,k^*}(\psi(t)) = \frac{\exp(\beta^T_{k,k^*} \psi)}{\sum_{k^+ \in K} \exp(\beta^T_{k^+,k} \psi)}. 
$$

(15b)

We use Scikit-learn for estimating parameters $\beta$ based on data. Fig. 3 shows an example for a process with two product demands $\psi = [\delta_{1,t}, \delta_{2,t}]^T$. The shaded areas are the frequencies $n_{j,k}$ predicted by logistic regression for a particular $k$ and $j$ (the $n_{j,k}$ with the largest $\eta_{n,j,k}(\psi)$) while the points are training data. We use logistic regression in this work because of its simplicity and interpretability, but it could be replaced by any classification method capable of probability estimation, e.g., Artificial Neural Networks, Support Vector Machines, k-Nearest Neighbours, Decision Trees, etc.

### 3 Optimizing the uncertainty set size

An important, non-trivial decision when using robust optimization is the size of the uncertainty set — or in this work the choice of parameter $\alpha$. It governs a trade-off between the robustness of the solution and its cost. A common approach is to use a-priori guarantees to determine an uncertainty set size that is guaranteed to have a probability of constraint violation below a predefined level. A-priori guarantees are, however, not guaranteed to be tight and uncertainty sets based on them can be overly conservative. As demonstrated by Li and Li, determining the optimal uncertainty set size can instead be seen as its own optimization problem. They minimize the uncertainty set size with the constraint that the solution remains feasible with a pre-defined probability. We propose a different formulation that does not require the decision maker to choose a probability of constraint satisfaction but is based purely on cost instead:

$$
\min_{\alpha} c^*(\alpha) + \sum_j p_{j}^f(\alpha) \cdot c_j^f,
$$

(16)

where $c^*(\alpha)$ is the minimal overall cost of the process as determined by solving Problem 3 for a given value of $\alpha$, $p_{j}^f(\alpha)$ is the corresponding probability of failure.
evaluated using Eqn. 12, and $c_f^j$ is the cost incurred in case of an unplanned failure of unit $j$, i.e., the cost of corrective maintenance. Effectively, Problem 16 minimizes the trade-off between preventive and corrective maintenance. Note that this formulation assumes that each unit fails no more than once in the evaluated horizon $T$. This is reasonable under the assumption that the cost of failure $c_f^j$ is high and therefore $P_{f_j}$ tends to be low.

Problem 16 is a one-dimensional optimization problem, but determining $c^*(\alpha)$ and $p_{f_j}(\alpha)$ can be computationally expensive because it requires solving a potentially large MILP problem and Monte-Carlo simulation. It can therefore be viewed as a black box optimization problem with expensive function evaluations. We propose Bayesian optimization, which is known to work well on expensive low dimensional objective functions, as an effective solution strategy. Bayesian optimization has the further advantage that it can handle noise well. Both $c^*$ and $p_{f_j}$ can be noisy because it may not be possible to solve Problem 9 to optimality in a reasonable time frame. Further noise is introduced by the Monte-Carlo simulation used to evaluate $p_{f_j}$.

4 Case study

![Figure 4: STN instance proposed by Kondili et al. Tasks are performed on four units: Heater, Reactor 1, Reactor 2, and Still.](image)
The model by Biondi et al.\textsuperscript{18}, an extension of the State-Task-Network (STN)\textsuperscript{19}, forms the basis of our case study. The classic STN is a scheduling problem in which a set of tasks $I$ has to be assigned to a set of units $J$. Biondi et al.\textsuperscript{18} extend the STN by allowing each task $i$ to be performed in a number of different operating modes $k \in K_i$. They add constraints reducing the residual lifetime $r_{j,t}$ of each unit $j$ every time a task is performed, and restore $r_{j,t}$ by performing maintenance. Because the scheduling problem can only be solved for a short time horizon $T_S$ but maintenance occurs infrequently, they add a planning horizon $T_P$ to the problem. For the planning horizon, instead of an exact schedule, only the number of times $n_{i,j,k,t}$ a task $i$ is performed on unit $j$ in operating mode $k$ in each planning period $t$ is calculated. Eqns.\textsuperscript{17} to \textsuperscript{20d} give the modified version used as a case study in this work:

Objective function:

$$\text{cost} = \sum_{j \in J} c_j^{\text{maint}} \left( s_{j}^{\text{fin}} / s_j^{\text{max}} + \sum_{t \in T} m_{j,t} \right)$$

$$+ c_s^{\text{storage}} \left( q_{s,t}^{\text{fin}} + \sum_{t \in T_P} q_{s,t} \right)$$

$$+ U \left( \sum_{s \in S} \phi_{s}^{d} + \sum_{t \in T_S} \phi_{s,t}^{g} \right)$$

(17)

Constraints scheduling horizon:

$$\sum_{k \in K_i} \sum_{i \in I_j} \sum_{t'} w_{i,j,k,t'} + \sum_{t'} m_{j,t'} \leq 1 \quad \forall J, t \in T_S$$

(18a)

$$v_{i,j}^{\text{min}} w_{i,j,k,t} \leq b_{i,j,k,t} \leq v_{i,j}^{\text{max}} w_{i,j,k,t} \quad \forall J, i \in I_j, k \in K_j, t \in T_S$$

(18b)

$$q_{s,t} = q_{s,t-1} + \sum_{i \in I_s} \rho_{i,s} \sum_{j \in J} \sum_{k \in K_j} b_{i,j,k,t-p_{i,j,k}}$$

$$- \sum_{i \in I_s} \rho_{i,s} \sum_{j \in J} \sum_{k \in K_j} b_{i,j,k,t}$$

$$\forall s, t \in T_S$$

(18c)

$$0 \leq q_{s,t} - \phi_{s,t}^{q} \leq c_s \quad \forall s, t \in T_S$$

(18d)

$$m_{j,t} s_{j,t}^{0} \leq s_{j,t} \leq s_{j,t}^{\text{max}} + m_{j,t} \cdot (s_{j,t}^{0} - s_{j,t}^{\text{max}}) \quad \forall t, j \in J, D \in U$$

(18e)

$$s_{j,t} \geq s_{j,t-\Delta t_S} + \sum_{k} w_{i,j,k,t} d_{j,k} + m_{j,t} \cdot (s_{j}^{0} - s_{j}^{\text{max}}) \quad \forall t, j \in J, D \in U$$

(18f)
\[ s_{j,t} \leq s_{j,t-\Delta t_S} + \sum_i \sum_k w_{i,j,k,t} \tilde{d}_{j,k} \quad \forall t, j \in J, D \in U, \quad (18g) \]

Constraints planning horizon:
\[ \sum_{i \in I_j} \sum_{k \in K_j} p_{i,j,k} n_{i,j,k,t} + \tau_j m_{j,t} \leq \Delta t_P \quad \forall J, t \in T_P \setminus \{\bar{t}_P\} \quad (19a) \]
\[ v_{i,j}^{\min} \sum_{k \in K_j} n_{i,j,k,t} \leq a_{i,j,t} \leq v_{i,j}^{\max} \sum_{k \in K_j} n_{i,j,k,t} \quad \forall J, i \in I_j, k \in K_j, t \in T_P \quad (19b) \]
\[ q_{s,t} = q_{s,t-1} + \sum_{i \in I_s} \sum_{j \in J} a_{i,j,t} - \sum_{i \in I_s} \rho_i s_{i,j,k,t} - \delta_{s,t} \quad \forall s, t \in T_P \setminus \{\bar{t}_P\} \quad (19c) \]
\[ 0 \leq q_{s,t} - c_s \quad \forall s, t \in T_P \quad (19d) \]
\[ n_{i,j,k,t} \leq U \cdot \omega_{j,k,t} \quad \forall J, i \in I_j, k \in K_j, t \in T_P \quad (19e) \]
\[ \sum_{k \in K_j} \omega_{j,k,t} = 1 \quad \forall J, t \in T_P \quad (19f) \]
\[ s_{j,t} \leq s_{j,t-\Delta t_S} \quad \forall t, j \in J \quad (19g) \]
\[ s_{j,t}^* \geq s_{j,t-\Delta t_P} + \sum_k n_{j,k,t} \tilde{d}_{j,k,t} + m_{j,t} \cdot (s_j^0 - s_{j,t}^*) \quad \forall t, j \in J \quad (19h) \]
\[ s_{j,t} \leq s_{j,t-\Delta t_P} + \sum_k n_{j,k,t} \tilde{d}_{j,k,t} \quad \forall t, j \in J \quad (19i) \]

Constraints interface between scheduling and planning:
\[ \sum_{i \in I_j} \sum_{k \in K_j} \sum_{i_j \in I_j} \sum_{i_j \in I_j} n_{i,j,k,t} \tilde{d}_{i,j,k,t} \quad \forall j \in J \quad (20a) \]
\[ q_{s,t}^{fin} = q_{s,t} + \sum_{i \in I_s} \sum_{j \in J} \sum_{k \in K_j} b_{i,j,k} \tilde{t}_{i,j,k,t} + \phi_{i,j,k,t} \quad \forall s \quad (20b) \]
The decision variables are $m_{j,t}$, $q_{s,t}$, $w_{i,j,k,t}$, $n_{i,j,k,t}$, $b_{i,j,k,t}$, $a_{i,j,t}$, $s_{j,t}$, $\phi_{d,s,t}$, $\phi_{q,s,t}$ and $\omega_{j,k,t}$.

The product demand $\delta_{s,t}$ has to be satisfied at the end of each planning period and at the end of any time interval in the scheduling horizon. In practice, this model would be solved regularly in a rolling horizon fashion using recent demand estimates and degradation signal measurements $s_{j,0}$.

In comparison to Biondi et al.\textsuperscript{18}, the residual lifetime constraints have been replaced with the degradation signal based health model developed above (Eqn. 9).

For the planning horizon, $s_{j,t}$ cannot be reset exactly to $s_{j,0}$, because the exact time at which maintenance is performed is unknown. Instead, it is merely enforced that $s_{j,t} \leq s_{j,max}$.

In addition, the objective function is slightly different. The term $c_{j}^{\text{maint}}(s_{j,\text{fin}}/s_{j,max})$ can be interpreted as a final cost of maintenance dependent on the final degradation signal $s_{j,\text{fin}}$ (state of health) of unit $j$. Similar to Biondi et al.'s\textsuperscript{18} penalty terms it avoids unnecessary degradation and ensures maintenance happens towards the end of a unit's residual lifetime.

Since the exact sequence of operating modes and maintenance actions is unknown in the planning horizon $T_P$, the probability of failure $p_j^f$ can only be evaluated over the scheduling horizon $T_S$. In order to still evaluate $p_j^f$ over a longer time period two possibilities exist: the schedule can be extended in length by solving the model repeatedly in a rolling horizon fashion or the Markov chain-based estimation approach in Algorithm\textsuperscript{2} can be used. We compare both approaches to show that the proposed Markov chain estimate is indeed accurate. Note that, in order to facilitate a rolling horizon based solution approach, slack variables have been introduced in Eqns.\textsuperscript{18a} and\textsuperscript{20b}. This is necessary because the rolling horizon framework does not guarantee feasibility in subsequent time periods. Production targets from the planning model may, for example, not be achievable in the scheduling model. The slack variables $\phi_{d,s,t}$ and $\phi_{q,s,t}$ are penalized in the objective function.

We assume that the frequencies of operating mode occurrence $n_{j,k}$ and the transition probabilities $\pi_{k,k'}$ depend on the product demands in each planning period.

\begin{align*}
0 \leq q_{s,\text{fin}}^{\text{in}} & \leq c_s \quad \forall s \quad (20c) \\
q_{s,t} = q_{s,\text{fin}}^{\text{in}} + \sum_{i \in I_S} \bar{\rho}_{i,s} \sum_{j \in J_i} \sum_{k \in K_j} \sum_{t' = \bar{t}_s + 2 - p_{i,j,k}} b_{i,j,k,t'} \\
& + \sum_{i \in I_S} \bar{\rho}_{i,s} \sum_{j \in J_i} a_{i,j,\bar{t}_p} \quad \forall s \quad (20d) \\
& - \sum_{i \in I_S} \bar{\rho}_{i,s} \sum_{j \in J_i} a_{i,j,\bar{t}_p} - \delta_{s,\bar{t}_p}
\end{align*}
\( \phi_t = [d_{s_1,t}, \ldots, d_{s_n,t}] \). We sample a range of demands using Latin Hypercube Sampling and solve just the scheduling horizon to generate data for estimating \( n_{j,k} (\psi_t) \) and \( \pi_{k,k} (\psi_t) \).

Notice that the model above fulfills the assumptions in Theorem 1 and solutions can be obtained by solving the deterministic approximation.

## 5 Results

The framework outlined above was evaluated on five instances of the STN (see Table 1 and Appendix C). The model was implemented in Pyomo and solved using CPLEX 12.7.1.0. All source code is publicly available under the MIT Licence.

Unless mentioned otherwise, we considered an evaluation horizon of 12 planning periods. The failure probability \( p^f_j \) for each unit \( j \) was evaluated for a range of values of the uncertainty set parameter \( \alpha \) using both the frequency and Markov chain estimates as well as rolling horizon. The termination criteria for each CPLEX run were a maximum time limit between 1 – 5 minutes (depending on the size of the instance) and a MIP gap of 2% (except for the toy instance which was solved to optimality). For each instance we considered a low, average, and high demand scenario where the high scenario was close to maximum process capacity. For Instance P1 both the robust and deterministic Problems 9 and 10 were solved a number of times to evaluate the quality of the deterministic approximation. For all other instances only the deterministic approach was used. All calculations were carried on an i7-6700 CPU with 8 × 3.4GHz and 16GB RAM.

Fig. 5 shows three maintenance schedules for the original STN instance (P1) by Kondili et al. with Biondi et al.’s demand scenario (average scenario) with
Figure 5: Comparison of maintenance schedules between deterministic solution ($\alpha = 0.5$) and two robust solutions with different values of $\alpha$ (Instance P19, average demand scenario by Biondi et al.18). The number of required maintenance actions increases with increasing uncertainty set size (decreasing $\alpha$).

different values for $\alpha$. The number of maintenance actions increases with increasing uncertainty set size (decreasing $\alpha$). Essentially, hedging against more uncertainty and ensuring solution robustness for a larger set of possible realizations requires earlier maintenance. In the average demand scenario, maintenance actions increase by 22% when hedging against some of the uncertainty ($\alpha = 0.26$) and by 56% when hedging against almost all uncertainty ($\alpha = 0.02$). However, this trend also depends on product demand: for the low demand scenario, only an increase of 25% is necessary for $\alpha = 0.02$, while an increase of 64% is necessary in the high demand scenario. A higher demand increases unit utilization and therefore also the absolute number of maintenance actions required in a given time period.

Fig. 6 shows the failure probability $p_j^f$ for Reactor 1 as a function of both total cost (cost of storage and cost of maintenance) and the uncertainty set parameter $\alpha$. As expected, $p_j^f$ increases for smaller uncertainty sets (large $\alpha$’s) and a low $p_j^f$ comes at a significant cost – the price of robustness. Notice that, while calculating $p_j^f$ using Monte-Carlo simulation only introduces modest noise, the calculated cost is very noisy due to the non-optimality of the solutions.

The results in Fig. 6 were obtained by solving the deterministic Problem 10. While Theorem 1 guarantees that these solutions are also feasible in the robust Problem 9, it does not prove that they are also optimal. Fig. 7 shows both total cost
Figure 6: Probability of Reactor 1 failing $p_f^j$ vs uncertainty set parameter $\alpha$ and cost (Instance P1, average demand scenario). Each point is a solution to Problem 10 obtained by CPLEX. The probability of failure $p_f^j$ was estimated using the Algorithm 2 Markov chain approach.

Figure 7: Robust vs. deterministic approach (Instance P1). Each model was solved 25 times with $\alpha = 0.41$ and a 120s time limit per rolling horizon iteration using out-of-the-box CPLEX. The robust model has 22514 variables and 14664 constraints while the deterministic model has 6122 variables and 7332 constraints.
and average optimality gap for a number of rolling horizon solutions to the deterministic and robust version of Instance P1\textsuperscript{19}. The uncertainty set size was $\alpha = 0.41$ and a maximum time limit of 120s was used for each CPLEX run. Within this time limit, out-of-the-box CPLEX achieves an average optimality gap of 12.1\% on the robust problem compared with 3.8\% for the deterministic approximation with maximum values for $\tilde{d}_{j,k}$. Similarly, the deterministic approximation achieves significantly lower objective values. While many approaches could improve solution quality of the robust problem, e.g., solver parameter tuning or leveraging Satisfiability Modulo Theory\textsuperscript{58}, Constraint Programming\textsuperscript{59}, or Approximation Algorithms\textsuperscript{60}, it is likely that the deterministic approximation will remain favorable as it has significantly fewer variables and constraints (6122 vs. 22514 and 7332 vs. 14664 respectively). Assuming a box uncertainty set, we view it as a reasonable approximation for instances which cannot be solved to optimality in a reasonable amount of time. In the case of a more complex uncertainty set, replacing $\tilde{d}_{j,k}$ with its maximum value may lead to conservative solutions. General uncertainty sets require solving the robust problem.

Note that the large range of solution values in Fig. 7 is not only due to the differing MIP gaps, but also the rolling horizon approach which does not guarantee optimality.

Logistic regressions for the Frequency and Monte-Carlo approaches were trained based on 200 scheduling horizon only solutions. For the Frequency approach, the training points and their predicted values for Reaction 1 in mode Normal of the toy instance are shown in Fig. 8. Logistic regression predicts $n_{i,j,k}$ reasonably well but the rigid, linear classifier cannot capture some of the details. This is, however, not a major problem as the entire predicted probability distribution $\eta_{n_{i,j,k}}$ of operating mode occurrence frequencies $n_{i,j,k}$ is used in estimating $\bar{p}_{j}^f$. Near the predicted boundaries, $\eta_{n_{i,j,k}}$ of adjacent frequencies will be non-zero and they will be sampled in a significant number of operating mode sequences in Algorithm 1.

Fig. 9 shows the probability of failure $p_{j}^f$ for each unit in the toy instance as a function of the uncertainty set parameter $\alpha$ for three different demand scenarios (average, high, and low). Since the rolling horizon framework does not guarantee optimality, solving the problem repeatedly for the same value of $\alpha$ can lead to different solutions and failure probabilities. The problem was therefore solved 10 times for each value of $\alpha$. It can be seen that the probability of failure generally increases with demand. The figure furthermore shows the two bounds obtained using the Frequency and Markov chain based approaches, i.e. Algorithm 1 versus 2. For the reactor both approaches provide good upper bounds. For the heater, the frequency based approach performs very well, while the Markov chain approach underestimates $p_{j}^f$ for the high demand scenario and overestimates it for the average and low demand
Figure 8: Toy instance: Frequency $n_{i,j,k}$ of Reaction 1 occurring in normal mode on unit Reactor within one scheduling horizon. Points are training data generated by solving the scheduling model repeatedly and shaded areas are predictions by logistic regression.

Figure 9: Toy instance: Frequency vs. Markov chain approach. Points are rolling horizon solutions. Colored lines are bounds from the Frequency and Markov chain approach. The dotted black lines show a-priori bound B4 by Li et al.}\[300x113\]
scenarios. Finally notice that the apriori bound given by the dotted lines greatly overestimates $p^f_j$. Fig. 10 shows similar trends for Instance P1 (Kondili). Both approaches provide reasonable bounds for all units and scenarios except the average demand scenario on the Heater, for which the frequency approach underestimates $p^f_j$. Notice that $p^f_j$ is nearly zero for both the Heater and Reactor 2 at low demand irrespective of $\alpha$. This is because for this scenario no maintenance occurs on either unit and $s_{j,t}$ does not get close to $s^{max}_j$.

![Figure 10: Instance P1: Frequency vs. Markov chain approach. Points are rolling horizon solutions. Colored lines are bounds from the Frequency and Markov chain approach. The dotted black lines show a-priori bound B4 by Li et al.]

The performance of the Frequency and Markov chain based probability estimates
was assessed using three metrics:

\[ \text{rms}_{\text{all}}^2 = \frac{1}{N \cdot |A|} \sum_{n \in \{1..N\}, \alpha \in A} \left( \left[ p^f_j \right]_{n,\alpha} - \bar{p}^f_j \right)^2, \]  

(21a)

\[ p_{\text{out}} = \frac{1}{N \cdot |A|} \sum_{n \in \{1..N\}, \alpha \in A} \mathbb{1} \left( \left[ p^f_j \right]_{n,\alpha} > \bar{p}^f_j \right), \text{ and} \]  

(21b)

\[ \text{rms}_{\text{out}}^2 = \frac{1}{p_{\text{out}} \cdot N \cdot |A|} \sum_{n \in \{1..N\}, \alpha \in A} \mathbb{1} \left( \left[ p^f_j \right]_{n,\alpha} > \bar{p}^f_j \right) \left( \left[ p^f_j \right]_{n,\alpha} - \bar{p}^f_j \right)^2, \]  

(21c)

where \( \text{rms}_{\text{all}} \) is the root-mean-squared deviation between the estimate and all rolling horizon solutions, \( p_{\text{out}} \) is the percentage of rolling horizon solutions with a larger \( p^f_j \) than the estimated bound, and \( \text{rms}_{\text{out}} \) is the root-mean-squared deviation of all underestimated points. While \( \text{rms}_{\text{all}} \) evaluates the estimate \( \bar{p}^f_j \)'s quality as a predictor of \( p^f_j \), \( p_{\text{out}} \) and \( \text{rms}_{\text{out}} \) assess its quality as an upper bound.

| instance | bound | rms_{all} | p_{out} | rms_{out} |
|----------|-------|-----------|--------|-----------|
| toy      | freq  | 8.00      | 17.54  | 0.90      |
| toy      | mc    | 10.41     | 9.62   | 2.86      |
| P1_{19}  | freq  | 12.61     | 18.08  | 5.80      |
| P1       | mc    | 17.25     | 10.13  | 1.81      |
| P2_{25}  | freq  | 7.40      | 48.19  | 2.24      |
| P2       | mc    | 13.68     | 40.56  | 1.10      |
| P4_{26}  | freq  | 10.09     | 13.77  | 4.10      |
| P4       | mc    | 11.40     | 11.91  | 2.67      |
| P6_{27}  | freq  | 16.35     | 29.40  | 4.48      |
| P6       | mc    | 20.16     | 21.27  | 3.23      |
| all      | freq  | 10.89     | 25.40  | 3.50      |
| all      | mc    | 14.58     | 18.70  | 2.34      |

Table 2: Average performance metrics for probability estimates - all instances

Table 2 shows values for all three instances averaged over demand scenarios and units for all tested STN instances. It can be seen that the frequency approach is generally a better estimator for \( p^f_j \) than the Markov chain approach (smaller values of \( \text{rms}_{\text{all}} \)) but also has a larger rate of misclassification \( p_{\text{out}} \). While \( \text{rms}_{\text{all}} \) can be large due to noise in the rolling horizon solutions and \( p_{\text{out}} \) values of up to 48% show that \( \bar{p}^f_j \) is not a perfect upper bound, \( \text{rms}_{\text{out}} \) is generally small with average values.
of 3.50 and 2.34% for the Frequency and Markov chain approach respectively. This means that, when \( \bar{p}_j^f \) underestimates \( p_j^f \), it does not do so by much. Considering the noise introduced by non-optimal solutions and the rolling horizon framework, the error introduced by estimating \( p_j^f \) through \( \bar{p}_j^f \) is small. Because it is a slightly better upper bound, the Markov chain approach was used for all subsequent experiments unless mentioned otherwise.

![Figure 11: Effect of number of Monte-Carlo samples \( N \) on failure probability \( p_j^f \) of Reactor 1 (Instance P1\textsuperscript{19}).](image)

Both probability estimation approaches are dependent on the number \( N \) of operating mode sequences generated. Fig. 11 shows that increasing \( N \) from 100 to 1000 for Reactor 1 in Instance P1\textsuperscript{19} only has a small effect on \( p_j^f \), especially for the Markov chain based approach. \( N = 100 \) is therefore deemed sufficient.

Figs. 12 and 13 compare Bayesian optimization (BO) with random search for Instance P1\textsuperscript{19}. Overall cost (Eqn. 16) was evaluated over a horizon of 24 weeks and both Bayesian optimization and random search were repeated five times. For the Bayesian optimization, four points were sampled evenly from the interval \( \alpha \in [0.02, 0.5] \) initially. Fig. 12 shows the obtained objective values as a function of \( \alpha \). There is clearly a trade-off between high cost of preventive maintenance in conservative solutions (small \( \alpha \)) and high cost of corrective maintenance for less conservative but also less robust solutions (large \( \alpha \)). Bayesian optimization very efficiently samples
Figure 12: Bayesian optimization vs. random search. Five runs of BO and random search were conducted. BO efficiently explores values near the optimal $\alpha$.

Figure 13: Bayesian optimization vs. random search. Points are individual values obtained at a given iteration. Lines represent the best previously achieved solution value averaged over five runs. BO consistently finds better solutions.
from the area around the optimal $\alpha \approx 0.3$ while random search naturally samples from the entire interval. Fig 13 shows the lowest objective value previously obtained as a function of the number of samples (averaged over five runs). Bayesian optimization consistently finds lower cost solutions than random search and achieves a good compromise between preventive and corrective maintenance within about 20 iterations.

6 Conclusion

This work integrates equipment degradation effects in process level optimization problems. The demonstrated methodology is summarized in Fig. 14. We combine commonly used methods from the Degradation Modeling literature, which allow unit health characteristics to be estimated and updated from data, with Robust Optimization. This is highly relevant since, realistically, almost all equipment in chemical and manufacturing processes will be subject to performance degradation and failures.

Solving realistic integrated maintenance and production scheduling and planning problems is a hard task by itself, because models tend to be large and computationally expensive. Combining such models with robust optimization increases the need for solving problems efficiently. Furthermore, the scheduling task is highly repetitive and should become easier as historical data is collected. To reduce computational...
expense, we show conditions where robust optimization problems can be solved by solving a deterministic approximation and develop data-based methods for estimating failure probabilities.

In the context of computationally expensive models, we show that Bayesian Optimization can be used effectively to optimize the uncertainty set in Robust optimization and balance the trade-off between preventive and corrective maintenance.

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A Formulating the robust counterpart

The reformulation of the semi-infinite constraints

\[ m_{j,t} s^0_j \leq s_{j,t} \quad \forall t, j \in J, \tilde{d}_{j,k} \in \mathcal{D} \quad (22a) \]

\[ s_{j,t} \leq s_{j}^{\text{max}} + m_{j,t} \cdot (s^0_j - s_{j}^{\text{max}}) \quad \forall t, j \in J, \tilde{d}_{j,k} \in \mathcal{U} \quad (22b) \]

\[ s_{j,t} \geq s_{j,t-\Delta t} + \sum_k x_{j,k,t} \tilde{d}_{j,k} + m_{j,t} \cdot (s^0_j - s_{j}^{\text{max}}) \quad \forall t, j \in J, \tilde{d}_{j,k} \in \mathcal{U} \quad (22c) \]

\[ s_{j,t} \leq s_{j,t-\Delta t} + \sum_k x_{j,k,t} \tilde{d}_{j,k} \quad \forall t, j \in J, \tilde{d}_{j,k} \in \mathcal{U} \quad (22d) \]

into a deterministic robust counterpart in this work is based on the approach by Lappas and Gounaris\textsuperscript{24}. \( s_{j,t} \) is replaced by the affine decision rule

\[ s_{j,t} = [s_{j,t}]_0 + \sum_k [s_{j,t}]_k \tilde{d}_{j,k} \]

in all constraints, where \([s_{j,t}]_0\) and \([s_{j,t}]_k\) are coefficients which become new variables in the reformulated constraints. The first constraint (Eqn. 22a) can be reformulate
in the following way:

\[ m_{j,t}s^0_j \leq [s_{j,t}]_0 + \sum_k [s_{j,t}]_k \tilde{d}_{j,k} \]

\[ \Rightarrow -\sum_k [s_{j,t}]_k \tilde{d}_{j,k} \leq [s_{j,t}]_0 - m_{j,t}s^0_j \]

\[ \Rightarrow \Theta^* \leq [s_{j,t}]_0 - m_{j,t}s^0_j, \]

where

\[ \Theta^* = \max_{\tilde{d}_{j,k}} \quad -\sum_k [s_{j,t}]_k \tilde{d}_{j,k} \]

s.t

\[ -\tilde{d}_{j,k} \leq -\tilde{d}_{j,k}(1 - \epsilon) \quad \forall k \]

\[ \tilde{d}_{j,k} \leq \tilde{d}_{j,k}(1 + \epsilon) \quad \forall k. \]

The dual of this is

\[ \Theta^* = \min_{u^1_{k,j,t},l^1_{k,j,t}} \quad \sum_k \bar{d}_{j,k} \left[(1 + \epsilon)u^1_{k,j,t} - (1 - \epsilon)l^1_{k,j,t}\right] \]

s.t

\[ u^1_{k,j,t} - l^1_{k,j,t} \geq -[s_{j,t}]_k \quad \forall k, \]

with dual variables \(u^1_{k,j,t}\) and \(l^1_{k,j,t}\). Dropping the minimization leads to the final reformulation:

\[ \sum_k \bar{d}_{j,k} \left[(1 + \epsilon)u^1_{k,j,t} - (1 - \epsilon)l^1_{k,j,t}\right] \leq [s_{j,t}]_0 - m_{j,t}s^0_j \quad \forall t, j \in J \]

\[ u^1_{k,j,t} - l^1_{k,j,t} \geq -[s_{j,t}]_k \quad \forall j, t, k \]

Similar analysis for the second inequality (Eqn. 22b) leads to reformulation

\[ \sum_k \bar{d}_{j,k} \left[(1 + \epsilon)u^2_{k,j,t} - (1 - \epsilon)l^2_{k,j,t}\right] \leq s^\max_j - [s_{j,t}]_0 + m_{j,t} \cdot (s^0_j - s^\max_j) \quad \forall t, j \in J \]

\[ u^2_{k,j,t} - l^2_{k,j,t} \geq [s_{j,t}]_k \quad \forall j, t, k, \]

the third inequality (Eqn. 22c) yields

\[ \sum_k \bar{d}_{j,k} \left[(1 + \epsilon)u^3_{k,j,t} - (1 - \epsilon)l^3_{k,j,t}\right] \leq [s_{j,t}]_0 - [s_{j,t-\Delta}]_0 + m_{j,t}s^\max_j \quad \forall t, j \in J \]

\[ u^3_{k,j,t} - l^3_{k,j,t} \geq [s_{j,t-\Delta}]_k - [s_{j,t}]_k + \bar{x}_{j,k,t} \quad \forall j, t, k, \]
and the fourth (Eqn. 22d)
\[
\sum_k \bar{d}_{j,k} [(1 + \epsilon) u_{k}^{4,j,t} - (1 - \epsilon) l_{k}^{4,j,t}] \\
\leq -[s_{j,t}]_0 + [s_{j,t-\Delta t}]_0 \quad \forall t, j \in J \\
u_{k}^{4,j,t} - l_{k}^{4,j,t} \geq -[s_{j,t-\Delta t}]_k + [s_{j,t}]_k - x_{j,k,t} \quad \forall j, t, k.
\]

B Equivalence to deterministic optimization with maximal parameters

Note that for convenience and readability the index \( j \) has been dropped in all equations in this appendix.

Consider the case where the cost, process model, and maintenance model in Problem 9 are not functions of the uncertain parameters \( \tilde{d}_k \):

\[
\begin{align*}
\min_{x, m} \quad & \text{cost}(x, m) \quad \quad & (23a) \\
\text{s.t} \quad & \text{process model}(x, m) \quad \quad & (23b) \\
& \text{maintenance model}(x, m) \quad \quad & (23c) \\
& m_t s_0 \leq [s_t]_0 + \sum [s_t]_k \tilde{d}_k, \quad \forall t, \tilde{d}_k \in \mathcal{U} \quad & (23d) \\
& [s_t]_0 + \sum [s_t]_k \tilde{d}_k \leq s_{\text{max}} + m_t (s^0 - s_{\text{max}}), \quad \forall t, \tilde{d}_k \in \mathcal{U} \quad & (23e) \\
& [s_t]_0 + \sum [s_t]_k \tilde{d}_k \geq [s_{t-1}]_0 + \sum [s_{t-1}]_k \tilde{d}_k \\
& \quad + \sum_k x_{k,t} \tilde{d}_k \quad \forall t, \tilde{d}_k \in \mathcal{U} \quad & (23f) \\
& \quad + m_t (s^0 - s_{\text{max}}), \\
& [s_t]_0 + \sum [s_t]_k \tilde{d}_k [s_{t-1}]_0 + \sum [s_{t-1}]_k \tilde{d}_k + \sum_k x_{k,t-1} \tilde{d}_k, \quad \forall t, \tilde{d}_k \in \mathcal{U} \quad & (23g)
\end{align*}
\]

Furthermore consider a deterministic version of Problem 23

\[
\begin{align*}
\min_{x, m} \quad & \text{cost}(x, m) \quad \quad & (24a) \\
\text{s.t} \quad & \text{process model}(x, m) \quad \quad & (24b) \\
& \text{maintenance model}(x, m) \quad \quad & (24c) \\
& m_t s^0 \leq s_t, \quad \forall t \quad & (24d) \\
& s_t \leq s_{\text{max}} + m_t (s^0 - s_{\text{max}}), \quad \forall t \quad & (24e)
\end{align*}
\]
\[ s_t \geq s_{t-1} + \sum_k x_{k,t}d_{k}^{\text{max}} + m_t(s^0 - s^{\text{max}}), \quad \forall t \quad (24f) \]
\[ s_t \leq s_{t-1} + \sum_k x_{k,t}d_{k}^{\text{max}}, \quad \forall t \quad (24g) \]
in which \( \tilde{d}_k \) has been replaced by
\[ d_{k}^{\text{max}} = \max_{\tilde{d}_k \in \mathcal{U}} \tilde{d}_k. \]

**Theorem 2.** Given that cost, process model, and maintenance model are not functions of \( \tilde{d}_{j,k} \) and that \( s^0_j \leq s^{\text{init}}_j = s_{j,t=t_0} \leq s^{\text{max}}_j \) and \( \tilde{d}_{j,k} \geq 0, \forall \tilde{d}_{j,k} \in \mathcal{U} \), then a feasible solution \((x = [x_{k,t}, \ldots], m = [m_t, \ldots], h = [s_t])\) to Problem 24 forms a feasible solution \((x = [x_{k,t}, \ldots], m = [m_t, \ldots], h = [s_t])\) to Problem 23 with

\[ [s_t]_0 = \begin{cases} s^{\text{init}}_t & t < t_{m,0} \\ s^0_t & t \geq t_{m,0} \end{cases} \quad (25a) \]
\[ [s_t]_k = \sum_{t'=t_{m,t}}^t x_{k,t}, \quad (25b) \]

where \( s^{\text{init}} = s(t = 0) \), \( t_{m,0} \) is the first point in time at which maintenance is performed, and \( t_{m,t} \) is the most recent point in time at which maintenance was performed.

**Proof.** First we show that the Inequality 23d
\[ m_t s^0 \leq [s_t]_0 + \sum [s_t]_k \tilde{d}_k \quad (23d) \]
holds for any \( \tilde{d}_k \geq 0 \) given \((x = [x_{k,t}, \ldots], m = [m_t, \ldots], h = [s_t])\): From the assumption \( s^0 \leq s^{\text{init}} \leq s^{\text{max}} \) and Eqn. 25a it follows that \( s^0 \leq [s_t]_0 \leq s^{\text{max}} \). Furthermore, it directly follows from Eqn. 25b that \( [s_t]_k \geq 0 \). Eqn. 23d is therefore guaranteed to hold for any \( \tilde{d}_k \in \mathcal{U}, \tilde{d}_k \geq 0 \).

Next, we show that Inequalities 23f and 23g
\[ [s_t]_0 + \sum [s_t]_k \tilde{d}_k \geq [s_{t-1}]_0 + \sum [s_{t-1}]_k \tilde{d}_k + \sum_k x_{k,t} \tilde{d}_k + m_t(s^0 - s^{\text{max}}) \quad (23f) \]
and
\[ [s_t]_0 + \sum [s_t]_k \tilde{d}_k \leq [s_{t-1}]_0 + \sum [s_{t-1}]_k \tilde{d}_k + \sum_k x_{k,t} \tilde{d}_k \quad (23g) \]
respectively, hold for any $\tilde{d}_k \in \mathcal{U}$ as long as Inequality 23e is satisfied. We first assume that $m_t = 0$. In this case $[s_{t-1}]_k = [s_{t-1}]_k + x_{k,t}$ (from Eqn. 25b), $[s_t]_0 = [s_{t-1}]_0$ (from Eqn. 25a) and Eqns. 23f and 23g simplify to

$$[s_t]_0 \geq [s_{t-1}]_0$$

and

$$[s_t]_0 \leq [s_{t-1}]_0,$$

which is true for any $\tilde{d}_k$. Next we assume that $m_t = 1$. In this case $[s_t]_0 = s^0$ (from Eqn. 25a), $[s_t]_k = 0$ (from Eqn. 25b), and $x_{k,t} = 0$ (assuming that a unit can not be operated while maintenance is performed). Substituting this into Eqns. 23f and 23g and rearranging yields

$$[s_{t-1}]_0 + \sum [s_{t-1}]_k \tilde{d}_k \leq s^{\max}$$

and

$$s^0 \leq [s_{t-1}]_0 + \sum [s_{t-1}]_k \tilde{d}_k$$

respectively. Eqn. 26 is guaranteed to be satisfied as long as Inequality 23e holds for $t = t - 1$ and Eqn. 27 holds for any $\tilde{d}_k \in \mathcal{U}, \tilde{d}_k \geq 0$ since $[s_{t-1}]_0 \geq S_0$ and $[s_{t-1}]_k \geq 0$.

Finally we show that the Inequality 23e

$$[s_t]_0 + \sum [s_t]_k \tilde{d}_k \leq s^{\max} + m_t(s^0 - s^{\max})$$

holds for any $\tilde{d}_k \in \mathcal{U}$. To this end we notice that

$$\arg \max_{\tilde{d}_k \in \mathcal{U}} [s_t]_0 + \sum [s_t]_k \tilde{d}_k = d_k^{\max}$$

since $[s_t]_k \geq 0$. Therefore, if Eqn. 23e holds for $\tilde{d}_k = d_k^{\max}$, it holds for any $\tilde{d}_k \in \mathcal{U}$. Since $(x = [x_{k,t}, \ldots], m = [m_{t}, \ldots], h = [s_t])$ is a solution to Problem 24

$$s_t \leq s^{\max} + m_t(s^0 - s^{\max}),$$

Lastly, noticing that the definition of $[s_t]_0$ and $[s_t]_k$ (Eqns. 25a and 25b) ensure that $s_t$ can always be decomposed as

$$s_t = [s_t]_0 + \sum [s_t]_k d_k^{\max}$$

if $s_t$ satisfies Problem 24 it follows that

$$s_t = [s_t]_0 + \sum [s_t]_k d_k^{\max} \leq s^{\max} + m_t(s^0 - s^{\max})$$

and Eqn. 23e holds for all $\tilde{d}_k \in \mathcal{U}$. $\Box$
## C Instances of the STN

| States | Capacity [kg] | Initial [kg] | Storage cost | Product 1 | Product 2 | Product 3 | Product 4 |
|--------|---------------|--------------|--------------|-----------|-----------|-----------|-----------|
| Feed A | ∞             | ∞            | ∞            | 100       | 200       | 100       | ∞         |
| Feed B | ∞             | ∞            | ∞            | 0         | 0         | 0         | 0         |
| Feed C | ∞             | ∞            | 1            | 1         | 1         | 1         | 5         |
| Hot A  | 100           | 0            | 0            | 1         | 1         | 1         | 1         |
| Int. BC| 200           | 0            | 0            | 1         | 1         | 1         | 1         |
| Int. AB| 150           | 0            | 0            | 1         | 1         | 1         | 1         |
| Impure E| 100          | 0            | 0            | 1         | 1         | 1         | 1         |

| Capacity [kg] | Initial [kg] | Storage cost |
|---------------|--------------|--------------|
| Feed A        | ∞            | ∞            |
| Feed B        | ∞            | ∞            |
| Feed C        | ∞            | 1            |
| Hot A         | 100          | 0            |
| Int. BC       | 200          | 0            |
| Int. AB       | 150          | 0            |
| Impure E      | 100          | 0            |

### Units and Operations

| Units        | Heater | Reactor 1 | Reactor 2 | Still |
|--------------|--------|-----------|-----------|-------|
| v_min [kg]   | 40     | 32        | 20        | 80    |
| v_max [kg]   | 100    | 80        | 50        | 200   |
| s_min [hr]   | 30     | 50        | 120       | 40    |
| c_main [kg]  | 300    | 900       | 2000      | 1200  |
| c_f [kg]     | 2000   | 3000      | 3000      | 1500  |

### Task Modes and Periods

| Period | Scenario | Low | Average | High |
|--------|----------|-----|---------|------|
| 1      | Product 1| 76  | 136     | 190  |
| 2      | Product 2| 116 | 162     | 180  |
| 3      | Product 1| 101 | 115     | 125  |
| 4      | Product 2| 91  | 141     | 167  |
| 5      | Product 1| 60  | 147     | 166  |
| 6      | Product 2| 60  | 103     | 203  |
| 7      | Product 1| 54  | 148     | 90   |
| 8      | Product 2| 110 | 113     | 224  |
| 9      | Product 1| 92  | 105     | 174  |
| 10     | Product 2| 99  | 175     | 126  |
| 11     | Product 1| 51  | 177     | 66   |
| 12     | Product 2| 117 | 164     | 119  |
| 13     | Product 1| 108 | 124     | 234  |
| 14     | Product 2| 64  | 107     | 64   |
| 15     | Product 1| 62  | 154     | 103  |
| 16     | Product 2| 62  | 135     | 77   |
| 17     | Product 1| 71  | 109     | 112  |
| 18     | Product 2| 86  | 139     | 186  |
| 19     | Product 1| 80  | 102     | 174  |
| 20     | Product 2| 70  | 172     | 239  |
| 21     | Product 1| 92  | 120     | 124  |
| 22     | Product 2| 59  | 153     | 194  |
| 23     | Product 1| 70  | 124     | 91   |
| 24     | Product 2| 75  | 141     | 228  |

| Task Mode | Unit |
|-----------|------|
| Heating   | Heater | p | d/σ |
| Slow      | 9      | 1 | 0.27 |
| Normal    | 6      | 2 | 0.54 |
| Fast      | 3      | 3.81 |
| Reaction 1| Slow   | 27 | 4 | 1.08 |
| Normal    | 15     | 5 | 1.35 |
| Fast      | 8      | 8 | 2.43 |
| Reaction 2| Slow   | 36 | 1 | 0.27 |
| Normal    | 21     | 3 | 0.81 |
| Fast      | 15     | 5 | 1.35 |
| Reaction 3| Slow   | 30 | 3 | 0.81 |
| Normal    | 18     | 7 | 1.35 |
| Fast      | 6      | 8 | 2.43 |
| Separation| Slow   | 15 | 2 | 0.54 |
| Normal    | 9      | 5 | 1.35 |
| Fast      | 6      | 6 | 1.62 |

| Product 1 | Product 2 | Product 1 | Product 2 | Product 1 | Product 2 |
|-----------|-----------|-----------|-----------|-----------|-----------|
| Low       | 76        | 139       | 240       | 294       | 294       |
| Average   | 116       | 162       | 180       | 323       | 323       |
| High      | 100       | 200       | 217       | 335       | 335       |

Table 3: Instance P1
States: S1 S2 S3 S4

Capacity [kg]: ∞ ∞ ∞ ∞
Initial [kg]: ∞ 0 0 0
Storage cost: 0 1 1 1

Units:
| Task | Mode | Unit | p | d/σ | p | d/σ | p | d/σ |
|------|------|------|---|-----|---|-----|---|-----|
| T1   | Slow | U1   | 33| 3/0.66 | 30| 3/0.66 |
| T1   | Normal | U2   | 25| 5/1.35 | 21| 6/1.62 |
| T1   | Fast | U3   | 15| 7/2.17 | 12| 9/2.79 |
| T2   | Slow | U4   | 24| 4/0.88 |
| T2   | Normal | U5   | 18| 6/1.62 |
| T3   | Fast | U1   | 12| 10/3.1 |
| T3   | Slow | U2   | 21| 2/0.44 | 18| 2/0.44 |
| T3   | Normal | U3   | 15| 4/1.08 | 12| 4/1.08 |
| T3   | Fast | U4   | 9 | 7/2.17 | 6 | 6/1.86 |

Table 4: Instance P225
### States

| States | F1 | F2 | I1 | I2 | I3 | P1 | P2 |
|--------|----|----|----|----|----|----|----|
| Capacity [kg] | ∞ | ∞ | 200 | 100 | 500 | 1000 | 1000 |
| Initial [kg] | ∞ | ∞ | 0 | 0 | 0 | 0 | 0 |
| Storage cost | 0 | 0 | 1 | 1 | 5 | 5 | 5 |

### Units

| Units | R1 | R2 | R3 |
|-------|----|----|----|
| \( x^{\text{min}} \) [kg] | 40 | 25 | 40 |
| \( x^{\text{max}} \) [kg] | 80 | 50 | 80 |
| \( s^{\text{max}} \) | 70 | 120 | 70 |
| \( s^{\text{inst}} \) | 10 | 10 | 10 |
| \( \tau_j \) [hr] | 21 | 21 | 21 |
| \( c_{\text{maint}} \) | 600 | 600 | 600 |

### Task Mode Unit

| Task | Mode | R1 | R2 | R3 |
|------|------|----|----|----|
| \( p_{i,j,k} \) | \( d_{i,j,k} / \sigma_{i,j,k} \) | \( p / \sigma \) | \( d / \sigma \) |
| T1   | Slow | 24 | 3/0.66 | 24 | 3/0.66 |
|      | Normal | 15 | 5/1.35 | 15 | 5/1.35 |
|      | Fast  | 9 | 8/2.16 | 9 | 8/2.16 |
| T2   | Slow | 36 | 3/0.66 | 36 | 3/0.66 |
|      | Normal | 24 | 5/1.35 | 24 | 5/1.35 |
|      | Fast  | 15 | 8/2.16 | 15 | 8/2.16 |
| T3   | Slow | 12 | 3/0.66 |
|      | Normal | 9 | 5/1.35 |
|      | Fast  | 6 | 8/2.16 |
| T4   | Slow | 24 | 3/0.66 |
|      | Normal | 15 | 5/1.35 |
|      | Fast  | 9 | 8/2.16 |

### Period

| Period | Scenario | Low | Average | High | Period | Scenario | Low | Average | High |
|--------|----------|-----|---------|------|--------|----------|-----|---------|------|
|        |          | P1  | P2      | P1   | P2     | P1      | P2  | P1      | P2   |
| 1      |          | 190 | 102     | 271  | 231    | 311     | 305 | 13      |      |
| 2      |          | 172 | 156     | 230  | 282    | 381     | 347 | 14      |      |
| 3      |          | 102 | 103     | 274  | 226    | 381     | 321 | 15      |      |
| 4      |          | 130 | 172     | 289  | 281    | 310     | 310 | 16      |      |
| 5      |          | 130 | 104     | 270  | 212    | 317     | 371 | 17      |      |
| 6      |          | 174 | 192     | 205  | 205    | 339     | 328 | 18      |      |
| 7      |          | 167 | 194     | 250  | 248    | 379     | 348 | 19      |      |
| 8      |          | 185 | 175     | 259  | 282    | 317     | 392 | 20      |      |
| 9      |          | 179 | 180     | 211  | 233    | 300     | 387 | 21      |      |
| 10     |          | 131 | 120     | 261  | 292    | 346     | 326 | 22      |      |
| 11     |          | 104 | 196     | 271  | 212    | 364     | 364 | 23      |      |
| 12     |          | 104 | 188     | 202  | 289    | 309     | 346 | 24      |      |

Table 5: Instance P4

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Table 6: Instance P6
| Period | Scenario | Low   | Average | High   |
|--------|----------|-------|---------|--------|
|        |          | P1    | P2      | P3     | P4     | P1    | P2    | P3    | P4     | P1    | P2    | P3    | P4     |
| 1      |          | 715   | 501     | 801    | 1277   | 1356  | 1739  | 1349  | 1605   | 1844  | 1898  | 1631  |
| 2      |          | 593   | 878     | 888    | 739    | 1533  | 1361  | 1384  | 1374   | 1687  | 1882  | 1650  | 1732  |
| 3      |          | 743   | 995     | 817    | 563    | 1727  | 1400  | 1323  | 1351   | 1510  | 1805  | 1893  | 1699  |
| 4      |          | 620   | 963     | 636    | 698    | 1702  | 1701  | 1260  | 1605   | 1557  | 1717  | 1693  | 1908  |
| 5      |          | 991   | 612     | 535    | 686    | 1521  | 1424  | 1600  | 1315   | 1929  | 1769  | 1657  | 1918  |
| 6      |          | 919   | 819     | 914    | 626    | 1451  | 1412  | 1667  | 1406   | 1539  | 1818  | 1676  | 1521  |
| 7      |          | 648   | 799     | 920    | 549    | 1447  | 1471  | 1732  | 1620   | 1999  | 1663  | 1632  | 1603  |
| 8      |          | 609   | 728     | 969    | 925    | 1746  | 1444  | 1694  | 1512   | 1673  | 1987  | 1924  | 1742  |
| 9      |          | 741   | 575     | 604    | 814    | 1691  | 1456  | 1384  | 1305   | 1826  | 1559  | 1982  | 1882  |
| 10     |          | 968   | 682     | 853    | 532    | 1436  | 1297  | 1564  | 1356   | 1987  | 1737  | 1598  | 1910  |
| 11     |          | 624   | 789     | 816    | 728    | 1357  | 1730  | 1441  | 1638   | 1696  | 1660  | 1761  | 1778  |
| 12     |          | 840   | 929     | 700    | 733    | 1384  | 1283  | 1461  | 1423   | 1779  | 1722  | 1558  | 1655  |
| 13     |          | 516   | 790     | 705    | 743    | 1387  | 1594  | 1696  | 1533   | 1596  | 1528  | 1857  | 1745  |
| 14     |          | 556   | 643     | 974    | 890    | 1722  | 1493  | 1528  | 1533   | 1782  | 1829  | 1994  | 1512  |
| 15     |          | 940   | 715     | 797    | 638    | 1470  | 1377  | 1635  | 1303   | 1949  | 1738  | 1933  | 1782  |
| 16     |          | 894   | 896     | 693    | 853    | 1563  | 1467  | 1526  | 1565   | 1837  | 1593  | 1938  | 1852  |
| 17     |          | 792   | 994     | 509    | 647    | 1561  | 1593  | 1614  | 1531   | 1694  | 1869  | 1879  | 1593  |
| 18     |          | 725   | 718     | 856    | 789    | 1739  | 1681  | 1373  | 1255   | 1902  | 1663  | 1814  | 1953  |
| 19     |          | 820   | 886     | 971    | 531    | 1576  | 1706  | 1635  | 1628   | 1875  | 1988  | 1648  | 1512  |
| 20     |          | 950   | 788     | 580    | 859    | 1627  | 1358  | 1469  | 1694   | 1642  | 1519  | 1999  | 1595  |
| 21     |          | 641   | 773     | 681    | 877    | 1257  | 1433  | 1581  | 1420   | 1890  | 1942  | 1854  | 1826  |
| 22     |          | 793   | 963     | 950    | 634    | 1250  | 1641  | 1644  | 1404   | 1795  | 1628  | 1658  | 1961  |
| 23     |          | 504   | 741     | 531    | 671    | 1472  | 1617  | 1311  | 1519   | 1967  | 1768  | 1877  | 1739  |
| 24     |          | 830   | 529     | 819    | 594    | 1390  | 1645  | 1632  | 1614   | 1844  | 1945  | 1620  | 1563  |

Table 7: Instance P6 continued
Table 8: Toy instance
Except for the toy instance, all instances are taken from the benchmark collection by Lappas and Gounaris\textsuperscript{24}. All parameters were converted to a discrete time formulation and degradation parameters were added. For Instance P1\textsuperscript{19} parameters from Biondi et al.\textsuperscript{18} were used. The time steps and horizons used in each instance are given in Table 9.

| Instance  | Toy | P1\textsuperscript{19} | P2\textsuperscript{25} | P4\textsuperscript{26} | P6\textsuperscript{27} |
|-----------|-----|-------------------------|-------------------------|-------------------------|-------------------------|
| $T_S$     | 30  | 168                     | 168                     | 168                     | 168                     |
| $\Delta t_S$ | 1   | 3                       | 3                       | 3                       | 3                       |
| $T_P$     | 720 | 4032                    | 4032                    | 4032                    | 4032                    |
| $\Delta t_P$ | 30  | 168                     | 168                     | 168                     | 168                     |

Table 9: Time horizons of STN instances

The degradation of all units is assumed to follow a Wiener process. The distribution of increments is

$$S_{j,t+p_i,j,k} - S_{j,t} = D_{i,j,k}, \quad D_{i,j,k} \sim \mathcal{N}(\bar{d}_{i,j,k}, \sigma^2_{i,j,k}),$$

where $\bar{d}_{i,j,k}$ is the nominal amount of degradation when task $i$ is performed on unit $j$ in mode $k$. When no task is being processed the degradation signal is assumed to vary with zero mean and a small variance:

$$S_{j,t} + \Delta t - S_{j,t} = D_{0,\Delta t}, \quad D_{0,\Delta t} \sim \mathcal{N}(0, 0.05^2 \Delta t). \quad (29)$$

A detailed list of all parameter values used in each case study can be found in Tables 3 through 8.

D Crossing probabilities of a Brownian motion for a piecewise linear boundary

When the Wiener process is used as a degradation model, the failure probability $p_f^j$ can be calculated efficiently based on analytical result\textsuperscript{15,41,62}. The probability of a Wiener process with piecewise constant parameters $\theta_{j,k} = [\mu_{j,k}, \sigma_{j,k}]$ crossing a fixed threshold $s^\text{max}_j$ is equivalent to the probability of a standard Brownian motion $W(t)$ (a Wiener process with $\mathcal{N}(0, 1)$ distributed increments) crossing a piecewise linear boundary. The probability of $W(t)$ crossing a linear boundary $at + b$ is known to be inverse gaussian distributed

$$P(W(t) \geq at + b, t \leq T) = 1 - \Phi\left(\frac{aT + b}{\sqrt{T}}\right) + \exp^{-2ab} \Phi\left(\frac{aT - b}{\sqrt{T}}\right), \quad (30)$$
where \( \Phi(\cdot) \) is the standard normal distribution function. Based on this, the probability of failure \( p^j_{u,v} \) between two consecutive maintenance times \( t_{m,u} \) and \( t_{m,v} \) can be calculated as

\[
p^j_{u,v} = 1 - \mathbb{E} h(y) = 1 - \prod_{l=1}^{n} \mathbb{1}(y_l > 0) \left( 1 - \exp \left( -\frac{2y_{t_{l-1}}y_l}{t_l - t_{l-1}} \right) \right),
\]

where \( t_l, l \in \{1, \ldots, n\} \) are the \( n \) points in time between \( t_{m,u} \) and \( t_{m,v} \) at which the operating mode \( k \) changes.

Here \( y \) is a vector representing the values of \( W(t) \) at each \( t_l \). It is defined as

\[
y = c + MD^{1/2}u,
\]

where \( M \) is a lower triangular matrix of ones,

\[
D^{1/2} = \text{diag}(\sqrt{t_1 - t_{m,u}}, \sqrt{t_2 - t_1}, \ldots, \sqrt{t_{m,v} - t_n}),
\]

\( u \) is a random vector with \( u_l \sim \mathcal{N}(0, \sigma^2_{j,k}(t_l)) \), and \( c \) is the piecewise linear boundary

\[
c = (s^{\text{max}}_j - s^{\text{init}}_j) \cdot [1, \ldots, 1]^{\top} - M \text{diag}(0, \mu_{j,k}(t_1), \ldots, \mu_{j,k}(t_n)) \Delta t
\]

with

\[
\Delta t = [0, t_1 - t_0, \ldots, t_n - t_{n-1}]^{\top}.
\]

The overall probability of failure over the evaluation horizon \( T \) can then be calculated as

\[
p^f_j = 1 - \prod_{u=1}^{n+1} \left( 1 - p^u_{j,u-1} \right),
\]

where \( t_{m,0} = 0, t_{m,n+1} = T \), and \( t_{m,u} \in \{1, \ldots, n\} \) are the \( n \) points in time at which maintenance is carried out on unit \( j \) in the evaluation horizon.

### E Nomenclature

- \( h \) health variables
- \( m \) maintenance variables
- \( x \) process variables

### Indices
\begin{itemize}
\item $i$ task
\item $j$ unit
\item $k$ operating mode
\item $s$ state
\item $t$ time
\end{itemize}

\textbf{Sets}

$I$ set of tasks
$I_j$ set of tasks $i$ available on unit $j$
$I_s$ set of tasks $i$ consuming state $s$
$I_\bar{s}$ set of tasks $i$ producing state $\bar{s}$
$J$ set of process units
$J_i$ set of units $j$ on which task $i$ can be performed
$K_i$ set of operating modes allowed for task $i$
$K_j$ set of operating modes $k$ available on unit $j$
$T$ evaluation horizon
$T_P$ planning horizon
$T_S$ scheduling horizon
$\mathcal{U}$ uncertainty set
$\mathcal{X}$ set of operating mode sequences $x_j^k$

\textbf{Discrete Variables}

$m_{j,t}$ 1 if maintenance is performed on unit $j$ at time $t$
$n_{i,j,k,t}$ number of times task $i$ is performed on unit $j$ in mode $k$ in time period $t$
$w_{i,j,k,t}$ 1 if task $i$ starts on unit $j$ in mode $k$ at time $t$, 0 otherwise
$x_{j,k,t}$ 1 if unit $j$ is operated in mode $k$ at time $t$
$x_j^k$ sequence of operating modes $[k_1, k_2, \ldots, k_T]$
$\omega_{j,k,t}$ 1 if unit $j$ operates in mode $k$ in period $t$, 0 otherwise

\textbf{Continuous Variables}

$a_{i,j,k,t}$ amount of material processed by task $i$ in unit $j$ in mode $k$ in time period $t$
$b_{i,j,k,t}$ amount of material committed to task $i$ on unit $j$ in mode $k$ at time $t$
$c^*$ minimal cost determined by solving Problem 9
$c_{j}^f$ cost of unit $j$ failing
$\mathcal{D}$ random variable modeling increment of $S(t)$
$N_{j,k}$ random variable modeling $n_{j,k}$
\(n_{j,k}\) number of times mode \(k\) occurs on unit \(j\) in a given \(\Delta t\)

\(p_f^j\) probability of failure

\(\hat{p}_f^j\) estimated upper bound on \(p_f^j\)

\(q_{s,t}^{fin}\) quantity of state \(s\) stored at end of planning horizon

\(q_{s,t}\) quantity of state \(s\) stored at time \(t\)

\(S(t)\) stochastic process modeling \(s^{meas}(t)\)

\(s^n_{j,t}\) realization of \(S_{j}(t)\) at time \(t\)

\(s^{meas}(t)\) value of degradation signal at end of planning horizon

\(S_t\) random variable modeling \(s^{meas}(t)\) at time \(t\)

\(X^k_j(t)\) memoryless Markov chain modeling \(x^k_j\)

\(X^k_{j,t}\) state of Markov chain at time \(t\)

\(\phi^d_s\) slack variable for unfulfilled demand of state \(s\)

\(\phi^q_{s,t}\) slack variable for storage capacity violation of state \(s\) at time \(t\)

\(\psi\) process/environmental parameters

**Parameters**

\(c_{j,\text{maint}}\) cost of maintenance for unit \(j\)

\(c_s^{\text{storage}}\) per unit cost of storage for state \(s\)

\(c_s\) storage capacity of state \(s\)

\(D\) distribution of \(D\)

\(\tilde{d}_{j,k}\) nominal value of \(\tilde{d}_{j,k}\)

\(\tilde{d}_{j,k}\) uncertain parameter modeling increment of \(S(t)\)

\(q_{j,k}^{max}\) maximum of \(\tilde{d}_{j,k}\) in \(U\)

\(N\) number of samples in Monte-Carlo simulation

\(p_{i,j,k}\) processing time of task \(i\) on unit \(j\) in mode \(k\)

\(r_{j,t}\) residual lifetime of unit \(j\) at time \(t\)

\([s_{j,t}]_0, [s_{j,t}]_k\) parameters for affine decision rule

\(s^0\) reset value degradation signal

\(s^{\text{init}}\) initial value of degradation signal

\(s^{\text{max}}\) failure threshold degradation signal

\(\bar{t}_P\) first time period in planning horizon

\(\bar{t}_S\) last time period in scheduling horizon

\(\Delta t_P\) length of planning period

\(\Delta t_S\) length of scheduling period

\(U\) large number

\(v_{i,j}^{\text{max}}\) maximum batch size for task \(i\) on unit \(j\)

\(v_{i,j}^{\text{min}}\) minimum batch size for task \(i\) on unit \(j\)

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\[ \alpha \] size parameter of \( \mathcal{U} \)

\[ \delta_{s,t} \] demand for \( s \) at time \( t \)

\[ \epsilon_{j,k} \] size parameter of \( \mathcal{U} \)

\[ \eta_{j,k} \] probability of \( k \) occurring \( n_{j,k} \) times

\[ \theta \] parameter vector of \( \mathcal{D} \)

\[ \mu_{j,k} \] mean of \( \mathcal{D}_{j,k} \)

\[ \pi_{k,k^*} \] transition probability Markov chain

\[ \bar{\rho}_{i,s} \] fraction of state \( s \) of material produced by task \( i \)

\[ \rho_{i,s} \] fraction of state \( s \) of material consumed by task \( i \)

\[ \sigma_{j,k} \] standard deviation of \( \mathcal{D}_{j,k} \)

\[ \tau_j \] duration of maintenance on unit \( j \)

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