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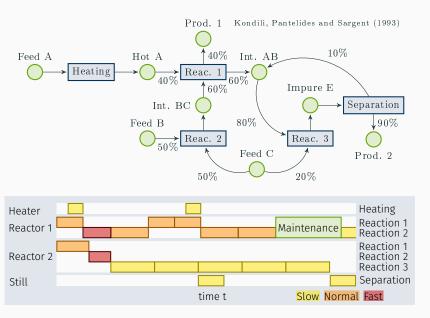
# Data-driven optimization of processes with degrading equipment

Johannes Wiebe<sup>1</sup>, Inês Cecílio<sup>2</sup>, Ruth Misener<sup>1</sup> Tuesday 11<sup>th</sup> September, 2018

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### Motivation: Why degradation matters



```
\begin{array}{ccc} \min & \cos(\boldsymbol{x}, \boldsymbol{m} &) \\ \text{s.t.} & \operatorname{process} \operatorname{model}(\boldsymbol{x}, \boldsymbol{m} &) & \text{(eg. balance equations)} \\ & & \operatorname{maintenance} \operatorname{model}(\boldsymbol{x}, \boldsymbol{m} &) & \text{(eg. types of maint.)} \end{array}
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where  $\boldsymbol{x}$  are process variables,  $\boldsymbol{m}$  are maintenance variables

```
\begin{array}{ll} \min \limits_{\boldsymbol{x},\boldsymbol{m},\boldsymbol{h}} & \operatorname{cost}(\boldsymbol{x},\boldsymbol{m},\boldsymbol{h}) \\ \text{s.t.} & \operatorname{process\ model}(\boldsymbol{x},\boldsymbol{m},\boldsymbol{h}) & (\text{eg. balance\ equations}) \\ & \operatorname{maintenance\ model}(\boldsymbol{x},\boldsymbol{m},\boldsymbol{h}) & (\text{eg. types\ of\ maint.}) \\ & \operatorname{health\ model}(\boldsymbol{x},\boldsymbol{m},\boldsymbol{h}), & (\text{eq. prognosis\ model}) \end{array}
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where x are process variables, m are maintenance variables, and h are health related variables.

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#### **Related Work**

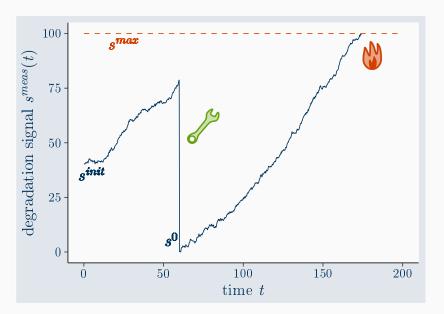
Vassiliadis and Pistikopoulos (2001); Liu, Yahia and Papageorgiou (2014); Xenos, et int, Thornhill (2016); Aguirre and Papageorgiou (2018); Biondi, Sand and Harjunkoski (2017); Yildirim, Gebraeel and Sun (2017); Başçiftci, Ahmed, Gebraeel and Yildirim (2018)

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```

where x are process variables, m are maintenance variables, and h are health related variables.

#### Idea

Combine process level MI(N)LP scheduling & planning with more sophisticated (stochastic) degradation modelling and robust optimization.



The degradation signal  $s^{meas}(t)$  can be modelled by a stochastic process :

$$S(t) = \{S_t : t \in T\},\$$

where  $S_t$  is a random variable (Alaswad and Xiang, 2017).

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# Often used: Lévy type processes (Applebaum, 2004)

- Independent increments:  $S_{t_2} S_{t_1}, ..., S_{t_n} S_{t_{n-1}}$  are independent for any  $0 < t_1 < t_2 < ... < t_n < \infty$
- Stationary increments:  $S_t S_s$  and  $S_{t-s}$  have the same distribution for any s < t

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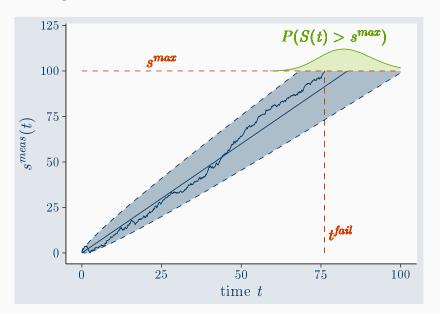
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- Stationary increments:  $S_t S_s$  and  $S_{t-s}$  have the same distribution for any s < t

Therefore  $S_t - S_{t-\Delta t} = D \sim \mathcal{D}(\Theta, \Delta t)$ , where  $\Theta$  are parameters of distribution  $\mathcal{D}$ .

### Calculating failure probabilities



### A health model based on Lévy processes

### **Assumption**

The health of each unit j can be described by a Lévy process  $S_j(t)$  with increments  $S_{j,t} - S_{j,t-\Delta t} = D_j \sim \mathcal{D}_j(\Theta, \Delta t)$ .

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$$\min_{\boldsymbol{x}, \boldsymbol{m}, \boldsymbol{h}} \quad \text{cost}(\boldsymbol{x}, \boldsymbol{m}, \boldsymbol{h})$$

s.t. process  $model(\boldsymbol{x}, \boldsymbol{m}, \boldsymbol{h})$ 

 $\text{maintenance model}(\boldsymbol{x},\boldsymbol{m},\boldsymbol{h})$ 

$$S_{j,t} \le s_j^{max} \qquad \forall t, j \in J$$

$$S_{j,t} = \begin{cases} S_{j,t-1} + D_j & , & \text{if } m_{j,t} = 0 \\ s_j^0, & \text{otherwise} \end{cases} \qquad \forall t, j \in J$$

where  $m_{j,t} = 1$  if maintenance is performed on unit j at time t.

# Accounting for effects of process variables

# Assumption (Liao and Tian, 2013)

All relevant operating variables are piecewise constant – i.e. the process has a set of discrete operating modes  $k \in K$ .

$$\min_{\boldsymbol{x}, \boldsymbol{m}, \boldsymbol{h}} \quad \operatorname{cost}(\boldsymbol{x}, \boldsymbol{m}, \boldsymbol{h})$$

s.t. process model(x, m, h)

maintenance model(x, m, h)

$$S_{j,t} \leq s_j^{max} \qquad \forall t, j \in J$$

$$S_{j,t} = \begin{cases} S_{j,t-1} + \sum_{\mathbf{k} \in \mathcal{K}} \mathbf{x}_{j,\mathbf{k},t} \cdot D_{j,\mathbf{k}}, & \text{if } m_{j,t} = 0 \\ s_j^0, & \text{otherwise} \end{cases} \quad \forall t, j \in J$$

where  $x_{j,k,t} = 1$  if unit j operates in mode k at time t.

# Deriving a robust counterpart (Lappas and Gounaris, 2016)

#### Idea

Replace random variables  $D_{j,k}$  and  $S_{j,t}$  by uncertain parameter  $\tilde{d}_{j,k} \in \mathcal{U}$  and second stage variable  $s_{j,t}(\tilde{d}_{j,k})$ .

$$\min_{x,m,h} \quad \cos(x,m,h)$$

s.t. process model(x, m, h)

maintenance model(x, m, h)

$$s_{j,t}(\tilde{d}_{j,k}) \le s_j^{max}$$

$$\forall t, j \in J$$

$$\mathbf{s}_{j,t} = \begin{cases} \mathbf{s}_{j,t-1} + \sum_{k \in \mathcal{K}} x_{j,k,t} \cdot \tilde{\mathbf{d}}_{j,k} , & \text{if } m_{j,t} = 0 \\ s_j^0, & \text{otherwise} \end{cases} \forall t, j \in J$$

$$\forall \tilde{d}_{i,k} \in \mathcal{U}.$$

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$$\min_{\boldsymbol{x}, \boldsymbol{m}, \boldsymbol{h}} \quad \text{cost}(\boldsymbol{x}, \boldsymbol{m}, \boldsymbol{h})$$

s.t. process model(x, m, h)

maintenance model(x, m, h)

$$s_{j,t}(\tilde{d}_{j,k}) \leq s_j^{max}$$

 $\forall t, j \in J$ 

$$\mathbf{s}_{j,t} = \begin{cases} \mathbf{s}_{j,t-1} + \sum_{k \in \mathcal{K}} x_{j,k,t} \cdot \tilde{\mathbf{d}}_{j,k}, & \text{if } m_{j,t} = 0 \\ s_j^0, & \text{otherwise} \end{cases} \forall t, j \in J$$

 $\forall \tilde{d}_{j,k} \in \mathcal{U}$ . Approximate  $s_{j,t}(\tilde{d}_{j,k})$  by linear decision rule. Utilize Robust Optimization reformulation techniques.

### Deriving a robust counterpart (Lappas and Gounaris, 2016)

### In special cases

Solve an approximate deterministic model with an order of magnitude fewer variables/constraints.

$$\begin{aligned} & \min_{\boldsymbol{x}, \boldsymbol{m}, \boldsymbol{h}} & \operatorname{cost}(\boldsymbol{x}, \boldsymbol{m}, \boldsymbol{h}) \\ & \text{s.t.} & \operatorname{process} & \operatorname{model}(\boldsymbol{x}, \boldsymbol{m}, \boldsymbol{h}) \\ & & \operatorname{maintenance} & \operatorname{model}(\boldsymbol{x}, \boldsymbol{m}, \boldsymbol{h}) \\ & & s_{j,t}(\tilde{\boldsymbol{d}}_{j,k}) \leq s_{j}^{max} & \forall t, j \in J \\ & s_{j,t} &= \begin{cases} s_{j,t-1} + \sum\limits_{k \in \mathcal{K}} x_{j,k,t} \cdot \tilde{\boldsymbol{d}}_{j,k} , & \text{if } m_{j,t} = 0 \\ s_{j}^{0}, & \text{otherwise} \end{cases} & \forall t, j \in J \end{aligned}$$

 $\forall \tilde{d}_{j,k} \in \mathcal{U}$ . Approximate  $s_{j,t}(\tilde{d}_{j,k})$  by linear decision rule. Utilize Robust Optimization reformulation techniques.

#### How do we choose $\mathcal{U}$ ?

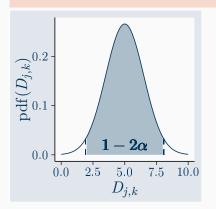
### Assumption: $\mathcal{U}$ is a box uncertainty set

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

#### How do we choose $\mathcal{U}$ ?

### Assumption: U is a box uncertainty set

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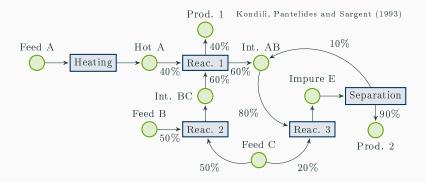


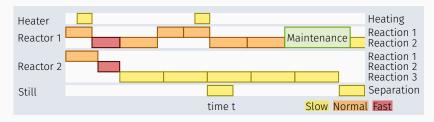
Choose  $\epsilon_{j,k}$  from distribution  $\mathcal{D}_{j,k}$  (Ning and You, 2017):

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

Size of  $\mathcal{U}$  depends on a single parameter  $\alpha$ !

### Case study: State-Task-Network (Kondili et al., 1993)

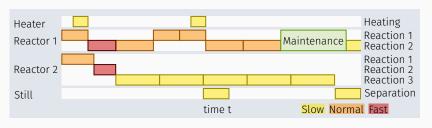




### Case study: State-Task-Network (Kondili et al., 1993)

Biondi, Sand and Harjunkoski (2017) extend the STN to include...

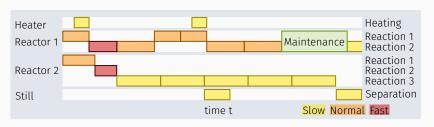
- ...unit health and maintenance scheduling,
- ...integrated scheduling and planning,
- ... multiple operating modes per task.



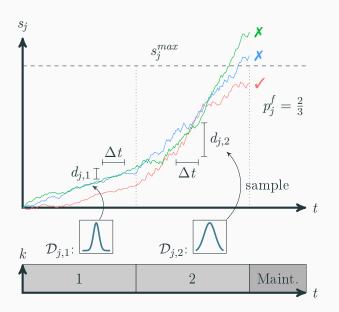
# Case study: State-Task-Network (Kondili et al., 1993)

#### This work...

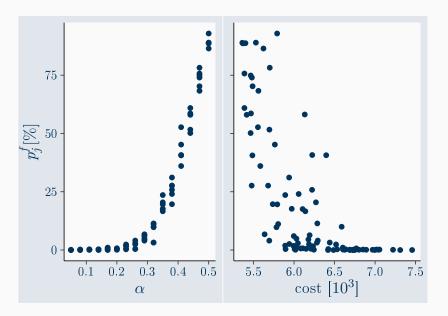
- ...replaces their deterministic health model by the proposed approach based on degradation modelling,
- ... utilizes robust optimization to obtain a solution that is likely to remain feasible,
- ...analyzes the price of robustness.



### Evaluating solution robustness



### The price of robustness



# Choosing $\alpha$ is its own optimization problem

We optimize  $\alpha$  by solving

$$\min_{\alpha} c^*(\alpha) + \sum_{j} p_j^f(\alpha) \cdot c_j^f$$

- $c^*(\alpha)$  is the objective value of a MILP solution given  $\alpha$ .
- $p_j^f(\alpha)$  is the corresponding probability of failure (of unit j).
- $c_i^f$  is the cost of an unexpected failure.

Alternative objective: Li and Li (2015)

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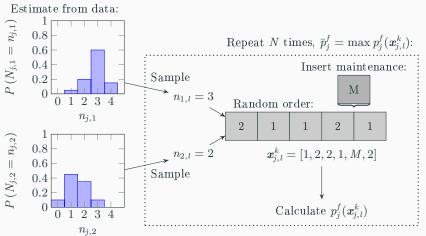
Alternative objective: Li and Li (2015)

### Idea: Use Bayesian Optimization (BO)

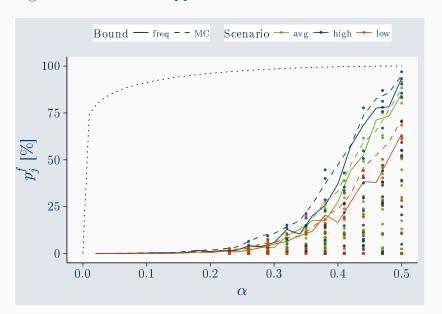
Both  $c^*$  and  $p_j^f$  can be viewed as expensive black box functions. BO is very suitable for this setting (Jones et al., 1998).

# Saving time: data-driven approximations

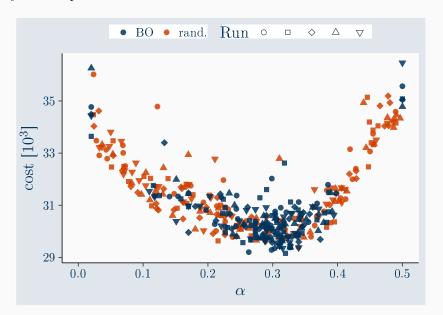
An upper bound on the probability of failure  $p_j^f$  can be estimated from data (using logistic regression).



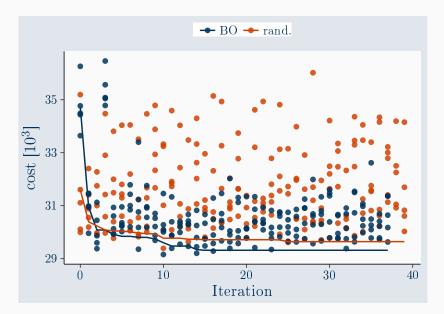
### Saving time: data-driven approximations



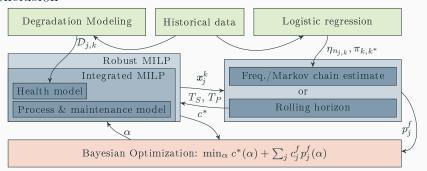
### Bayesian Optimization



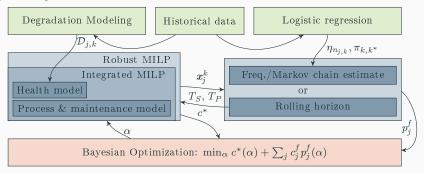
### Bayesian Optimization



#### Conclusion



#### Conclusion



# Thank You!

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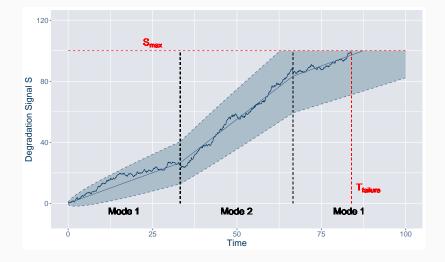
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# Degradation modelling with multiple operating modes



Saving time: a deterministic approximation

### **Assumption**

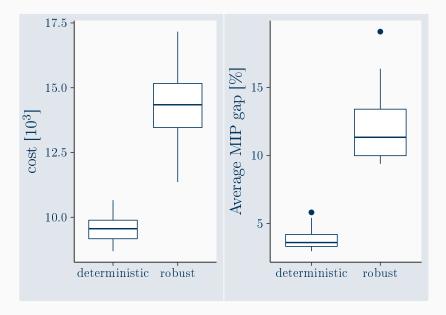
Only the health model depends on  $\tilde{d}_{j,k}$  and  $\tilde{d}_{j,k} \geq 0$ .

Then we can prove that a solution to

$$\begin{aligned} & \min_{\boldsymbol{x}, \boldsymbol{m}, \boldsymbol{h}} & \operatorname{cost}(\boldsymbol{x}, \boldsymbol{m}, \boldsymbol{h}) \\ & \text{s.t.} & & \operatorname{process model, maint. model}(\boldsymbol{x}, \boldsymbol{m}, \boldsymbol{h}) \\ & & s_{j,t} \leq s_{j}^{max} & \forall t, j \in J \\ & s_{j,t} = \begin{cases} s_{j,t-1} + \sum\limits_{k \in \mathcal{K}} x_{j,k,t} \cdot \boldsymbol{d}_{j,k}^{max}, & \text{if } m_{j,t} = 0 \\ s_{j}^{0}, & \text{otherwise} \end{cases} & \forall t, j \in J$$

with  $d_{j,k}^{max} = \max_{\mathcal{U}} \tilde{d}_{j,k}$  is also feasible in the robust problem.

# Saving time: a deterministic approximation



How does robust optimization work?

#### General idea

- · Make constraints hold for all values in  $\mathcal{U}$ :  $\sum_{i} \tilde{a}_{ij} x_j \leq b_i, \forall \tilde{a}_{ij} \in \mathcal{U}$
- Reformulate semi-infinite constraint:  $\sum_{i} a_{ij} x_j + \text{protection } (\mathcal{U}) \leq b_i$
- · How do we choose the right protection level?

## Example: Soyster's method (worst case) [1973]

$$\max_{x_1, x_2} x_1 + x_2 \qquad \max_{x_1, x_2} x_1 + x_2$$
s.t. 
$$\tilde{a}_{11}x_1 + \tilde{a}_{12}x_2 \le b_1, \qquad \text{s.t.} \qquad a_{11}x_1 + a_{12}x_2 + \sum_j \hat{a}_{ij} |x_j| \le b_1$$

$$\forall \tilde{a}_{ij} \in \mathcal{U}$$
Given:  $[a_{11}, a_{12}] = [1, 2], [\hat{a}_{11}, \hat{a}_{12}] = [0.1, 0.2], [b_1] = [2]$ 

#### Formulation

### Scheduling

$$M_{j,t}S_{j,0} \leq S_{j,t} \leq S_{j,max} + M_{j,t} \cdot (S_{j,0} - S_{j,max}) \qquad \forall t, j \in J, D \in \mathcal{D}$$

$$S_{j,t} \geq S_{j,t-\Delta t} + \sum_{k} Z_{j,k,t}D_{j,k,t} + M_{j,t} \cdot (S_{j,0} - S_{j,max}) \qquad \forall t, j \in J, D \in \mathcal{D}$$

$$S_{j,t} \leq S_{j,t-\Delta t} + \sum_{k} Z_{j,k,t}D_{j,k,t} \qquad \forall t, j \in J, D \in \mathcal{D}$$

### **Planning**

$$S_{j,t} \leq S_{j,max} \qquad \forall t, j \in J$$

$$S_{j,t} \geq S_{j,t-\Delta t} + \sum_{k} N_{j,k,t} D_{j,k,t} + M_{j,t} \cdot (S_{j,0} - S_{j,max}) \quad \forall t, j \in J$$

$$S_{j,t} \leq S_{j,t-\Delta t} + \sum_{k} N_{j,k,t} D_{j,k,t} \qquad \forall t, j \in J$$

Adjustable robust optimization

#### Affine decision rule

$$S_{j,t} = [S_{j,t}]_0 + \sum_k \sum_{t'=0}^t [S_{j,t}]_{k,t'} D_{j,k,t'}.$$

# Size of toy problem

	deterministic	robust $D \neq f(t)$	robust $D = f(t)$
# vars	913	3011	27719
# binaries	338	338	338
# constraints	1198	2356	13300
time to solve [s]	2	0.3-10	0.3-10
gap [%]	0	0	0
scheduling periods	30	30	30
planning periods	8	8	8
task-unit-op. mode	6	6	6
combinations	U	0	U

# Size of realistic problem

	deterministic	robust $D \neq f(t)$	robust $D = f(t)$
# vars	5389		397361
# binaries	2492		2492
# constraints	6798		180858
time to solve [s]	7883		16756
gap [%]	3.62		31.02
scheduling periods	56	56	56
planning periods	24	24	24
task-unit-op. mode combinations	24	24	24

### Deriving a robust counterpart

Replace  $D_{j,k}$  by an uncertain parameter  $\tilde{d}_{j,k}$  bounded by a set  $\mathcal{U}$ :

$$\begin{aligned} s_{j,t} &\leq s_j^{max} & \forall t,j \in J \\ s_{j,t} &= \begin{cases} s_{j,t-1} + \sum_{k \in \mathcal{K}} x_{j,k,t} \cdot \tilde{d}_{j,k}, & \text{if } m_{j,t} = 0 \\ s_j^0, & \text{otherwise} \end{cases} & \forall \tilde{d}_{j,k} \in \mathcal{U}, t,j \in J \end{aligned}$$

Reformulate:

$$m_{j,t}s_{j}^{0} \leq s_{j,t} \leq s_{j}^{max} + m_{j,t} \cdot (s_{j}^{0} - s_{j,max}) \qquad \forall t, j \in J, \tilde{d}_{j,k} \in \mathcal{U}$$

$$s_{j,t} \geq s_{j,t-\Delta t} + \sum_{k} x_{j,k,t} \tilde{d}_{j,k} + m_{j,t} \cdot (s_{j}^{0} - s_{j}^{max}) \qquad \forall t, j \in J, \tilde{d}_{j,k} \in \mathcal{U}$$

$$s_{j,t} \leq s_{j,t-\Delta t} + \sum_{k} x_{j,k,t} \tilde{d}_{j,k} \qquad \forall t, j \in J, \tilde{d}_{j,k} \in \mathcal{U},$$

Replace  $s_{j,t}$  by linear decision rule  $s_{j,t} = [s_{j,t}]_0 + \sum_k [s_{j,t}]_k \tilde{d}_{j,k}$ .

Objective function:

$$cost = \sum_{j \in J} c_j^{maint} \left( s_j^{fin} / s_j^{max} + \sum_{t \in T} m_{j,t} \right) + c_s^{storage} \left( q_s^{fin} + \sum_{t \in T_p} q_{s,t} \right) + U \left( \sum_{s \in S} \phi_s^d + \sum_{t \in T_S} \phi_{s,t}^q \right)$$

Constraints scheduling horizon:

$$\sum_{k \in K_j} \sum_{i \in I_j} \sum_{t' = t - p_{i,j,k} + \Delta t_S}^t w_{i,j,k,t'} + \sum_{t' = t - \tau_i + \Delta t_S}^t m_{j,t'} \le 1 \quad \forall J, t \in T_S$$
 (2a)

$$v_{i,j}^{min}w_{i,j,k,t} \leq b_{i,j,k,t} \leq v_{i,j}^{max}w_{i,j,k,t} \qquad \qquad \forall J,i \in I_j, k \in K_j, t \in T_S \qquad (2b)$$

$$q_{s,t} = q_{s,t-1} + \sum_{i \in \overline{I}_s} \bar{\rho}_{i,s} \sum_{j \in J_i} \sum_{k \in K_j} b_{i,j,k,t-p_{i,j,k}}$$

$$-\sum_{i \in I_s} \rho_{i,s} \sum_{i \in J_i} \sum_{k \in K_i} b_{i,j,k,t}$$
  $\forall s, t \in T_S$  (2c)

$$0 \le q_{s,t} - \phi_{s,t}^q \le c_s \tag{2d}$$

$$m_{j,t}s_j^0 \le s_{j,t} \le s_j^{max} + m_{j,t} \cdot (s_j^0 - s_j^{max}) \qquad \forall t, j \in J, D \in \mathcal{U}$$
 (2e)

$$s_{j,t} \ge s_{j,t-\Delta t_S} + \sum_{i} \sum_{k} w_{i,j,k,t} \tilde{d}_{j,k} + m_{j,t} \cdot (s_j^0 - s_j^{max}) \qquad \forall t, j \in J, D \in \mathcal{U}$$
 (2f)

$$s_{j,t} \le s_{j,t-\Delta t_S} + \sum_{i} \sum_{k} w_{i,j,k,t} \tilde{d}_{j,k} \qquad \forall t, j \in J, D \in \mathcal{U},$$
 (2g)

Constraints planning horizon:

$$\sum_{i \in I_j} \sum_{k \in K_j} p_{i,j,k} n_{i,j,k,t} + \tau_j m_{j,t} \le \Delta t_P \qquad \forall J, t \in T_P \setminus \{\bar{t}_P\}$$
 (2a)

$$v_{i,j}^{min} \sum_{k \in K_j} n_{i,j,k,t} \leq a_{i,j,t} \leq v_{i,j}^{max} \sum_{k \in K_j} n_{i,j,k,t} \qquad \qquad \forall J, i \in I_j, k \in K_j, t \in T_P \quad \text{(2b)}$$

$$q_{s,t} = q_{s,t-1} + \sum_{i \in \overline{I}_s} \bar{\rho}_{i,s} \sum_{j \in J_i} a_{i,j,t} - \sum_{i \in I_s} \rho_{i,s} \sum_{j \in J_i} a_{i,j,t} - \delta_{s,t} \quad \forall s,t \in T_P \backslash \{\overline{t}_P\}$$
 (2c)

$$0 \le q_{s,t} \le c_s \qquad \qquad \forall s,t \in T_P \tag{2d}$$

$$n_{i,j,k,t} \leq U \cdot \omega_{j,k,t} \qquad \forall J, i \in I_j, k \in K_j, t \in T_P \quad (2e)$$

$$\sum_{k \in K_j} \omega_{j,k,t} = 1 \qquad \qquad \forall J, t \in T_P$$
 (2f)

$$s_{j,t} \le s_j^{max}$$
  $\forall t, j \in J$  (2g)

$$s_j^t \ge s_{j,t-\Delta t_P} + \sum_k n_{j,k,t} \tilde{d}_{j,k,t} + m_{j,t} \cdot (s_j^0 - s_j^{max}) \qquad \forall t, j \in J$$
 (2h)

$$s_{j,t} \le s_{j,t-\Delta t_P} + \sum_{i} n_{j,k,t} \tilde{d}_{j,k,t} \qquad \forall t, j \in J$$
 (2i)

Constraints interface between scheduling and planning:

$$\begin{split} \sum_{k \in K_j} \sum_{i \in I_j} \sum_{t' = \overline{t}_S + 2\Delta t_S - p_{i,j,k}}^{\overline{t}_S} w_{i,j,k,t'} \left[ p_{i,j,k} - (\overline{t}_S - t' + \Delta t_S) \right] \\ + \sum_{t' = \overline{t}_S + 2\Delta t_S - \tau_j}^{\overline{t}_S} m_{j,t'} \left[ \tau_j - (\overline{t}_S - t' + \Delta t_S) \right] \\ + \sum_{t' = \overline{t}_S + 2\Delta t_S - \tau_j}^{\overline{t}_S} m_{j,t'} \left[ \tau_j - (\overline{t}_S - t' + \Delta t_S) \right] \\ + \sum_{i \in I_j} \sum_{k \in K_j} p_{i,j,k} n_{i,j,k,\overline{t}_P} + \tau_j m_{j,\overline{t}_P} \le \Delta t_P, \\ q_s^{fin} = q_{s,\overline{t}_S} + \sum_{i \in \overline{t}_s} \bar{\rho}_{i,s} \sum_{j \in J_i} \sum_{k \in K_j} b_{i,j,k,\overline{t}_S + 1 - p_{i,j,k}} \\ - d_{s,\overline{t}_S} + \phi_s^d \\ 0 \le q_s^{fin} \le c_s \\ q_{s,\overline{t}_P} = q_s^{fin} + \sum_{i \in \overline{t}_S} \bar{\rho}_{i,s} \sum_{j \in J_i} \sum_{k \in K_j} \sum_{t' = \overline{t}_S + 2 - p_{i,j,k}} b_{i,j,k,t'} \\ + \sum_{i \in \overline{t}_S} \bar{\rho}_{i,s} \sum_{j,J_i} a_{i,j,\overline{t}_P} \\ - \sum_{i,I_s} \rho_{i,s} \sum_{j \in J_i} a_{i,j,\overline{t}_P} - d_{s,\overline{t}_P} \end{split}$$

Results: instances

Instance	Toy	P1	P2	P4	P6
Units	2	4	5	3	6
Tasks	3	5	3	4	8
Op. modes	2	3	3	2	2
Products	2	2	1	2	4
Discrete vars	518	2492	1930	1869	1993
Continuous vars	1033	3630	2371	2777	4084
Constraints	1860	7332	5705	5699	7994
Avg. MIP gap [%]	0.0	3.0	5.8	10.9	1.02

Table 1: Evaluated STN instances

P1: Kondili et al. (1993), P2: Karimi and McDonald (1997), P4: Maravelias and Grossmann (2003), P6: Ierapetritou and Floudas (1998)

## Results: metrics data-driven approximation

$$\operatorname{rms}_{all}^{2} = \frac{1}{N \cdot |A|} \sum_{n \in \{1..N\}, \alpha \in A} \left( \left[ p_{j}^{f} \right]_{n,\alpha} - \bar{p}_{j}^{f} \right)^{2}, \tag{3a}$$

$$p_{out} = \frac{1}{N \cdot |A|} \sum_{n \in \{1..N\}, \alpha \in A} \mathbb{1} \left( \left[ p_{j}^{f} \right]_{n,\alpha} > \bar{p}_{j}^{f} \right), \text{ and} \tag{3b}$$

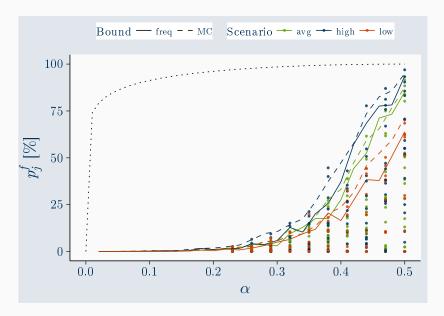
$$\operatorname{rms}_{out}^2 = \frac{1}{p_{out} \cdot N \cdot |A|} \sum_{n \in \{1..N\}, \alpha \in A} \mathbb{1}\left(\left[p_j^f\right]_{n,\alpha} > \bar{p}_j^f\right) \left(\left[p_j^f\right]_{n,\alpha} - \bar{p}_j^f\right)^2, \quad (3c^2)$$

Results: metrics data-driven approximation

instance	bound	${\rm rms\_all}$	${ m rms\_max}$	p_out
toy	freq	8.00	1.53	29.40
toy	mc	10.41	3.08	21.27
P1	freq	12.61	3.52	17.54
P1	mc	17.25	4.39	9.62
P2	freq	7.40	2.31	18.08
P2	mc	13.68	4.98	10.13
P4	freq	9.17	3.27	47.78
P4	mc	11.43	2.84	32.50
P6	freq	18.75	8.94	12.17
P6	mc	20.84	10.09	10.98
all	freq	11.19	3.91	24.99
all	$\mathrm{mc}$	14.72	5.08	16.90

P1: Kondili et al. (1993), P2: Karimi and McDonald (1997), P4: Maravelias and Grossmann (2003), P6: Ierapetritou and Floudas (1998)

# Results: metrics data-driven approximation



Results: metrics data-driven approximation

