Adjustable Robust Optimization for Chemical Production Scheduling[1]

Dhruv Gupta

Department of Chemical and Biological Engineering

University of Wisconsin – Madison

November 4, 2016

[1]Lappas, N.H. & Gounaris, C.E., 2016. Multi-stage adjustable robust optimization for process scheduling under uncertainty. *AIChE Journal*, 62(5), pp.1646–1667.

Robust Optimization (RO)

$$\min_{x \in X} f(x,\xi) \quad \text{s.t. } g_i(x,\xi) \le 0 \ \forall i \quad \xrightarrow[\text{Counterpart}]{\text{Robust}} \quad \min_{x \in X} \max_{\xi \in \Xi} f(x,\xi) \quad \text{s.t. } g_i(x,\xi) \le 0 \ \forall \xi \in \Xi, i$$

- RO seeks to identify solutions that remain feasible under any realization of the parameters within an uncertainty set $\xi \in \Xi$.
- Selects the best solution for the "worst-case".
- Particularly suitable where loss of feasibility cannot be tolerated
  - Safety concerns
  - Equipment physical limitations
- Advantages (over stochastic optimization)
  - Typically RO counterpart belongs to same problem class as the original deterministic problem $\Rightarrow$ Similar computational tractability.
  - Applicable even when probability distribution of parameters not available, but bounds available.
- Limitations
  - "Too conservative" due to focus on "worst-case".
  - Restricted to single-stage decision-making.
- Modeling the uncertainty set
  - $\Xi = \{\xi \in \mathbb{R}^n \mid \|\xi\|_p \le \alpha\}$ p=1,p=2 (ellipsoid), p=∞ (box)
  - $\Xi = \{\xi \in \mathbb{R}^n \mid \sum_{i=1}^n h_{ji}\xi_i \le g_j, \forall j\}$ (polyhedral set)
  - $\Xi = \{\xi \in \mathbb{R}^n \mid \sum_{i=1}^n h_{ji}(x)\xi_i \le g_j(x), \forall j\}$ (decision-dependent; endogenous)

Adjustable (Multi-stage) Robust Optimization (ARO)

$$x^1 \rightarrow \xi^1 \rightarrow x^2(\xi^1) \ldots \rightarrow \xi^{T-1} \rightarrow x^T(\xi^1, \ldots \xi^{T-1})$$

- Parameters realize gradually at different points in time, decisions are to be taken at each time interval in between
  - Multi-period problems (Vehicle routing, production scheduling, etc.)
- Special case: Two-stage
  - "Here and now" decisions, "Wait and see" decisions
  - For example, "invest capacities –observe demands –operate network" or "plan production –observe demands –buy/sell excess"
  - Exact solution methods: Benders dual cutting-plane approach (Thiele et al., 2010) and Constraint-and-column generation procedure (Zeng and Zhao, 2013)
- An approximate method to tackle the multi-stage problem
  - Static Robust Optimization (SRO) where all $x^t(\xi)$ are chosen at t=0
  - Adjustable (to parameter realizations) robust optimization (Ben-Tal et al. 2004)
  - Further research ongoing to find better approximations (Bertsimas and Caramanis, 2010; Bertsimas et al., 2011; Postek and den Hertog, 2016; …)
- Why approximate? Imperfect non-anticipativity.
- Decide now $[x^t]$ (the default/nominal value) and $[\Delta x^t]$ (the proportional adjustment)
  - $x_t = [x^t] + [\Delta x^t]\xi^t$ (Optimal "policy" for continuous decisions)
  - For integer recourse: piecewise-constant rules (Bertsimas and Georghiou, 2015)

Advantages of ARO over SRO

- Enables modeling time-dependent parameter values
  - e.g. Processing times $\alpha_i \rightarrow \alpha_{in}$ (tasks: *i*, time-point: *n*)
  - A task run in the morning could be 30 mins, afternoon can be 35 mins.
  - Hence, no implicit assumption at decision making step that realizations are identical with time

- Better "worst-case" performance
  - SRO solution subset of ARO solution
  - Accounts for correlation $\sum_i \sum_n h_{fin}\alpha_{in} \leq g_f \; \forall f \in F$

- Better performance on the average
  - Capitalizes on realizations, through recourse

- Can directly handle equality constraints
  - Hence, applicable to a broader set of models
  - Useful in the case of e.g. Zero-wait materials

- Can also be solved as a single optimization (retains problem class)

- Choice: Which variables are adjustable.
  - No adjustable decisions $\Rightarrow$ SRO
  - Adjustable decisions and their bounds dictate advantage of ARO over SRO

Scheduling Deterministic Model[1]

- Continuous time, global (floating) event points T_n; decide N apriori
- S_{sn} denotes inventory of material *s* between points *n* and *n*+1
- P_S denotes price of material *s*
- $W_{inn'}$ when 1 denotes task *i* starts at point *n* and ends on/before *n'*
- $B_{inn'}$ denotes batch-size of task *i* that starts at point *n* and ends on/before *n'*
- G_{jn} when 1 denotes utilization of unit *j* at point *n*

$$\min_{\substack{W,T,B\\S,G,z}} z$$

-ve of Profit $z = \sum_{s\in S} P_s(S_{s0} - S_{sN})$ $\quad T_N = H$

Makespan $z = T_N - T_1$ $\quad S_{sN} \geq D_s$

$$T_{n'} - T_n \geq \sum_{i\in I_j}(\alpha_i W_{inn'} + \beta_i B_{inn'}) \ \forall j \in J, n \in N, n' \in N_n^+$$

$$T_{n'} - T_n \leq \bar{M}[1 - \sum_{i\in I_j \cap I^{zw}} W_{inn'}] + \sum_{i\in I_j}(\alpha_i W_{inn'} + \beta_i B_{inn'}) \ \forall j \in J, n \in N, n' \in N_n^+$$

$$T_N - T_n \geq \sum_{i\in I_j}\sum_{n'\in N:\{n'\geq n\}}\sum_{n''\in N_{n'}^+}(\alpha_i W_{inn'} + \beta_i B_{inn'}) \ \forall j \in J, n \in N$$

$$G_{jn} = G_{j(n-1)} + \sum_{i\in I_j}[\sum_{n'\in N_n^+} W_{inn'} - \sum_{n'\in N_n^-} W_{in'n}] \quad \forall j \in J, n \in N$$

$$S_{sn} = S_{s(n-1)} + \sum_{i\in I_s^p} \rho_{is} \sum_{n'\in N_n^-} B_{in'n} - \sum_{i\in I_s^C} \rho_{is} \sum_{n'\in N_n^+} B_{inn'} \quad \forall j \in J, n \in N$$

$$W_{inn'} B_i^{min} \leq B_{inn'} \leq W_{inn'} B_i^{max} \quad \forall j \in J, n \in N, n' \in N_n^+$$

$$0 \leq G_{jn} \leq 1 \forall j \in J, n \in N \qquad 0 \leq S_{sn} \leq S_s^{max} \forall s \in S, n \in N$$

$$G_{jN} = 0 \ \forall j \in J \qquad T_1 = 0$$

$$W_{inn'} = 0, B_{inn'} = 0 \ \forall i \in I, n \in N, n' \in N \backslash N_n^+$$

$$W_{inn'} \in \{0,1\} \ \forall i \in I, n \in N, n' \in N$$

[1]Castro P et al., 2004. Ind. Eng. Chem. Res. 43(1):105-118

ARO Counterpart Preliminaries

Endogenous uncertainty set for expanded α in time n

$$A(W) = \left\{ \alpha \in R_+^{|I||N|} : \begin{array}{l} \sum_{i\in I}\sum_{n\in N} h_{fin}\left(\sum_{n'\in N_n^-} W_{in'n}\right)\alpha_{in} \le \sum_{i\in I}\sum_{n\in N} g_{fin}\left(\sum_{n'\in N_n^-} W_{in'n}\right) \forall f\in F \\ \alpha_{in}^{lb} \le \alpha_{in} \le \alpha_{in}^{ub} \quad \forall\, i\in I, n\in N \end{array} \right\}$$

Can adjust decisions that are not multiplied with an uncertain parameter

$$T_n \rightarrow [T_n]_0 + \sum_{i\in I}\sum_{n'\in N}[\Delta T_n]_{in'}\alpha_{in'}$$
$$B_{inn''} \rightarrow [B_{inn''}]_0 + \sum_{i'\in I}\sum_{n'\in N}[\Delta B_{inn''}]_{i'n'}\alpha_{i'n'}$$
$$S_{sn} \rightarrow [S_{sn}]_0 + \sum_{i\in I}\sum_{n'\in N}[\Delta S_{sn}]_{in'}\alpha_{in'}$$

Non-anticipativity: Cannot utilize value of some uncertain parameter realization not yet occurred to adjust present decisions

$$[\Delta T_n]_{in'} = 0 \quad \forall i\in I, n'\in N: n' > n$$
$$[\Delta B_{inn'}]_{i'n''} = 0 \quad \forall i,i'\in I, n,n',n''\in N: n'' > n' \ge n$$
$$[\Delta S_{sn}]_{in'} = 0 \quad \forall i\in I, s\in S, n'\in N: n' > n$$

Observability: Cannot adjust decisions due to uncertainty that never realized

$$\sum_{n''\in N_{n'}^-} W_{in''n'} = 0 \Rightarrow [\Delta T_n]_{in'} = 0 \quad \forall i\in I, n'\in N: n' \le n$$
$$\sum_{n''\in N_{n'}^-} W_{in''n'} = 0 \Rightarrow [\Delta B_{inn'''}]_{in'} = 0 \quad \forall i\in I, n'\in N: n' \le n$$
$$\sum_{n''\in N_{n'}^-} W_{in''n'} = 0 \Rightarrow [\Delta S_{sn}]_{in'} = 0 \quad \forall i\in I, n'\in N: n' \le n$$

Constraints

- M_I: Inequalities involving uncertain parameters and/or adjustable variables
- M_E: Equalities involving uncertain parameters and/or adjustable variables
- M_C: Remaining constraints (stay unchanged)

ARO Counterpart for M_E Equalities

Original equality constraint

$$S_{sn} = S_{s(n-1)} + \sum_{i\in I_s^p} \rho_{is} \sum_{n'\in N_n^-} B_{in'n} - \sum_{i\in I_s^C} \rho_{is} \sum_{n'\in N_n^+} B_{inn'} \quad \forall\, \alpha \in A(W)$$

New adjustable variables definitions

$$B_{inn''} \to [B_{inn''}]_0 + \sum_{i'\in I}\sum_{n'\in N}[\Delta B_{inn''}]_{i'n'}\alpha_{i'n'}$$
$$S_{sn} \to [S_{sn}]_0 + \sum_{i\in I}\sum_{n'\in N}[\Delta S_{sn}]_{in'}\alpha_{in'}$$

Robust Counterpart

Substitute in original equality constraints and collect terms multiplied with α_{in}

$$\sum_{i'\in I}\sum_{n''\in N}\left([\Delta S_{sn}]_{i'n''} - [\Delta S_{s(n-1)}]_{i'n''} - \sum_{i\in I_s^p}\rho_{is}\sum_{n'\in N_n^-}[\Delta B_{in'n}]_{i'n''} + \sum_{i\in I_s^C}\rho_{is}\sum_{n'\in N_n^+}[\Delta B_{inn'}]_{i'n''}\right)\alpha_{i'n''}$$
$$= -[S_{sn}]_0 + [S_{s(n-1)}]_0 + \sum_{i\in I_s^p}\rho_{is}\sum_{n'\in N_n^-}[B_{in'n}]_0 - \sum_{i\in I_s^C}\rho_{is}\sum_{n'\in N_n^+}[B_{inn'}]_0 \quad \forall \alpha \in A(W)$$

To accommodate all $\alpha \in A(W)$, both terms individually need to go to zero

$$[S_{sn}]_0 = [S_{s(n-1)}]_0 + \sum_{i\in I_s^p}\rho_{is}\sum_{n'\in N_n^-}[B_{in'n}]_0 - \sum_{i\in I_s^C}\rho_{is}\sum_{n'\in N_n^+}[B_{inn'}]_0$$
$$[\Delta S_{sn}]_{i'n''} = [\Delta S_{s(n-1)}]_{i'n''} + \sum_{i\in I_s^p}\rho_{is}\sum_{n'\in N_n^-}[\Delta B_{in'n}]_{i'n''} - \sum_{i\in I_s^C}\rho_{is}\sum_{n'\in N_n^+}[\Delta B_{inn'}]_{i'n''}$$

ARO Counterpart for M_I Inequalities

Original inequality constraint

$$T_{n'} - T_n \geq \sum_{i\in I_j}(\alpha_i W_{inn'} + \beta_i B_{inn'}) \ \forall j \in J, n \in N, n' \in N_n^+$$

New adjustable variables definitions

$$T_n \rightarrow [T_n]_0 + \sum_{i\in I}\sum_{n'\in N}[\Delta T_n]_{in'}\alpha_{in'}$$

$$B_{inn''} \rightarrow [B_{inn''}]_0 + \sum_{i'\in I}\sum_{n'\in N}[\Delta B_{inn''}]_{i'n'}\alpha_{i'n'}$$

Robust Counterpart

Substitute in original inequality constraints and collect terms multiplied with α_{in}

$$\theta^* = \sum_{i\in I_j}\alpha_{in}W_{inn'} + \sum_{i'\in I}\sum_{n''\in N}(-[\Delta T_{n'}]_{i'n''} + [\Delta T_n]_{i'n''} + \sum_{i\in I_j}\beta_i[\Delta B_{inn'}]_{i'n''})\alpha_{i'n''}$$
$$\leq [T_{n'}]_0 - [T_n]_0 - \sum_{i\in I_j}\beta_i[B_{inn'}]_0 \quad \forall \alpha \in A(W)\ \forall j \in J, n \in N, n' \in N_n^+$$

To accommodate all $\alpha \in A(W)$, we can equivalently find max of the left side expression θ^*

$$\theta^* = \max_{\alpha\in R_+^{|I||N|}} \sum_{i\in I_j}\alpha_{in}W_{inn'} + \sum_{i'\in I}\sum_{n''\in N}(-[\Delta T_{n'}]_{i'n''} + [\Delta T_n]_{i'n''} + \sum_{i\in I_j}\beta_i[\Delta B_{inn'}]_{i'n''})\alpha_{i'n''}$$
$$\text{s.t. } \left.\begin{array}{l}\sum_{i\in I}\sum_{n\in N}h_{fin}\left(\sum_{n'\in N_n^-}W_{in'n}\right)\alpha_{in} \leq \sum_{i\in I}\sum_{n\in N}g_{fin}\left(\sum_{n'\in N_n^-}W_{in'n}\right)\forall f \in F \\ \alpha_{in}^{lb} \leq \alpha_{in} \leq \alpha_{in}^{ub} \quad \forall\, i \in I, n \in N\end{array}\right\} \forall \alpha \in A(W)$$

Equivalently, we can solve the dual LP

$$\theta^* = \min_{\substack{p^{jnn'}\in R_+^{|F|} \\ q^{jnn'}\in R_+^{|I||N|} \\ r^{jnn'}\in R_+^{|I||N}}} \sum_{i\in I_j}\sum_{n"\in N}(\sum_{f\in F}g_{fi'n"}\left(\sum_{n'''\in N_{n"}^-}W_{i'n'''n"}\right)p_f^{jnn'} - \alpha_{i'n"}^{lb}q_{i'n"}^{jnn'} + \alpha_{i'n"}^{ub}r_{i'n"}^{jnn'})$$
$$\text{s.t. } \sum_{f\in F}h_{fi'n"}\left(\sum_{n'''\in N_{n"}^-}W_{i'n'''n"}\right)p_f^{jnn'} - q_{i'n"}^{jnn'} + r_{i'n"}^{jnn'}$$
$$\geq 1_{\{i'\in I_j\}}1_{\{n"=n\}}W_{i'n"n'} - [\Delta T_{n'}]_{i'n"} + [\Delta T_n]_{i'n"} + \sum_{i\in I_j}\beta_i[\Delta B_{inn'}]_{i'n''}\ \forall i' \in I, n" \in N$$

Finally, any feasible solution of the dual LP is acceptable, and we use McCormick exact linearization for bilinear terms

$$\sum_{i\in I_j}\sum_{n"\in N}(\sum_{f\in F}g_{fi'n"}s_{fi'n"}^{jnn'} - \alpha_{i'n"}^{lb}q_{i'n"}^{jnn'} + \alpha_{i'n"}^{ub}r_{i'n"}^{jnn'}) \leq [T_{n'}]_0 - [T_n]_0 - \sum_{i\in I_j}\beta_i[B_{inn'}]_0$$

$$\left.\begin{array}{l}\sum_{f\in F}h_{fi'n"}s_{fi'n"}^{jnn'} - q_{i'n"}^{jnn'} + r_{i'n"}^{jnn'} \geq 1_{\{i'\in I_j\}}1_{\{n"=n\}}W_{i'n"n'} - [\Delta T_{n'}]_{i'n"} + [\Delta T_n]_{i'n"} + \sum_{i\in I_j}\beta_i[\Delta B_{inn'}]_{i'n''} \\ \left.\begin{array}{l}\sum_{n'''\in N_{n"}^-}W_{i'n'''n"} = 1 \Rightarrow s_{fi'n"}^{jnn'} \geq p_f^{jnn'} \\ \sum_{n'''\in N_{n"}^-}W_{i'n'''n"} = 0 \Rightarrow s_{fi'n"}^{jnn'} \leq 0 \\ s_{fi'n"}^{jnn'} \leq p_f^{jnn'}\end{array}\right\} \forall f \in F\end{array}\right\} \forall i' \in I, n" \in N$$

Solution under nominal realization

SRO

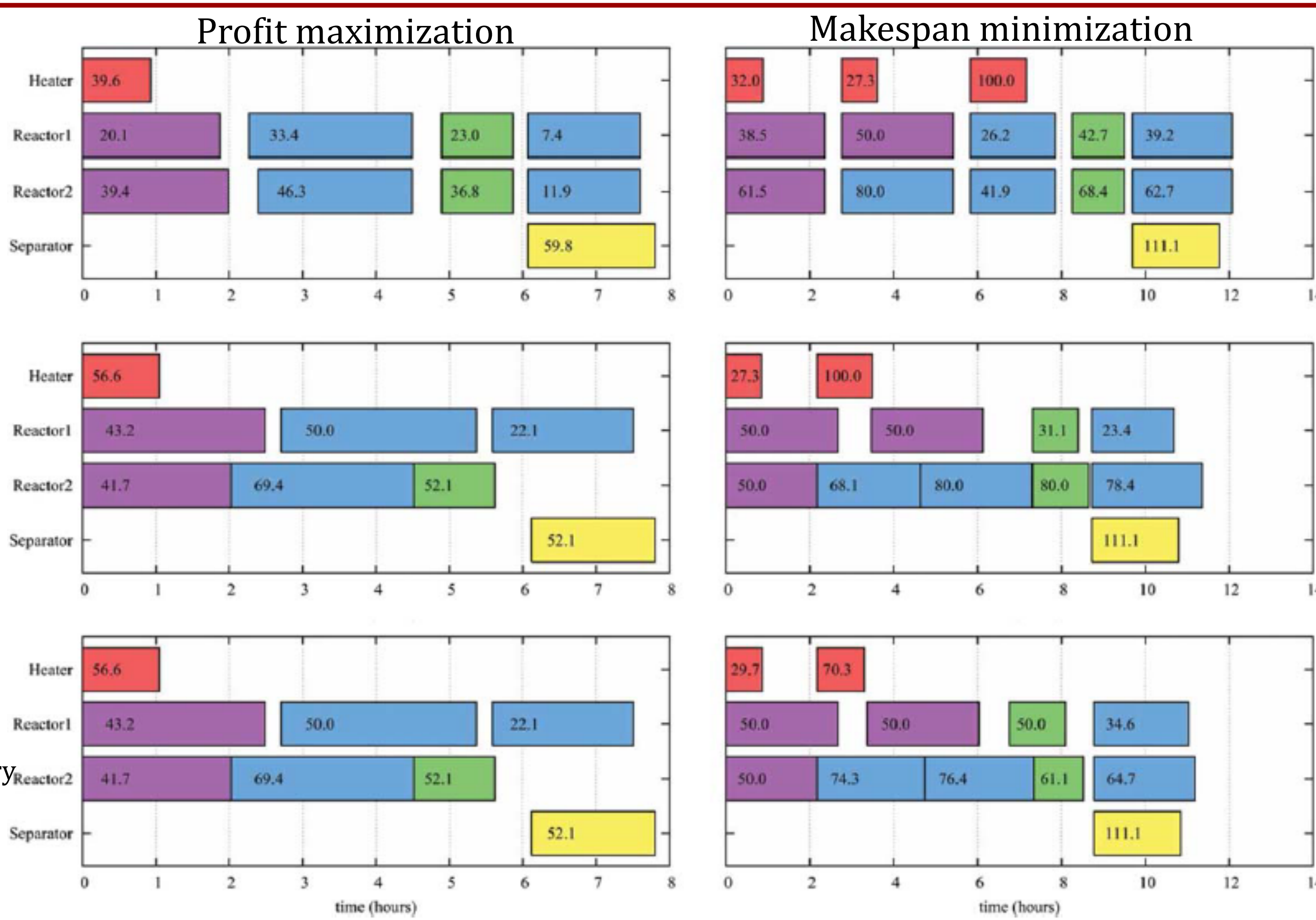
No adjustable decisions

ARO

Timing decisions adjustable

ARO

Timing, batch-sizes, and inventory decisions adjustable



- SRO introduces idle times/gaps to accommodate worst-case realization at every possible realization
- ARO features smaller gaps
- SRO solution is one of the candidate ARO solution; All realizations cannot be worst-case. => ARO is better even in the worst-case.

Further comparing SRO and AROs

	Max Profit			Min Makespan		
	SRO	ARO	ARO	SRO	ARO	ARO
Adjustable variables	–	T	T, B, S	–	T	T, B, S
# Event points	7	7	7	8	8	8
CPU time (s)	72	269	32,925	91	324	75,129
# Nodes	16,289	14,924	17,367	44,502	40,453	62,642
# Variables (cont.)	3,812	7,385	43,322	5,188	12,290	64,171
# Variables (bin.)	78	78	78	94	94	94
# Constraints	8,421	12,276	76,373	12,876	18,607	112,177
Worst-case objective	934.1	1,034.7	1,034.7	12.46	12.15	12.08

- Computational cost increases considerably with additional adjustable variables
- ARO solution marginally improves, for the makespan case with additional adjustment variables
- Adjusting "few but important" variables can be the right trade-off

- To measure conservatism, Recovery ratio: $RR = \frac{\zeta^*_{SRO} - \zeta^*_{ARO}}{\zeta^*_{SRO} - \zeta^*_{WCD}}$

Makespan minimization

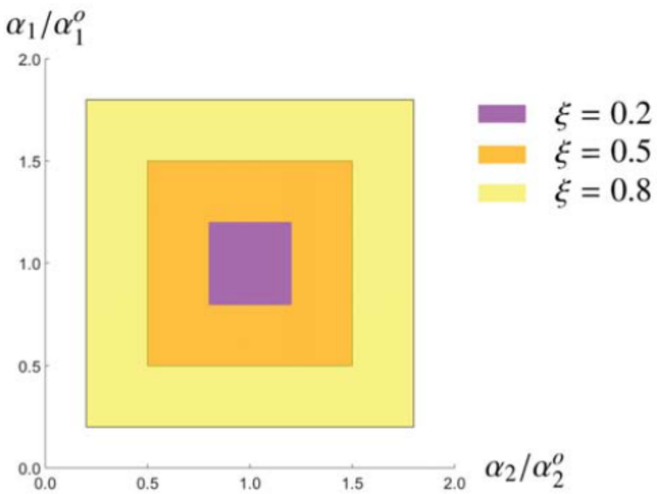
Instance	SRO	ARO	EDO	ERR
P1	12.47	11.64	10.66	45.9
P2	8.36	7.99	7.06	28.5
P3	16.03	15.58	13.36	16.9
P4	6.60	6.34	6.00	43.3
P5	–	12.66	11.00	–
P6	16.58	16.28	14.38	13.6
P7	29.39	26.53	23.50	48.6
Avg.				32.8

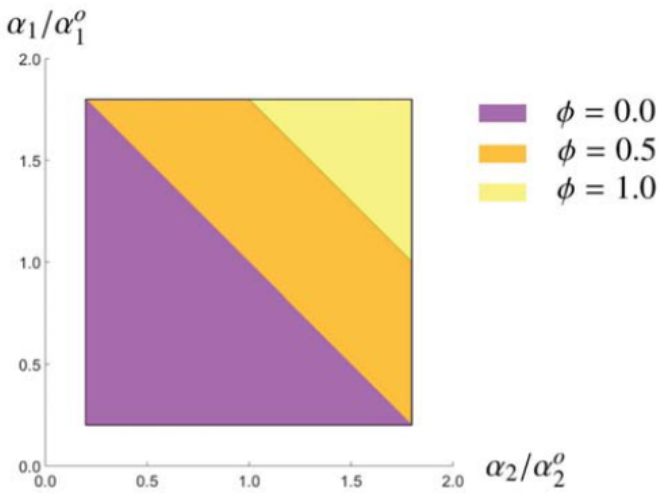
Expectations computed across a uniform sampling of the uncertainty set.

Zero-wait SRO N/A ← (P5)

Performance given an uncertainty set

$$A(W) = \left\{ \alpha \in R_+^{|I||N|} : \begin{array}{l} \sum_{i \in I} \sum_{n \in N} \left(\sum_{n' \in N_n^-} W_{in'n} \right) \alpha_{in} \leq \sum_{i \in I} \sum_{n \in N} (1 + \xi\phi) \alpha_i^0 \left(\sum_{n' \in N_n^-} W_{in'n} \right) \forall j \in J \\ (1 - \xi)\alpha_i^0 \leq \alpha_{in} \leq (1 + \xi)\alpha_i^0 \quad \forall\, i \in I, n \in N \end{array} \right\}$$





RR: Profit maximization

		ϕ				
		0.00	0.25	0.50	0.75	1.00
ξ	0.00	–	–	–	–	–
	0.10	41	19	0	0	–
	0.20	36	26	7	0	–
	0.30	40	47	35	13	–
	0.40	48	53	47	23	–
	0.50	51	55	48	13	–

RR: Makespan minimization

		ϕ				
		0.00	0.25	0.50	0.75	1.00
ξ	0.00	–	–	–	–	–
	0.10	97	86	67	63	–
	0.20	78	59	41	36	–
	0.30	72	55	32	26	–
	0.40	66	47	27	13	–
	0.50	60	36	23	19	–

- ARO is even more advantageous when uncertain parameters are correlated ($\phi \rightarrow 0$)

Summary (Multi-stage ARO)

- Generates an optimal policy (not a schedule) for continuous decisions
  - $x_t = [x^t] + [\Delta x^t]\xi^t$
- Better "average" and "worst-case" performance
  - SRO solution subset of ARO solution
  - Accounts for correlation $\sum_i \sum_n h_{fin}\alpha_{in} \leq g_f \; \forall \, f$
  - Capitalizes on realizations
- Can directly handle equality constraints
  - Hence, applicable to a broader set of models
  - Useful in the case of e.g. Zero-wait materials
- Suitable for endogenous uncertainties
- Adjusting few "important" variables can be a good trade-off between solution quality and computational time