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Modern Robust Optimization: Opportunities for Enterprise-Wide Optimization

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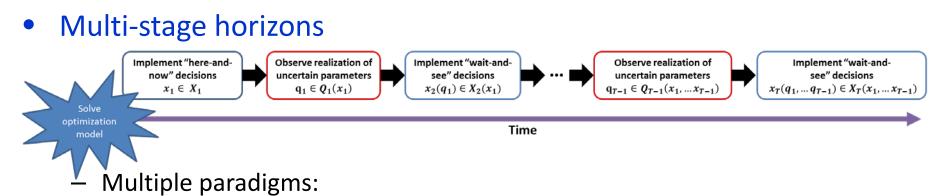


Uncertainty in EWO Setting

- Uncertainty is inherent in virtually all EWO settings, both strategic and operational ones
- Typical sources of uncertainty:
 - Market behavior
 - e.g., prices, customer demands
 - Unexpected events
 - e.g., disruptions
 - Model-system mismatch
 - e.g., unknown thermodynamics and/or kinetics
- Optimization in view of only the nominal case can lead to suboptimal/infeasible solutions
 - \rightarrow Need for risk-averse decision-making

Carnegie Mellon III ENGINEERING Challenges for EWO under Uncertainty

- Large combinatorial component
 - Mixed-integer models with lots of discrete decisions
 - Often custom-built approaches (decomposition, branch-and-cut/price, etc.)
 - Discreteness also prevalent on the side of uncertain parameters



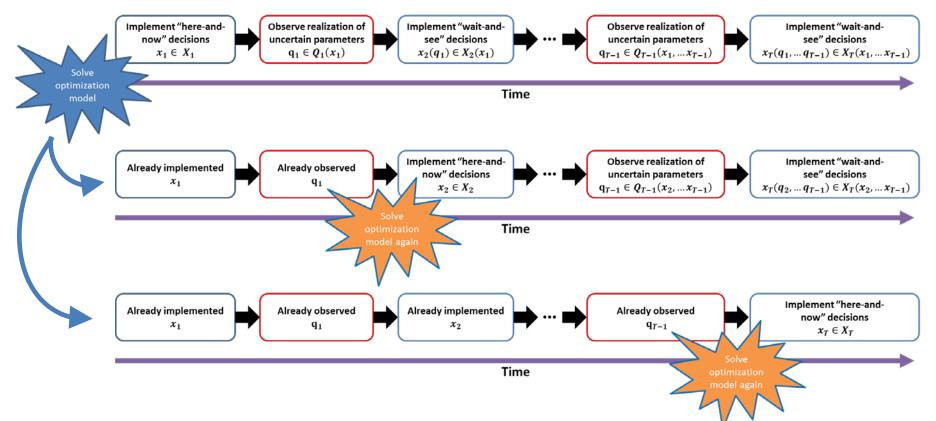
- Invest now, then operate every fiscal year
- Place/receive order now, then route material through the supply chain
- Decide control actions for the whole control horizon
- Set up a DSS to work autonomously in a rolling horizon fashion
 - Re-optimization round-the-clock, as often as you can afford





Multi-stage Horizons (cont'd)

- Re-optimization frequency dictated by tractability
- Number of stages dictated by need to locate "better solutions"



- Need high-quality "wait-and-see" decisions (prepare to adopt them!)
- "Closed-loop feasibility" is more likely as you account for more stages





Robust Optimization

- Game theory interpretation:
 - Player 1 (decision-maker) tries to minimize the objective
 - Player 2 (adversary nature) tries to minimize feasibility margin
- Foundations in "pessimistic optimization" (Wald, Soyster)
 - Attempts to find the solution that would perform best in the "worst-case"
 - The above implies that the solution must remain feasible under all cases we want to insure against (uncertainty set)

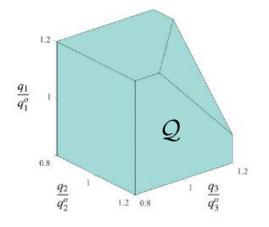
• Some references to start with:

- A. Ben-Tal, L. El Ghaoui and A. Nemirovski (2009). Robust Optimization. Princeton University Press
- D. Bertsimas, D.B. Brown and C. Caramanis (2011). Theory and Applications of Robust Optimization. SIAM Review, 53(3):464
- B.L. Gorissen, I. Yanikoglu and D. den Hertog (2015). A Practical Guide to Robust Optimization. Omega, 53:124
- C.E. Gounaris (2017). Advances in Robust Optimization and Opportunities for Process Operations. In: Proceedings of FOCAPO 2017/CPC IX, Paper ID IF110





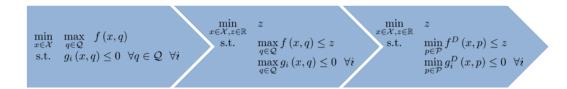
• a.k.a. "Static" Robust Optimization





Reformulation Approach

 Address semi-infinite formulation via duality-based treatment of inner problems



Robust Cutting-Plane Approach¹

- Given a (feasible or relaxed) solution, solve a separation problem to identify realizations from within the uncertainty set for which this solution violates a constraint
- Gradually enforce robustness by adding select deterministic constraints using violating realizations

The problem can be solved "monolithically," via direct call to an appropriate optimization solver

- Restricted to settings where strong duality holds
- The size of the problem grows a lot (unnecessarily?) as the uncertainty set dimensionality grows

- Can accommodate non-standard settings, e.g.,
 - discrete uncertain parameters
 - non MathOpt-based solvers
- Requires more elaborate implementation (and lots of "tuning")





Robust Optimization

- When to consider:
 - When you can routinely solve the deterministic problem
 - Feasibility is important
 - Safety reasons
 - Cannot monetize infeasibility
 - Large number of parameters that only sparsely participate in constraints
 - Stochastic description of uncertainty meets certain criteria
 - No detailed (joint) probability distributions
 - Well-motivated, strong correlations among parameters
- Size and shape of uncertainty set is chosen by the modeler
 - Usually some norm-based set (e.g., interval, ellipsoid, box)
 - No explicit requirement for scenarios and/or probability distributions
 - If distributional information exists, uncertainty sets can be related to confidence intervals



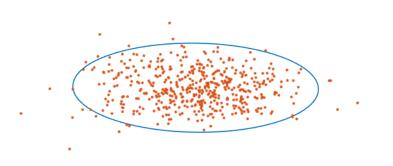
Examples of Uncertainty Sets

Ellipsoids

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Gaussian confidence intervals

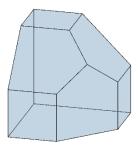
$$\mathcal{Q}_E = \left\{ \boldsymbol{q} \in \mathbb{R}^n : (\boldsymbol{q} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\boldsymbol{q} - \boldsymbol{\mu}) \leq \beta \right\}$$



Budget sets

aggregate forecasts at various hierarchies

$$\mathcal{Q}_{B} = \left\{ \boldsymbol{q} \in \left[\boldsymbol{q}, \boldsymbol{\bar{q}} \right]^{n} : \sum_{i \in B_{l}} \boldsymbol{q}_{i} \leq b_{l}, \ \forall l \in \{1, \dots, L\} \right\}$$

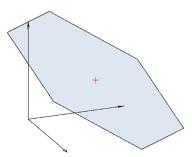


Factor models

bounded disturbances around nominal values

$$\mathcal{Q}_F = \left\{ q \in \mathbb{R}^n : q = q^0 + \Phi \boldsymbol{\xi} \text{ for some } \boldsymbol{\xi} \in \boldsymbol{\Xi} \right\}$$
$$\boldsymbol{\Xi} = \left\{ \boldsymbol{\xi} \in [-1, 1]^F : \left| e^\top \boldsymbol{\xi} \right| \le \beta F \right\}, \quad F \ll n$$

- "zero-net-alpha" models in portfolio optimization

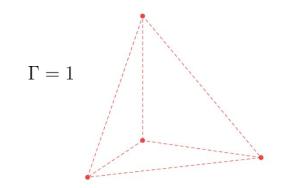


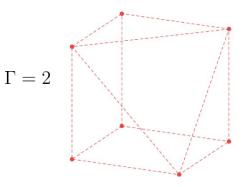


Examples of Uncertainty Sets

- Cardinality-constrained sets
 - "Gamma" sets (Bertsimas & Sim, 2004)

 $\mathcal{Q}_{\Gamma} = \left\{ q \in \left[q^0, q^0 + \hat{q} \right] : \exists W \subseteq \{1, \dots, n\}, \ |W| \le \Gamma : \mathbf{q}_i = \left\{ \begin{array}{cc} q_i^0 + \hat{q}_i, & \text{if } i \in W \\ q_i^0, & \text{if } i \notin W \end{array} \middle| \forall i \in \{1, \dots, n\} \right\} \right\}$





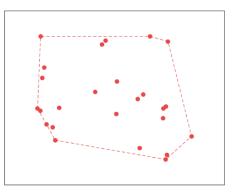
Discrete sets

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Collection of relevant scenarios

$$Q_S = \{q^{(1)}, q^{(2)}, \dots, q^{(M)}\}$$





Polyhedral Uncertainty Sets

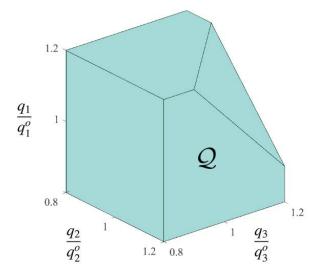
Advantages:

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- Numerically tractable, maintaining class of deterministic counterpart
- Derivable from historical data via machine learning techniques
- Can always be used as approximations of non-polyhedral sets

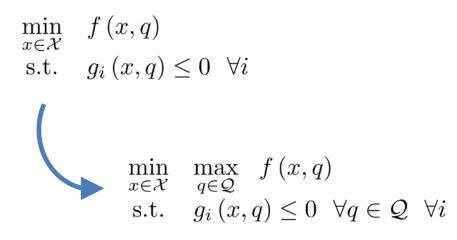
$$\mathcal{Q} = \left\{ \begin{array}{l} q \in \mathbb{R}^{nq}, \ p \in \left\{0,1\right\}^{np} : \\ Hq + Gp \le d \\ q^{L} \le q \le q^{U} \end{array} \right\}$$

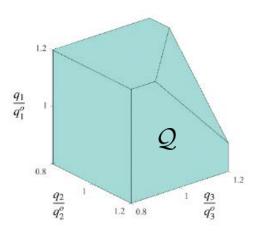




• a.k.a. "Static" Robust Optimization

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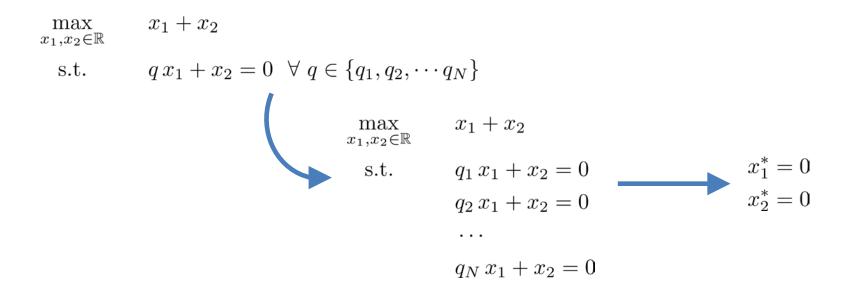




- <u>Main limitation</u>: All decisions are considered as "here-and-now" (irrespectively of whether the application mandates this or not)
- Consequently, we cannot enforce equalities involving uncertain parameters (e.g., mass balances with uncertain reaction rates)



• SRO affords us only a single value (solution) for each decision variable, making it hard to satisfy an equality constraint that references an uncertain parameter for all its realizations

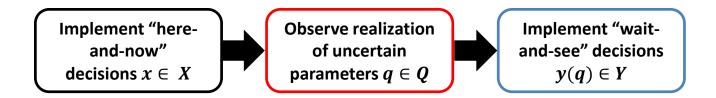


State-variable elimination could sometimes remedy the issue





• "Adjustable" Robust Optimization



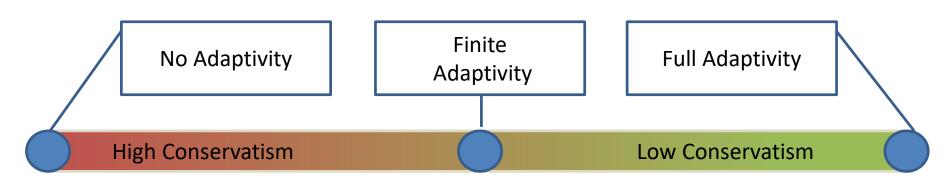
$$\min_{x \in \mathcal{X}} \max_{q \in \mathcal{Q}} \min_{y(q) \in \mathcal{Y}} \quad f(x, y, q)$$

s.t.
$$g_i(x, y, q) \le 0 \quad \forall q \in \mathcal{Q} \quad \forall i$$

- A specific y may be optimal for a scenario q, but suboptimal for a scenario q'
- Best y(q) may correspond to any arbitrary functional dependence
- Ideally we would like to identify the best feasible *y* for each possible *q*

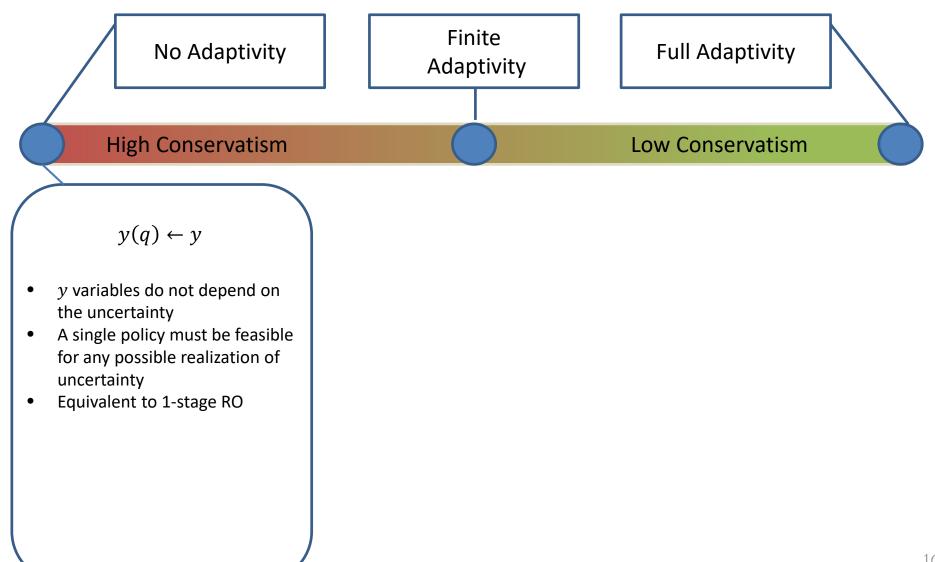






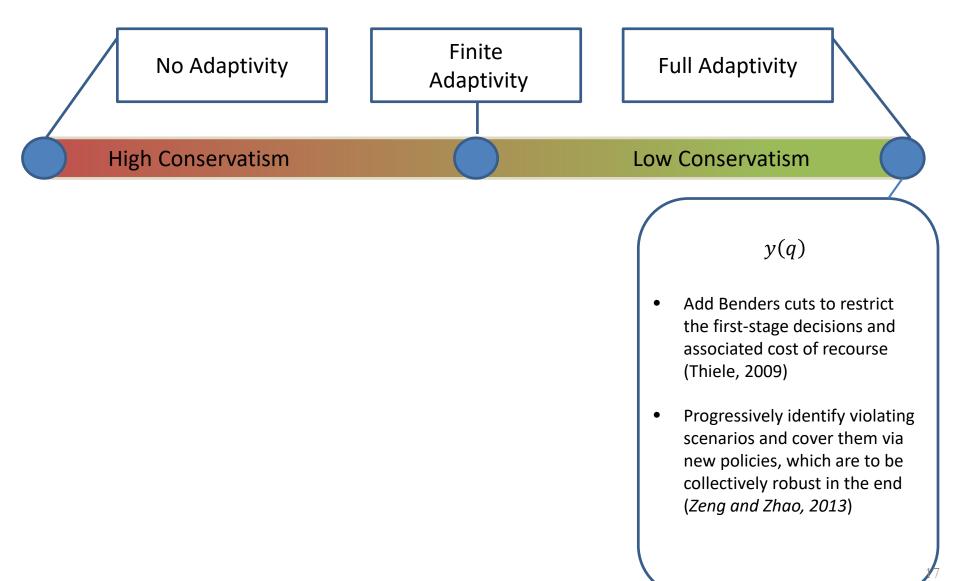








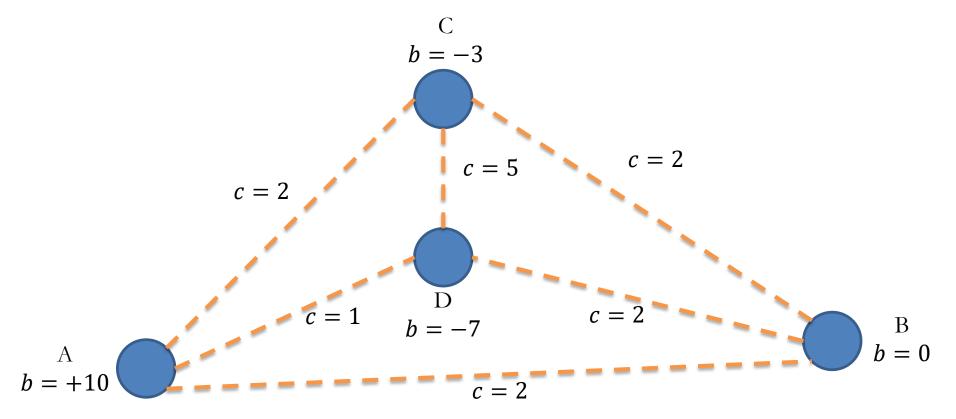








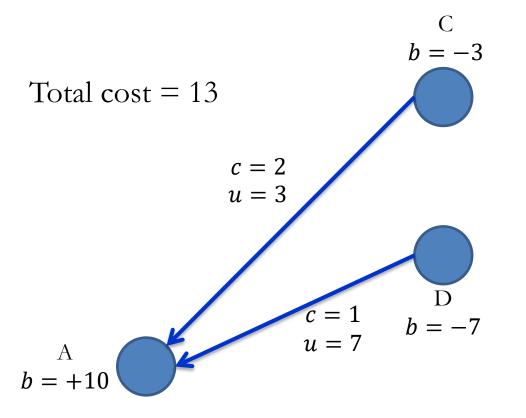
Consider the transportation of a commodity between four locations

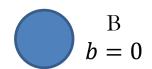






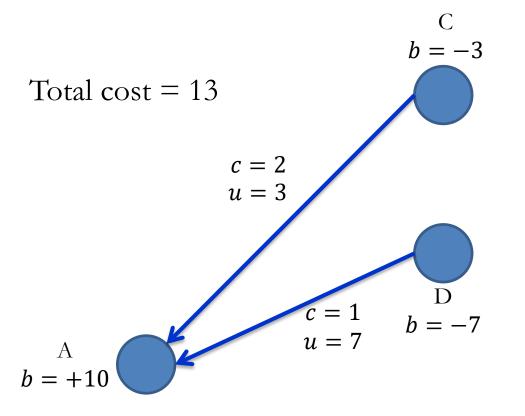
Optimal solution is to build exactly two links

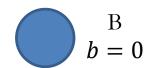






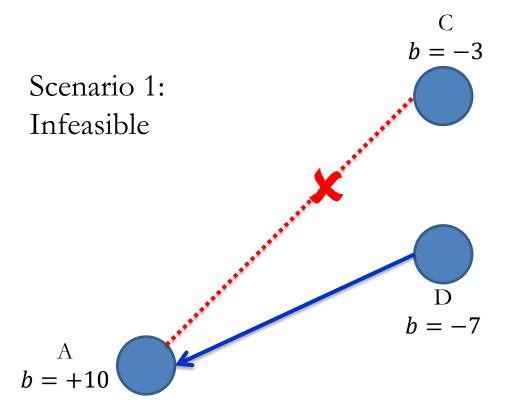


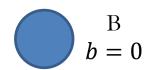






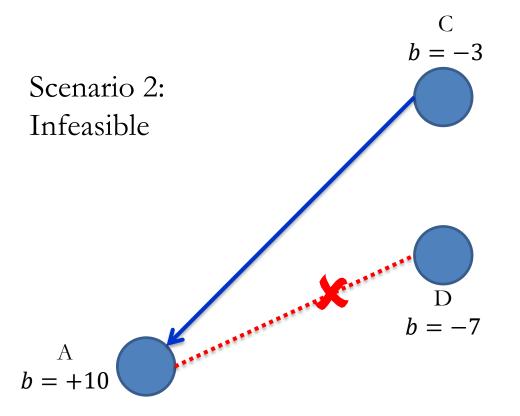


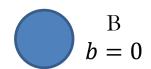






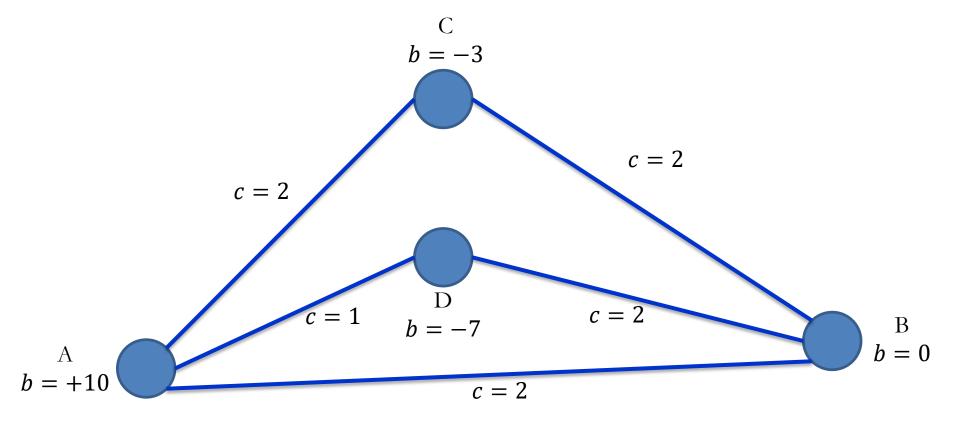






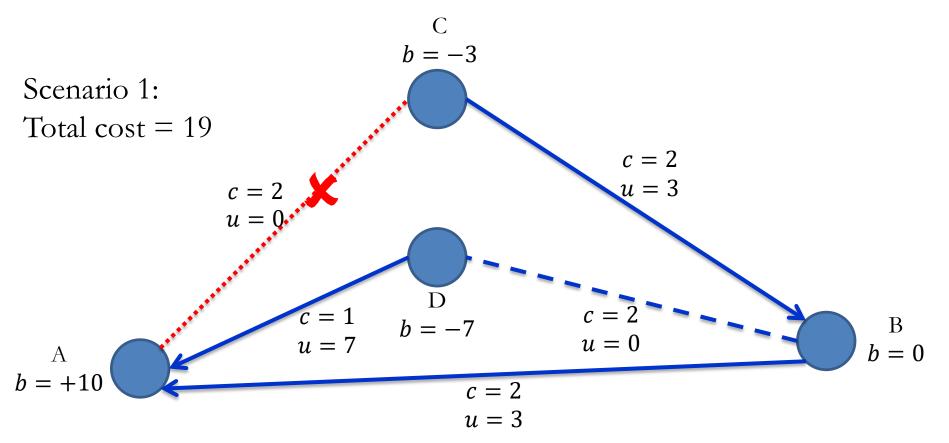






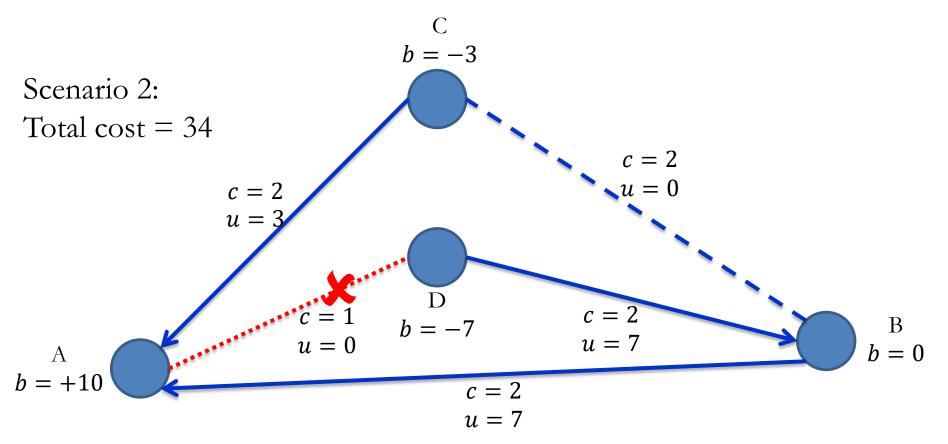






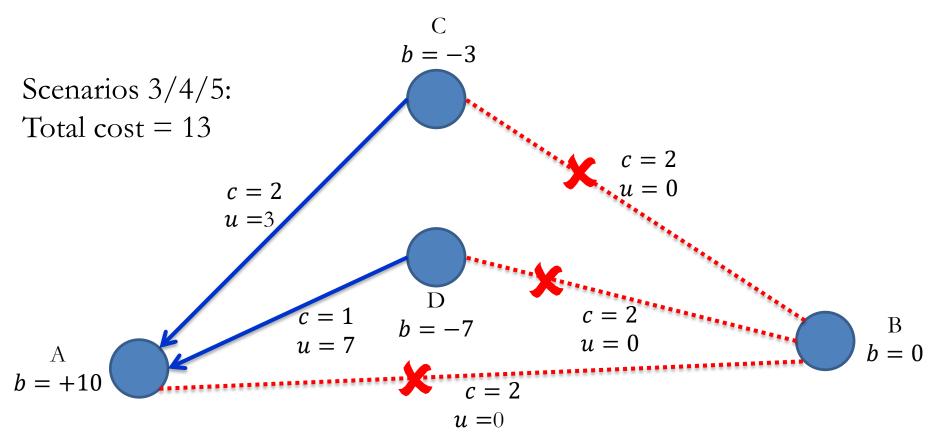








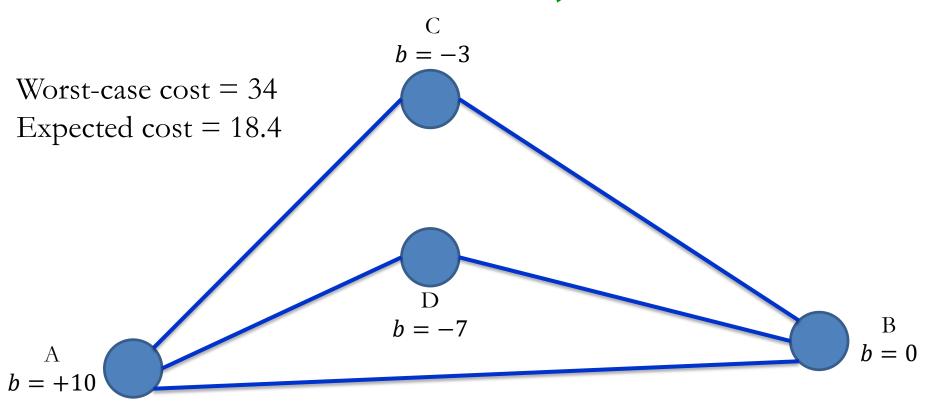








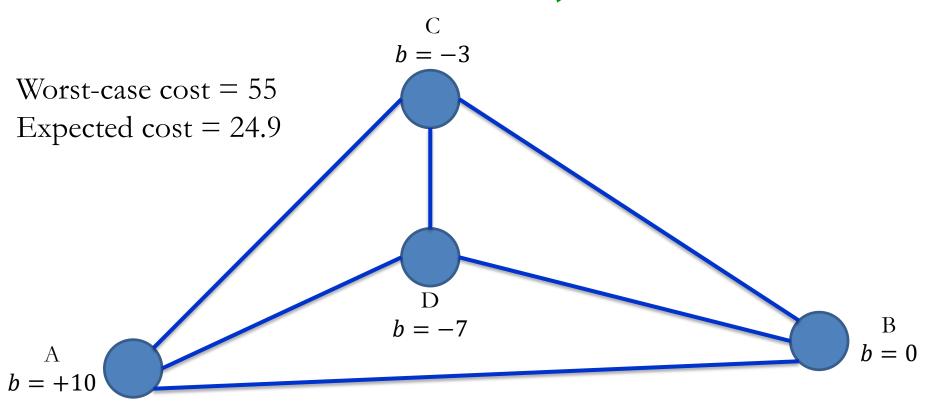
Robust (up to 1 disrupted links) Network







Robust (up to 2 disrupted links) Network

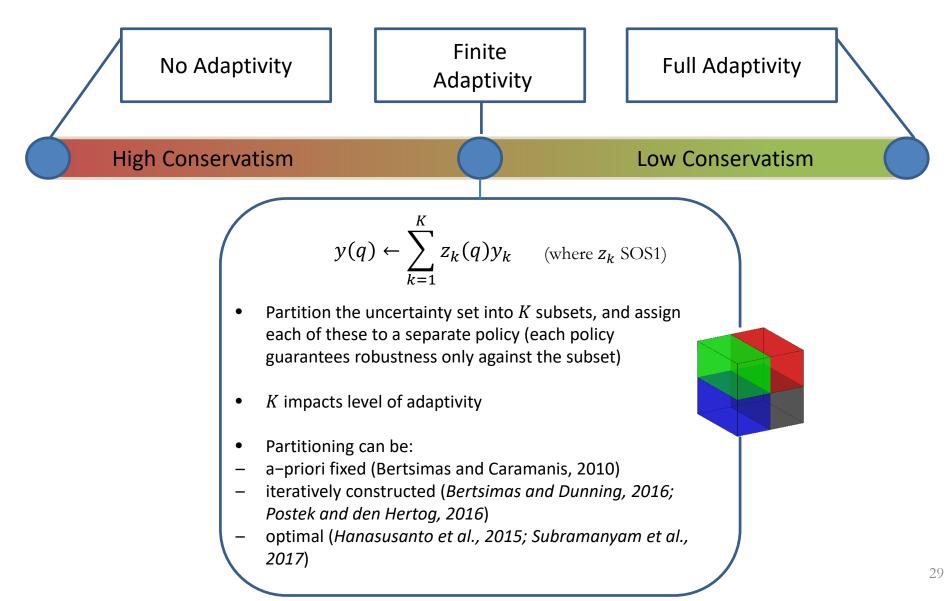


Apply C&CG to solve this problem on a larger scale!

L.R. Matthews, C.E. Gounaris and Y.G. Kevrekidis (2017). Designing Networks with Uncertain Edge Failures Using Two-Stage Robust Optimization. Under Review



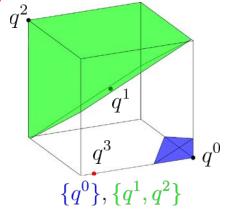








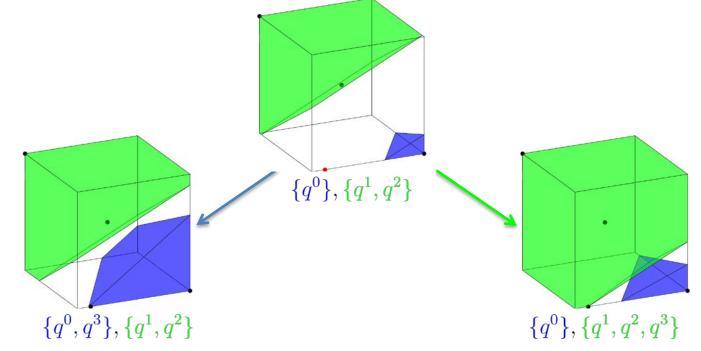
- Example with K = 2
 - Blue region = insured by policy 1, green region = insured by policy 2
 - Black points = scenarios enforced, red points = new scenarios identified







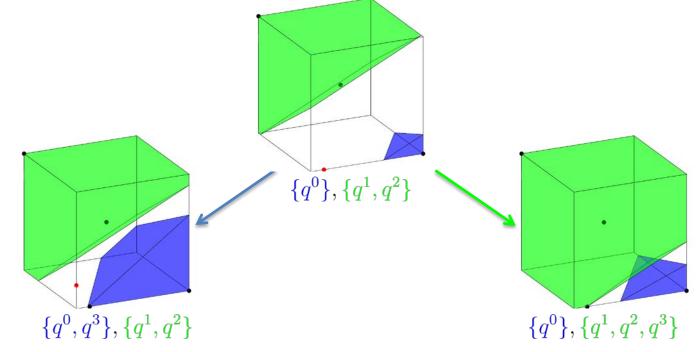
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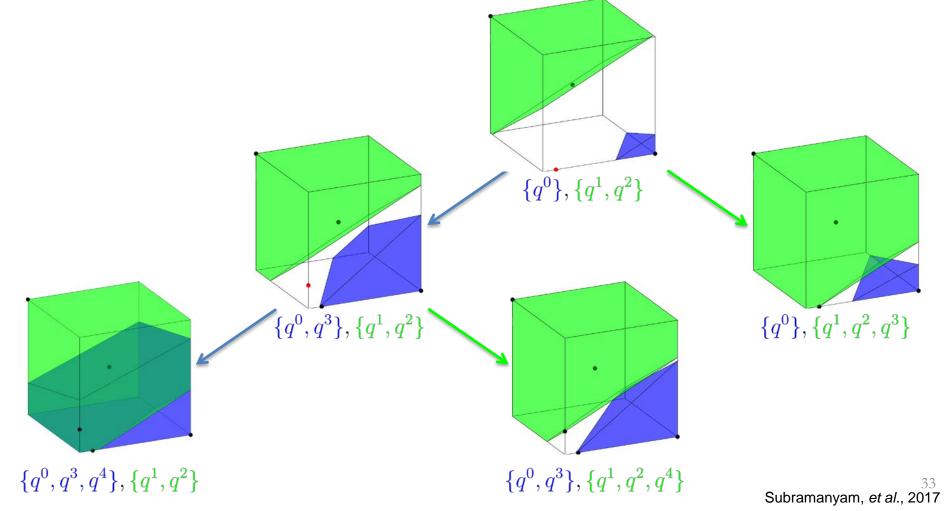
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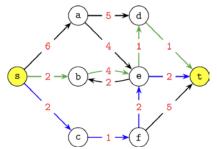
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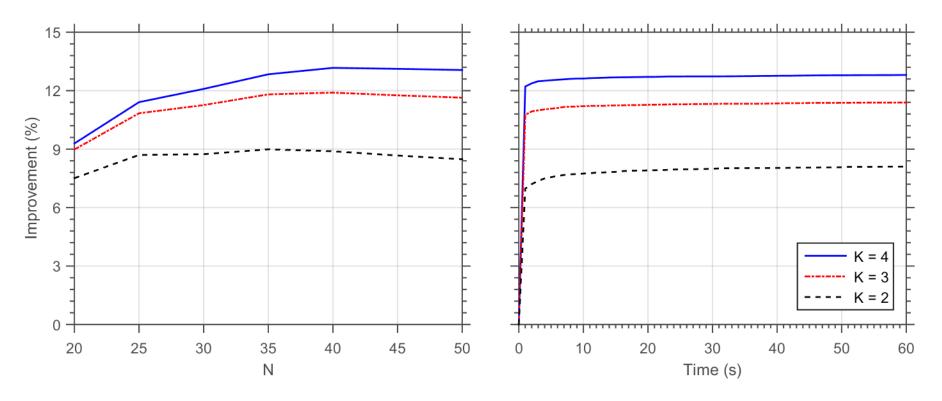






- Shortest Paths with Uncertain Costs
 - Low K suffices for maximal WC-objective gains
 - High quality solutions identified quickly





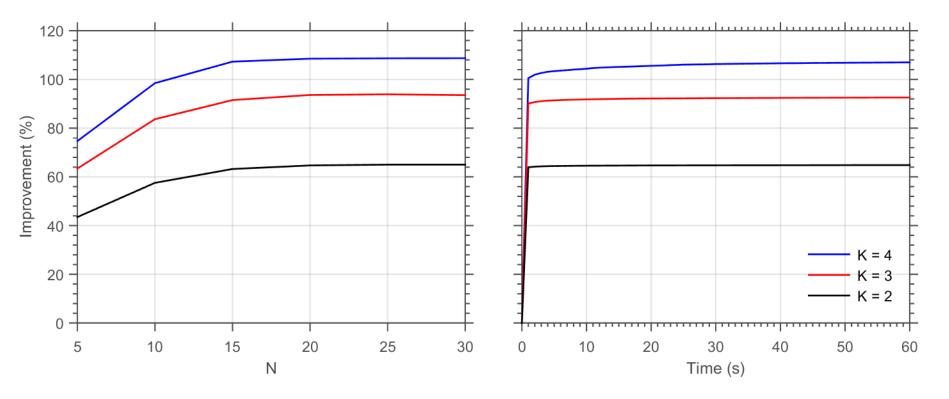
A. Subramanyam, C.E. Gounaris and W. Wiesemann (2017). K-Adaptability in Two-Stage Mixed-Integer Robust Optimization. Under Review. E₄ print available at: http://www.optimization-online.org/DB_HTML/2017/06/6093.html





- Capital Budgeting with Uncertain ROIs
 - Low K suffices for maximal WC-objective gains
 - High quality solutions identified quickly

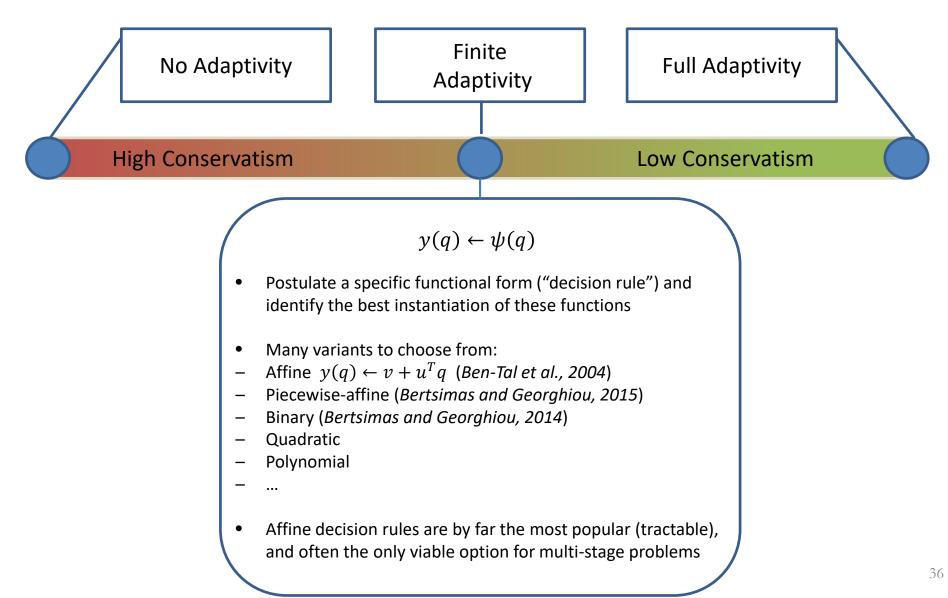




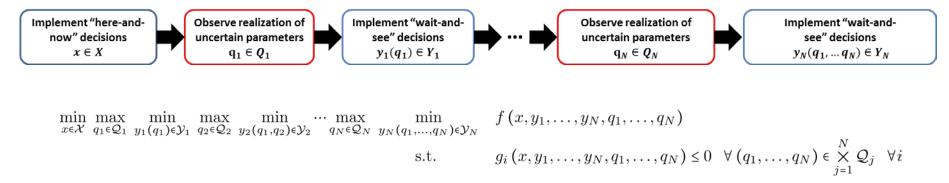
A. Subramanyam, C.E. Gounaris and W. Wiesemann (2017). K-Adaptability in Two-Stage Mixed-Integer Robust Optimization. Under Review. E₅ print available at: http://www.optimization-online.org/DB_HTML/2017/06/6093.html







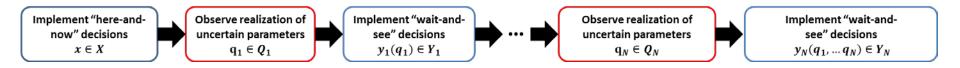




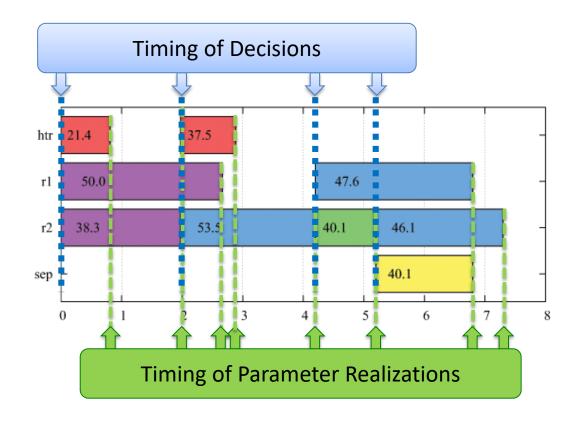
- Information gets revealed progressively
- Decisions have to be taken in between revelations
- Non-anticipativity must be obeyed
- Typical examples: Scheduling, Inventory planning, etc.



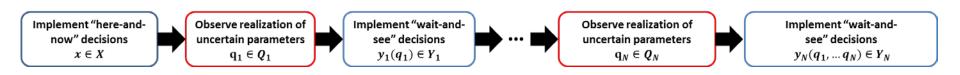




Typical examples: **Scheduling**, **Inventory planning**, etc.





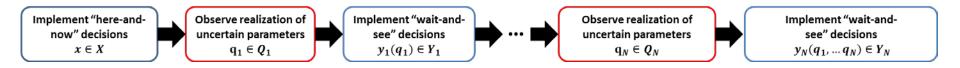


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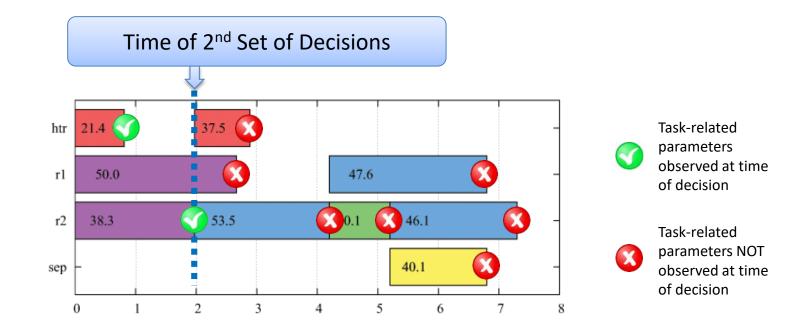






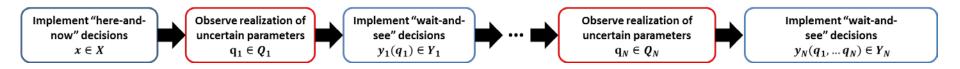


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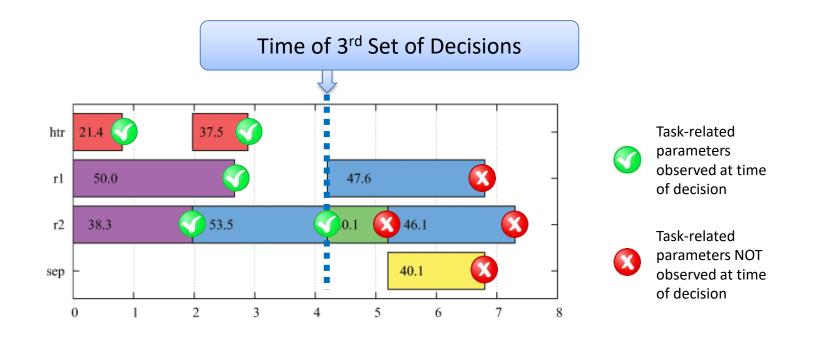






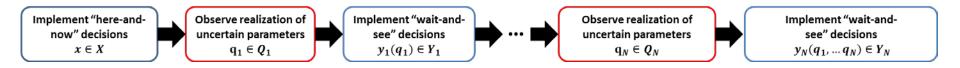


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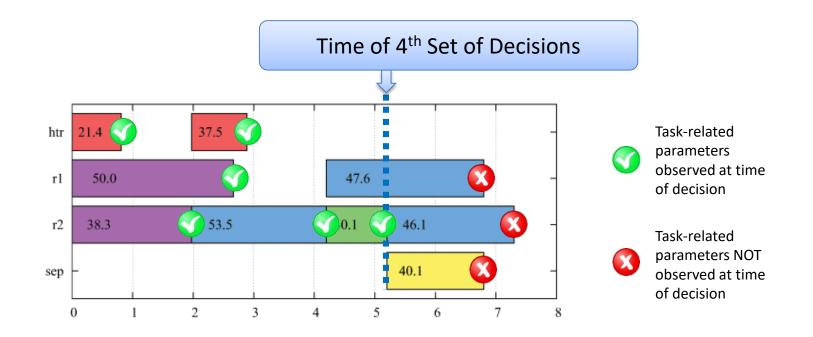




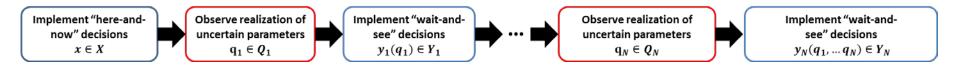




• Typical examples: **Scheduling, Inventory planning**, etc.







• Affine Decision Rules

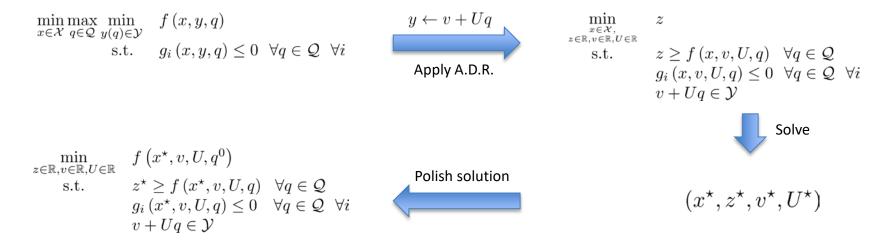
$$y_{1} \leftarrow v_{1} + u_{11}^{T} q_{1}$$

$$y_{2} \leftarrow v_{2} + u_{21}^{T} q_{1} + u_{22}^{T} q_{2}$$

$$y_{3} \leftarrow v_{3} + u_{31}^{T} q_{1} + u_{32}^{T} q_{2} + u_{33}^{T} q_{3}$$

$$\vdots$$

$$y_{N} \leftarrow v_{N} + u_{N1}^{T} q_{1} + u_{N2}^{T} q_{2} + u_{N3}^{T} q_{3} + \dots + u_{NN}^{T} q_{N}$$
Expect (lots of) degeneracy!

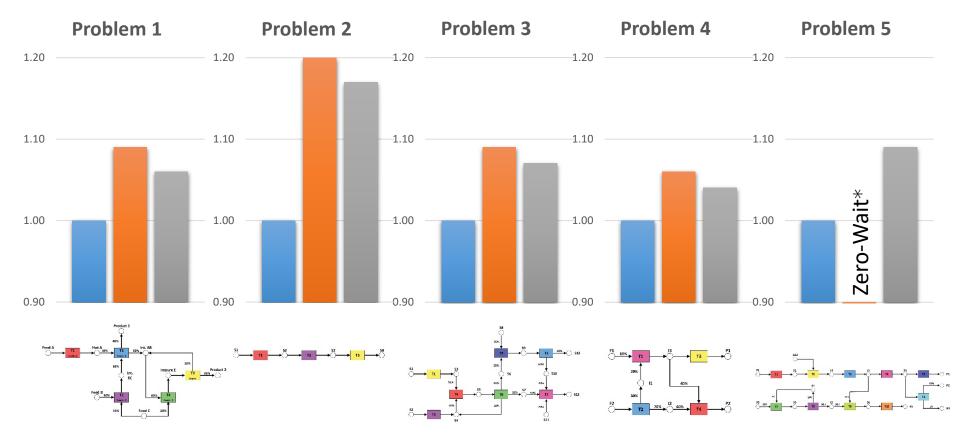




Worst-case Makespan (processing time uncertainty)

Static Robust

Adjustable Robust



N.H. Lappas and C.E. Gounaris (2016). Multi-stage Adjustable Robust Optimization for Process Scheduling Under Uncertainty. AIChE Journal, 62(5):1646-1667. Selected as Editor's Choice Paper. DOI 10.1002/aic.15183

*This instance cannot be solved with the static robust approach 44

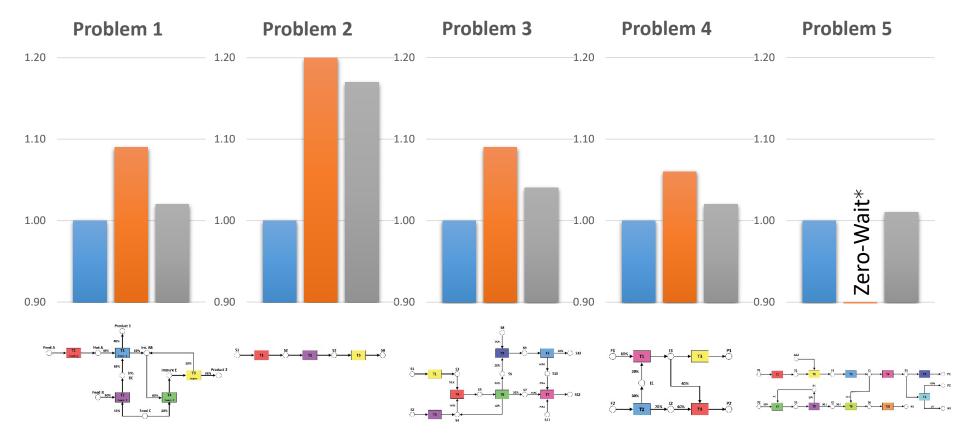
W.C. Deterministic



Expected Makespan (processing time uncertainty)

Static Robust

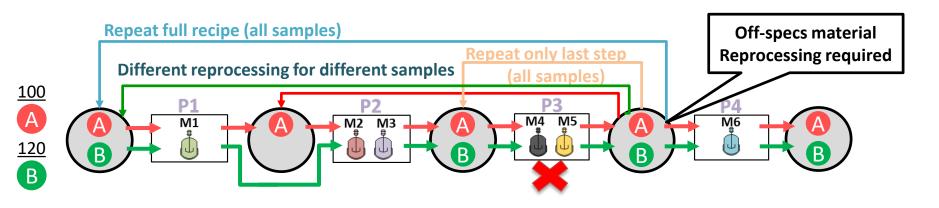
Adjustable Robust



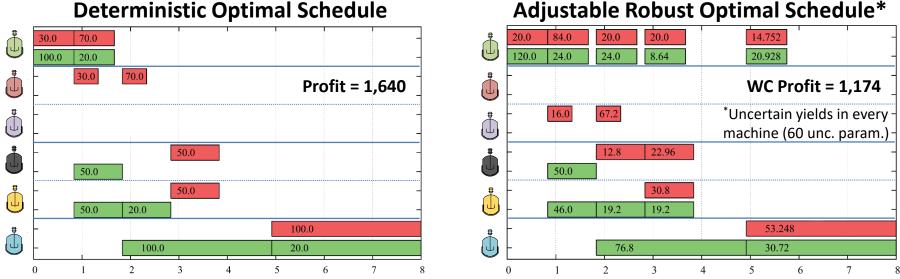
N.H. Lappas and C.E. Gounaris (2016). Multi-stage Adjustable Robust Optimization for Process Scheduling Under Uncertainty. AIChE Journal, 62(5):1646-1667. Selected as Editor's Choice Paper. DOI 10.1002/aic.15183 *This instance cannot be solved with the static robust approach 45

W.C. Deterministic





Deterministic Optimal Schedule



N.H. Lappas, L.A. Ricardez-Sandoval, R. Fukasawa and C.E. Gounaris (2017). Adjustable Robust Optimization for Multi-tasking Scheduling with Reprocessing of Imperfect Tasks. Under Review

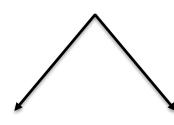




Endogenous Uncertainty

Flavors of endogeneity:

Uncertain parameters can be classified as:



Exogenous:

Parameter realizations do **not depend** on decisions (e.g., weather)

Endogenous:

Decisions **can affect** the realizations of uncertain parameters (e.g., maintenance decisions affect failure rates)

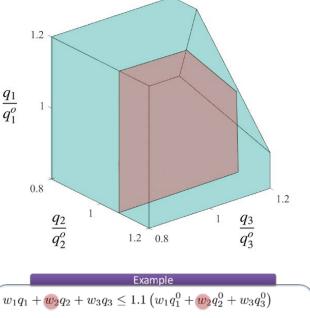
- Materialization: Decisions may make specific parameters lose their physical meaning (e.g., production yields of non-executed processes)
- Timing of realization:

Decisions can affect the time stage at which parameters are observed (e.g., demand for a new product will be revealed after the period it is launched)

 Distributional support: Decisions can affect the underlying distributions from which a parameter realization draws (e.g., technology decisions can affect the production yields)



- Avoids unnecessarily conservative solutions that attempt to insure against risk we are not really exposed to
- Provides for a considerable degree of modeling flexibility so as to capture the endogenous nature of parameters



If the binary decision $w_2 = 0$ prohibits parameter q_2 from materializing, then this parameter should not participate in the facet so as not to reduce the conservatism of the solution

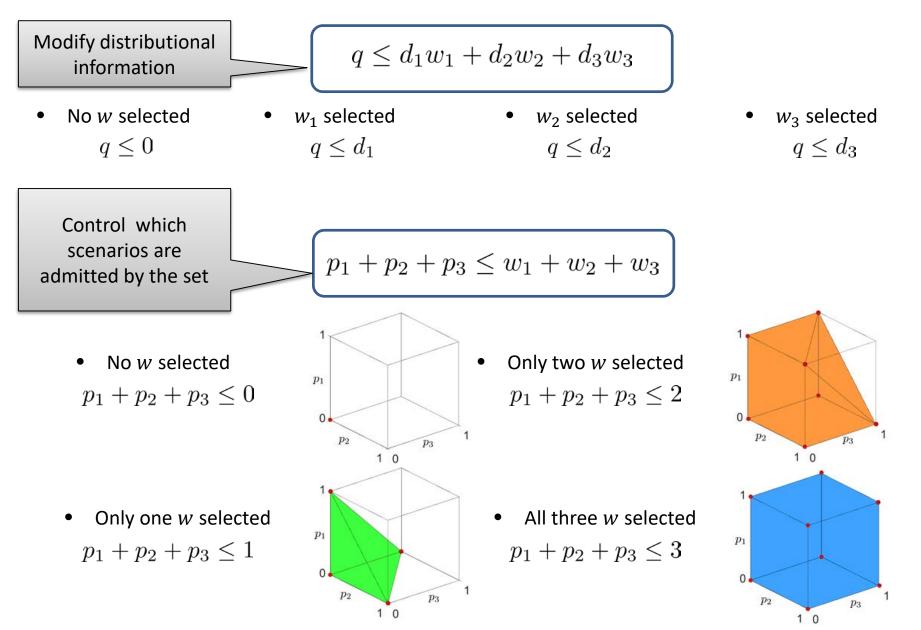
where: $v^{q}(w) \in \{0,1\}^{nq}$ and $v^{p}(w) \in \{0,1\}^{np}$



Modeling Capabilities



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Modeling Capabilities

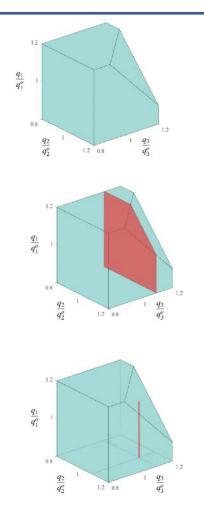
Remove the effect of non-materialized parameters

$$w_1q_1 + w_2q_2 + w_3q_3 \le (1+0.1)\left(w_1q_1^0 + w_2q_2^0 + w_3q_3^0\right)$$

• All three w_1, w_2, w_3 have been selected: $1 q_1 + 1 q_2 + 1 q_3 \le (1 + 0.1) (1 q_1^0 + 1 q_2^0 + 1 q_3^0)$

• Only w_1 , w_2 have been selected: $1 q_1 + 1 q_2 + 0 q_3 \le (1 + 0.1) (1 q_1^0 + 1 q_2^0 + 0 q_3^0)$

• Only w_1 has been selected: $1 q_1 + 0 q_2 + 0 q_3 \le (1 + 0.1) (1 q_1^0 + 0 q_2^0 + 0 q_3^0)$







Case Studies

I. Capacity Expansion

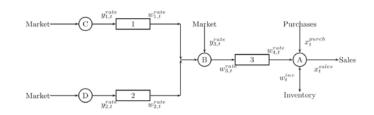
- Production yield of process i in time period t
 - Materialized, if process utilized in that period
- *Demand* for final product
 - Materialized always (exogenous)

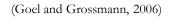
II. Offshore Oil Production

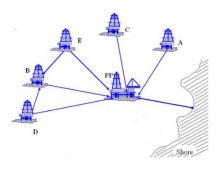
- Initial deliverability of field f
 - Materialized, if drilling occurs
 - Value depend on technology utilized
- *Reserve size* of field *f*
 - Materialized always (exogenous)

III. Clinical Trial Planning

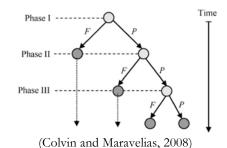
- Trial outcome of drug *i* in phase *j*
 - Materialized, if trial begins in some time period t







(Goel and Grossmann, 2004)







Benefits of Using DDUS

Normalized robust (max) objectives for 3 levels of uncertainty (low, medium, high)

Case Study	Deterministic	non-DDUS			
		L	М	Η	
Ι	100	71	65	44	
II	100	69	63	41	
III	100	57	45	36	





Benefits of Using DDUS

Normalized robust (max) objectives for 3 levels of uncertainty (low, medium, high)

Case Study	Deterministic	DDUS			non-DDUS			
		L	М	Η	L	Μ	Η	
Ι	100	90	84	79	71	65	44	
II	100	87	79	60	69	63	41	
III	100	71	65	54	57	45	36	





Opportunities = Challenges

MODERN ROBUST OPTIMIZATION CAN (in principle) ...

- Solve problems using "cutting-plane-like" approaches that progressively enforce the robustness of a solution
 - Capitalizes on deterministic optimization machinery
 - Provides more flexibility about what can be uncertain (e.g., disruptions)
 - Allows for better integration with custom-built solvers, including metaheuristics
- 2 Handle recourse (incl. mixed-integer recourse) in multi-stage decision making settings
 - Path to full adaptivity for 2-stage problems
 - Decision rules can be used (carefully) to address N-stage problems
 - Coping with equality constraints
 - Address endogenous uncertainty
 - Use of decision-dependent uncertainty sets





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