FRIEDRICH-ALEXANDER
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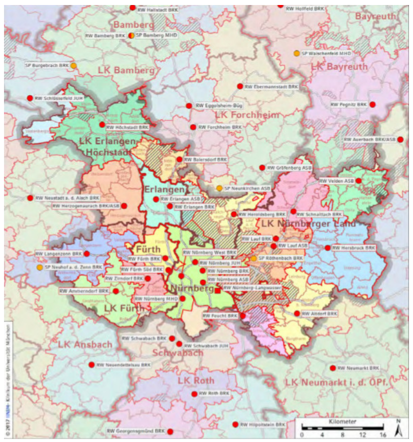
NATURWISSENSCHAFTLICHE
FAKULTÄT

Robust Protection against Uncertainties in Discrete-Continuous Optimization

Frauke Liers
FAU Erlangen-Nürnberg
Seminar DCN-AvH 29.04.2022, FAU

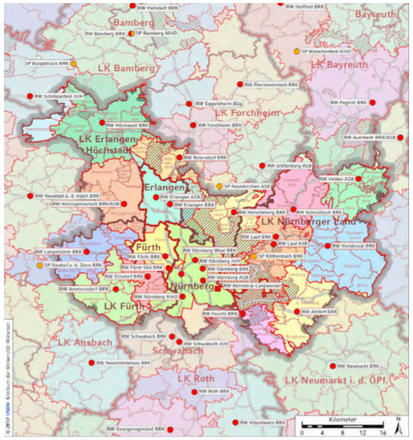
OPTIMIZATION
UNDER UNCERTAINTY
& DATA ANALYSIS

Optimization under Uncertainty



ambulance logistics

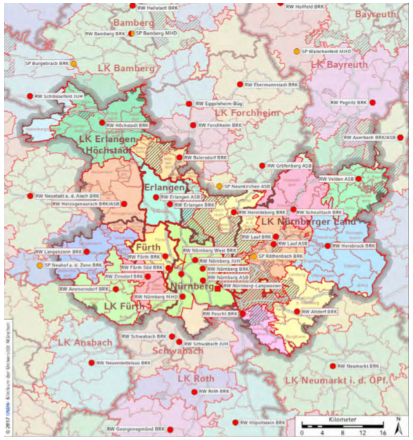
Optimization under Uncertainty



ambulance logistics

gas networks

Optimization under Uncertainty



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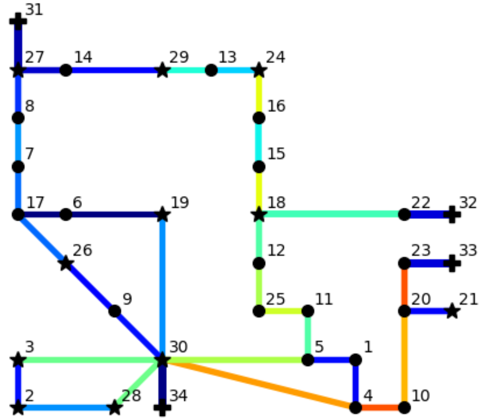
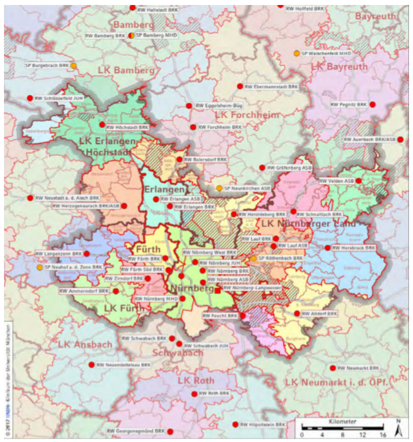


electricity networks

gas networks

Optimization under Uncertainty



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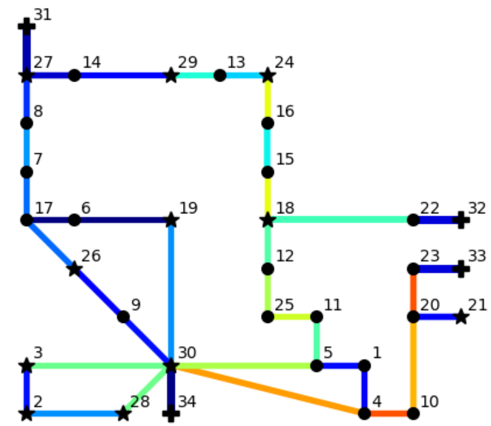

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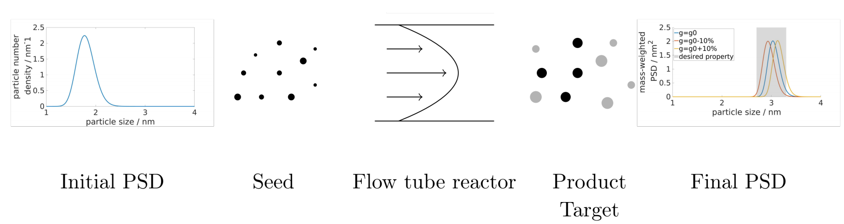


nanoparticle design

Optimization under Uncertainty

Handling of Uncertainties:

- ignore, solve nominal problem

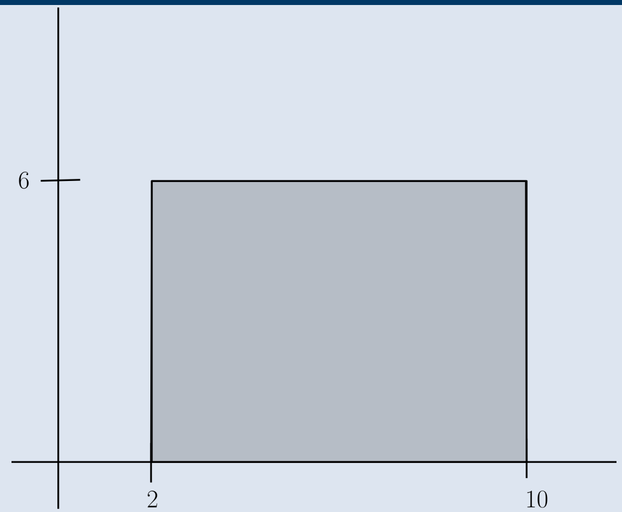
Optimization under Uncertainty

Handling of Uncertainties:

- ignore, solve nominal problem
- ex post: sensitivity analysis
- ex ante:
  - stochastic optimization
  - *robust optimization*

Robust Optimization

Modelling



Robust Optimization

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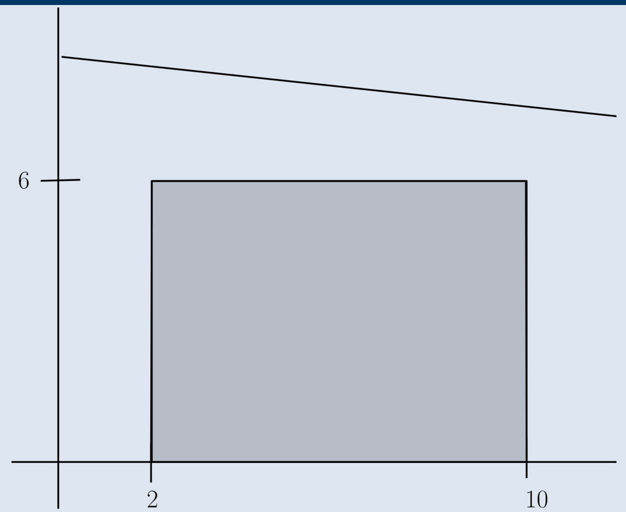

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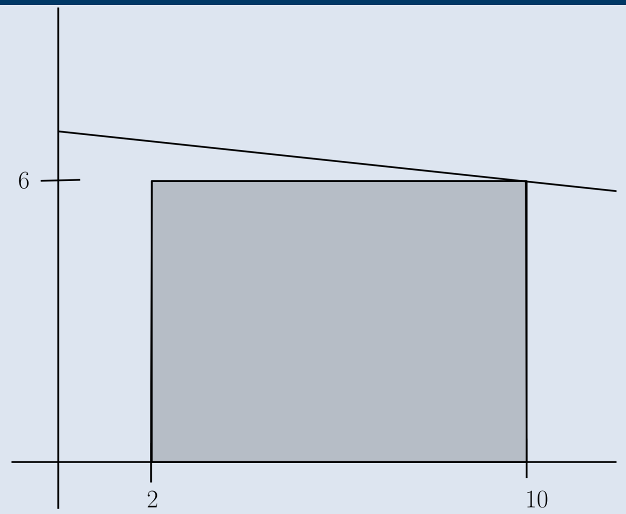

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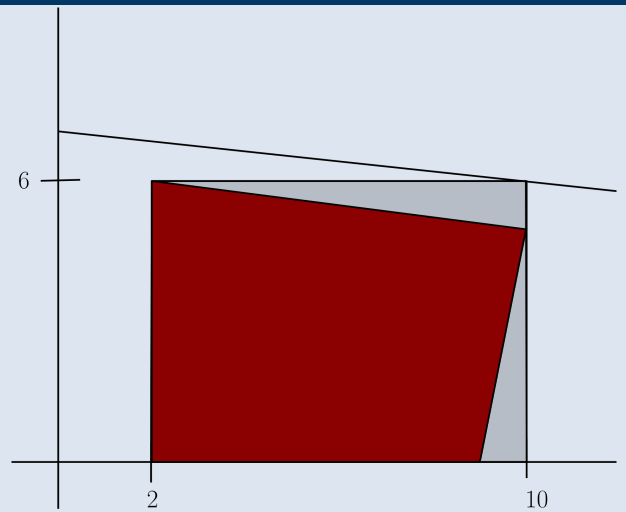
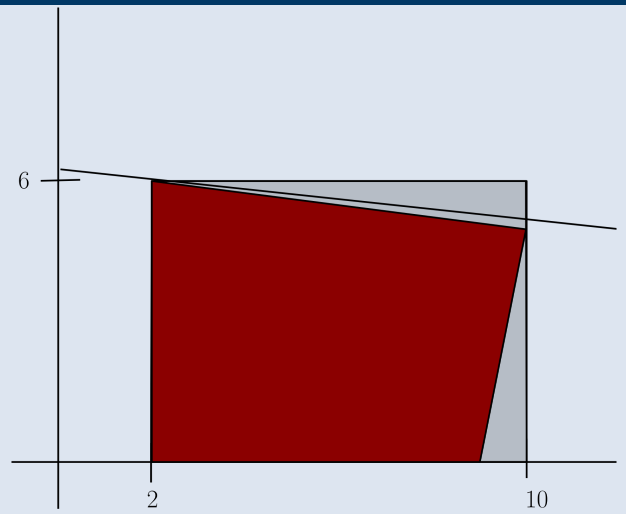


Robust Optimization

Modelling



Robustness: Protection Against the Worst Case

Modelling

- input: *uncertainty set* U (scenarios, intervals, etc.)
- *robust feasibility:* solution x has to be feasible for all $u \in U$ ('here-and-now')
- *robust optimality:* robust feasible x with best guaranteed solution value

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Evaluation

- robust and/or probabilistic protection? distributions known?
- mathematical tractability and conservatism?

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Solution Approaches

- approaches leading to stable solutions
- reformulation to algorithmically tractable robust counterpart (duality, scenario expansion, KKT, ...)
- decomposition (cutting plane algorithms, scenario generation, ...)
- approximation (Taylor expansion, linearization, safe approximation,...)

Overview

(Some of the) Contributions

- Soyster (1973), Kouvelis, Yu (1997), Ben-Tal, Nemirovski & co-authors (1997-), Bertsimas, Sim & co-authors, (2004 -), den Hertog & co-authors (2005 -), etc.

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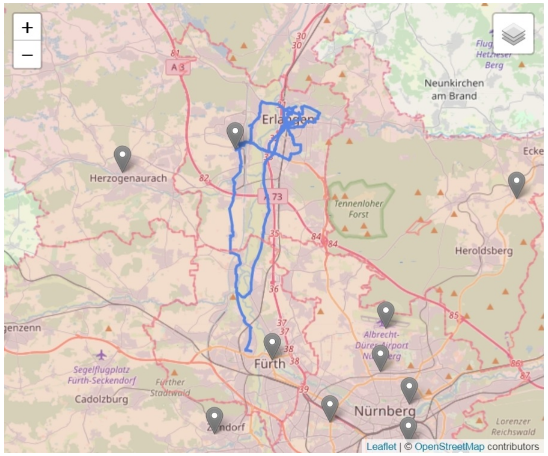
- some books / surveys: Ben-Tal, El Ghaoui, Nemirovski (2009), Gorissen, Yanikoglu, den Hertog (2015), Buchheim & Kurtz (2018), Yanikoglu, Gorissen, den Hertog (2019), Leyffer et al. (2019), etc.

Delay Minimization in Ambulance Logistics

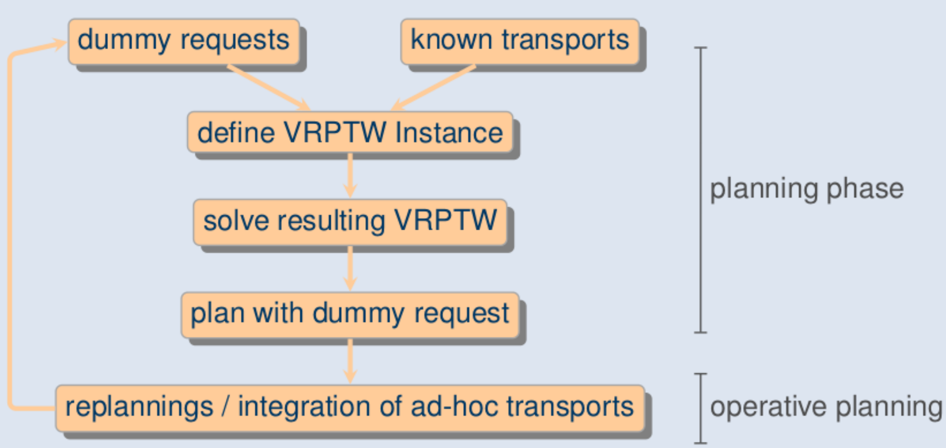
Adelhütte, Braun, L, Tschuppik (submitted)

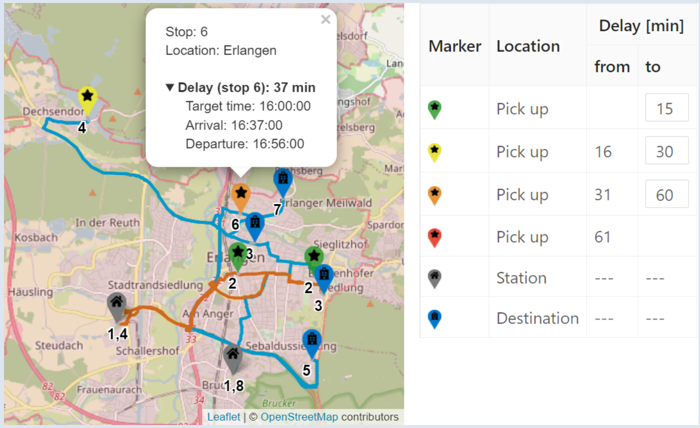


- robust logistics of (plannable) + ad-hoc transports
- ILS Nürnberg:
  - ca. 32,000 ambulance transports
  - ca. 30 % ad hoc
  - $\leq$ 44 KTWs
- vehicle routing problem with (soft + hard) time windows under uncertainty, e.g., Toth & Vigo (2014), Ibaraki et al (2005), Blauth, Traub & Vygen (2021), Agra et al (2013), Eufinger et al. (2020), ...

Algorithm Engineering for Optimized Routing

stable approach





Leithäuser et al., BMC Medical Informatics and Decision Making (2022)

- historical data: average daily improvement when compared to simulated reality: 421 min (total delay), 105 min (max delay)
- dummy requests for dialysis: reduces daily delay on avg. by 60 min
- extension to Covid-19, separate pools does not considerably increase delay

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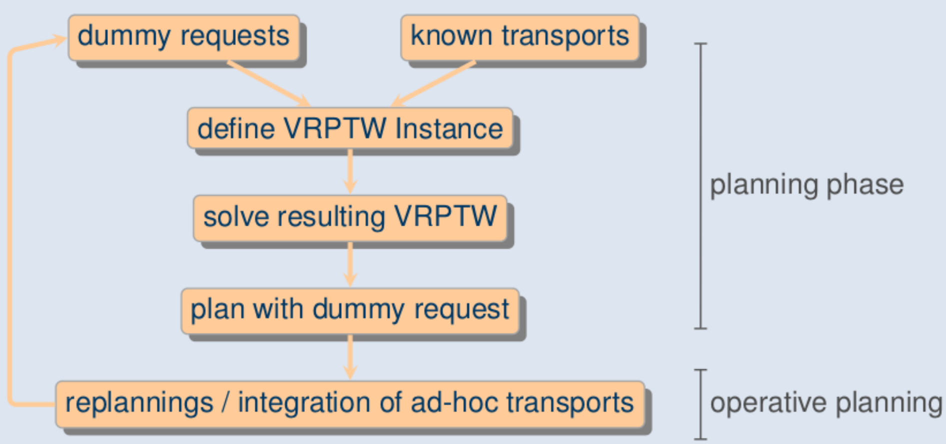

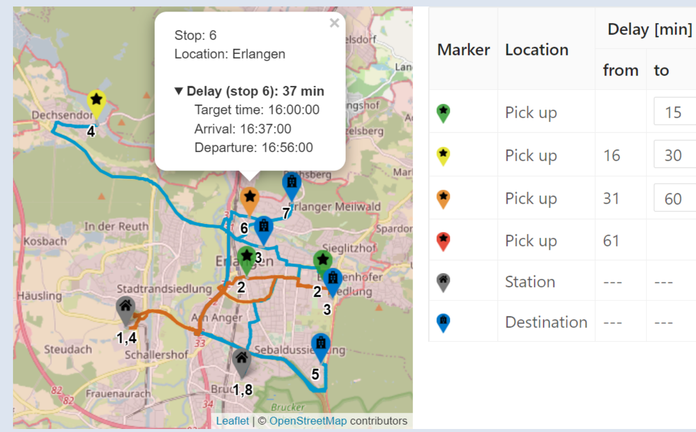

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Reformulation for Robust Linear Programs

Polyhedral Uncertainty Ben-Tal & Nemirovski

$$(\bar{a} + P\zeta)^T x \leq b \quad \forall \zeta : D\zeta \leq d \Leftrightarrow \tag{1}$$

$$\bar{a}^T x + \max_{\{\zeta : D\zeta \leq d\}} (P^T x)^T \zeta \leq b.$$

duality trick:

$$\max_{\zeta} \left\{ (P^T x)^T \zeta \mid D\zeta \leq d \right\} = \min_{y} \left\{ d^T y \mid D^T y = P^T x, y \geq 0 \right\}.$$

$$\bar{a}^T x + \min_{y} \left\{ d^T y \mid D^T y = P^T x, y \geq 0 \right\} \leq b.$$

If satisfied by a feasible y, then it is satisfied also for the minimum $\Rightarrow$ skip $\min \rightarrow$ x satisfies (1) iff $\exists\, y$ such that (x, y) satisfies

$$\bar{a}^T x + d^T y \leq b, \quad D^T y = P^T x, \; y \geq 0$$

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extendable to conic problems and to integral decisions x.

Robust Discrete / Combinatorial Optimization

- budgeted uncertainty, Γ-approach (Bertsimas, Sim (2004))

$$(\text{BP}) \quad \min_{x} \left\{ c^T x \mid x \in X \subseteq \{0,1\}^n \right\}$$

Uncertain cost $c_j \in [c_j, c_j + \Delta c_j]$, $\Delta c_j \geq 0$. Let $\Gamma \in \{0, \dots, n\} := N$. Determine solution that is robust against at most Γ disturbances.

$$(\text{RBP}) \quad \min_{x} \left\{ c^T x + \max_{S \subseteq N : |S| \leq \Gamma} \sum_{j \in S} \Delta c_j x_j \mid x \in X \subseteq \{0,1\}^n \right\}.$$

Let w.l.o.g. $\Delta c_1 \geq \Delta c_2 \ldots \geq \Delta c_n \geq 0$. Then optimum of (RBP) is

$$\min_{l=1,\dots,n+1} \left\{ \Gamma \Delta c_l + \min_{x \in X} \left\{ c^T x + \sum_{j=1}^{l} (\Delta c_j - \Delta c_l) x_j \right\} \right\}$$

with $\Delta c_{n+1} := 0$ and $x_{n+1} := 0$.
survey: Buchheim, Kurtz (2018)

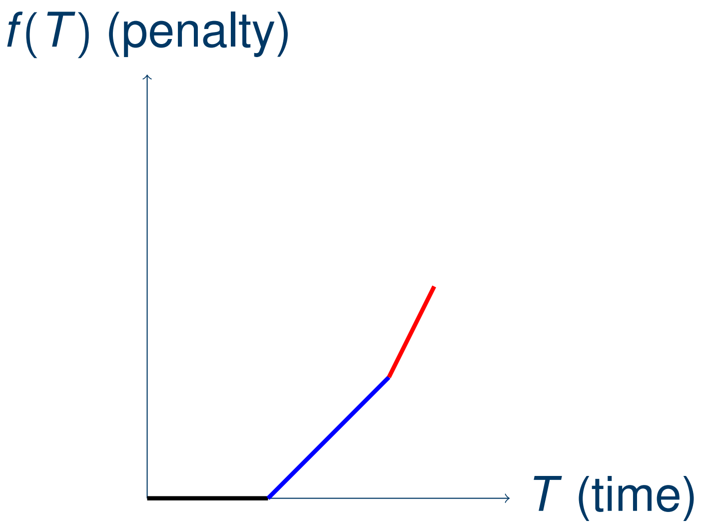
General Approach: Robust Vehicle Routing Problem

...with (Soft and Hard) Time Windows

- f_i is *penalty function*: punish delay for patient i

$$\min \sum_i f_i(T_i)$$

s.t. hard time windows satisfied



- ... transport on time: no penalty.
  ... transport with $\leq 1h$ delay: small penalty.
  ... with delay $> 1h$: high penalty.

Reformulations for Robust Nonlinear Mixed-Integer and Combinatorial Optimization

Adelhütte, L

- nominal problem

$$\min_{x\in\mathcal{X}} \sum_{i\in N} f_i(x,\overline{c}_i)$$

- $\forall i \in N$: uncertainty set $\mathcal{U}_i$, $c_i \in \mathcal{U}_i$
- Γ-robust counterpart: seek robust protection against $\leq \Gamma$ uncertainty realizations

$$\min_{x\in\mathcal{X}} \max_{S\subset N, |S|\leq\Gamma} \left\{ \sum_{i\in S} \max_{c_i\in\mathcal{U}_i} f_i(x,c_i) + \sum_{i\in N\setminus S} f_i(x,\overline{c}_i) \right\}$$

- semi-infinite Γ-robust counterpart can be reformulated in wide MINLP contexts for convex $\mathcal{U}_i$:
  - algorithmically tractable finite reformulations of Γ-robust counterpart possible for problems with nonlinear objective f that are concave (and also non-concave) in uncertainty
  - robust protection is often not costly

Theoretical Reformulations for Robust Counterpart

$$\min_{x,p,\theta} \Gamma\theta + \sum_{i\in[n]} f_i(x,\overline{u}^i) + p_i$$

$$\text{s.t.} x \in \mathcal{X}$$

$$p_i + \theta \geq \max_{u^i\in\mathcal{U}_i} f_i(x,u^i) - f_i(x,\overline{u}^i)$$

$$p,\theta \geq 0.$$

if f_i linear in uncertainty and $\mathcal{U}^i = \overline{u}^i + A^i \cdot \mathcal{Z}_i$, equivalent to

$$\min_{k\in\{0\}\cup N} \min_{x\in\mathcal{X}} \Gamma\theta^k(x) + \sum_{i\in N} (\overline{u}^i)^T l_i(x) + \max\{0, \theta^i(x) - \theta^k(x)\}$$

with $\theta^0(x) = 0$ and $\theta^k(x) = \sup_{y\in\mathcal{Z}_k} y^T x$.

Theoretical Reformulations for Robust Counterpart

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$$\text{s.t.} x \in \mathcal{X}$$
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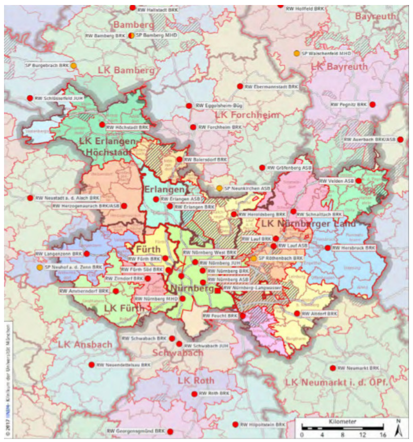
with $\theta^0(x) = 0$ and $\theta^k(x) = \sup_{y\in\mathcal{Z}_k} y^T x$.

example: robust VRP with piecewise linear objective:

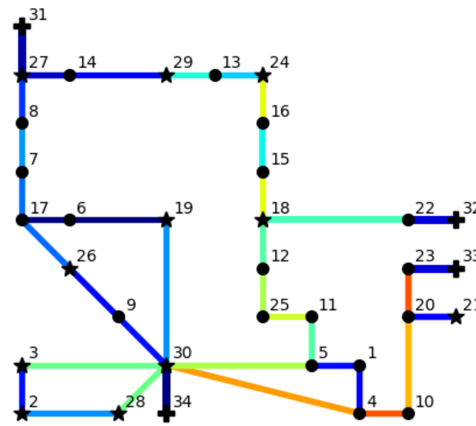
$$\min_{x\in\mathcal{X}} \sum_{i\in[n]} \max\{0, x_i - b_i\}.$$

the Γ-robust counterpart can be solved by $2[n]+1$ many piecewise linear nominal problems

Optimization under Uncertainty

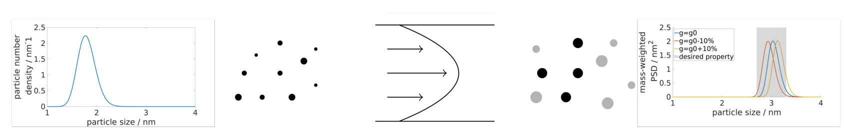


ambulance logistics



electricity networks

gas networks



Initial PSD · Seed · Flow tube reactor · Product Target · Final PSD

nanoparticle design

Robust Nomination Validation in Gas Networks

Problem

For each uncertainty, is there a configuration of the active elements leading to a feasible state?

min operating costs
flow conservation
pressure loss
pressure bounds
flow bounds
active elements

TRR 154

...this is a mixed-integer two-stage robust optimization problem with a non-convex quadratic lower level.

Nonlinear Robust Optimization

Kuchlbauer, L, Stingl INFORMS J Comput (2020)

formulation as minimax problem

$$\min_{x \in \mathbb{R}^n} \quad c(x)$$
$$\text{s. t.} \quad v(x, u) \leq 0 \quad \forall u \in \mathcal{U}.$$

minimax problem: $$\min_{x \in \mathbb{R}^n} \max_{u \in \mathcal{U}} v(x, u). \qquad \text{(RO)}$$

challenges:

- evaluation of worst case: global solution of $\max_{u \in \mathcal{U}} v(x, u)$
- nonlinear and non-convex
- few works only [Leyffer et al., 2020], no general approaches

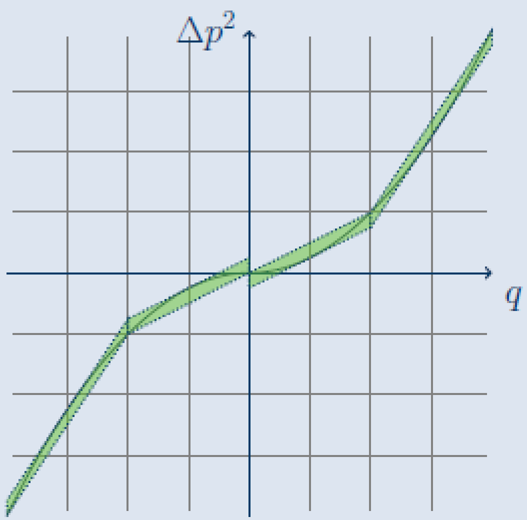
Our Solution Approach

adversarial problem

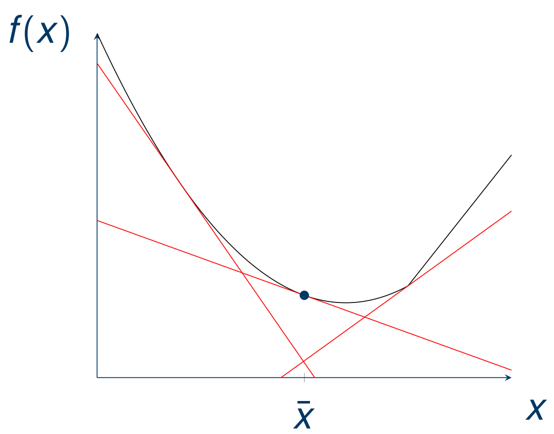
minimize the adversary's optimal value function

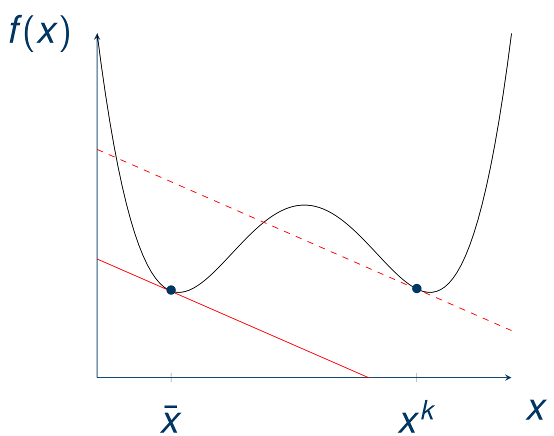
$$f(x) := \min_{x\in\mathbb{R}^n} \max_{u\in\mathcal{U}} v(x,u). \qquad \text{(RO)}$$

- bundle method for non-smooth and non-convex function $\min_{x\in\mathbb{R}^n} f(x)$
- piecewise linear relaxation for $\max_{u\in\mathcal{U}} v(x,u)$ with guaranteed error bound [Geißler, Martin, Morsi, Schewe, 2012]



Bundle Method





- approximate f by a piecewise linear model ϕ_k, using cutting planes
- use subgradients for nonsmooth functions
- find trial iterates around serious $\bar{x}$:

$$\min_{x^k \in \mathbb{R}^n} \phi_k(x^k) + \tau_k \|x^k - \bar{x}\|.$$

- downshift cutting planes to overcome lack of convexity
- e.g., nonconvex: [Kiwiel 2006], + *constant* error in subgradient: [Noll 2013]

Inexactness in the Adversarial Problem

$$\min_{x \in \mathbb{R}^n} f(x) = \min_{x \in \mathbb{R}^n} \max_{u \in \mathcal{U}} v(x,u). \qquad \text{(RO)}$$

inexact solution u_x to the adversarial problem:

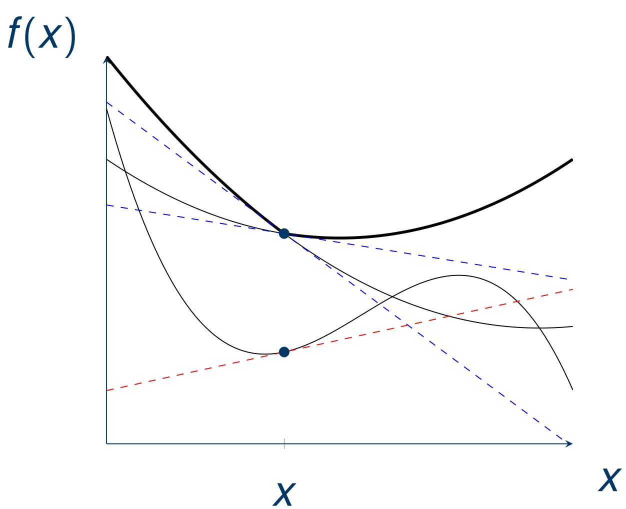
$$v(x, u_x) \geq \max_{u \in \mathcal{U}} v(x,u) - \varepsilon_x.$$

Clarke subdifferential of f at x: $\partial f(x) =$

$$\operatorname{conv}\{\partial_x v(x,u^*) \mid u^* \in \mathcal{U},\ v(x,u^*) = \max_{u \in \mathcal{U}} v(x,u)\}.$$

$$\tilde{\partial}_a f(x) := \operatorname{conv}\{\partial_x v(x,u) \mid u \in \mathcal{U},\ v(x,u) \geq v(x,u_x)\}.$$

approximate exact subdifferential from outside $\Rightarrow$ no constant error bound implied, *(no bundle concept available)!*



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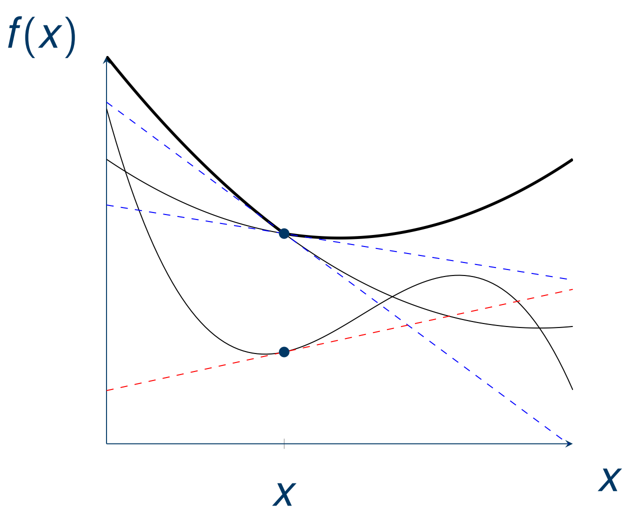

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approximate exact subdifferential from outside $\Rightarrow$ no constant error bound implied, *(no bundle concept available)!*

fix by adaptivity!

Adaptive Approximation of Function Value

approximate exact subdifferential (no access to subgradient with constant error):

$$\tilde{\partial}_a f(x) := \mathrm{conv}\{\partial_x v(x,u) \mid u \in \mathcal{U},\ v(x,u) \geq v(x,u_x)\}.$$

Definition

- $f : \mathbb{R}^n \to \mathbb{R}$ is approximate convex ($= LC^1$) if for every x and ε', there exists $\delta > 0$ s.t. f is ε'-convex on $B(x,\delta)$.
  (e.g., $\max_u f(x,u)$ with $f(.,u) \in C^1 \forall u$)
- $f : \mathbb{R}^n \to \mathbb{R}$ is ε'-convex if for any $x, x' \in X$ and $\lambda \in [0,1]$,

$$f(\lambda x + (1-\lambda)x') \leq \lambda f(x) + (1-\lambda) f(x') + \varepsilon' \lambda (1-\lambda)\|x - x'\|.$$

Lemma

Under the assumption of ε'-convexity, an approximate subgradient $g_k \in \tilde{\partial}_a f(x^k)$ fulfills

$$g_k{}^T(x - x^k) \leq f(x) - f(x^k) + \varepsilon_{x^k} + \varepsilon'\|x - x^k\|.$$

At trial iterates around a serious iterate $\bar{x}$, the adaptive approximation

$$f_a(x^k) := v(x^k, u_{x^k}) + \varepsilon_{x^k}, \quad g_k \in \partial_x v(x, u_x), \quad \varepsilon_{x^k} = \varepsilon'' \|\bar{x} - x^k\|$$

ensures the subgradient inequality

$${g_k}^T(\bar{x} - x^k) \leq f_a(\bar{x}) - f_a(x^k) + (\varepsilon' + \varepsilon'')\|\bar{x} - x^k\|.$$

$\Rightarrow$ Possibility to develop a bundle method

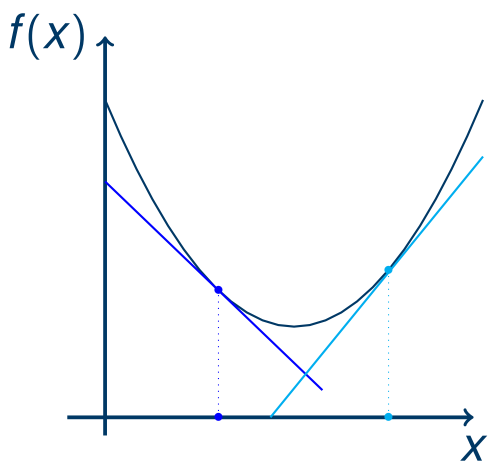
Convergence Result

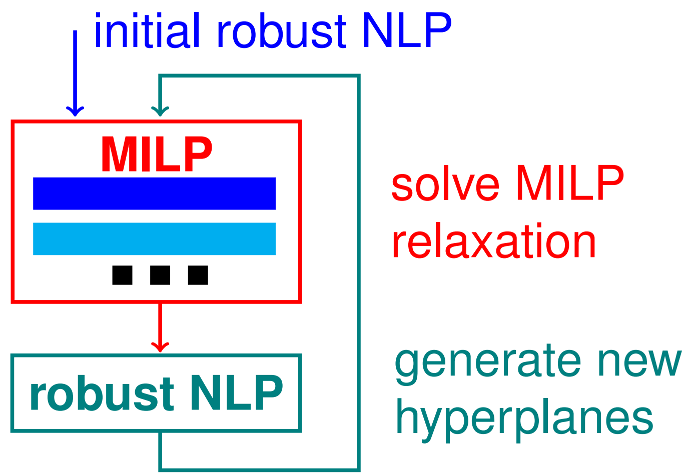
Theorem

Let x_1 be s.t. $\Omega := \{x \in \mathbb{R}^n : f(x) \leq f_a(x_1)\}$ is bounded, v be approximate convex (LC^1) and $\bar{x}$ be a solution obtained by the stopping criterion $0 \in \tilde{\partial}_a f(\bar{x})$ or an accumulation point of the sequence x_j. Further, let $\varepsilon_{x^k}(x_j) = \varepsilon''_{j,k}\|x^k - x_j\|$ with $\varepsilon''_{j,k} \in \mathcal{O}(\|x_j - x^k\|)$.
Then, it holds that

$$0 \in \tilde{\partial}_a f(\bar{x}).$$

Discrete-Continuous Robust Optimization via Outer Approximation

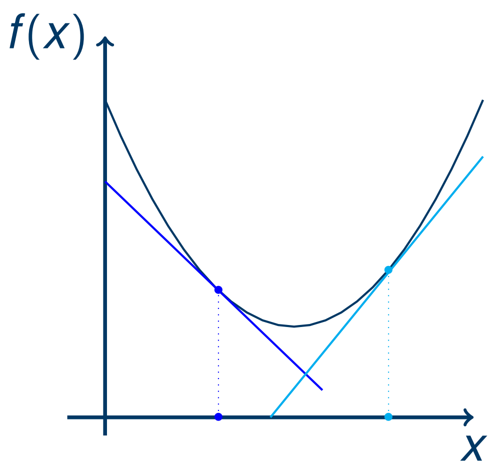


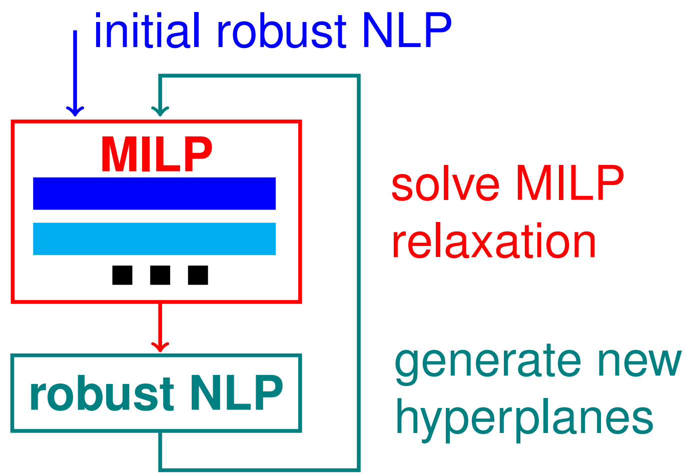


MILP $\Rightarrow$ lower bound

robust NLP $\Rightarrow$ upper bound

Discrete-Continuous Robust Optimization via Outer Approximation





MILP $\Rightarrow$ lower bound

robust NLP $\Rightarrow$ upper bound

- Solution of (nonlinear) robust subproblems?
  Kuchlbauer, L, Stingl INFORMS J Comput (2020)
- Valid inequalities for master problems?
  Kuchlbauer, L, in review J Opt Theory & Appl

Convex Mixed-Integer Robustness

$$\begin{aligned} \min_{x,y} \quad & C(x,y) \\ \text{s.t.} \quad & G(x,y) := \max_{u \in \mathcal{U}} \sum_{i=1}^{n} V_i^+(x,y,u) \leq 0, \\ & x \in X, y \in Y \cap \mathbb{Z}^{n_y}. \end{aligned}$$

C convex in x, y, allow non-convex adversarial

bundle method$\rightarrow$ function value $\tilde{G}(x^k, y^k)$, limiting aggregate subgradient

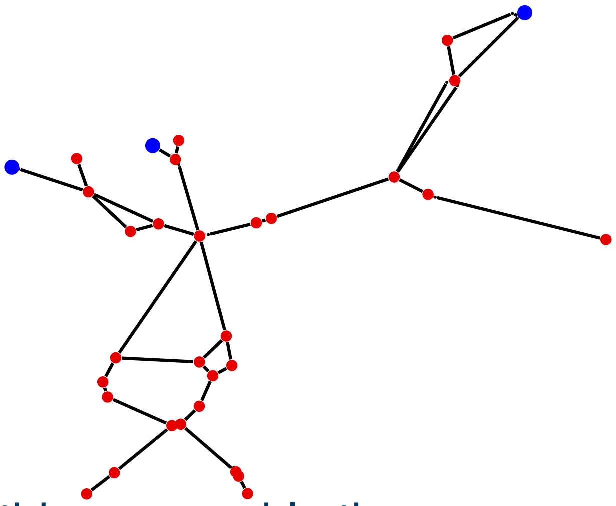
generates valid (feasibility and optimality)cuts

Theorem

The outer approximation method together with the adaptive bundle method terminates after finitely many outer approximation iterations and either detects infeasibility or outputs a solution (x^k, y^k) that is ε_k-feasible and ε_{oa}-optimal.

Numerical Results on Realistic Instances

nodes × arcs	compr.	valves	runtime	error constr.
11×11	2	1	13	0
24×25	4	0	8	0
40×45	5	2	903	0
103×105	21	3	362	5e-5



General approach can go to realistic sizes within reasonable time.

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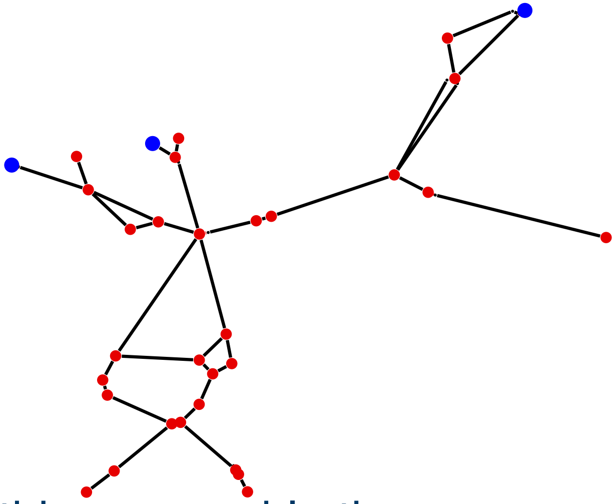
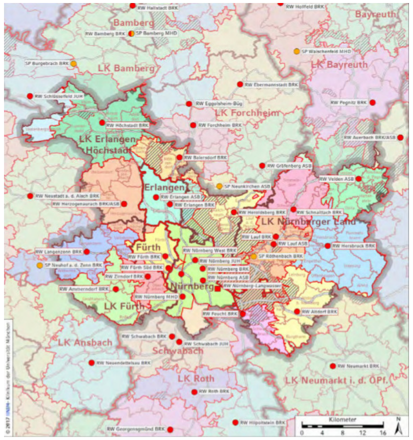


General approach can go to realistic sizes within reasonable time.

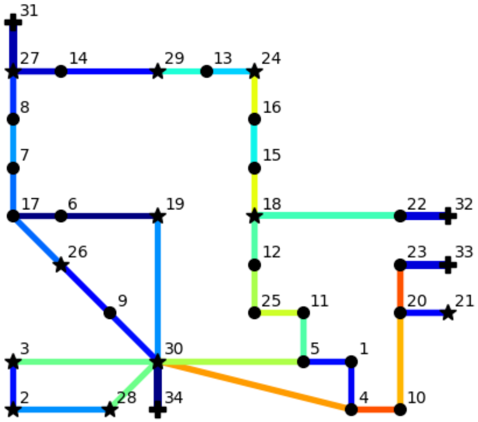
Currently

- Can we go beyond convexity in decisions?
- We only need: For any $x \in \mathbb{R}^N$ and any choice of ε_x, we have access to $u_x \in \mathcal{U}$ with $v(x, u_x) \geq \max_{u \in \mathcal{U}} v(x, u) - \varepsilon_x$ and to a $g_x \in \partial_x v(x, u_x)$

Optimization under Uncertainty

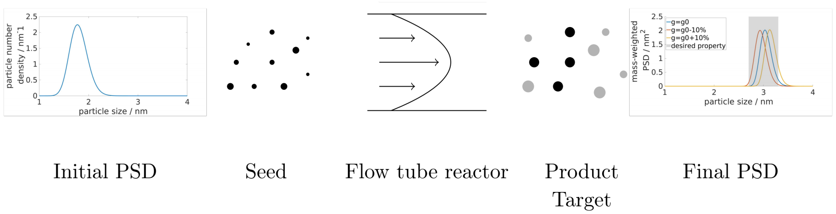


ambulance logistics



electricity networks

gas networks

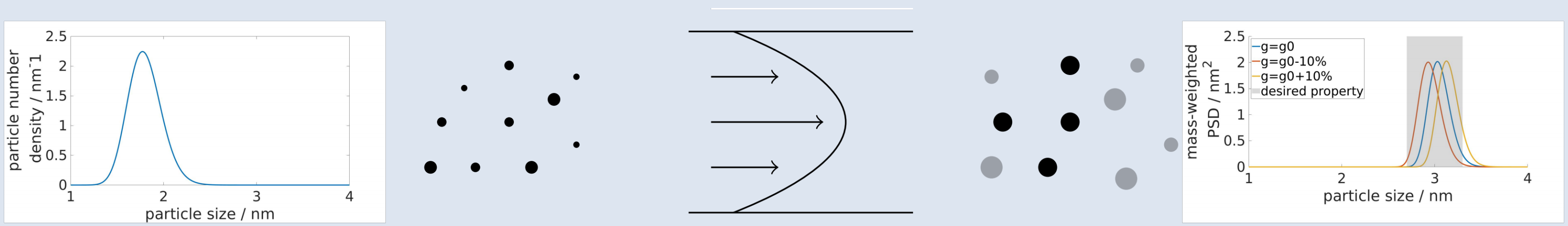


nanoparticle design

Quality Control in Nanoparticle Design

Dienstbier, Aigner, Pflug, Segets, Peukert, L

Particle synthesis process is ruled by PDEs



Initial PSD | Seed | Flow tube reactor | Product Target | Final PSD

Population-Balance equation: (x particle size, t time, G growth law, q particle number density, q_0 initial particle size distribution)

$$\partial_t q(t,x) + \partial_x \left(G_g(x) q(t,x) \right) = 0 \qquad \forall t > 0, x > 0,$$

$$q(0,x) = q_0(x) \quad \forall x > 0.$$

$$q(t,0) = 0 \qquad \forall t > 0.$$

Robust ZnO synthesis in a continous flow reactor

Diffusion-Limited Growth $G = \frac{c}{x}$

- (linear) PDE can be solved analytically with method of characteristics $q(t, x) = \frac{x}{\sqrt{x^2 - 2ct}} q_0(\sqrt{x^2 - 2ct})$.
- particle size distribution at reactor end:

$$q_c(t, x) = \int_0^{\infty} E_\tau(t, x) q(t, x),$$

  with residence time distribution $E\tau$
- Task: determine mean residence time τ (i.e., reactor length) such that synthesized volume

$$J_c(x_1, x_2, \tau) = \int_{x_1}^{x_2} x^3 \int_0^{\infty} E_\tau(t) q_c(x, t) dt dx,$$

  is optimized, even under uncertain c

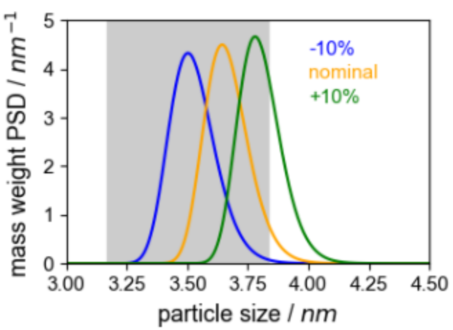
Robust ZnO synthesis in a continous flow reactor

Robust protection is algorithmically tractable and not costly

$$\max_{\tau>0} \quad \min_{c\in\mathcal{U}} \; J_{[q_c]}(\tau, x_1, x_2)$$

$$\text{s.t.} \quad \min_{c\in\mathcal{U}} \; \frac{J_{[q_c]}(\tau, x_1, x_2)}{J_{[q_c]}(\tau, 0, \infty)} \geq P_{min}.$$

- realistic: $c = 0.2\frac{nm}{min} \pm 10\%$, q_0: lognormal(1.8 nm), relative SD $\leq 10\%$
- goal: receive $x = 3.5nm \pm \frac{1}{3}$ at purity $P_{min} = 90\%$
- in these ranges, robust model is quasiconcave in c, can be reformulated and is tractable



Influence of variations in c by 10%.

	$c - 10\%$	c	$c + 10\%$
nominal ($\frac{g}{h}$)	1.390	1.498	infeasible
robust ($\frac{g}{h}$)	1.303	1.448	1.468

Synthesised mass

Price of robustness: $\frac{nominal - robust}{nominal} = 3.34\%$

- unprotected solution may become infeasible!

Summary

Solution Approaches

- approaches leading to stable solutions
- reformulation to algorithmically tractable robust counterpart (duality, scenario expansion, KKT, ...)
- decomposition (cutting plane algorithms, scenario generation, ...)
- approximation (Taylor expansion, linearization, safe approximation,...)

Summary

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Challenges

Development of further global algorithms (reformulations, decompositions, approximations, etc) for

- two-stage problems with integral and/or non-convex second stage
- finite-/and infinite-dimensional nonlinear robust problems
- algorithms for robust-probabilistic problems

Thank you for your attention!