Algorithms, Analysis, and Software for the Global Optimization of Chemical Process Systems under Uncertainty

Rohit Kannan

Process Systems Engineering Laboratory
Department of Chemical Engineering
Massachusetts Institute of Technology

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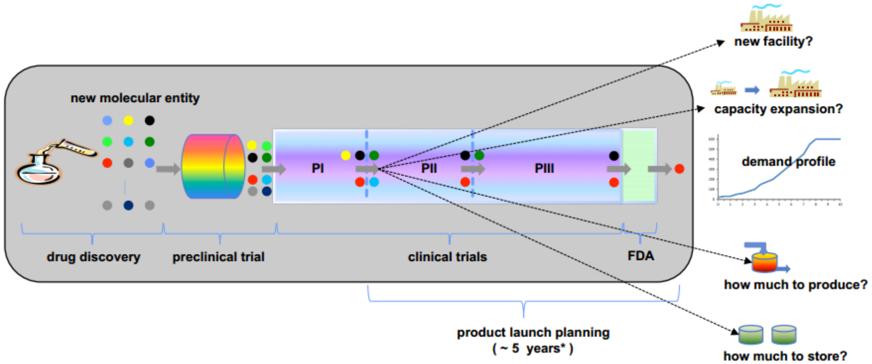
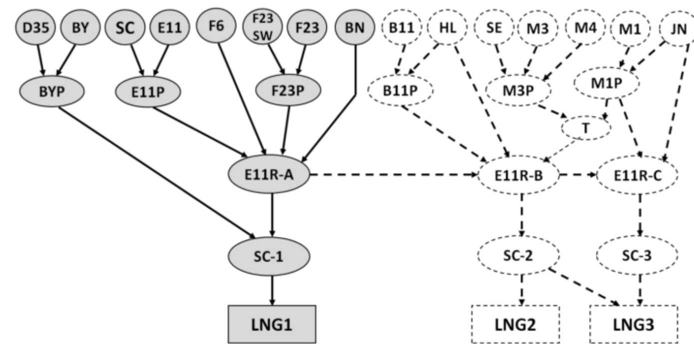
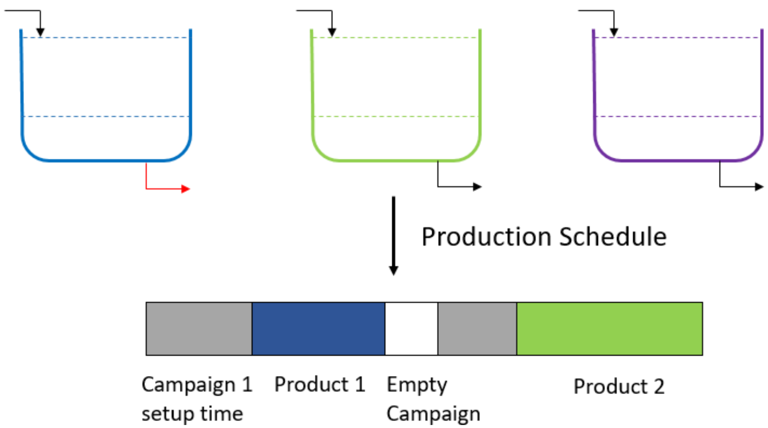
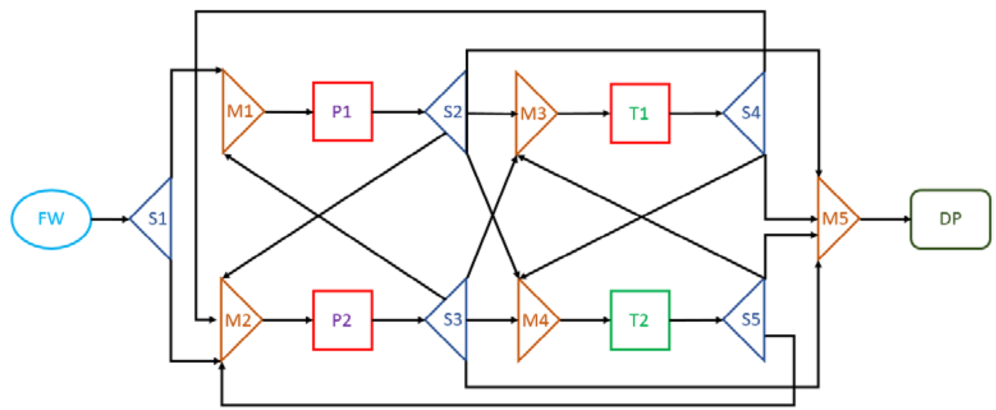
Motivation

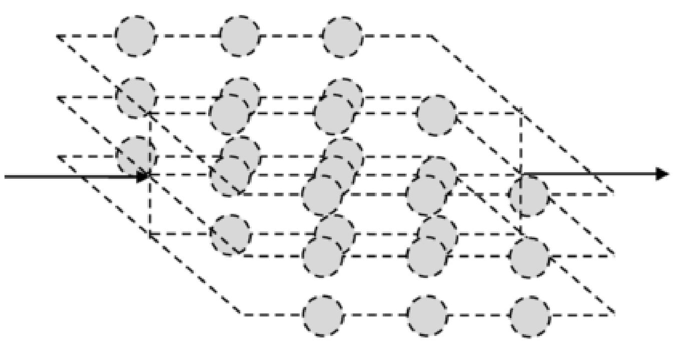
Engineering Applications

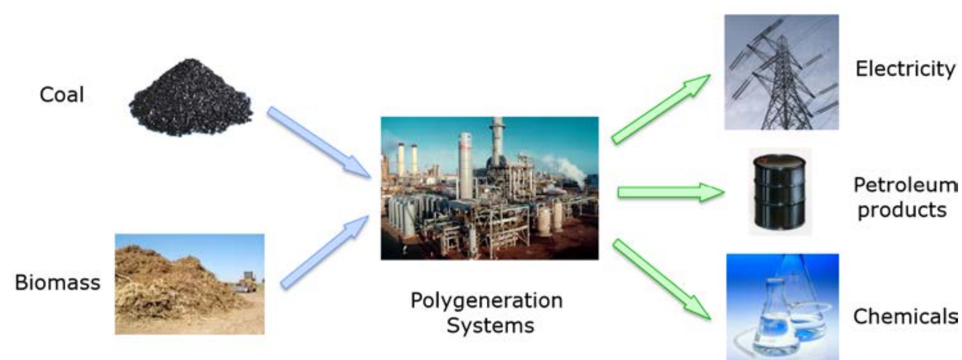






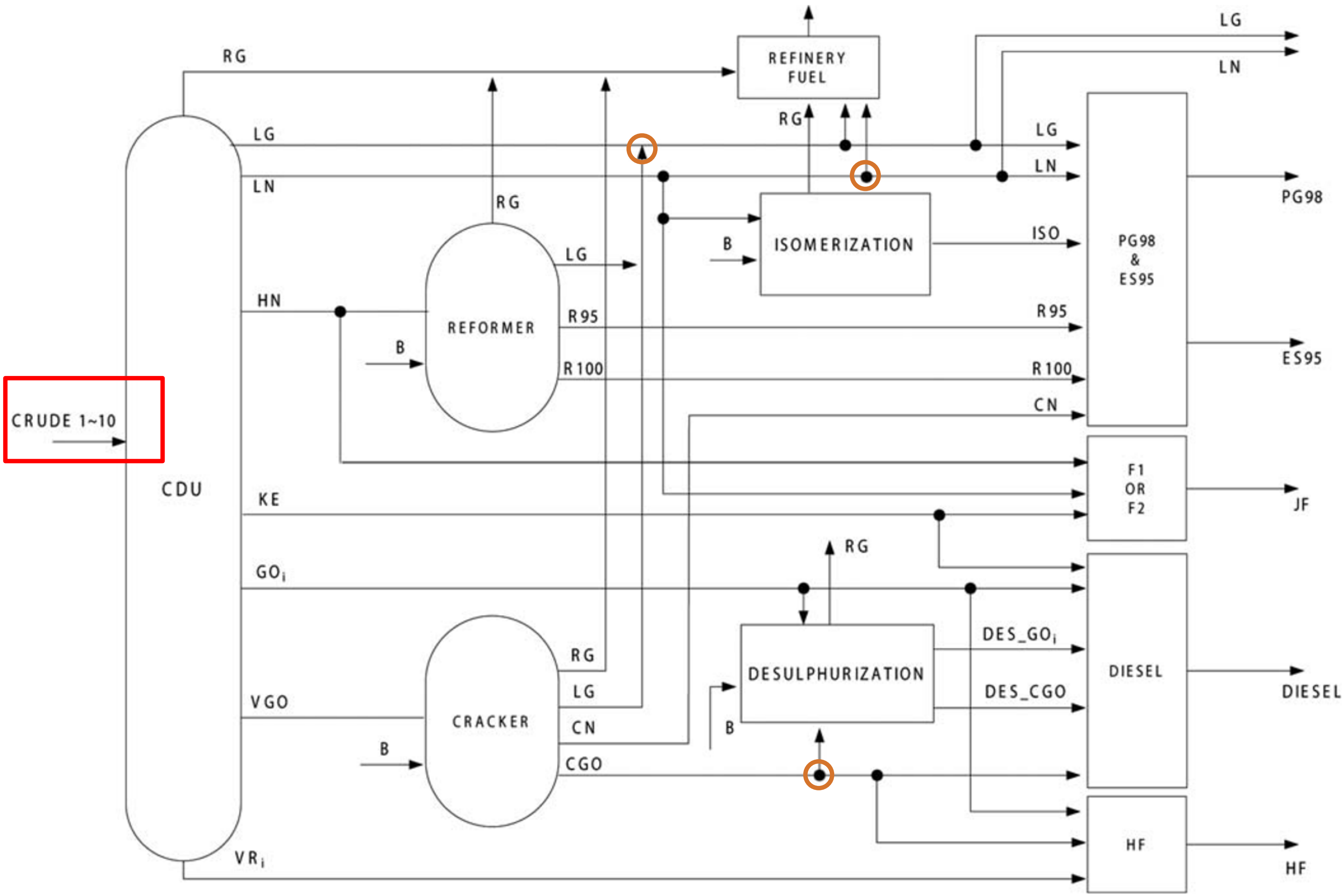






Motivation

Refinery Optimization Under Uncertainty



Quality Specifications

Vapor pressure
Octane number
Sensitivity

Sulfur: 15 ppm

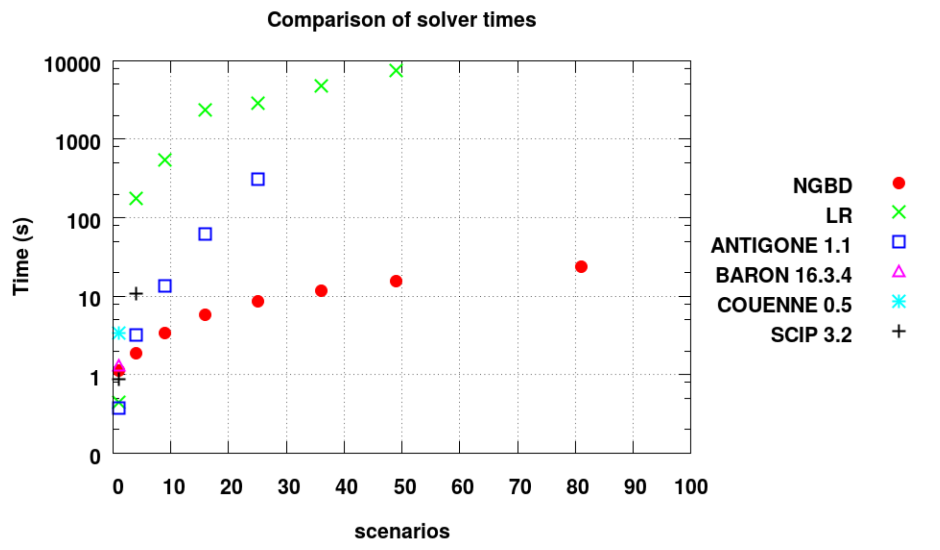
Viscosity index: 30-33

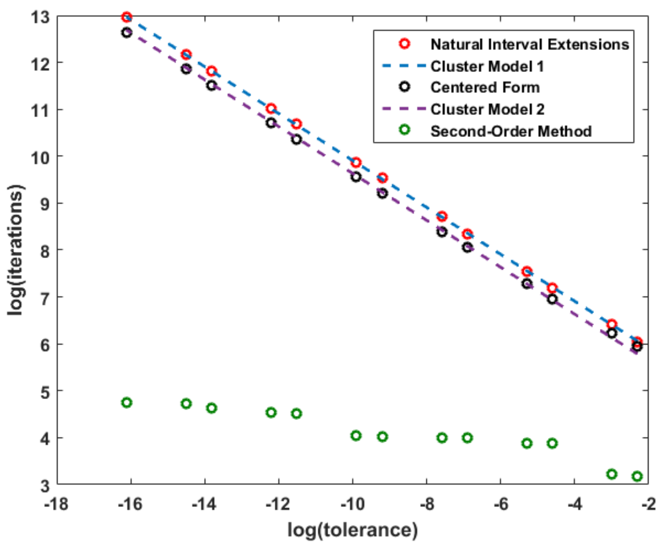
Sources of bilinear terms

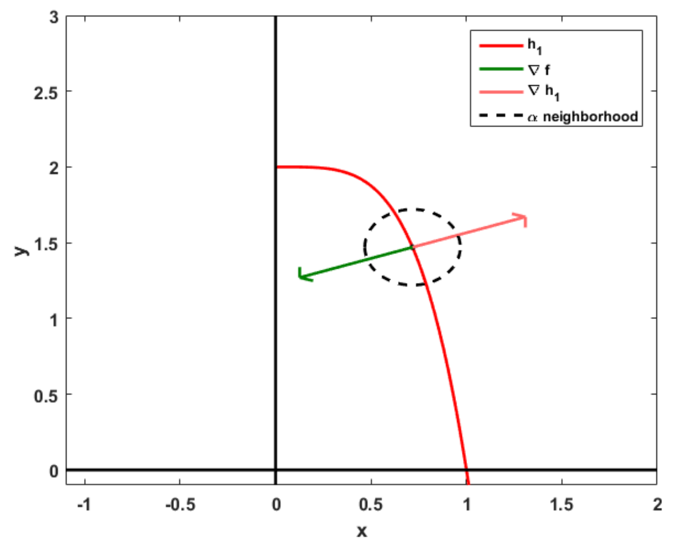
Outline

Inner minimization can be solved in a decomposable manner using NGBD

$$\sup_{\lambda_1,\cdots,\lambda_{s-1}} \boxed{\begin{aligned} \min_{\substack{x_1,\cdots,x_s,\\ y,z_1,\cdots,z_s}} \ & \sum_{h=1}^{s} p_h f_h(x_h, y, z_h) + \sum_{h=1}^{s-1} \lambda_h^T (z_h - z_{h+1}) \\ \text{s.t.} \ & g_h(x_h, y, z_h) \le 0, \ \forall h \in \{1,\cdots,s\}, \\ & x_h \in X_h, \ z_h \in Z, \ \forall h \in \{1,\cdots,s\}, \\ & y \in Y. \end{aligned}}$$







Outline

- Part 1: Algorithms & Software for Stochastic Programs
  - A fully-decomposable algorithm for two-stage stochastic mixed-integer nonlinear programs (MINLPs)
  - Implementation of decomposition algorithms in the software GOSSIP for solving such problems
  - Computational results that demonstrate the advantages of using the decomposition algorithms and GOSSIP

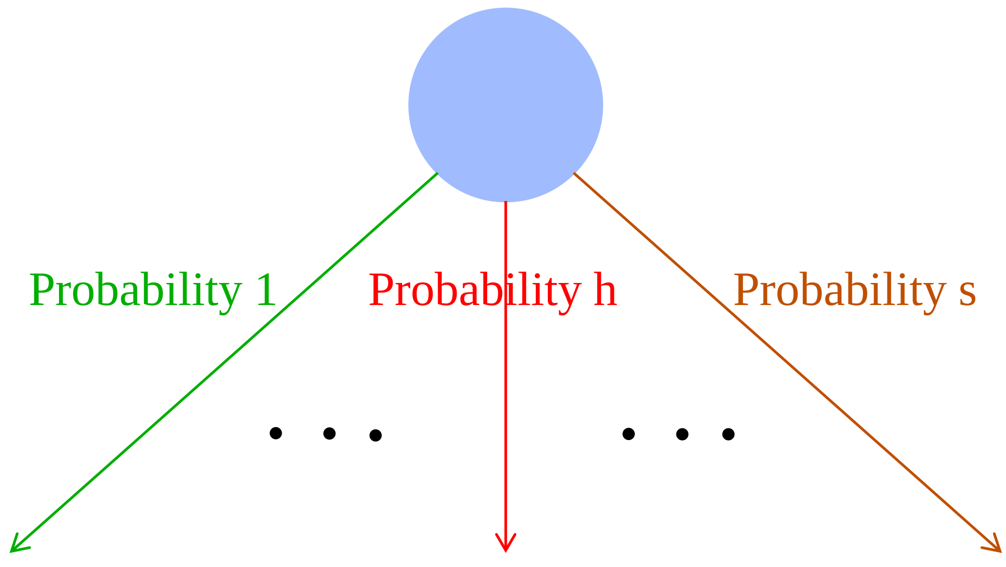
Two-Stage Stochastic Programming Framework

Two-Stage Stochastic Programming Framework

Stage 1 decisions (*y*, *z*)

- made before the realization of the uncertain parameters
- e.g., design decisions

Two-Stage Stochastic Programming Framework



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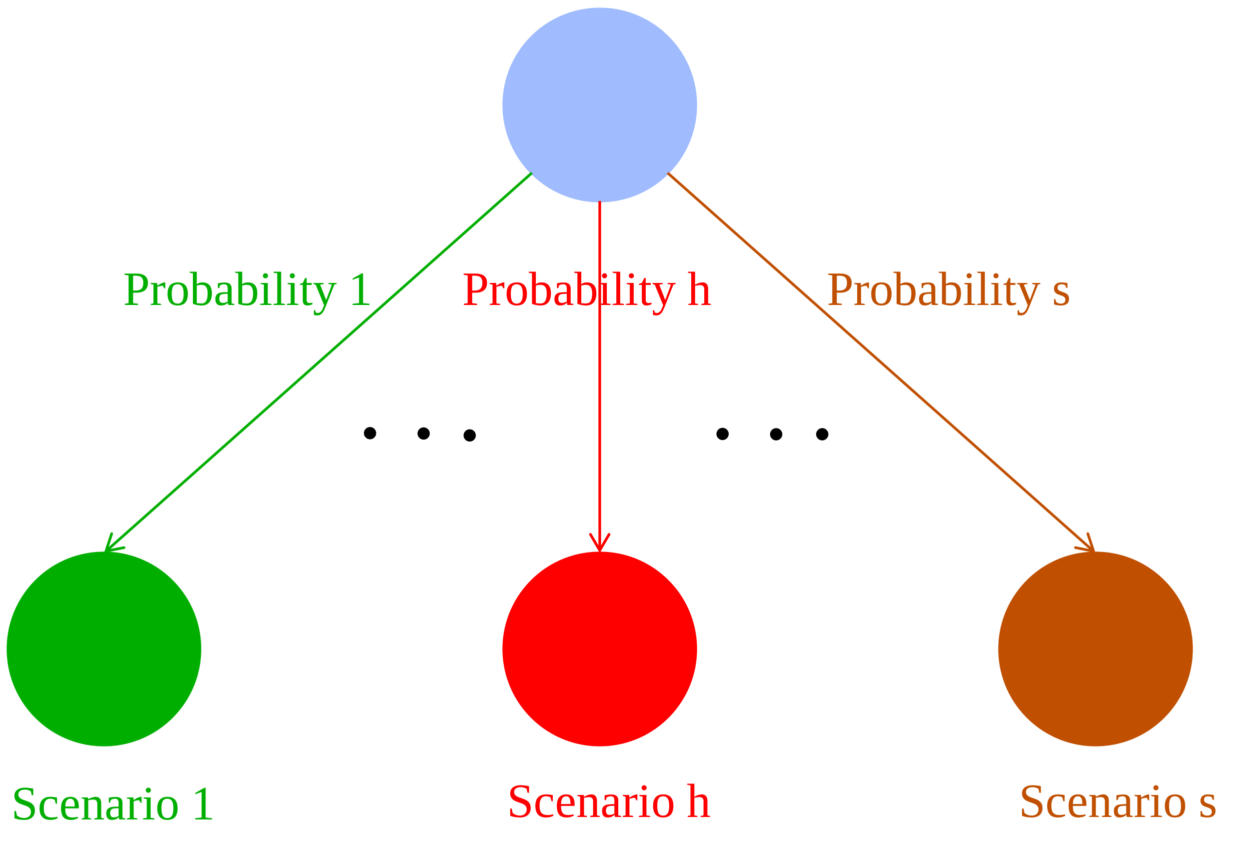
Realization of the uncertainty

- e.g., product demand

Two-Stage Stochastic Programming Framework



Stage 1 decisions (*y*, *z*)

- made before the realization of the uncertain parameters
- e.g., design decisions

Realization of the uncertainty

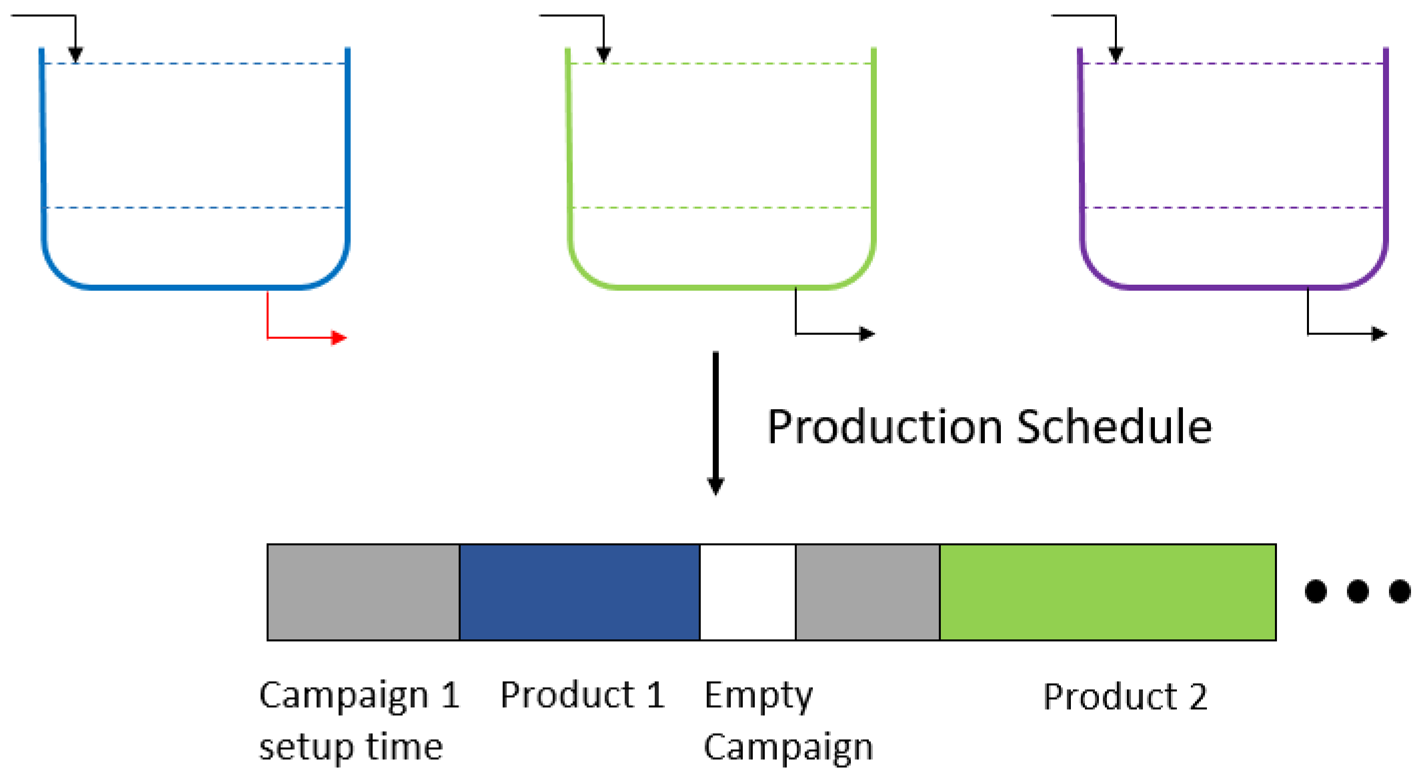
- e.g., product demand

Stage 2/Recourse decisions (x_h)

- made after the realization of the uncertain parameters
- e.g., operational decisions

Illustrative Example

Tank Sizing and Scheduling for a Chemical Plant



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Stage 1 decisions

- determine the sizes of the tanks for storing the products

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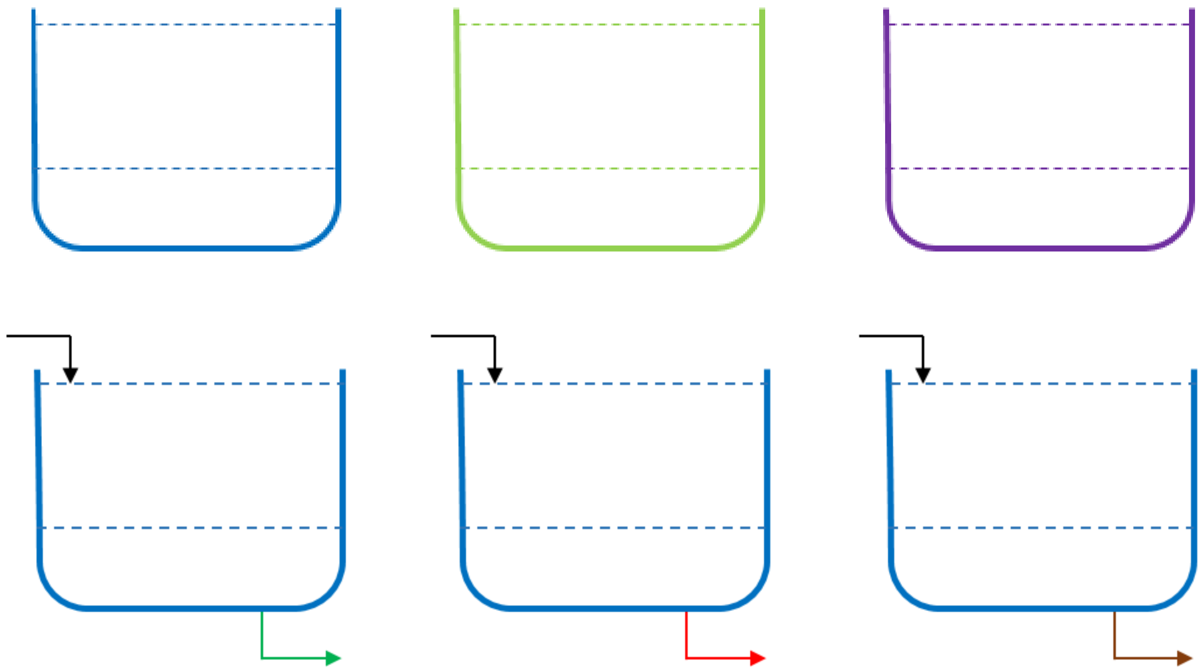

Stage 1 decisions

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Realization of the uncertainty

- demand of the first product

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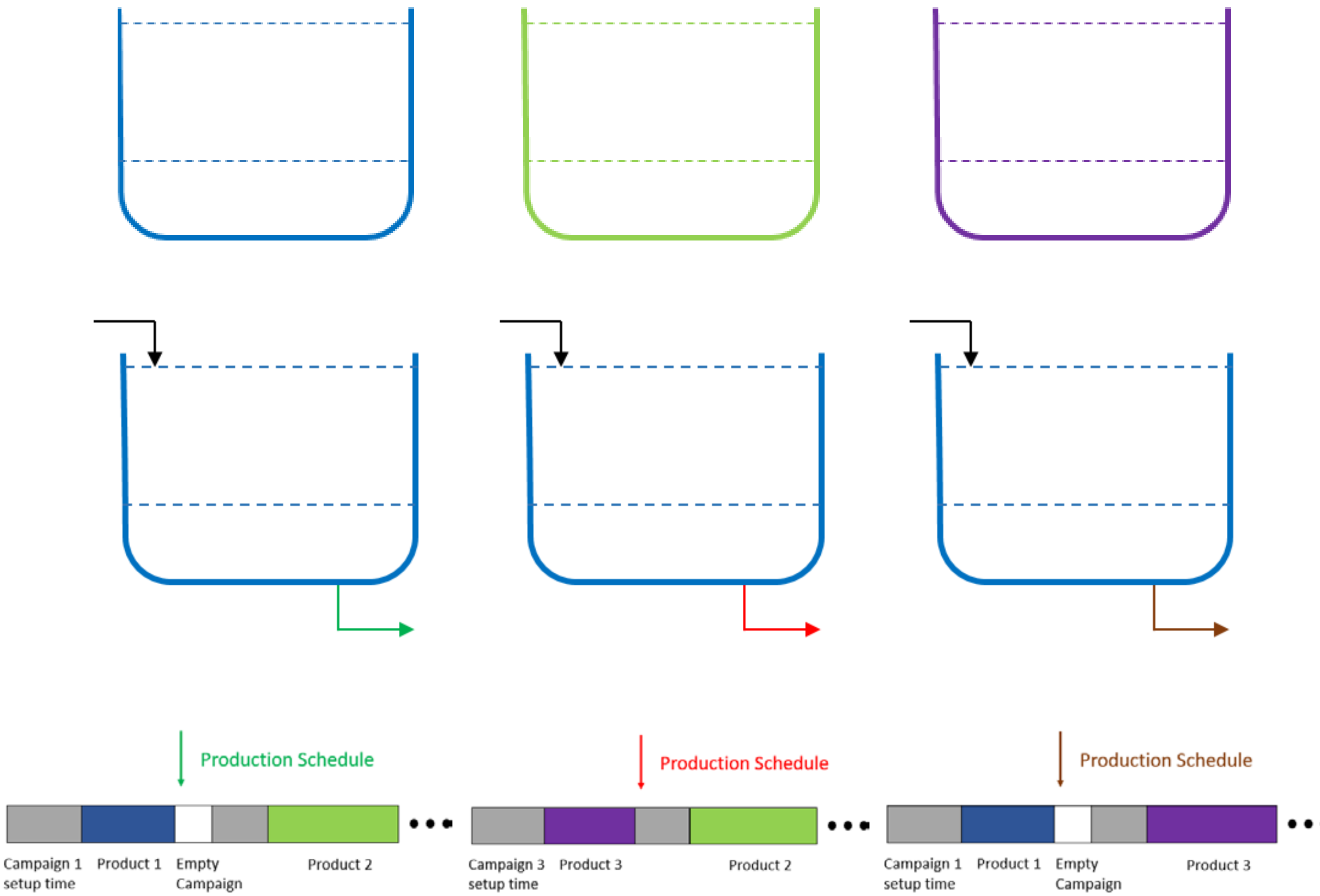


Stage 1 decisions

- determine the sizes of the tanks for storing the products

Realization of the uncertainty

- demand of the first product

Stage 2/Recourse decisions

- scheduling and campaign decisions

Two-stage stochastic MINLP framework

$$\min_{x_1,\cdots,x_s,y,z} \sum_{h=1}^{s} p_h f_h(x_h, y, z)$$

$$\text{s.t.} \quad g_h(x_h, y, z) \le 0, \ \forall h \in \{1,\cdots,s\},$$

$$x_h \in X_h \subset \{0,1\}^{n_{x_b}} \times \mathbb{R}^{n_{x_c}}, \ \forall h \in \{1,\cdots,s\},$$

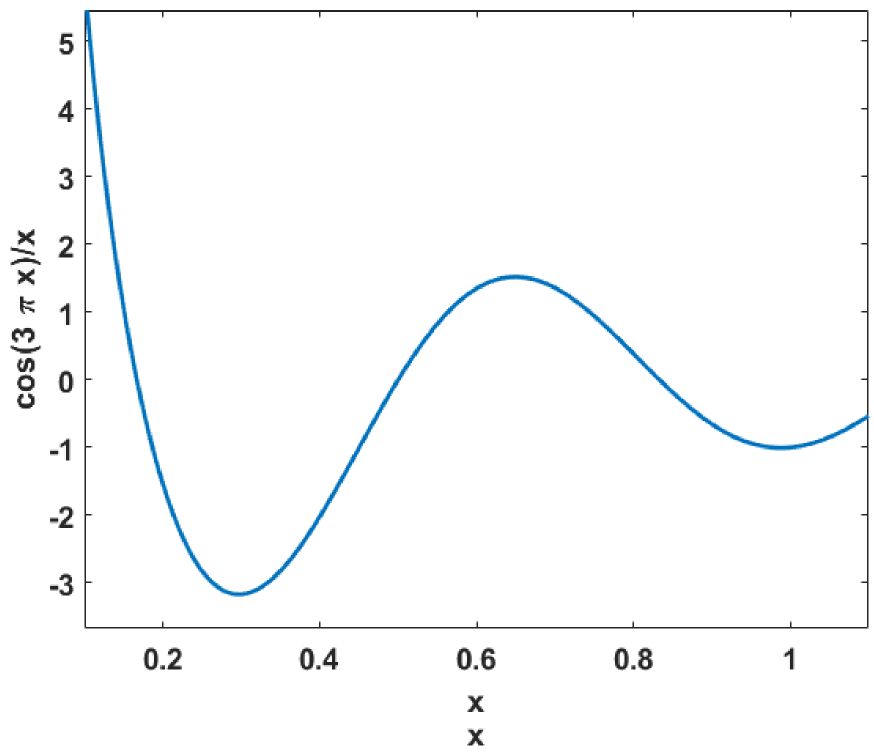
$$y \in Y \subset \{0,1\}^{n_y}, \ z \in Z \subset \mathbb{R}^{n_z}.$$

Notation

- p_h: probability of scenario h
- x_h: recourse decisions corresponding to scenario h
- y: binary first-stage decisions
- z: continuous first-stage decisions

Overview of Branch-and-Bound (B&B) Algorithms

Consider the problem $\min\limits_{x\in[0.1,1.1]} \dfrac{\cos(3\pi x)}{x}$



Overview of Branch-and-Bound (B&B) Algorithms

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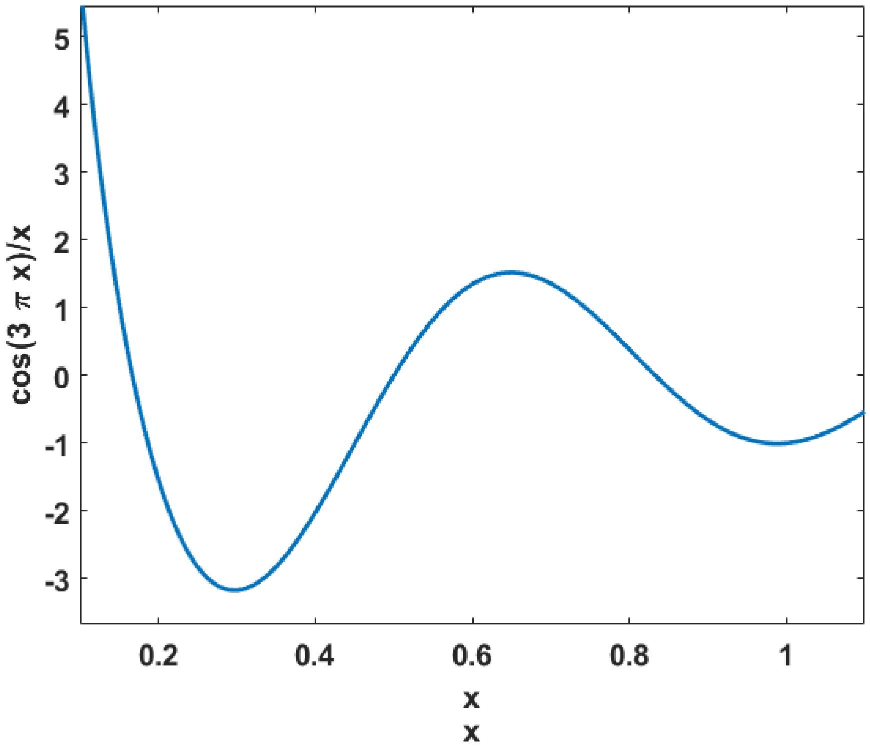
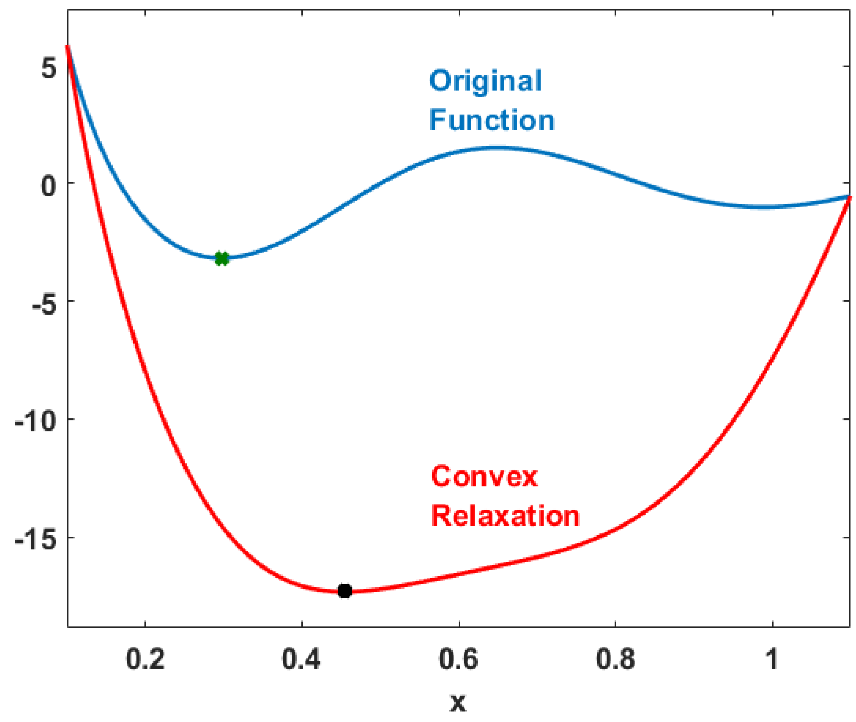
Since this function has multiple local minima, need global optimization techniques to guarantee finding its global solution



Overview of Branch-and-Bound (B&B) Algorithms

Consider the problem $\min_{x \in [0.1, 1.1]} \dfrac{\cos(3\pi x)}{x}$

The first step is to construct a convex relaxation of the function on the domain of interest



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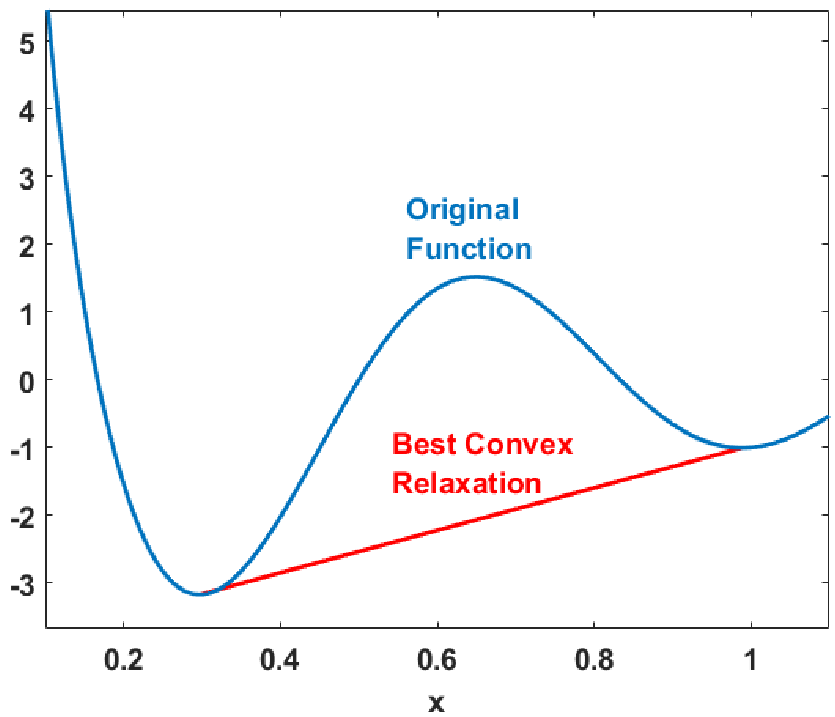
While we may be able to construct the best possible convex relaxation for simple functions, it is usually difficult (or even undesirable!) to construct for high-dimensional functions



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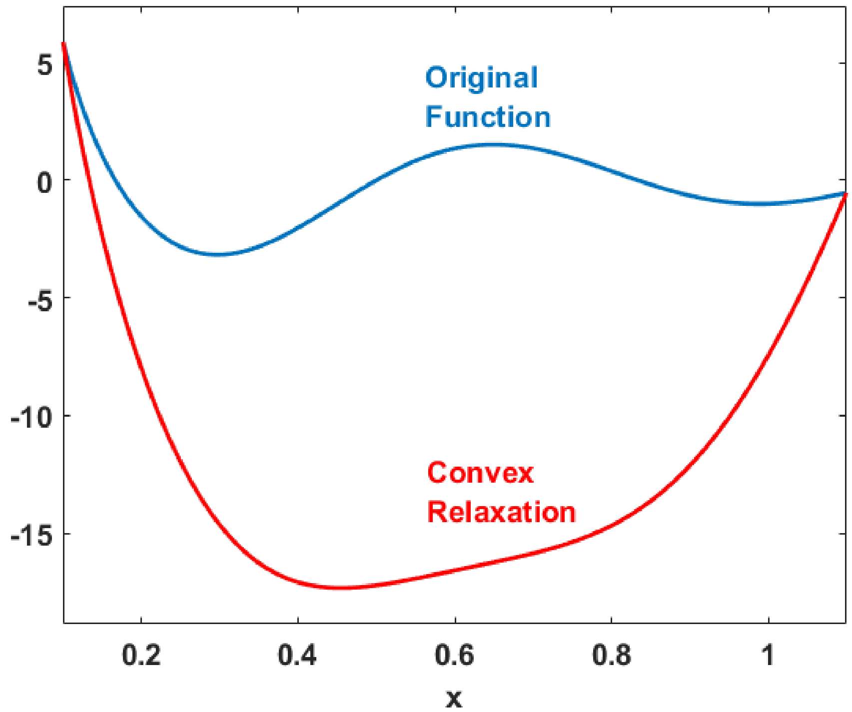
Once a convex relaxation is constructed, we can minimize this relaxation to obtain a lower bound on the minimum objective function value



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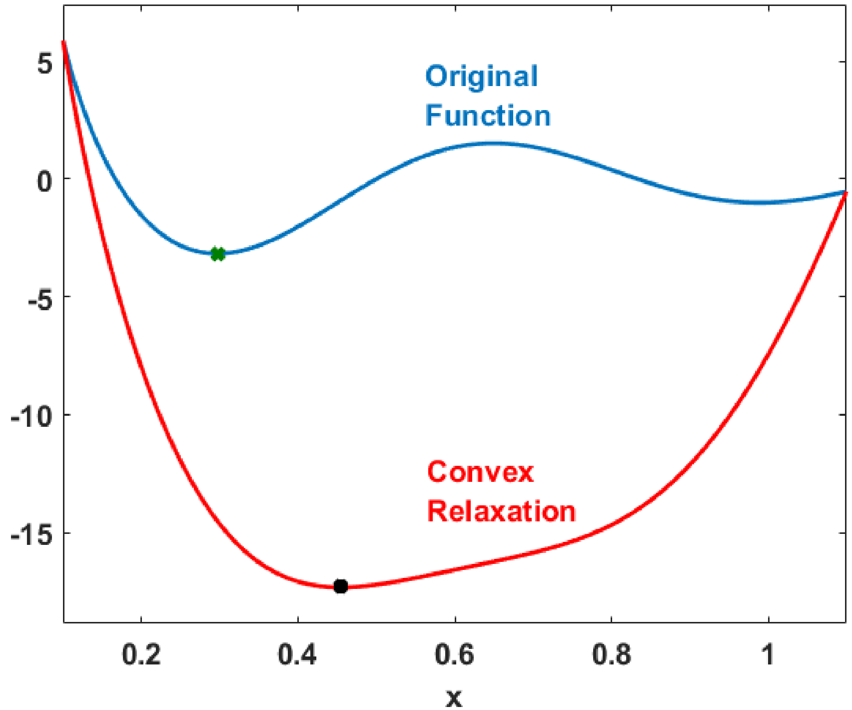
An upper bound on the minimum objective value can be obtained by using local optimization techniques (such as multi-start along with gradient descent)



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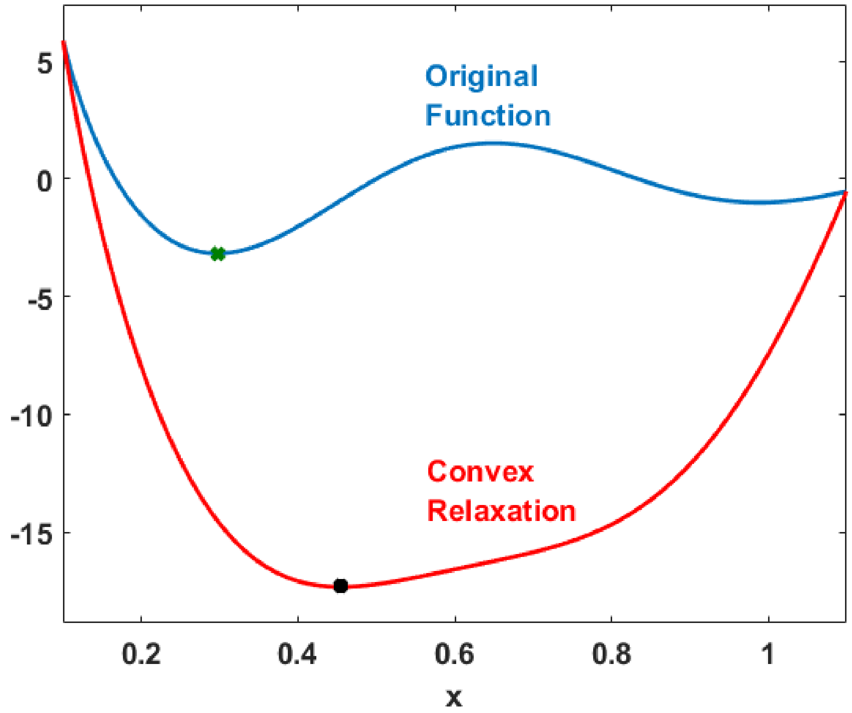

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To reduce the gap between the lower and upper bound, we use branch-and-bound

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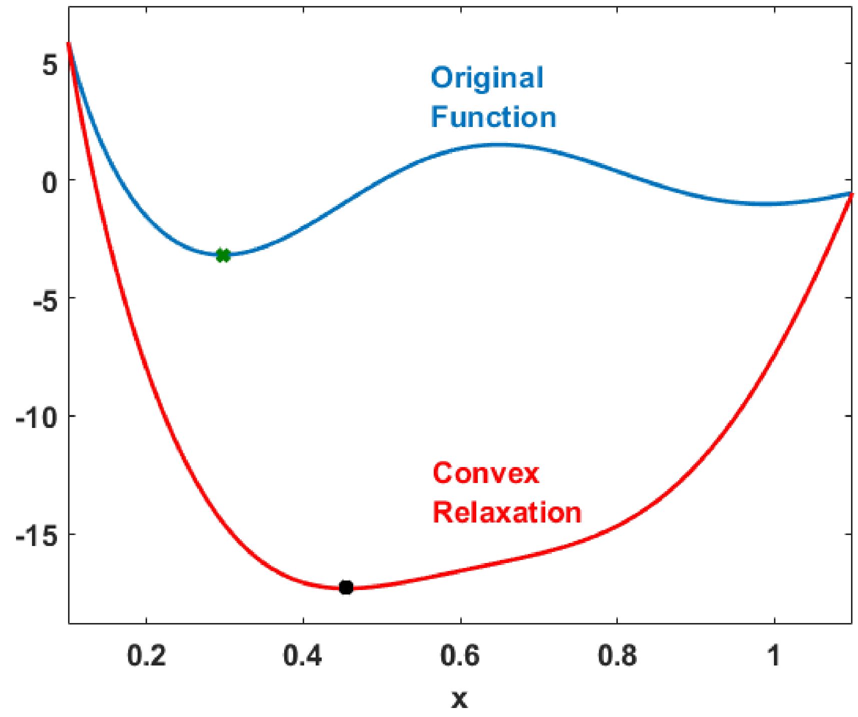
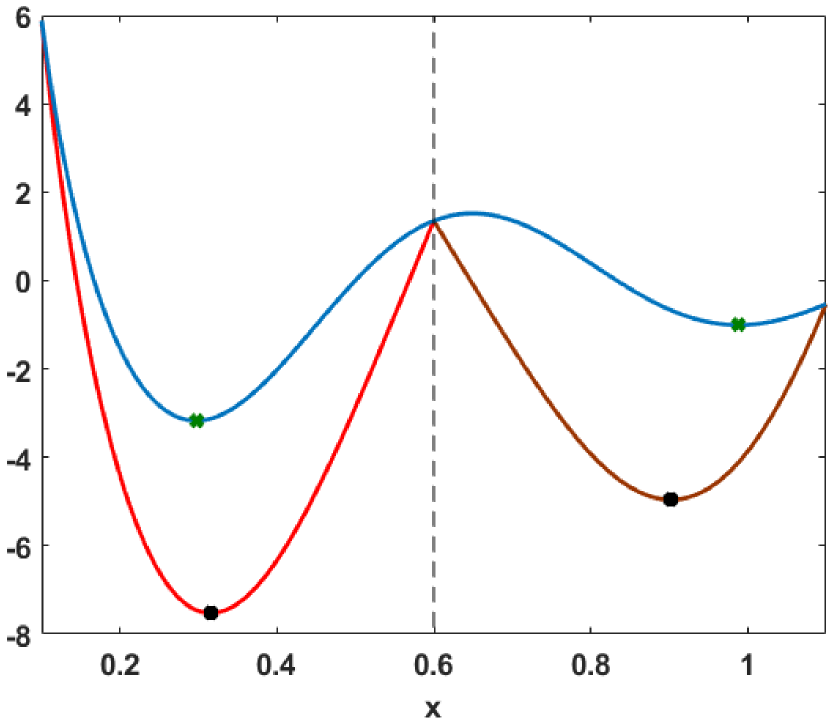


Overview of Branch-and-Bound (B&B) Algorithms

Consider the problem $\min\limits_{x \in [0.1, 1.1]} \dfrac{\cos(3\pi x)}{x}$

We split the domain of x into two regions, construct new and improved convex relaxations on each of those regions, and minimize the updated convex relaxations to obtain lower bounds on those particular regions



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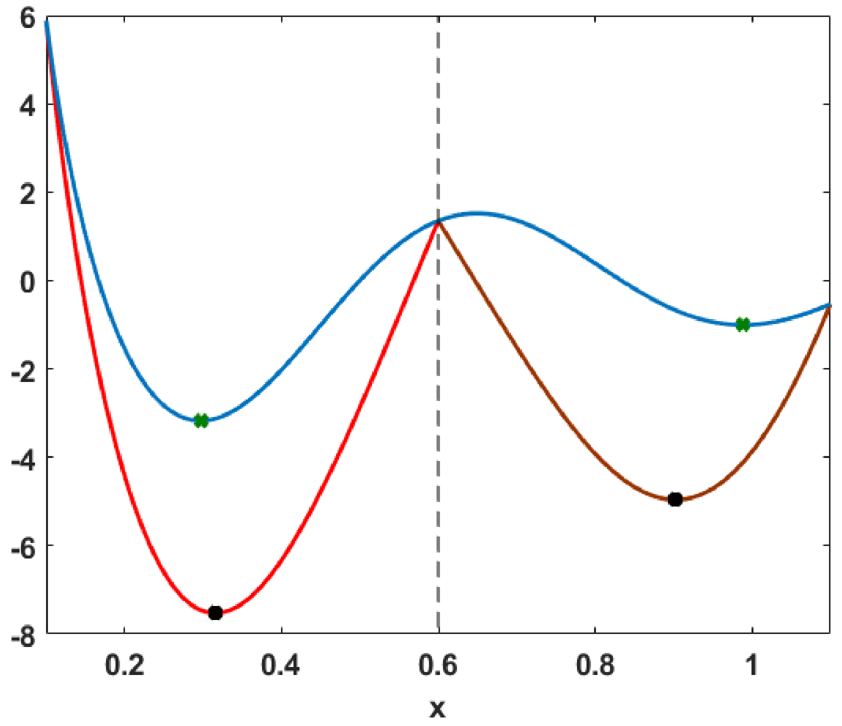
To converge the overall lower and upper bounds: branch and repeat



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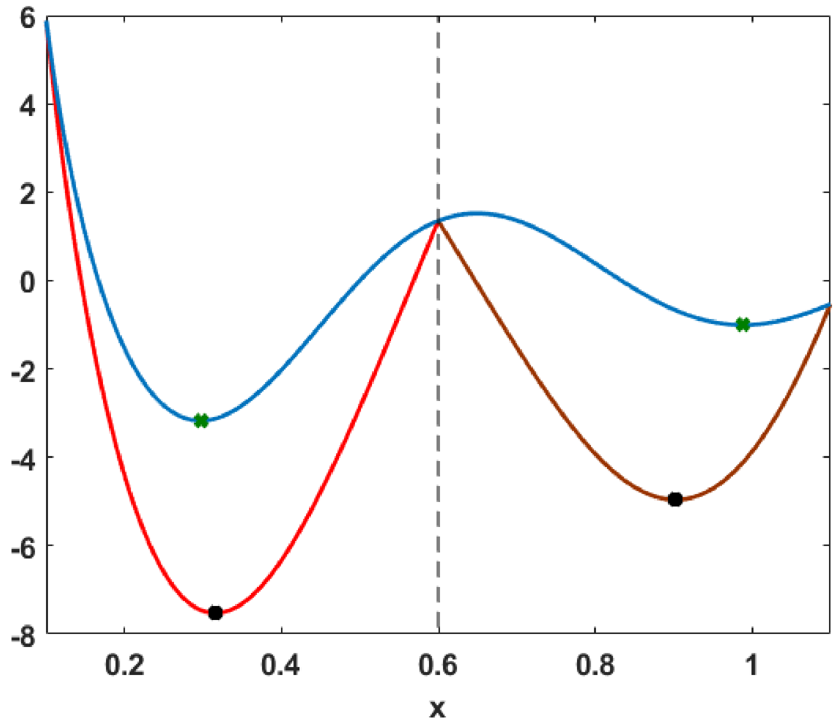
To converge the overall lower and upper bounds: branch and repeat

For constrained optimization problems, the procedure is similar with the understanding that we overestimate the feasible region by replacing the constraint functions with convex (and concave) relaxations



Overview of Branch-and-Bound (B&B) Algorithms

$$\min_{x\in[0.1,1.1]} \frac{\cos(3\pi x)}{x}$$

$$\text{s.t.} \quad 2x+\sin(12\pi x)=0,$$

$$0.04-x^2 \le 0.$$

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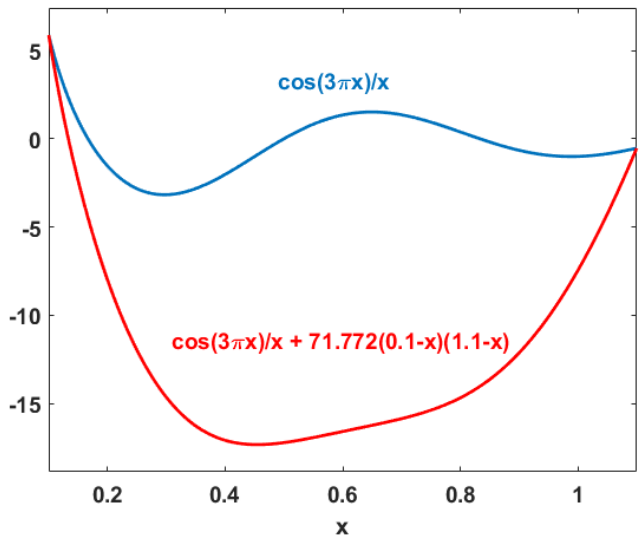

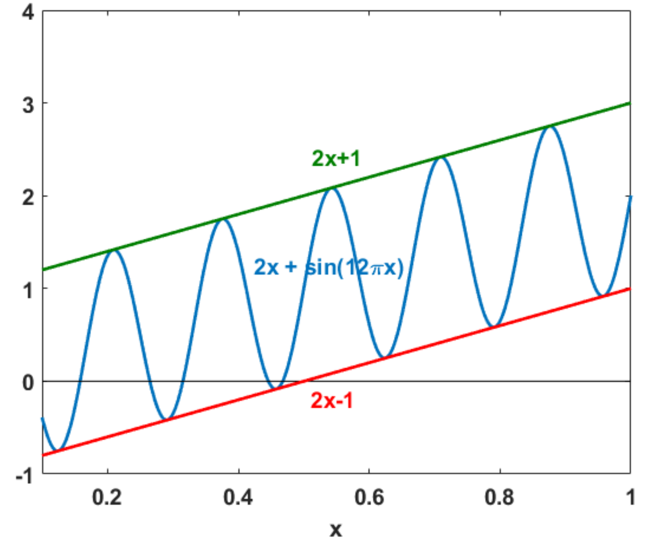

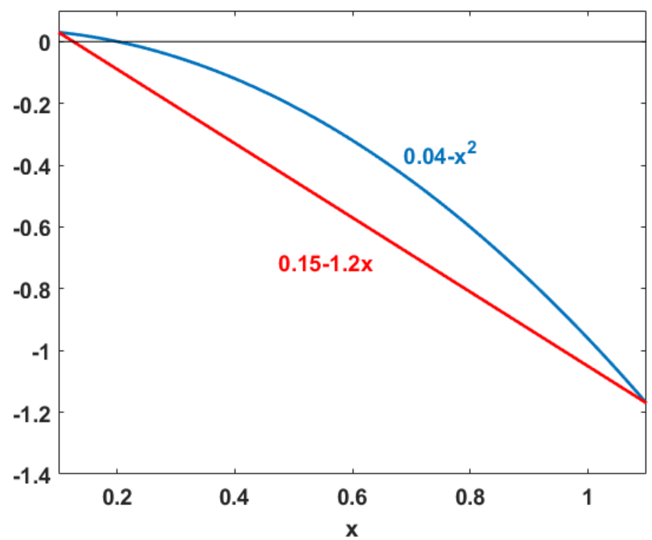

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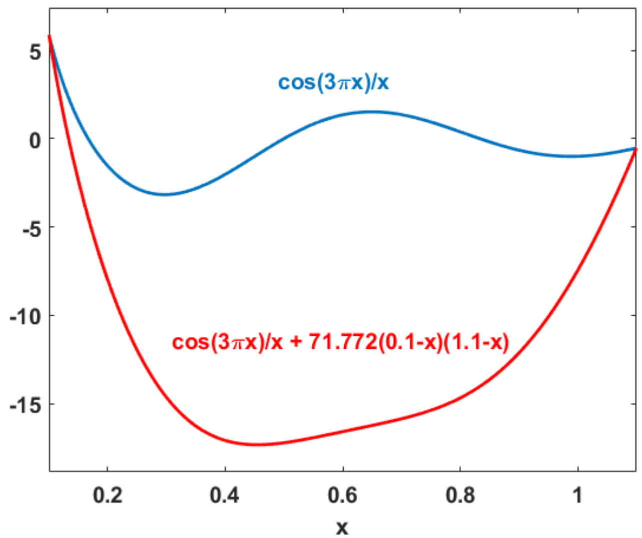
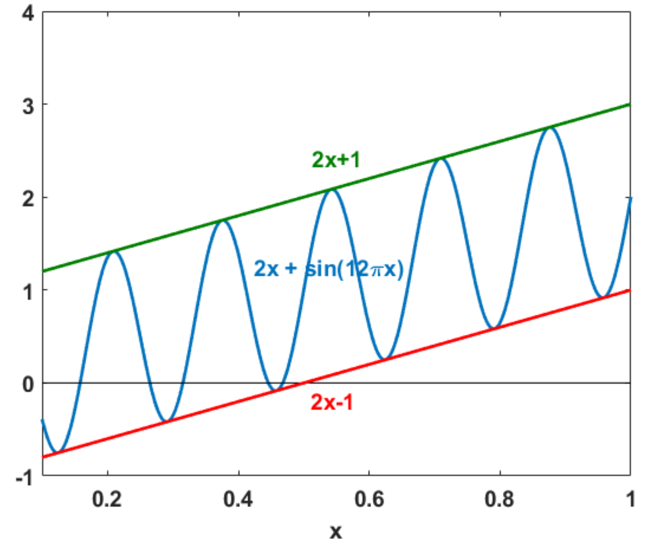
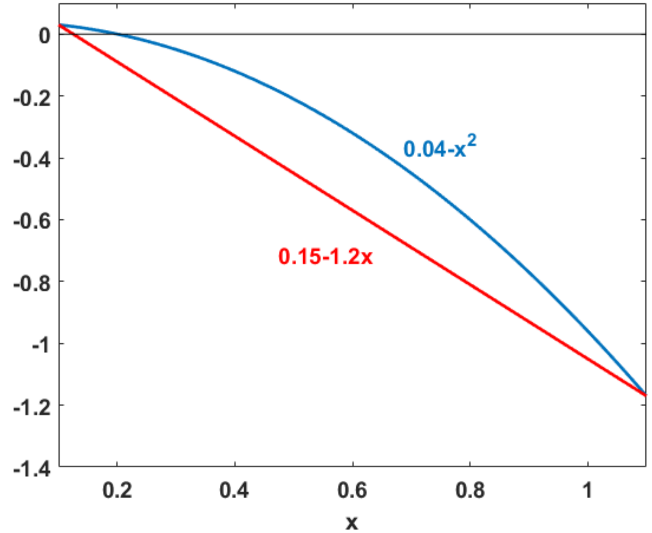


Can deduce tighter bounds on the variables using constraint information





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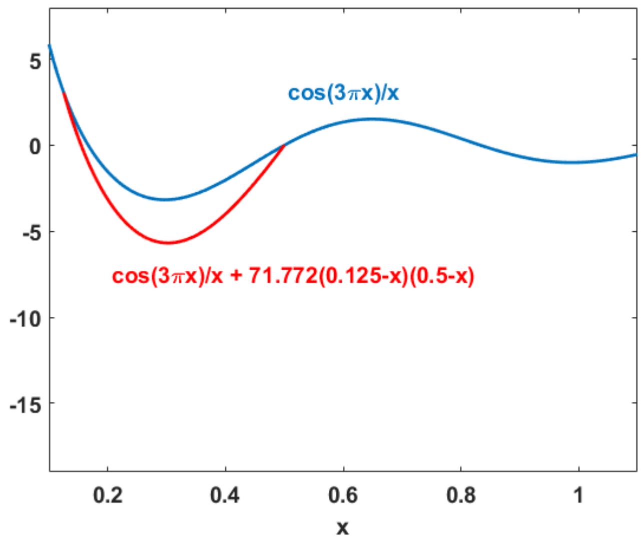
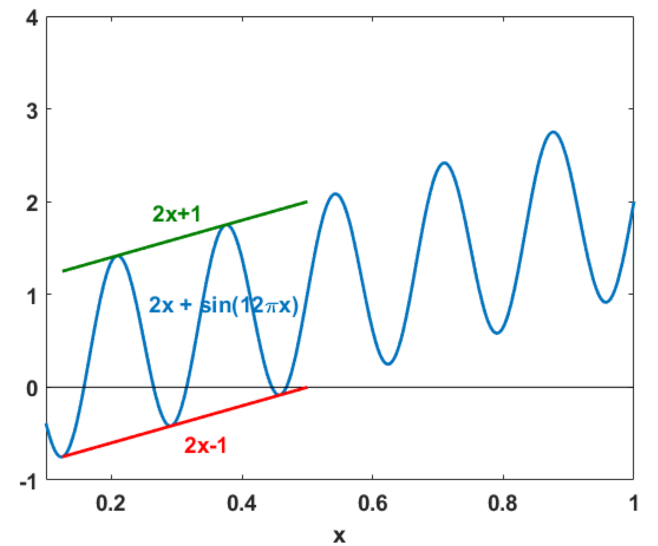
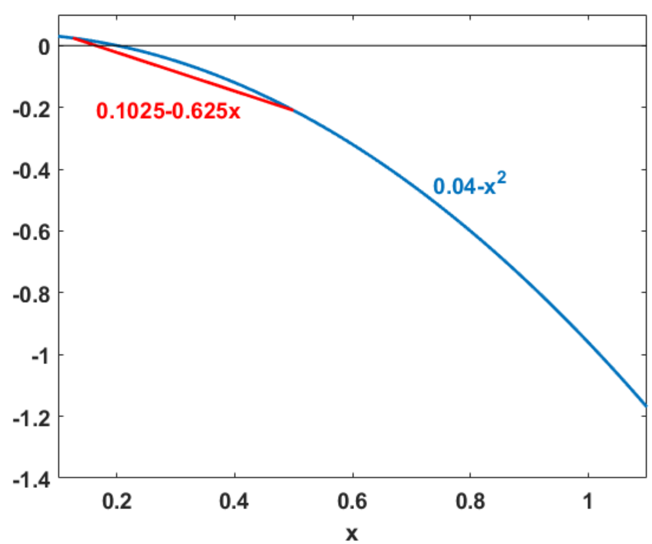


Can deduce tighter bounds on the variables using constraint information and construct tighter relaxations





Two-stage stochastic MINLP framework

$$\min_{x_1,\cdots,x_s,y,z} \sum_{h=1}^{s} p_h f_h(x_h, y, z)$$

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Notation

- p_h: probability of scenario h
- x_h: recourse decisions corresponding to scenario h
- y: binary first-stage decisions
- z: continuous first-stage decisions

Decomposition Approaches

Formulation

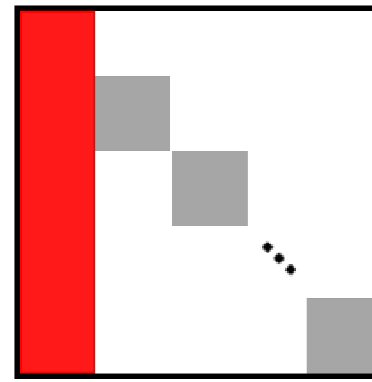
$$\min_{x_1,\cdots,x_s,\color{red}{y},\color{red}{z}} \sum_{h=1}^{s} p_h f_h(x_h, \color{red}{y}, \color{red}{z})$$

$$\text{s.t.} \quad g_h(x_h, \color{red}{y}, \color{red}{z}) \le 0, \ \forall h \in \{1,\cdots,s\},$$

$$x_h \in X_h \subset \{0,1\}^{n_{x_b}} \times \mathbb{R}^{n_{x_c}}, \ \forall h \in \{1,\cdots,s\},$$

Complicating variables

$$\color{red}{y} \in Y \subset \{0,1\}^{n_y}, \ \color{red}{z} \in Z \subset \mathbb{R}^{n_z}.$$



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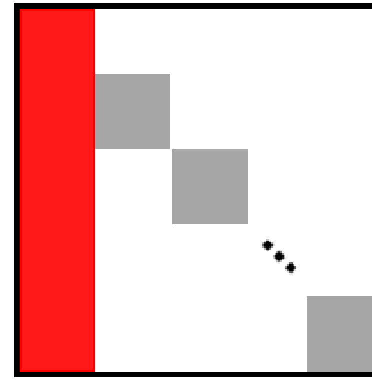


Equivalent Formulation

$$\min_{\substack{x_1,\cdots,x_s,\\ y_1,\cdots,y_s,\\ z_1,\cdots,z_s}} \sum_{h=1}^{s} p_h f_h(x_h, y_h, z_h)$$

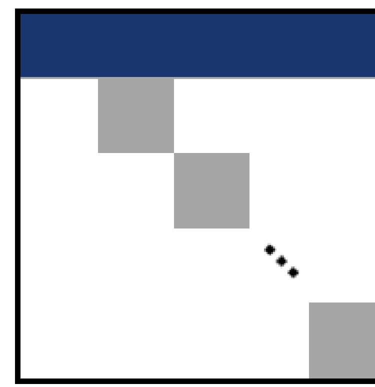
$$\text{s.t.} \quad g_h(x_h, y_h, z_h) \le 0, \ \forall h \in \{1,\cdots,s\},$$

Complicating constraints

$$y_h - y_{h+1} = 0, \ \forall h \in \{1,\cdots,s-1\},$$

$$z_h - z_{h+1} = 0, \ \forall h \in \{1,\cdots,s-1\},$$

$$x_h \in X_h, \ y_h \in Y, \ z_h \in Z, \ \forall h \in \{1,\cdots,s\}.$$



Prior Decomposition Approaches

Nonconvex Generalized Benders Decomposition

Fix the first-stage variables to generate upper bounds

$$\begin{aligned} \min_{x_1,\cdots,x_s} \quad & \sum_{h=1}^{s} p_h f_h(x_h, \overline{y}) \\ \text{s.t.} \quad & g_h(x_h, \overline{y}) \le 0, \ \forall h \in \{1,\cdots,s\}, \\ & x_h \in X_h, \ \forall h \in \{1,\cdots,s\}. \end{aligned}$$

Can solve the individual scenario problems independently

Li, X. et al., J. Optimiz. Theory. App., 2011.

Prior Decomposition Approaches

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Can solve the individual scenario problems independently

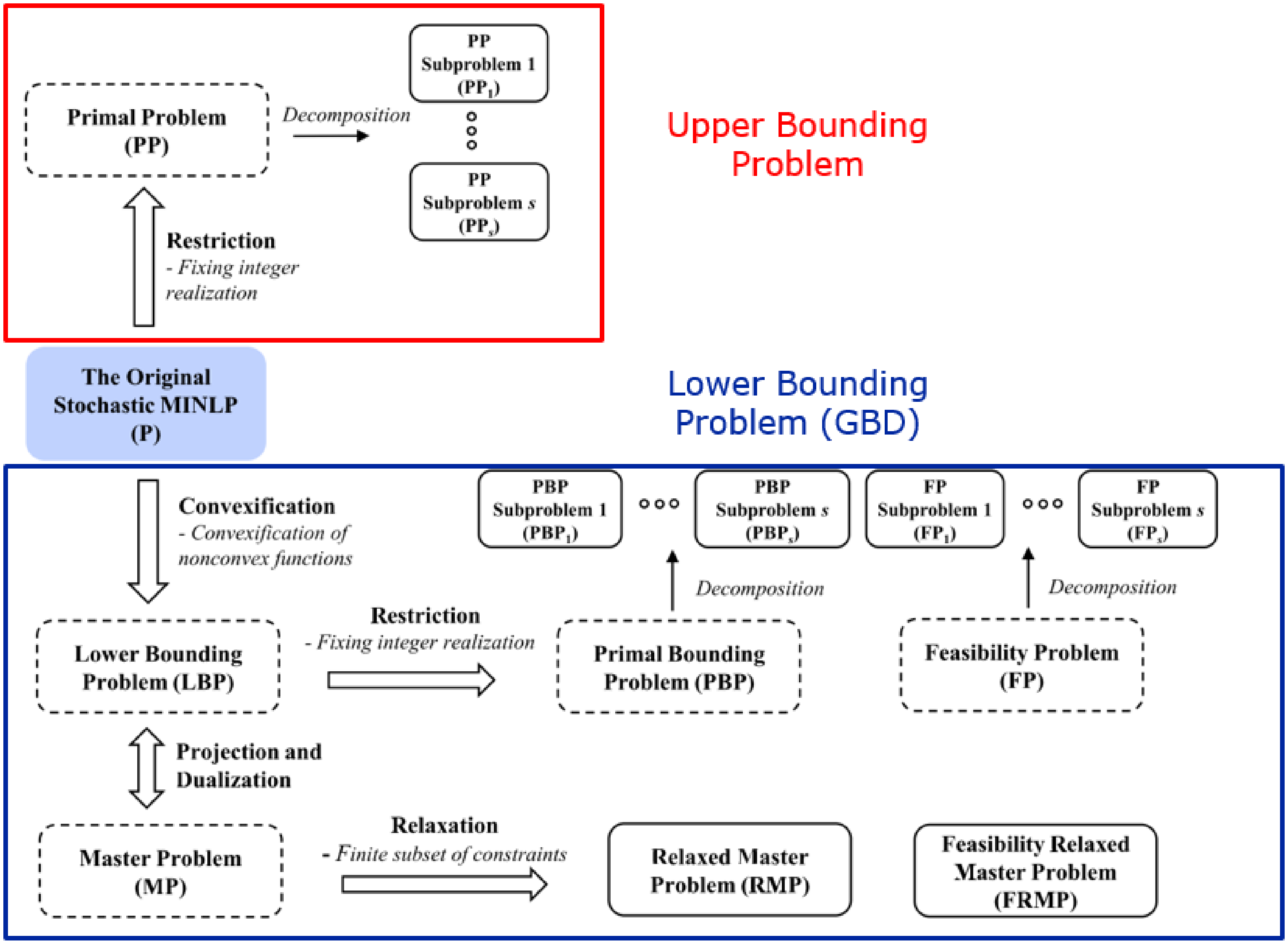
Construct a convex relaxation of the original problem to generate lower bounds

$$\begin{aligned} \min_{x_1,\cdots,x_s,y} \quad & \sum_{h=1}^{s} p_h \left[f_h^{\text{cv}}(x_h) + c_{y,h}^{\text{T}} y \right] \\ \text{s.t.} \quad & g_h^{\text{cv}}(x_h) + B_{y,h} y \le 0, \ \forall h \in \{1,\cdots,s\}, \\ & x_h \in \text{conv}(X_h), \ \forall h \in \{1,\cdots,s\}, \\ & y \in Y. \end{aligned}$$

Can solve the relaxed problem efficiently using GBD

Li, X. et al., J. Optimiz. Theory. App., 2011.

Prior Decomposition Approaches
Nonconvex Generalized Benders Decomposition



Li, X. et al., J. Optimiz. Theory. App., 2011.

Prior Decomposition Approaches

Lagrangian Relaxation

Upper bounds are generated using local optimization techniques

$$\min_{x_1,\cdots,x_s,y,z} \sum_{h=1}^{s} p_h f_h(x_h, y, z)$$

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Need to exploit the problem structure while solving large-scale instances

Guignard, M. et al., Math. Program., 1987.

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Need to exploit the problem structure while solving large-scale instances

To construct the lower bounding problem, consider:

$$\min_{\substack{x_1,\cdots,x_s,\\ y_1,\cdots,y_s,\\ z_1,\cdots,z_s}} \sum_{h=1}^{s} p_h f_h(x_h, y_h, z_h)$$
$$\text{s.t.} \quad g_h(x_h, y_h, z_h) \le 0, \ \forall h \in \{1,\cdots,s\},$$
$$y_h - y_{h+1} = 0, \ \forall h \in \{1,\cdots,s-1\},$$
$$z_h - z_{h+1} = 0, \ \forall h \in \{1,\cdots,s-1\},$$
$$x_h \in X_h, \ y_h \in Y, \ z_h \in Z, \ \forall h \in \{1,\cdots,s\}.$$

Guignard, M. et al., Math. Program., 1987.

Prior Decomposition Approaches
Lagrangian Relaxation

Upper bounds are generated using local optimization techniques

$$\min_{x_1,\cdots,x_s,y,z} \sum_{h=1}^{s} p_h f_h(x_h, y, z)$$
$$\text{s.t.} \quad g_h(x_h, y, z) \le 0, \ \forall h \in \{1,\cdots,s\},$$
$$x_h \in X_h, \ \forall h \in \{1,\cdots,s\},$$
$$y \in Y, \ z \in Z.$$

Need to exploit the problem structure while solving large-scale instances

Lower bounds are generated using (weak) Lagrangian duality

$$\sup_{\substack{\mu_1,\cdots,\mu_{s-1},\\ \lambda_1,\cdots,\lambda_{s-1}}} \ \min_{\substack{x_1,\cdots,x_s,\\ y_1,\cdots,y_s,\\ z_1,\cdots,z_s}} \sum_{h=1}^{s} p_h f_h(x_h, y_h, z_h) + \sum_{h=1}^{s-1} \mu_h^T (y_h - y_{h+1}) + \sum_{h=1}^{s-1} \lambda_h^T (z_h - z_{h+1})$$
$$\text{s.t.} \quad g_h(x_h, y_h, z_h) \le 0, \ \forall h \in \{1,\cdots,s\},$$
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Prior Decomposition Approaches
Lagrangian Relaxation

Upper bounds are generated using local optimization techniques

$$\begin{aligned}\min_{x_1,\cdots,x_s,y,z} \quad & \sum_{h=1}^{s} p_h f_h(x_h, y, z)\\ \text{s.t.} \quad & g_h(x_h, y, z) \le 0, \ \forall h \in \{1,\cdots,s\},\\ & x_h \in X_h, \ \forall h \in \{1,\cdots,s\},\\ & y \in Y, \ z \in Z.\end{aligned}$$

Need to exploit the problem structure while solving large-scale instances

Inner minimization can be decomposed into individual scenario subproblems

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Convergence is guaranteed by B&B, where it is sufficient to branch on the complicating variables y and z to converge

Guignard, M. et al., Math. Program., 1987.

Proposed Decomposition Approach
Modified Lagrangian Relaxation

Upper bounds can be generated either by fixing the continuous complicating variables, or by using local optimization techniques

$$\begin{aligned}
\min_{x_1,\cdots,x_s,y} \quad & \sum_{h=1}^{s} p_h f_h(x_h, y, \bar{z}) \\
\text{s.t.} \quad & g_h(x_h, y, \bar{z}) \le 0, \ \forall h \in \{1,\cdots,s\}, \\
& x_h \in X_h, \ \forall h \in \{1,\cdots,s\}, \\
& y \in Y.
\end{aligned}$$

Can solve this problem efficiently using NGBD

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\end{aligned}$$

Can solve this problem efficiently using NGBD

Lower bounds are generated by dualizing only a subset of the nonanticipativity constraints

$$\begin{aligned}
\sup_{\lambda_1,\cdots,\lambda_{s-1}} \ \min_{\substack{x_1,\cdots,x_s, \\ y,z_1,\cdots,z_s}} \quad & \sum_{h=1}^{s} p_h f_h(x_h, y, z_h) + \sum_{h=1}^{s-1} \lambda_h^T (z_h - z_{h+1}) \\
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Inner minimization can be solved in a decomposable manner using NGBD

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$$\sup_{\lambda_1,\cdots,\lambda_{s-1}} \boxed{\begin{aligned}
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& y \in Y.
\end{aligned}}$$

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Finite convergence of the B&B algorithm has been established, where it is sufficient to branch on the continuous complicating variables z to converge

GOSSIP

Overview and Motivation

- Software for the Global Optimization of nonconvex two-Stage Stochastic mixed-Integer nonlinear Programs
  - More than 50,000 lines of source code (primarily in C++)
  - Links to state-of-the-art solvers, e.g., CPLEX, IPOPT, ANTIGONE
  - Performs well on a diverse set of test cases from the literature

GOSSIP

Overview and Motivation

- Software for the Global Optimization of nonconvex two-Stage Stochastic mixed-Integer nonlinear Programs
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- Motivation

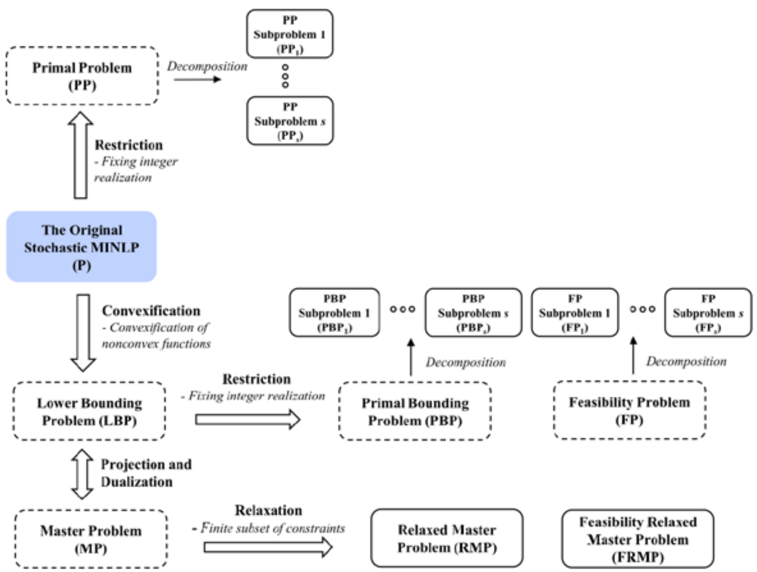
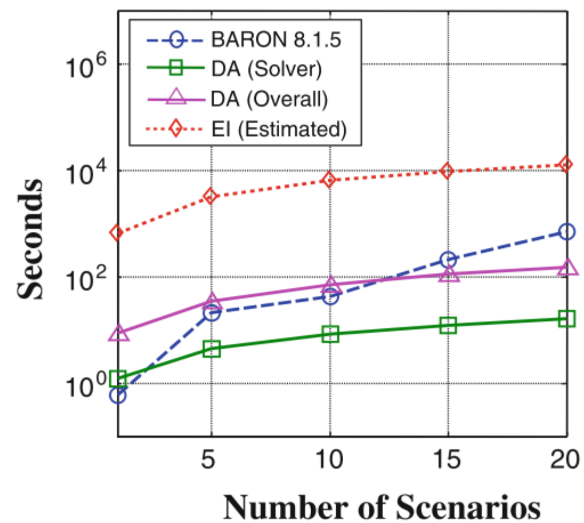


Image from Li et al., J. Global Optim., 2011

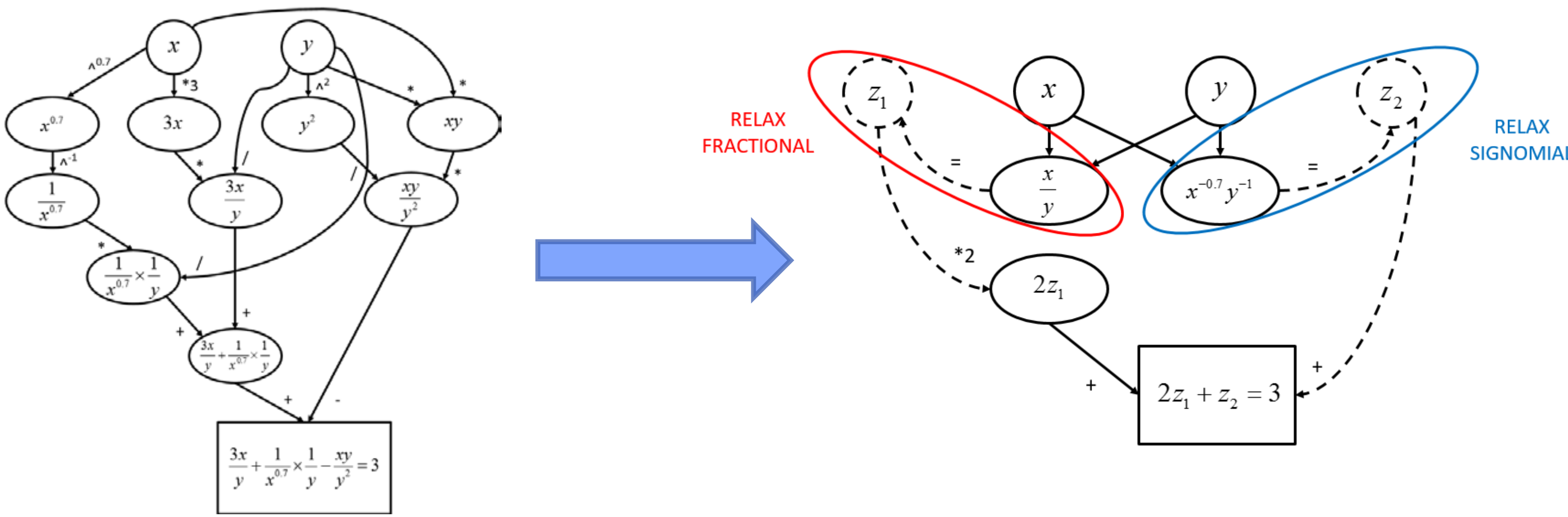


Implementing decomposition algorithms is a nontrivial task

Naïve implementations may result in significant overhead

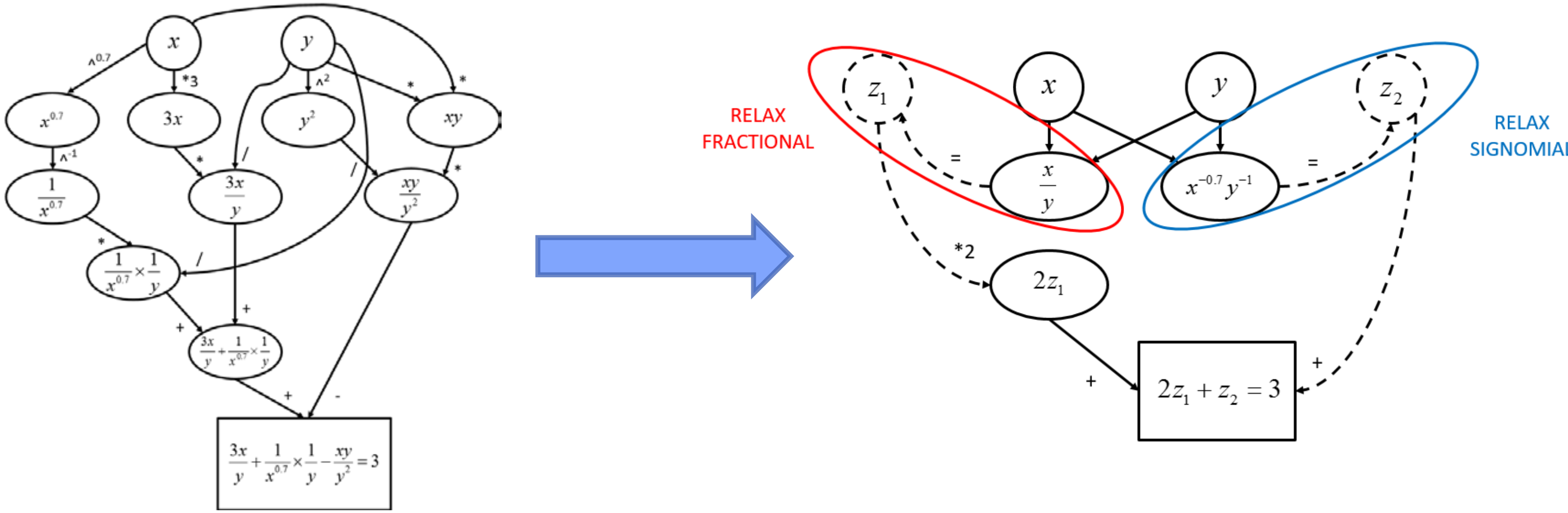
Select Features in GOSSIP

Automatic Structure Detection

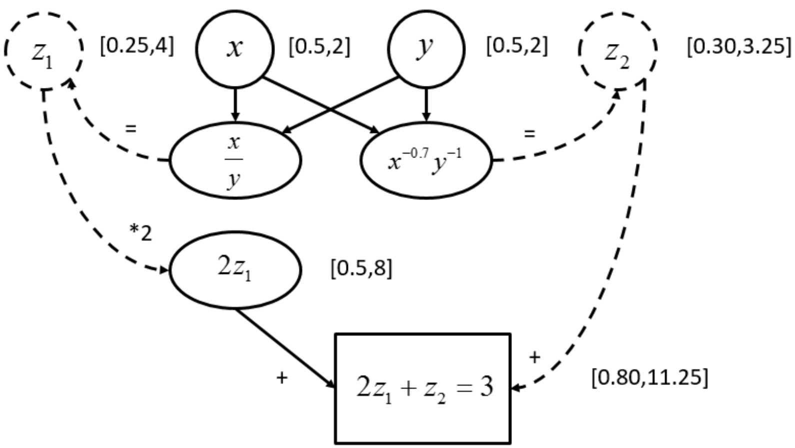


Select Features in GOSSIP

Automatic Structure Detection

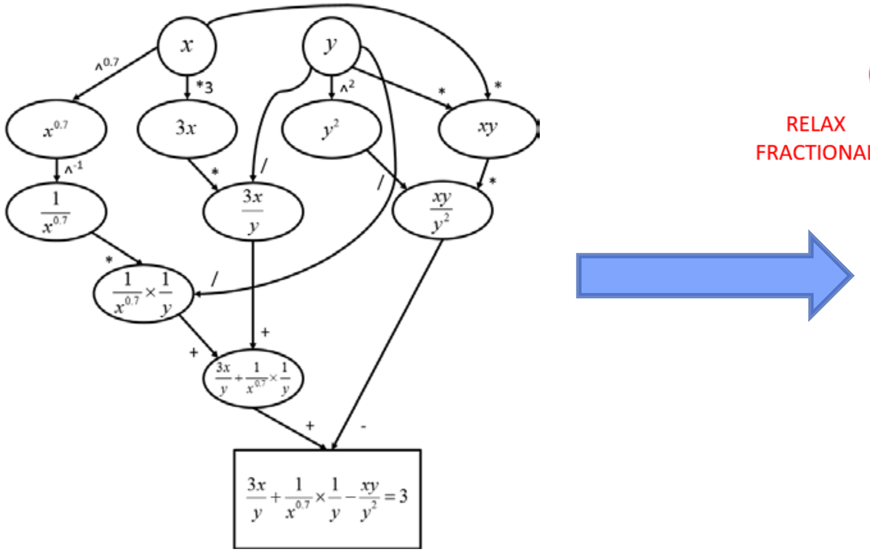


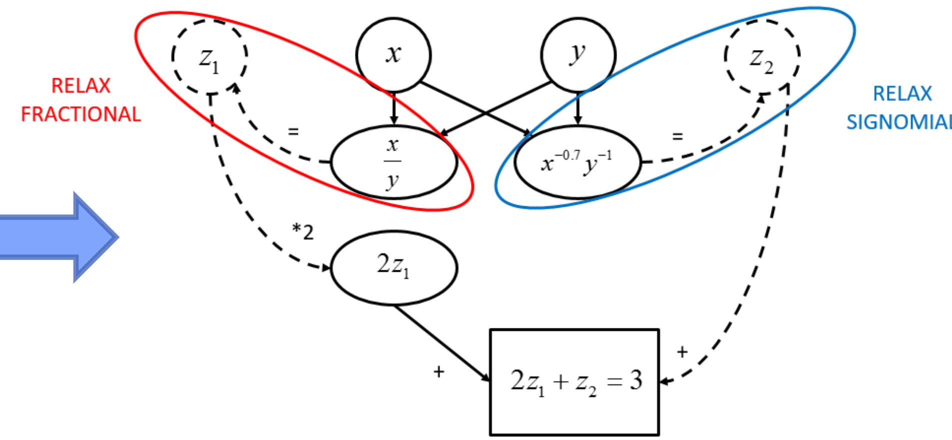
Scalable Bounds Tightening Techniques



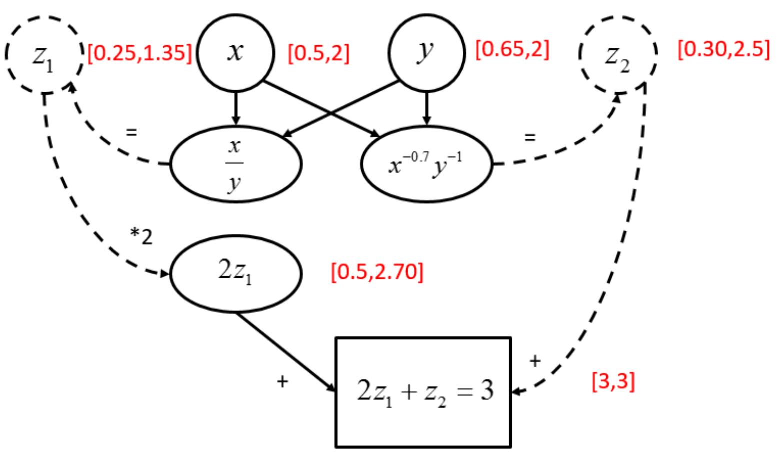
Select Features in GOSSIP

Automatic Structure Detection



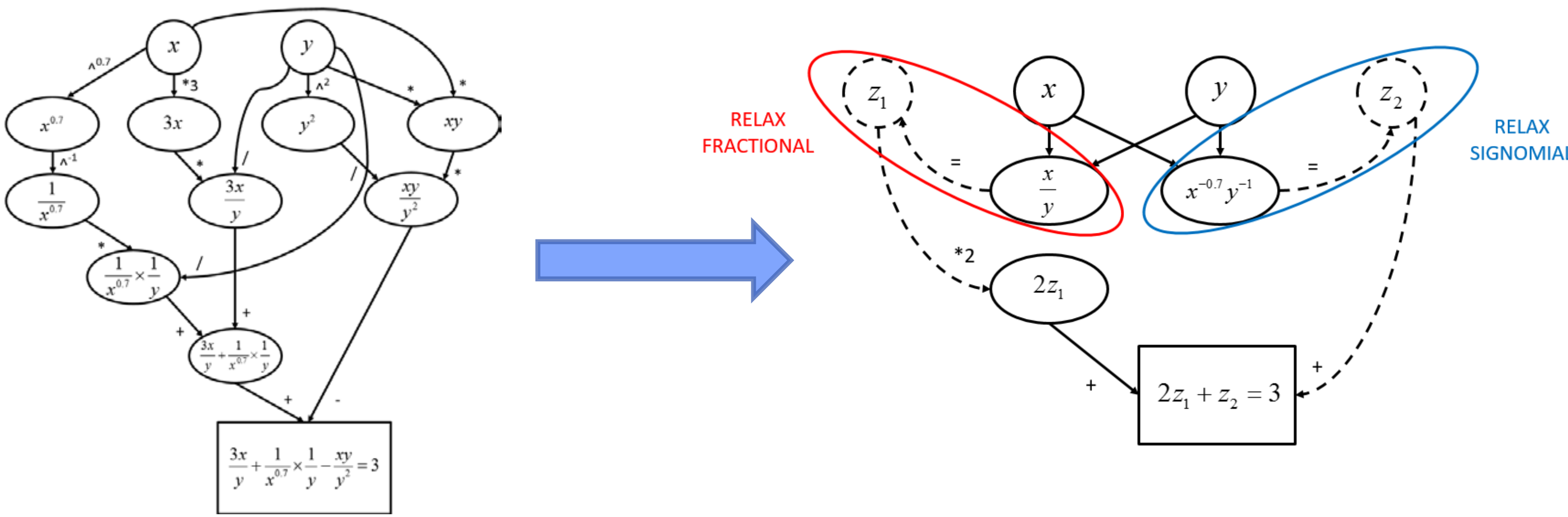


Scalable Bounds Tightening Techniques

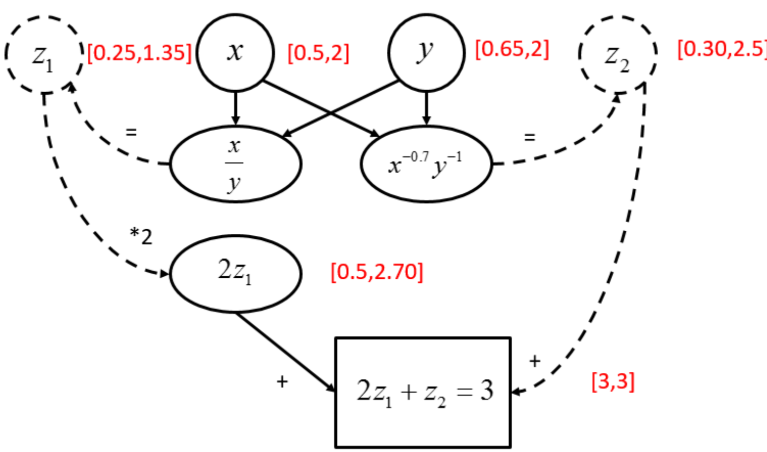


Select Features in GOSSIP

Automatic Structure Detection



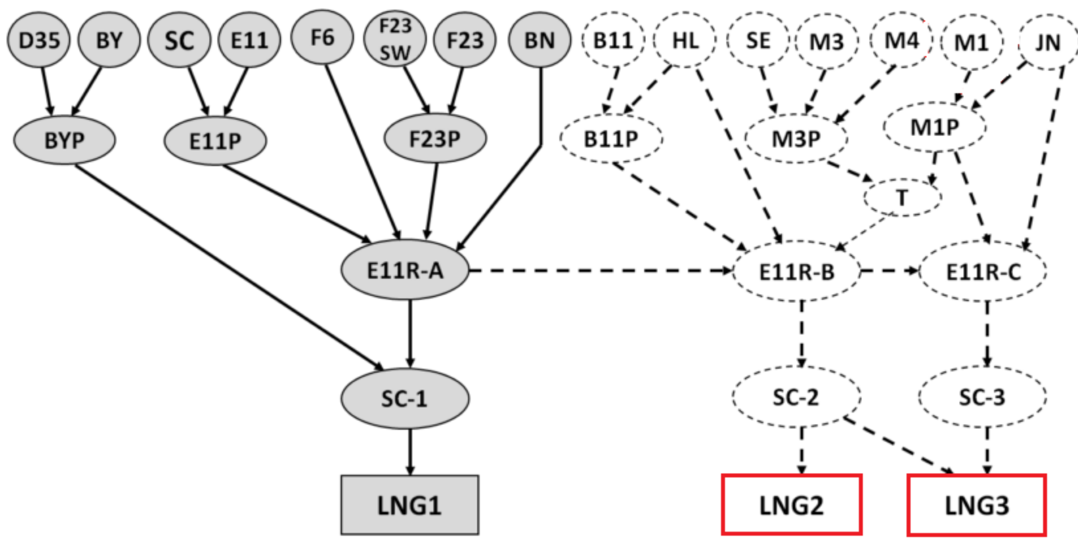
Scalable Bounds Tightening Techniques



$$
\begin{aligned}
z^{j,\mathrm{lo}} = \max_{h\in\{1,\cdots,s\}} \min_{x_h, y, z_h} \ & z_h^j \\
\text{s.t. } & g_h^{\mathrm{cv}}(x_h, y, z_h) \le 0, \\
& x_h \in \mathrm{conv}(X_h), \\
& y \in Y, \ z_h \in Z.
\end{aligned}
$$

Computational Study

Sarawak Gas Production System



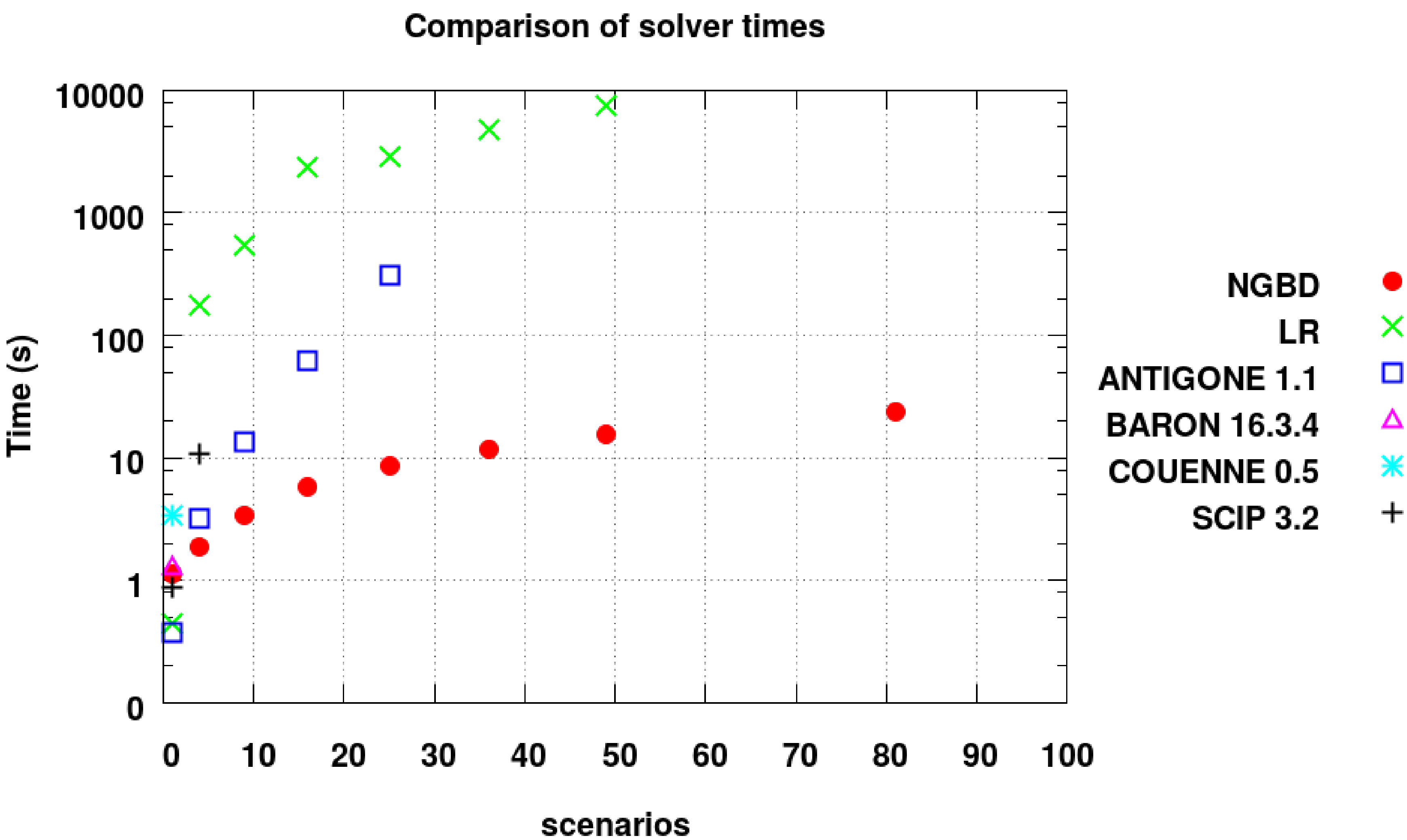
38 binary first-stage variables,
0 continuous first-stage variables,
93s continuous second-stage variables,
34s bilinear terms.

(s denotes the number of scenarios)

Li, X. et al., AIChE Journal, 2011.

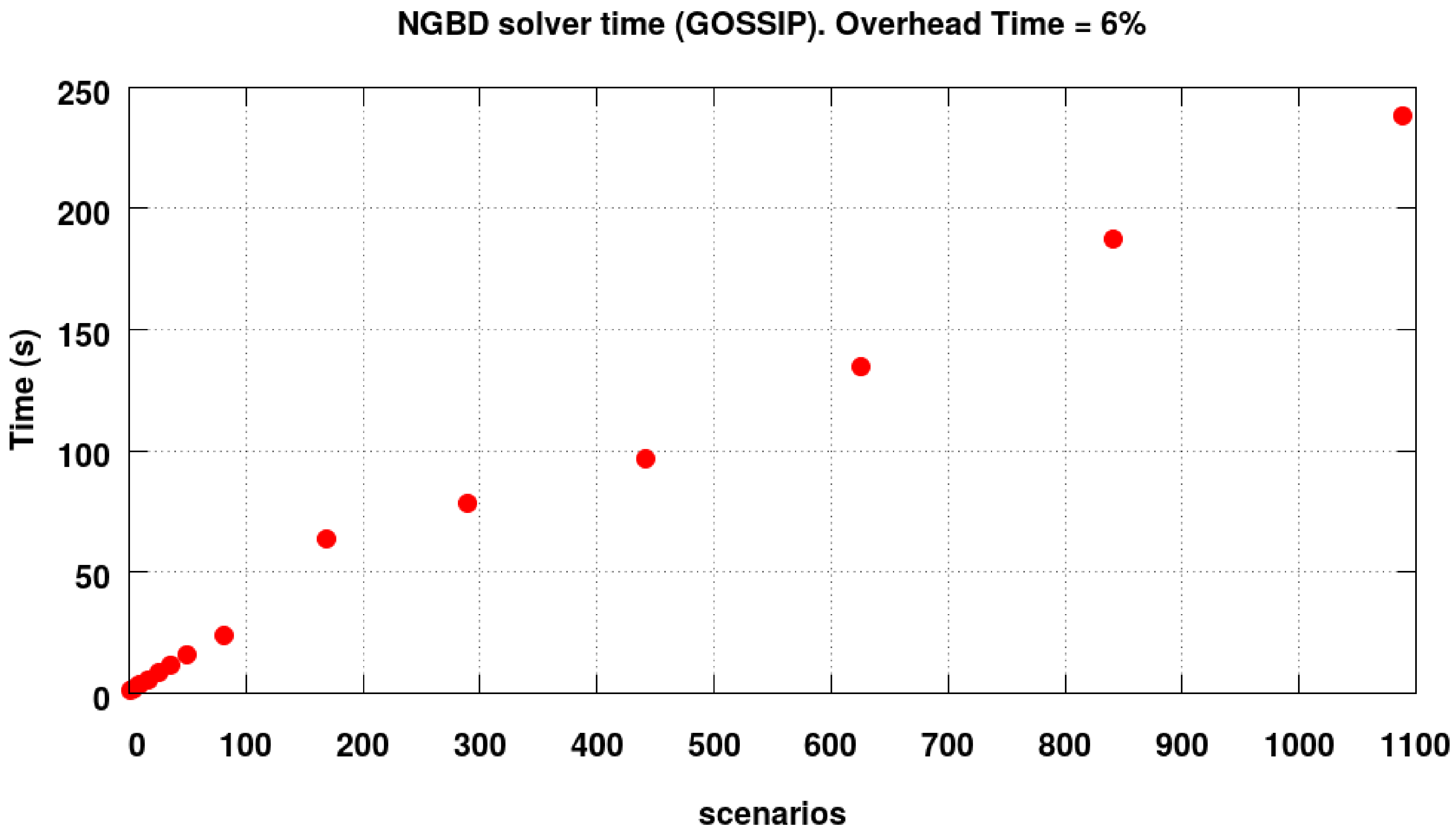
Computational Study

Sarawak Gas Production System

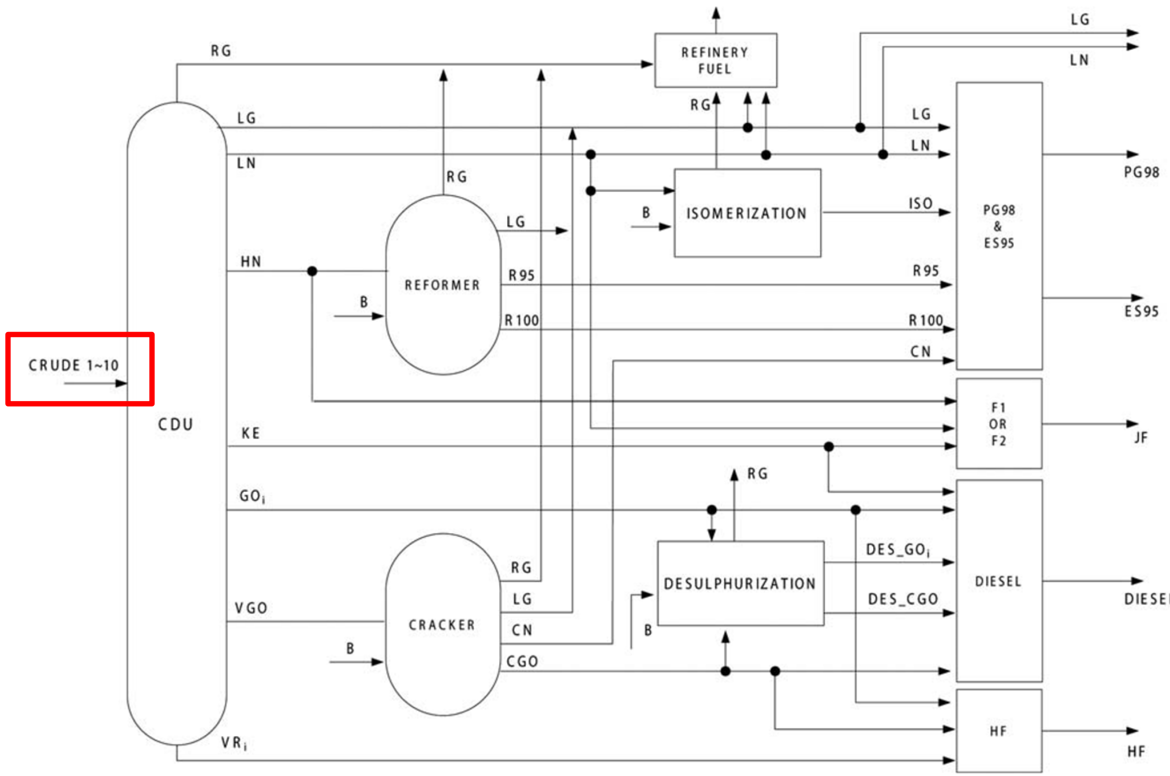


Absolute Tolerance: 1E-09, Relative Tolerance: 1E-03, Time Limit: 10,000 seconds

Computational Study
Sarawak Gas Production System



Computational Study
Refinery Model

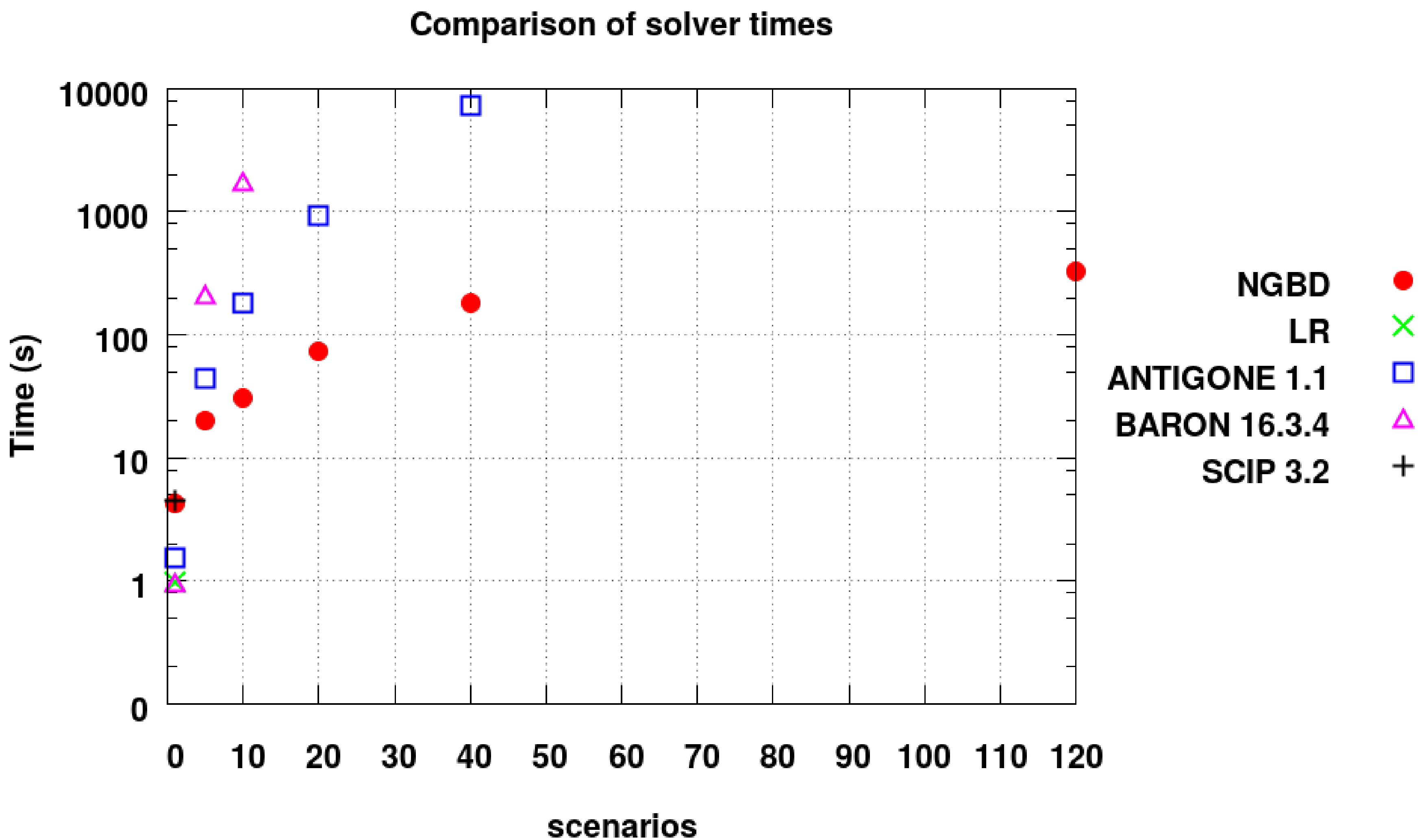


100 binary first-stage variables,
0 continuous first-stage variables,
122s continuous second-stage variables,
26s bilinear terms.

(s denotes the number of scenarios)

Yang, Y. et al., AIChE Journal, 2016.

Computational Study
Refinery Model



Absolute Tolerance: 1E-09, Relative Tolerance: 1E-03, Time Limit: 10,000 seconds

Computational Study
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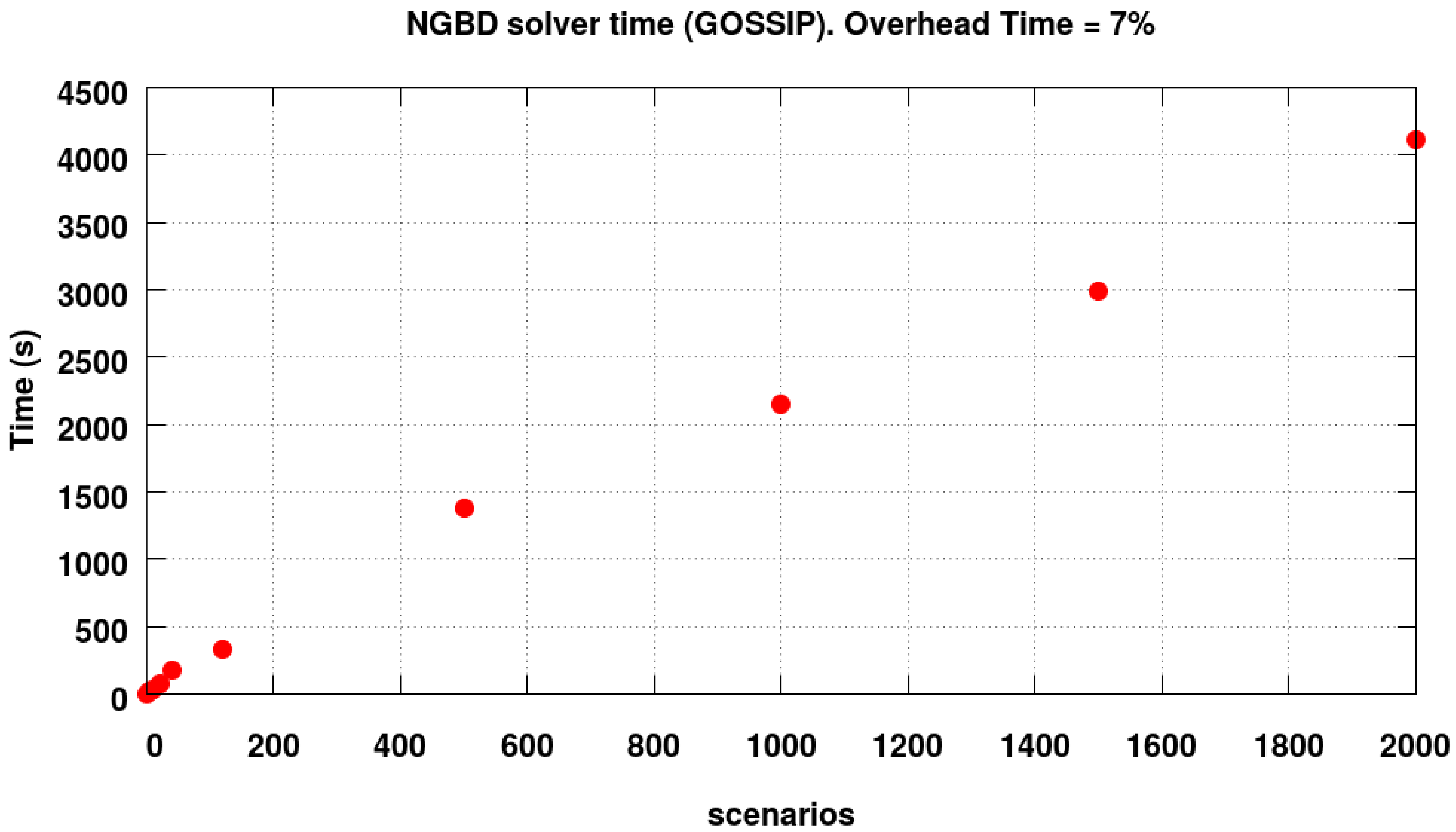
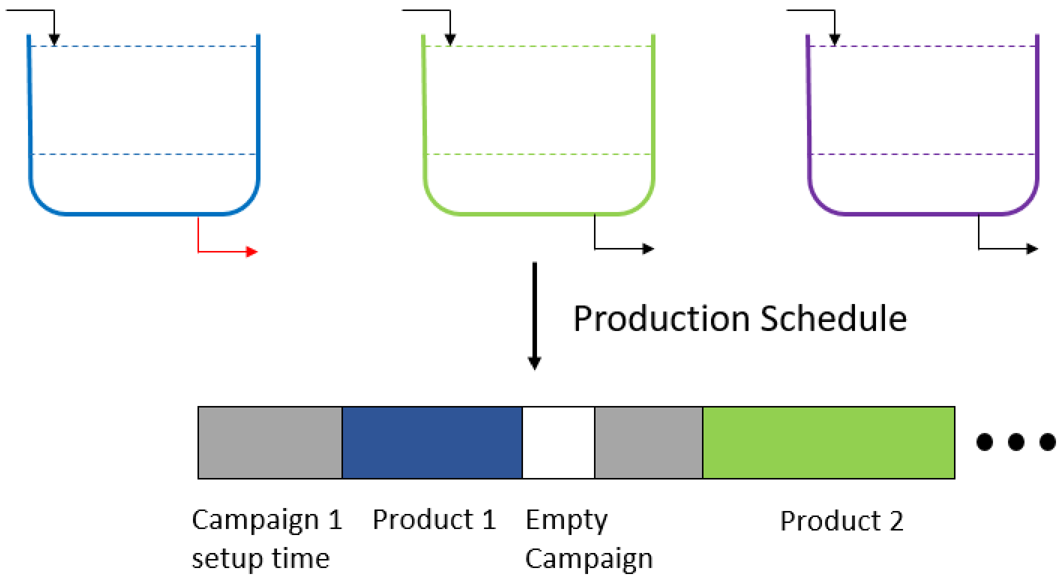


Computational Study

Tank Sizing Problem



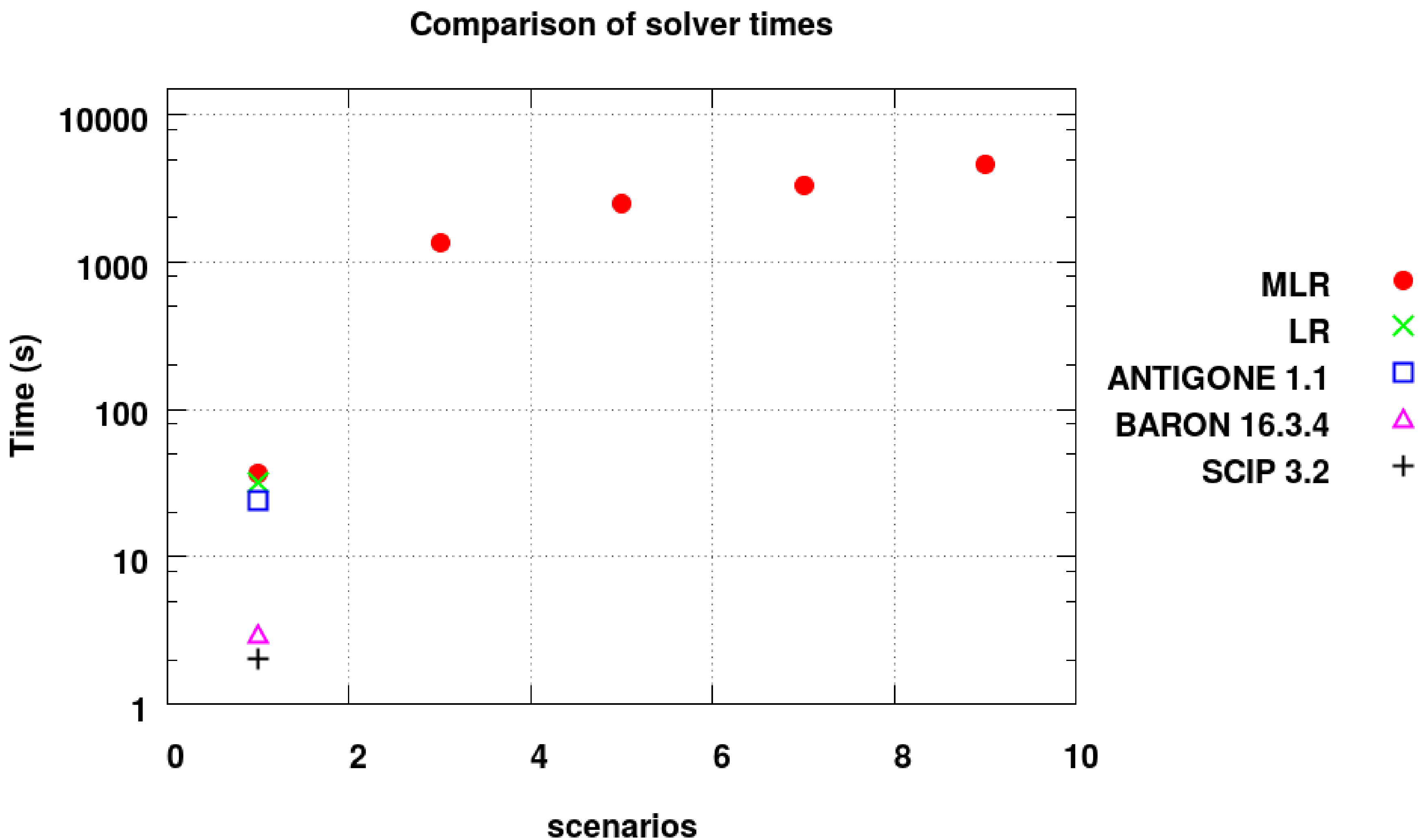
0 binary first-stage variables,
3 continuous first-stage variables,
9s binary second-stage variables,
38s continuous second-stage variables,
3 signomial terms,
47s bilinear terms.

(s denotes the number of scenarios)

Rebennack, S. et al., Comput. Chem. Eng., 2011.

Computational Study

Tank Sizing Problem



Absolute Tolerance: 1E-09, Relative Tolerance: 1E-03, Time Limit: 10,000 seconds

Computational Study
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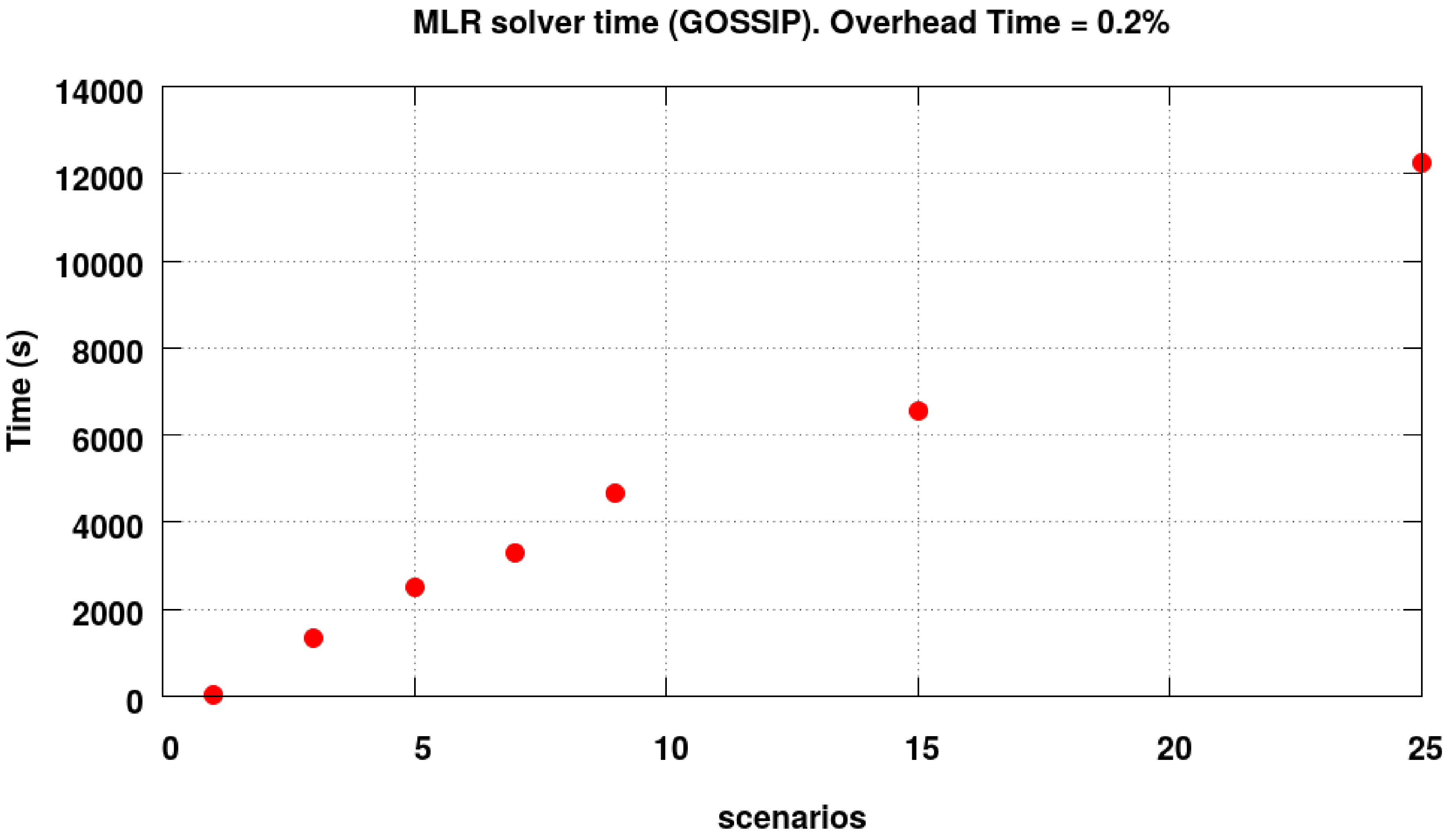


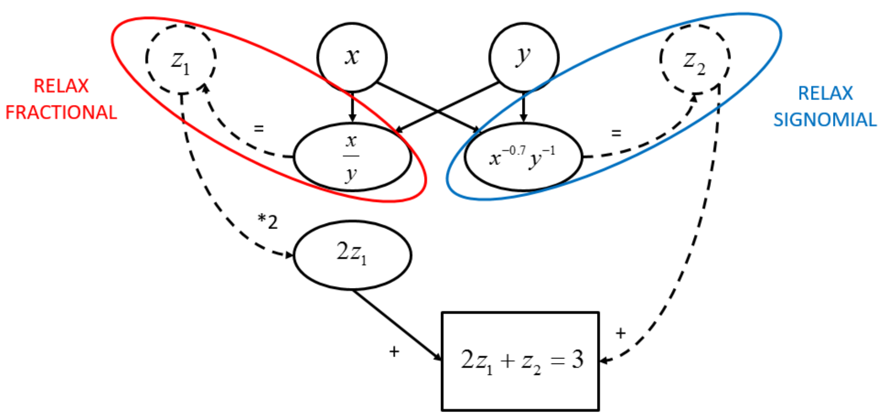
Summary of Part 1

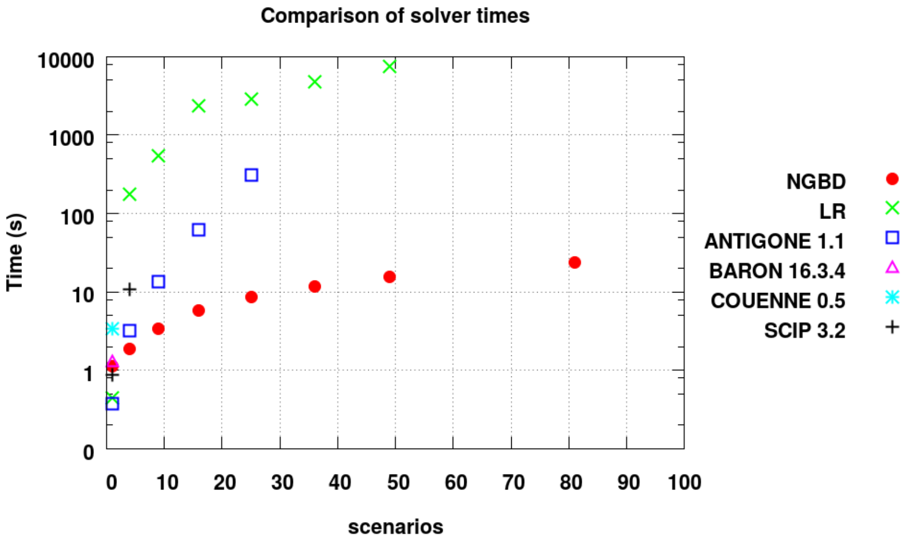
Inner minimization can be solved in a decomposable manner using NGBD

$$\sup_{\lambda_1,\cdots,\lambda_{s-1}} \boxed{\begin{aligned} \min_{\substack{x_1,\cdots,x_s,\\ y,z_1,\cdots,z_s}} \; & \sum_{h=1}^{s} p_h f_h(x_h,y,z_h) + \sum_{h=1}^{s-1} \lambda_h^T (z_h - z_{h+1}) \\ \text{s.t. } & g_h(x_h,y,z_h) \le 0, \; \forall h \in \{1,\cdots,s\}, \\ & x_h \in X_h, \; z_h \in Z, \; \forall h \in \{1,\cdots,s\}, \\ & y \in Y. \end{aligned}}$$

The branch-and-bound procedure can be accelerated using decomposable bounds tightening techniques

$$z^{j,\mathrm{lo}} = \max_{h\in\{1,\cdots,s\}} \boxed{\begin{aligned} \min_{x_h,y,z_h} \; & z_h^j \\ \text{s.t. } & g_h^{\mathrm{cv}}(x_h,y,z_h) \le 0, \\ & x_h \in \mathrm{conv}(X_h), \\ & y \in Y, \; z_h \in Z. \end{aligned}}$$

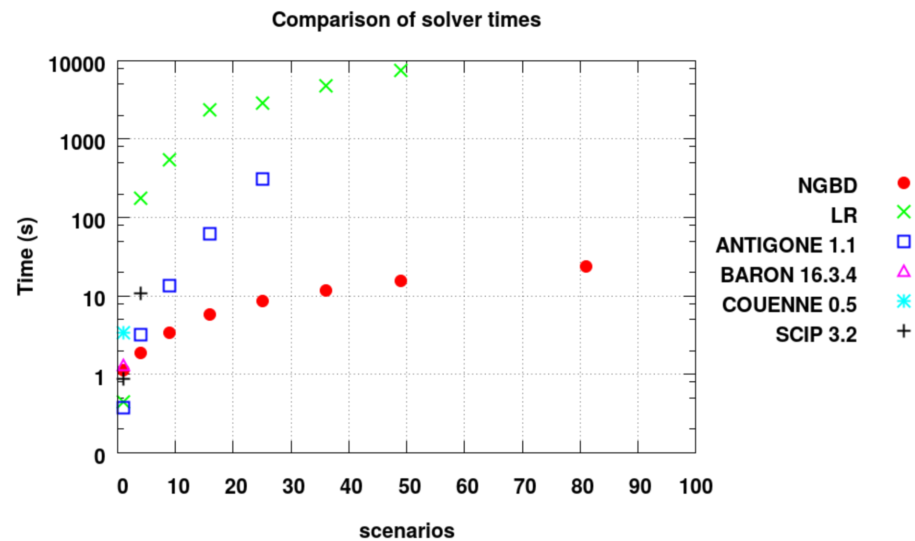


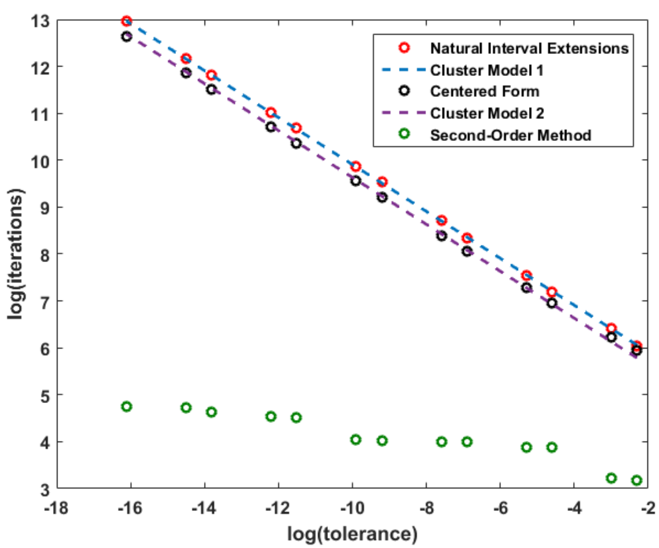


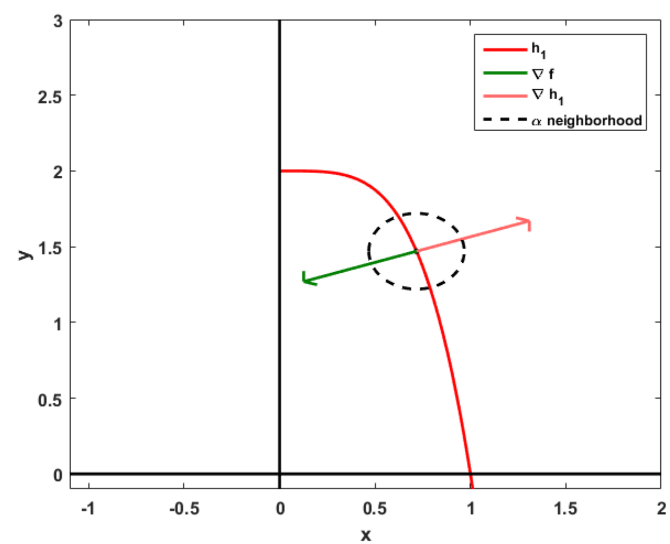
Outline

Inner minimization can be solved in a decomposable manner using NGBD

$$\sup_{\lambda_1,\cdots,\lambda_{s-1}} \boxed{\begin{aligned} &\min_{\substack{x_1,\cdots,x_s,\\ y,z_1,\cdots,z_s}} \sum_{h=1}^{s} p_h f_h(x_h,y,z_h) + \sum_{h=1}^{s-1} \lambda_h^T (z_h - z_{h+1}) \\ &\text{s.t. } g_h(x_h,y,z_h) \le 0, \ \forall h \in \{1,\cdots,s\}, \\ &\quad x_h \in X_h, \ z_h \in Z, \ \forall h \in \{1,\cdots,s\}, \\ &\quad y \in Y. \end{aligned}}$$







Outline

- Part 2: Theoretical Analysis of the Convergence Rate of Branch-and-Bound Algorithms
  - Analysis of the cluster problem in constrained optimization
  - Theory of convergence order for branch-and-bound algorithms for constrained optimization
  - An application of the above analyses through a case study

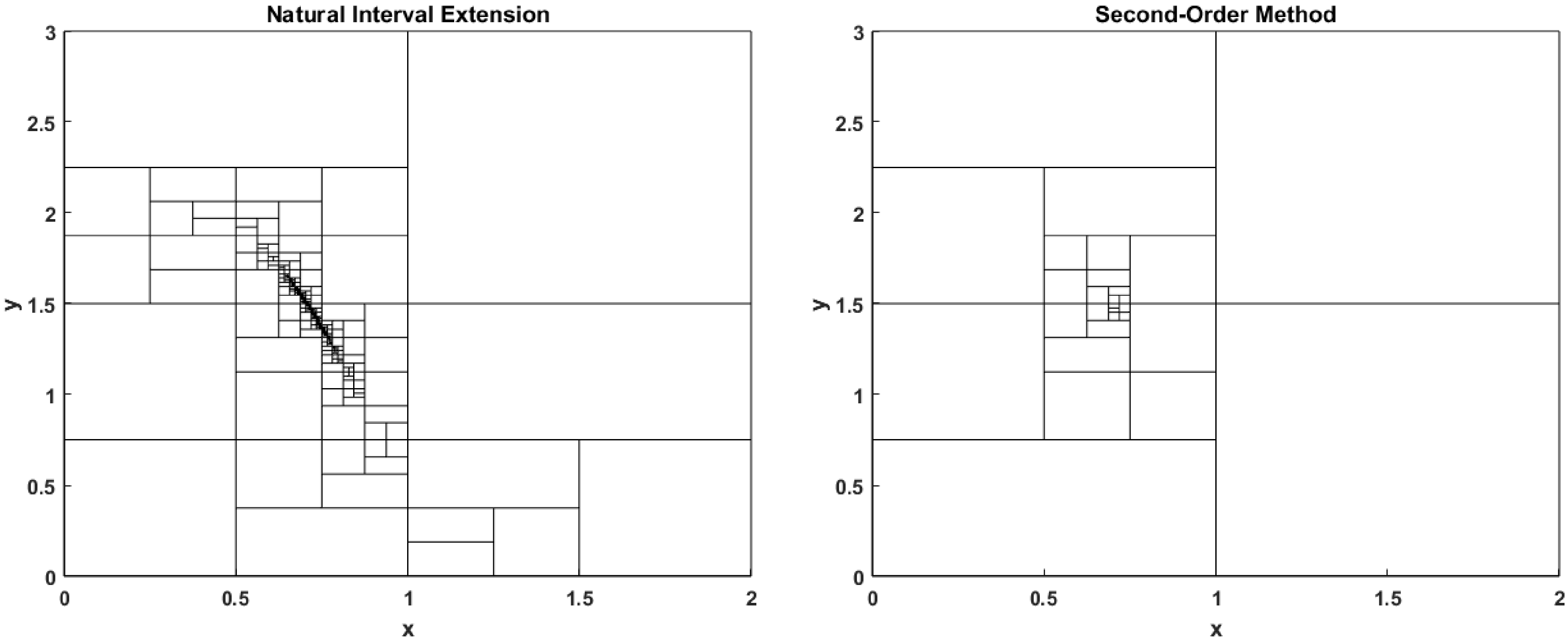
Motivation

Cluster Problem in Constrained Optimization

$$\min_{x,y}\ y^2 - 12x - 7y$$

$$\text{s.t. } y + 2x^4 - 2 = 0,$$

$$x \in [0,2],\ y \in [0,3].$$



Motivation

Cluster Problem in Constrained Optimization

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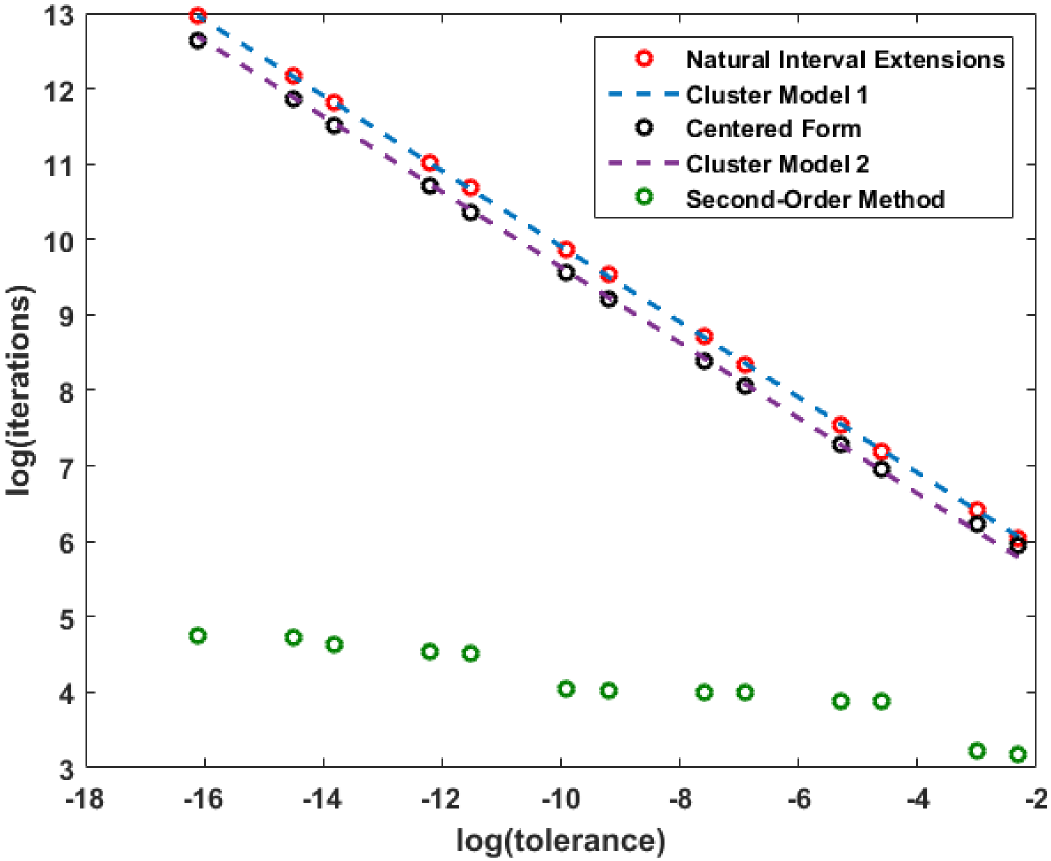
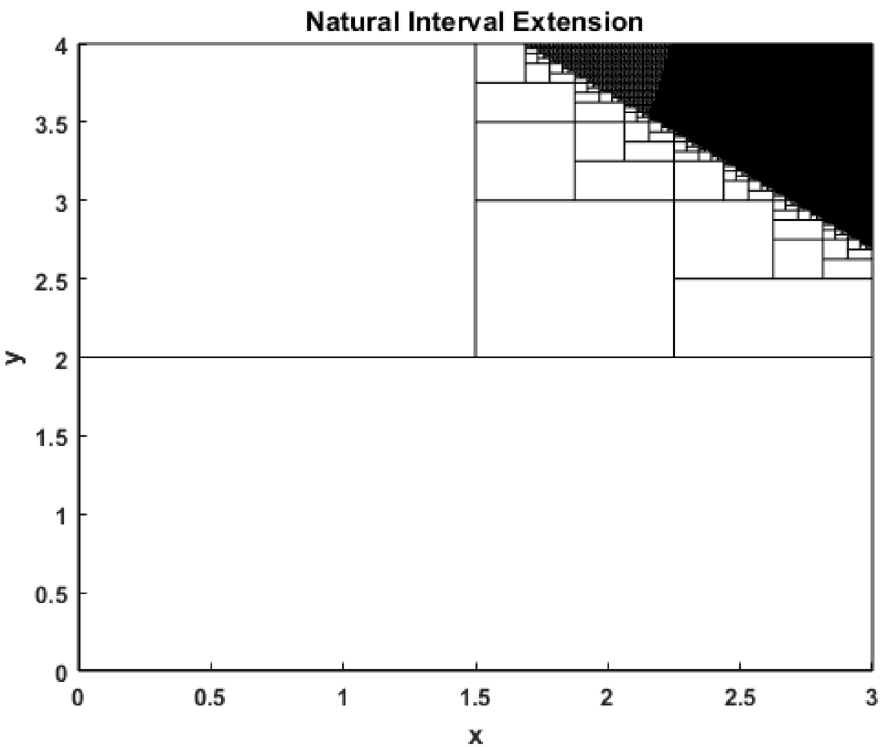
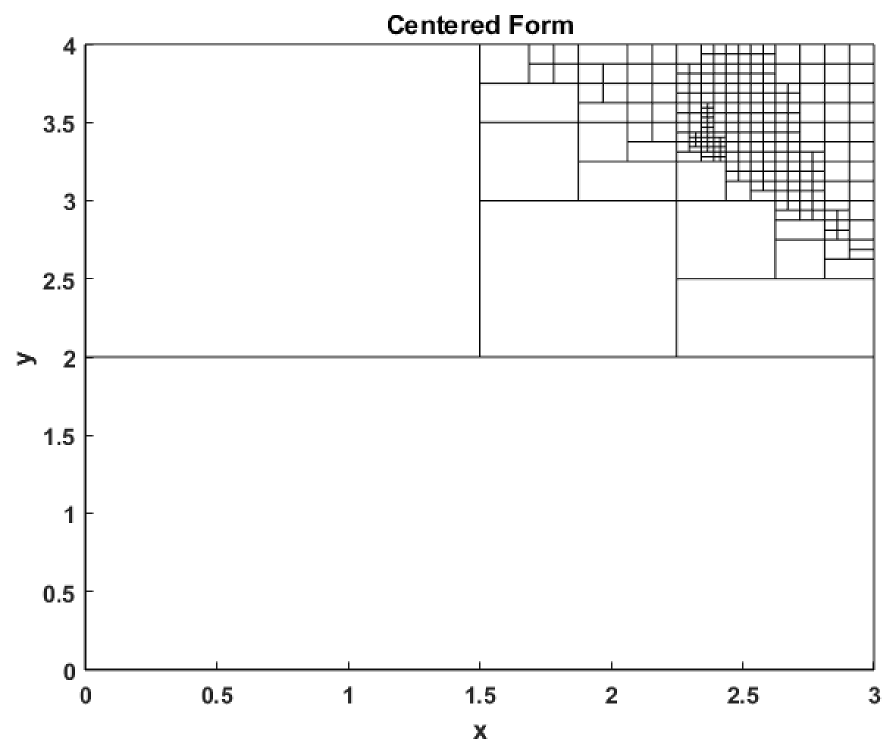


Motivation

Cluster Problem in Constrained Optimization

$$
\begin{aligned}
\min_{x,y} \quad & -x - y \\
\text{s.t.} \quad & y \le 2 + 2x^4 - 8x^3 + 8x^2, \\
& y \le 4x^4 - 32x^3 + 88x^2 - 96x + 36, \\
& x \in [0,3],\ y \in [0,4].
\end{aligned}
$$

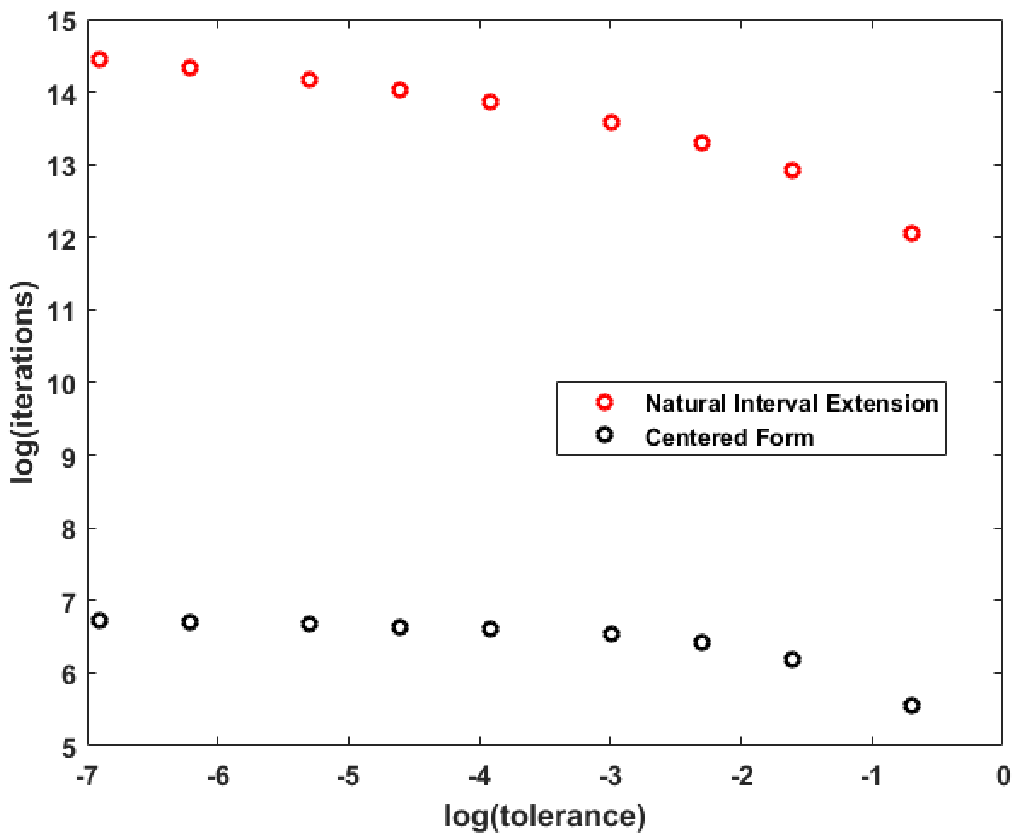




Motivation

Cluster Problem in Constrained Optimization

$$\min_{x,y} \; -x-y$$
$$\text{s.t. } y \le 2+2x^4-8x^3+8x^2,$$
$$y \le 4x^4-32x^3+88x^2-96x+36,$$
$$x\in[0,3],\; y\in[0,4].$$



The Cluster Problem Formulation

$$\begin{aligned} \min_{x \in X \subset \mathbb{R}^n} \ & f(x) \\ \text{s.t.} \ & g(x) \leq 0, \\ & h(x) = 0. \end{aligned}$$

The Cluster Problem Formulation

$$\min_{x \in X \subset \mathbb{R}^n} \; f(x)$$
$$\text{s.t.} \;\; g(x) \leq 0,$$
$$h(x) = 0.$$

- Assume that*:
  - The branch-and-bound algorithm finds an optimal solution early on in the branch-and-bound tree
  - The termination tolerance $\varepsilon \ll 1$

* We additionally assume that X is nonempty, open, bounded, and convex, and the functions f, g, and h are sufficiently smooth on X.

The Cluster Problem Formulation

$$\min_{x \in X \subset \mathbb{R}^n} f(x)$$
$$\text{s.t. } g(x) \leq 0,$$
$$h(x) = 0.$$

- Assume that*:
  - The branch-and-bound algorithm finds an optimal solution early on in the branch-and-bound tree
  - The termination tolerance $\varepsilon \ll 1$

- We wish to estimate the dependence of the number of boxes visited by the branch-and-bound algorithm** in a neighborhood of a global minimizer on the termination tolerance ε
  - Will help explain the computational results for the motivating examples

* We additionally assume that X is nonempty, open, bounded, and convex, and the functions f, g, and h are sufficiently smooth on X.

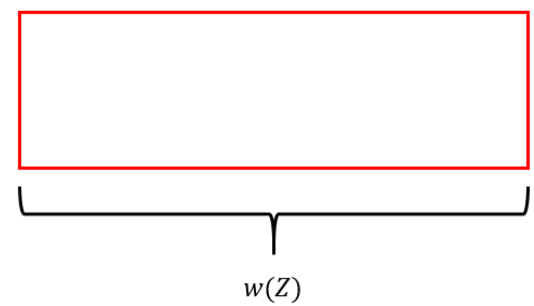
** In the worst case

Definitions

◆ Width of an interval

Let $Z = [z_1^{\mathrm{L}}, z_1^{\mathrm{U}}] \times \cdots \times [z_n^{\mathrm{L}}, z_n^{\mathrm{U}}] \in \mathbb{IR}^n$.

The width of Z is given by $w(Z) = \max\limits_{i=1,\cdots,n} (z_i^{\mathrm{U}} - z_i^{\mathrm{L}})$.



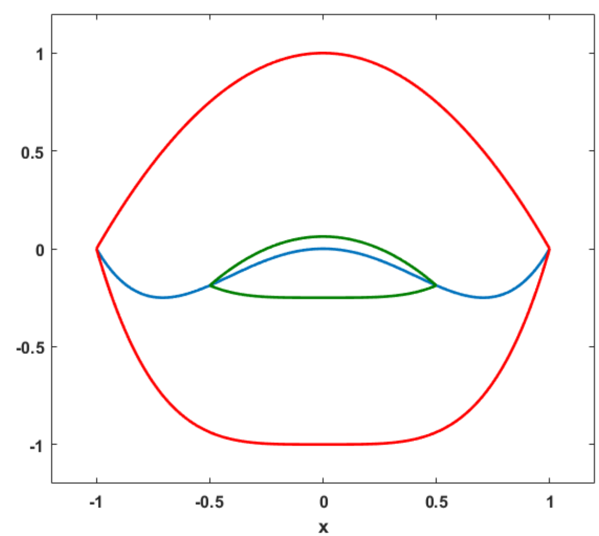
◆ Schemes of relaxations

Nonempty, bounded set $X \subset \mathbb{R}^n$, function $h : X \to \mathbb{R}$.

For each interval $Z \in \mathbb{I}X$, define convex relaxation $h_Z^{\mathrm{cv}} : Z \to \mathbb{R}$, concave relaxation $h_Z^{\mathrm{cc}} : Z \to \mathbb{R}$.

$\left(h_Z^{\mathrm{cv}}\right)\Big|_{Z \in \mathbb{I}X}$ defines a scheme of convex relaxations of h in X.

$\left(h_Z^{\mathrm{cc}}\right)\Big|_{Z \in \mathbb{I}X}$ defines a scheme of concave relaxations of h in X.

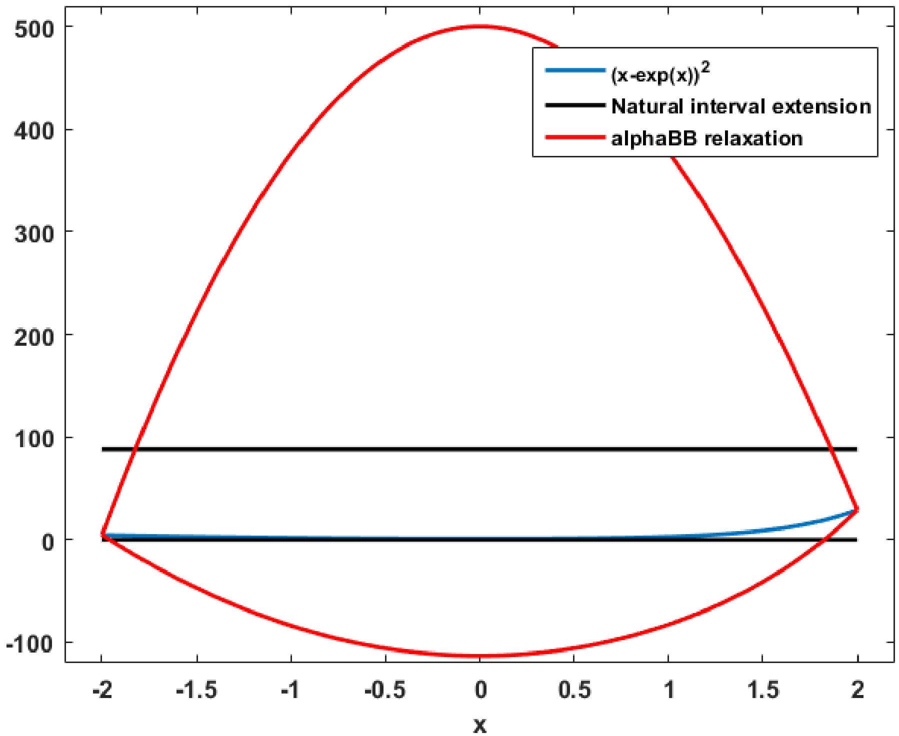


◆ Distance between sets

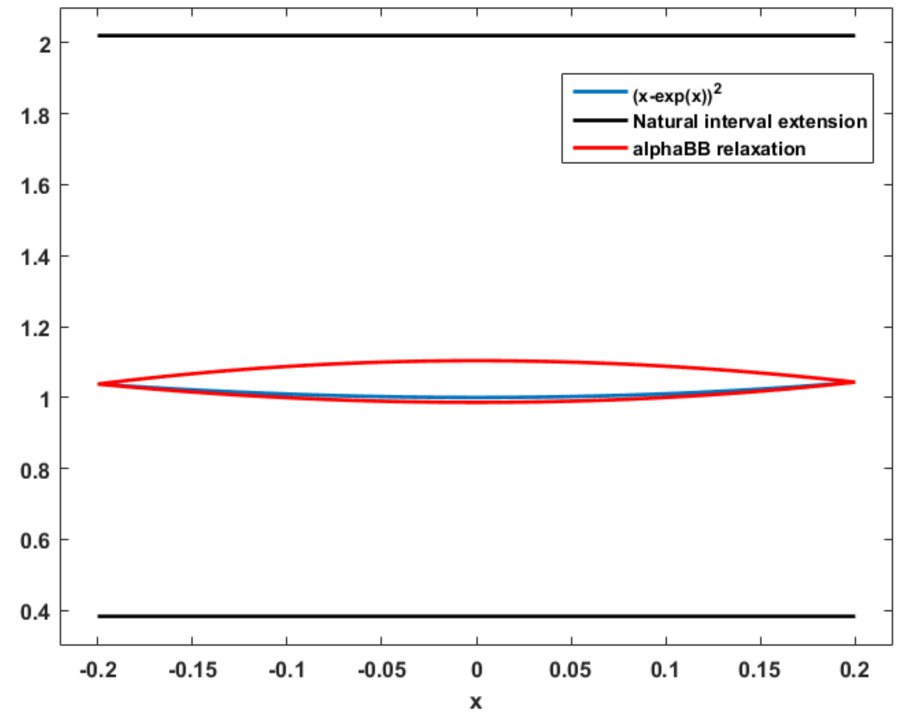
Let $Y, Z \subset \mathbb{R}^n$. The distance between Y and Z is defined as

$$d(Y, Z) := \inf_{\substack{y \in Y, \\ z \in Z}} \|y - z\|.$$

Introduction to Convergence Order



Relaxations on [-2,2]



Relaxations on [-0.2,0.2]

Convergence Order

Convex relaxation-based scheme

Original Problem
with x restricted to Z

$$\min_{x \in Z} f(x)$$
$$\text{s.t. } g(x) \le 0,$$
$$h(x) = 0.$$

Convex relaxation-based
lower bounding problem on Z

$$\mathcal{O}(Z) := \min_{x \in Z} f_Z^{\text{cv}}(x)$$
$$\text{s.t. } g_Z^{\text{cv}}(x) \le 0,$$
$$h_Z^{\text{cv}}(x) \le 0, \quad h_Z^{\text{cc}}(x) \ge 0.$$

$$\mathcal{F}(Z) := \left\{ x \in Z : g(x) \le 0, h(x) = 0 \right\}$$

$$\mathcal{F}^{\text{cv}}(Z) := \left\{ x \in Z : g_Z^{\text{cv}}(x) \le 0, h_Z^{\text{cv}}(x) \le 0, h_Z^{\text{cc}}(x) \ge 0 \right\}$$

Convergence Order

Convex relaxation-based scheme

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$$\min_{x \in Z} f(x)$$
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$$\mathcal{F}^{\text{cv}}(Z) := \{x \in Z : g_Z^{\text{cv}}(x) \leq 0, h_Z^{\text{cv}}(x) \leq 0, h_Z^{\text{cc}}(x) \geq 0\}$$

$$\mathcal{I}_C(Z) := \left\{(v, w) \in \mathbb{R}^{m_I} \times \mathbb{R}^{m_E} : v = g_Z^{\text{cv}}(x), h_Z^{\text{cv}}(x) \leq w \leq h_Z^{\text{cc}}(x) \text{ for some } x \in Z\right\}.$$

The convex relaxation-based lower bounding problem on Z is feasible if and only if $\mathcal{I}_C(Z) \cap \left(\mathbb{R}_-^{m_I} \times \{0_{m_E}\}\right) \neq \varnothing$

$(\mathcal{O}(Z))\big|_{Z \in \mathbb{I}X}$: scheme of lower bounds.

$(\mathcal{I}_C(Z))\big|_{Z \in \mathbb{I}X}$: scheme that determines feasibility of the lower bounding problem on Z.

Convergence Order
Convex relaxation-based scheme

The lower bounding scheme is said to have convergence of order $\beta > 0$ at

1. a feasible point $x \in X$ if $\exists \tau \geq 0$ s.t. $\forall Z \in \mathbb{I}X$ with $x \in Z$,

$$\min_{z \in \mathcal{F}(Z)} f(z) - \min_{z \in \mathcal{F}^{\mathrm{cv}}(Z)} f_Z^{\mathrm{cv}}(z) \leq \tau w(Z)^{\beta}.$$

2. an infeasible point $x \in X$ if $\exists \overline{\tau} \geq 0$ s.t. $\forall Z \in \mathbb{I}X$ with $x \in Z$,

$$d\left(\overline{\begin{bmatrix} g \\ h \end{bmatrix}}(Z), \mathbb{R}_-^{m_I} \times \{0\}\right) - d\left(\mathcal{I}_C(Z), \mathbb{R}_-^{m_I} \times \{0\}\right) \leq \overline{\tau} w(Z)^{\beta}.$$

Convergence Order

Convex relaxation-based scheme

The lower bounding scheme is said to have convergence of order $\beta > 0$ at

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"The lower bound has to converge to the minimum objective value with order at least β"

2. an infeasible point $x \in X$ if $\exists \overline{\tau} \geq 0$ s.t. $\forall Z \in \mathbb{I}X$ with $x \in Z$,

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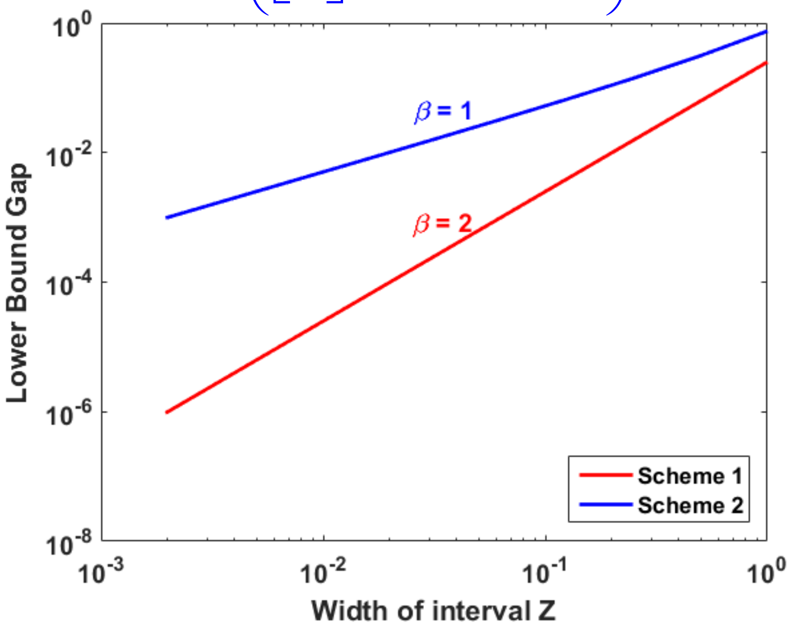

Convergence Order
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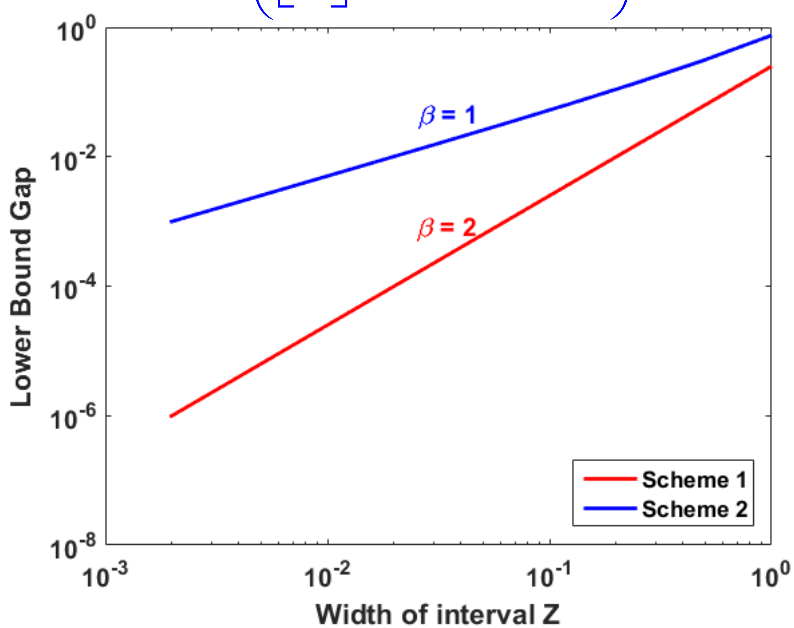
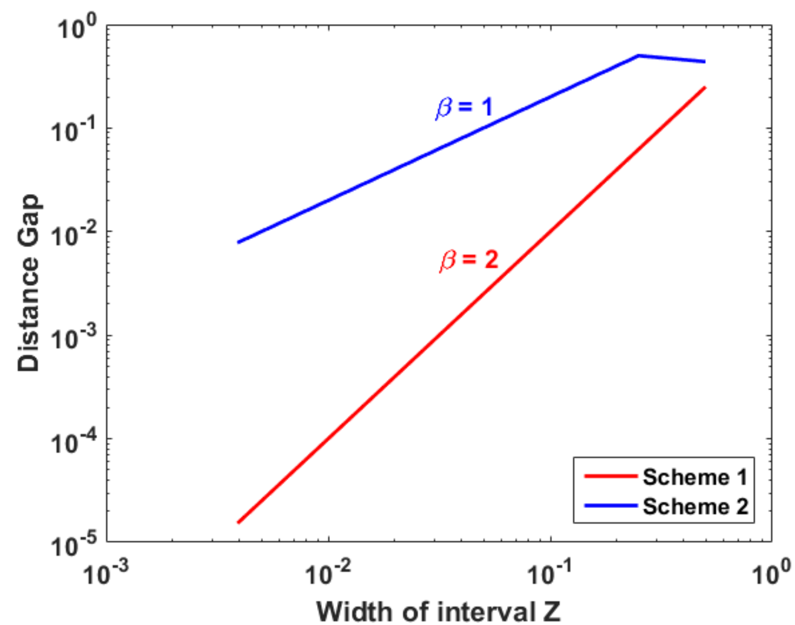
$$d\left(\overline{\begin{bmatrix} g \\ h \end{bmatrix}}(Z), \mathbb{R}_-^{m_I} \times \{0\}\right) - d\left(\mathcal{I}_C(Z), \mathbb{R}_-^{m_I} \times \{0\}\right) \leq \overline{\tau} w(Z)^{\beta}.$$

"The image of constraint relaxations has to converge (in distance) to the image of the true constraints with order at least β"





The Cluster Problem in Constrained Global Optimization

Suppose the lower bounding scheme

1. has convergence of order $\beta^* > 0$ at feasible points with a prefactor $\tau^* > 0$
2. has convergence of order $\beta^{\mathrm{I}} > 0$ at infeasible points with a prefactor $\tau^{\mathrm{I}} > 0$

Partition X into regions $X_1, \cdots, X_5$ such that

X_1 : points that are "quite infeasible"

X_2 : points that are "nearly feasible" but have "poor objective value"

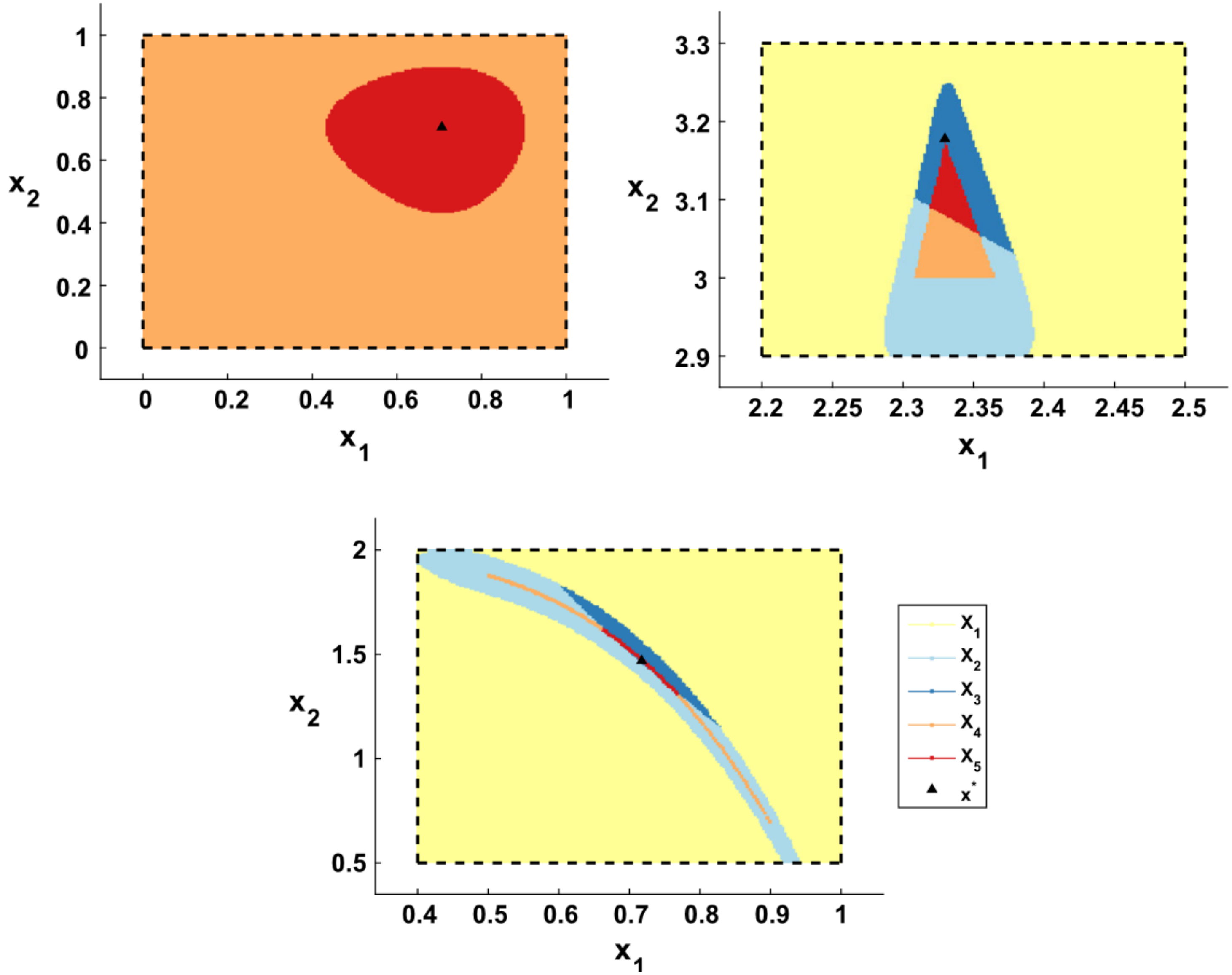
X_3 : points that are "nearly feasible" and have "good objective value"

X_4 : points that are feasible but "quite suboptimal"

X_5 : points that are feasible and "nearly optimal"

The precise definition of these regions depends on the termination tolerance ε

The Cluster Problem in Constrained Global Optimization

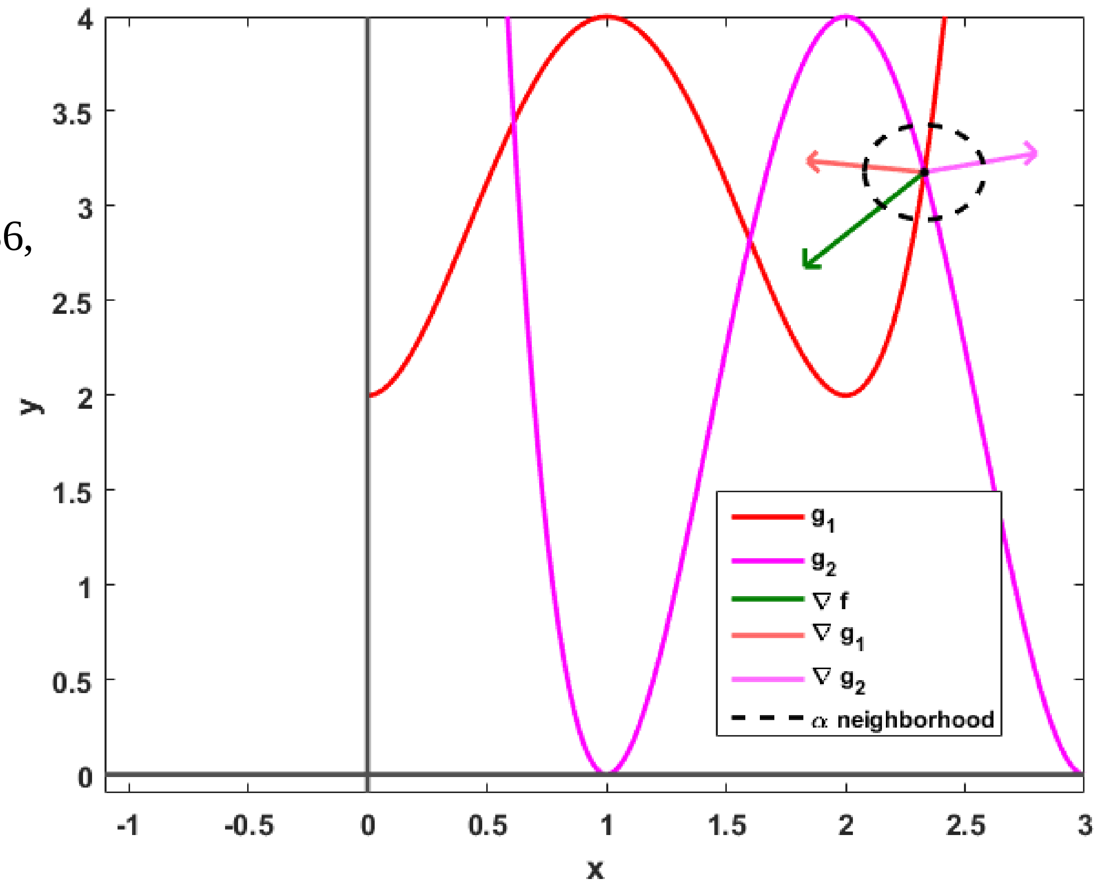


When first-order convergence is sufficient to avoid the cluster problem on X_5

$X_5 = \{x \in X \text{ which are feasible and "nearly optimal"}\}.$

The inner product of the objective gradient with any unit norm direction from x^* that locally leads to feasible points must be strictly positive

$$\min_{x,y} \; -x-y$$
$$\text{s.t. } y \le 2+2x^4-8x^3+8x^2,$$
$$y \le 4x^4-32x^3+88x^2-96x+36,$$
$$x \in [0,3],\; y \in [0,4].$$

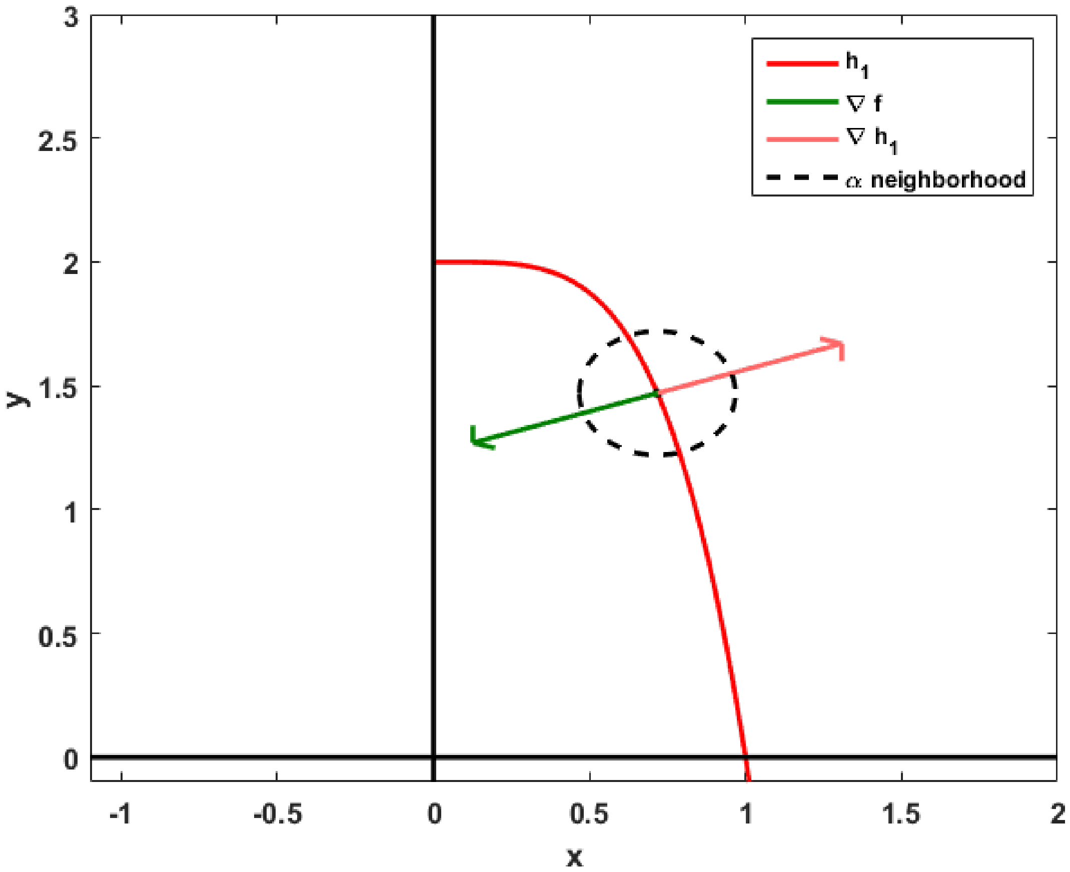


When first-order convergence is NOT sufficient to avoid the cluster problem on X_5

$X_5 = \{x \in X \text{ which are feasible and "nearly optimal"}\}$.

The inner product of the objective gradient with any unit norm direction from x^* that locally leads to feasible points must be strictly positive

$$\begin{aligned} \min_{x,y}\ & y^2 - 12x - 7y \\ \text{s.t. }\ & y + 2x^4 - 2 = 0, \\ & x \in [0,2],\ y \in [0,3]. \end{aligned}$$



When first-order convergence is sufficient to avoid the cluster problem on X_3

$X_3 = \{x \in X \text{ which are infeasible but have a "good objective value"}\}.$

For every unit norm direction from x^* that locally leads to infeasible points, either

1. the objective function grows linearly in that direction, or
2. the measure of constraint violation grows linearly in that direction

$$\min_{x,y} \ -x-y$$
$$\text{s.t. } y \le 2+2x^4-8x^3+8x^2,$$
$$y \le 4x^4-32x^3+88x^2-96x+36,$$
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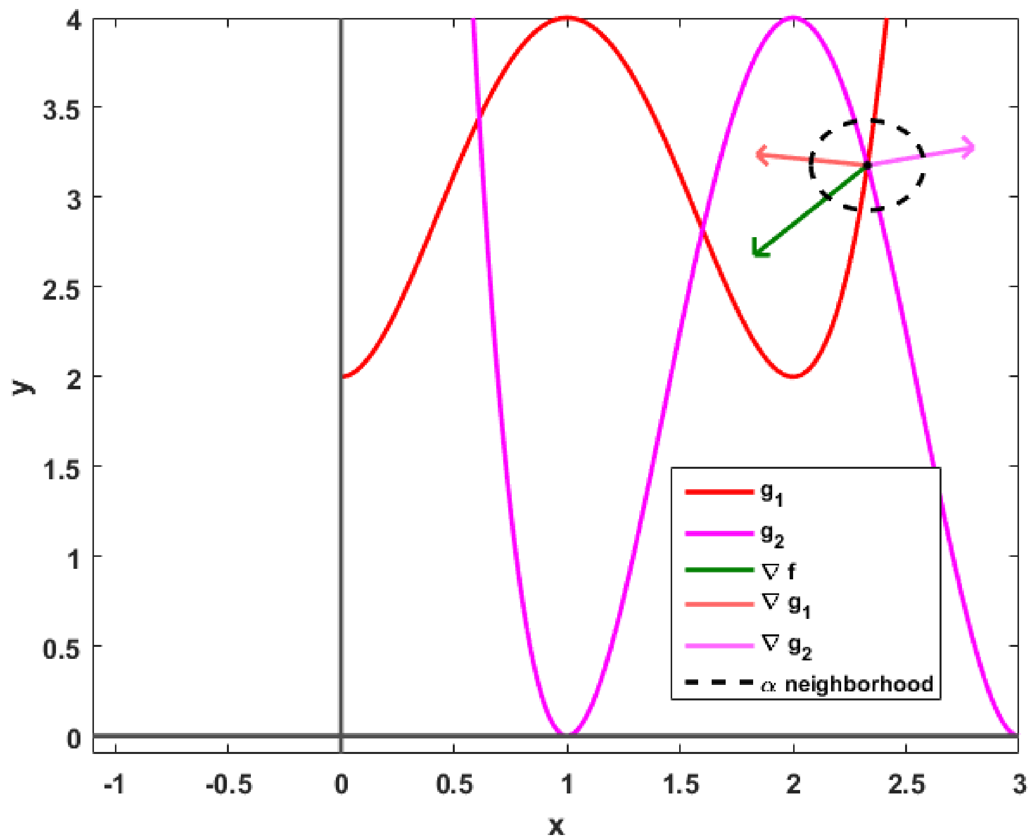

When first-order convergence is NOT sufficient to avoid the cluster problem on X_3

$X_3 = \{x \in X \text{ which are infeasible but have a "good objective value"}\}.$

For every unit norm direction from x^* that locally leads to infeasible points, either

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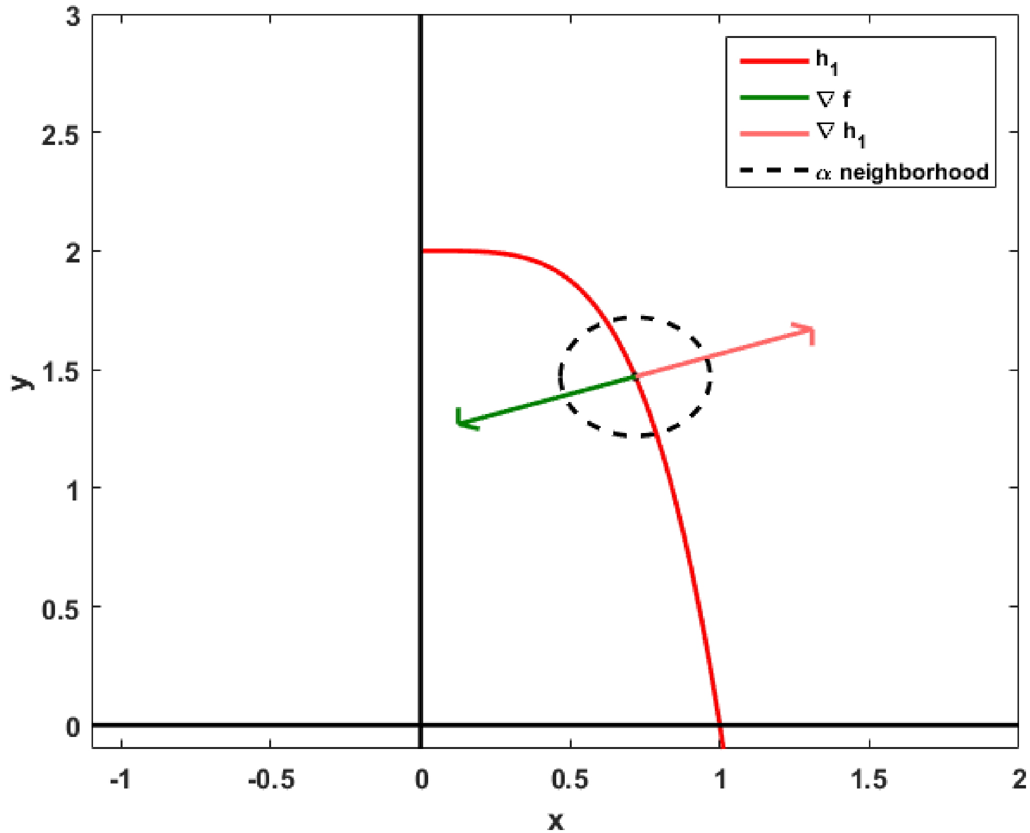
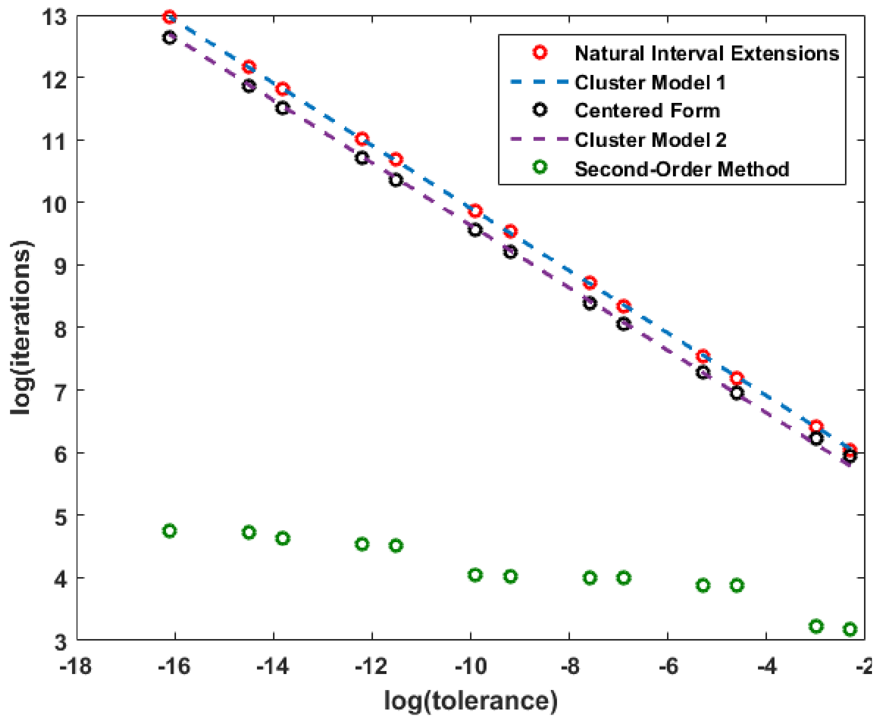
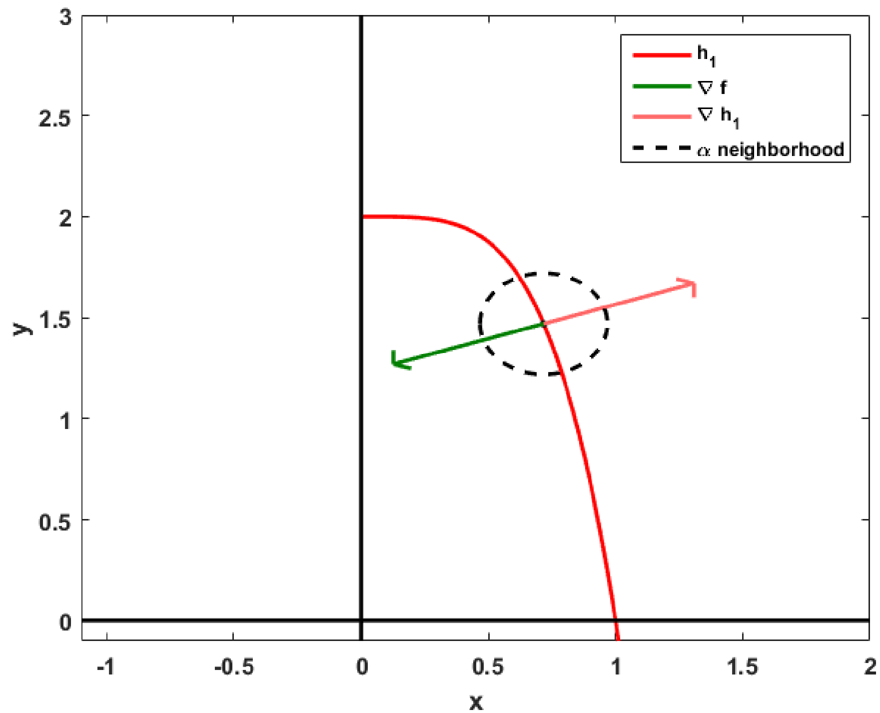


Revisiting the motivating examples

$$\min_{x,y}\ y^2 - 12x - 7y$$
$$\text{s.t.}\ \ y + 2x^4 - 2 = 0,$$
$$x \in [0,2],\ y \in [0,3].$$





Revisiting the motivating examples

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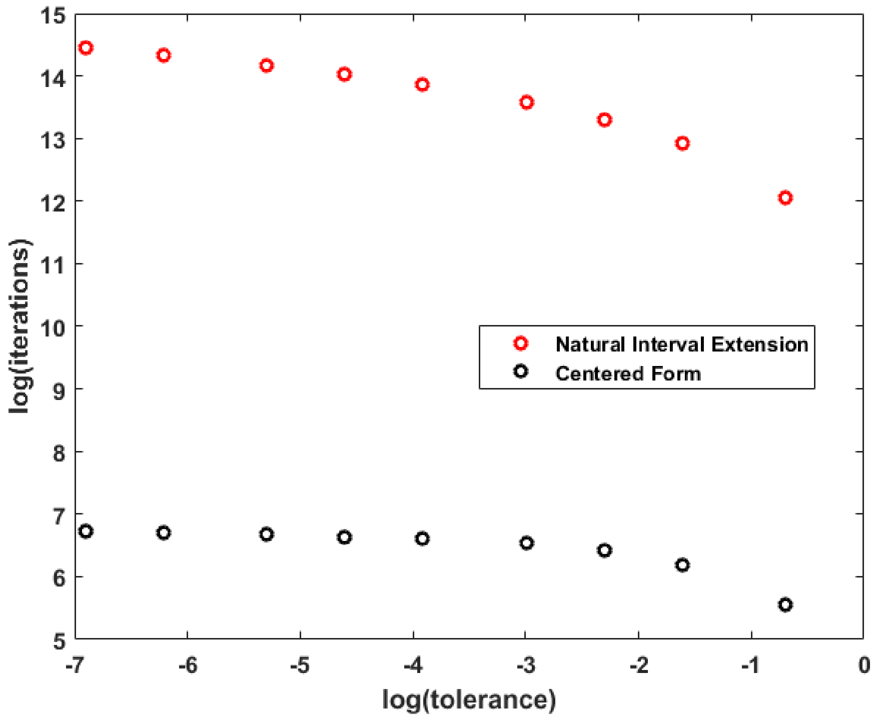
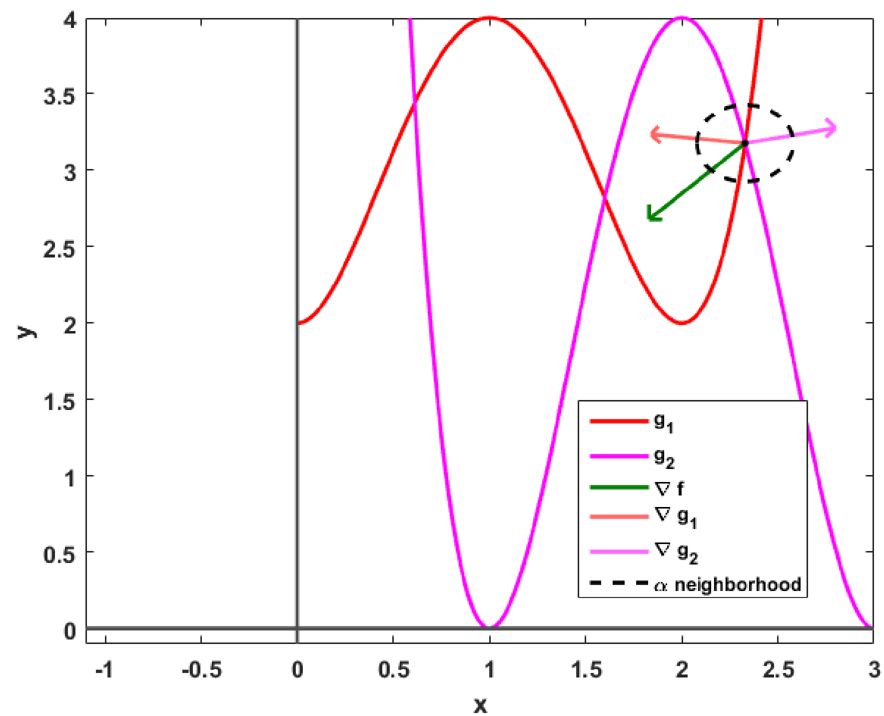




Reduced-space B&B algorithms

Consider the problem

$$\begin{aligned}\min_{x,y}\ & f(x,y) \\ \text{s.t. } & g(x,y) \le 0, \\ & h(x,y) = 0, \\ & x \in X, y \in Y,\end{aligned}$$

where X and Y are nonempty compact convex sets.

Assume

1. f and g are partly convex with respect to x on X, e.g. $x^2 + \exp(x)y^2 + x\sqrt{y} - y^2$
2. h is affine with respect to x on X, e.g. $(\log(y) - y^2 + y^3 + 1)x - y\exp(y^3)$

Epperly and Pistikopoulos proposed a reduced-space branch-and-bound algorithm that requires branching on only the y variables to converge

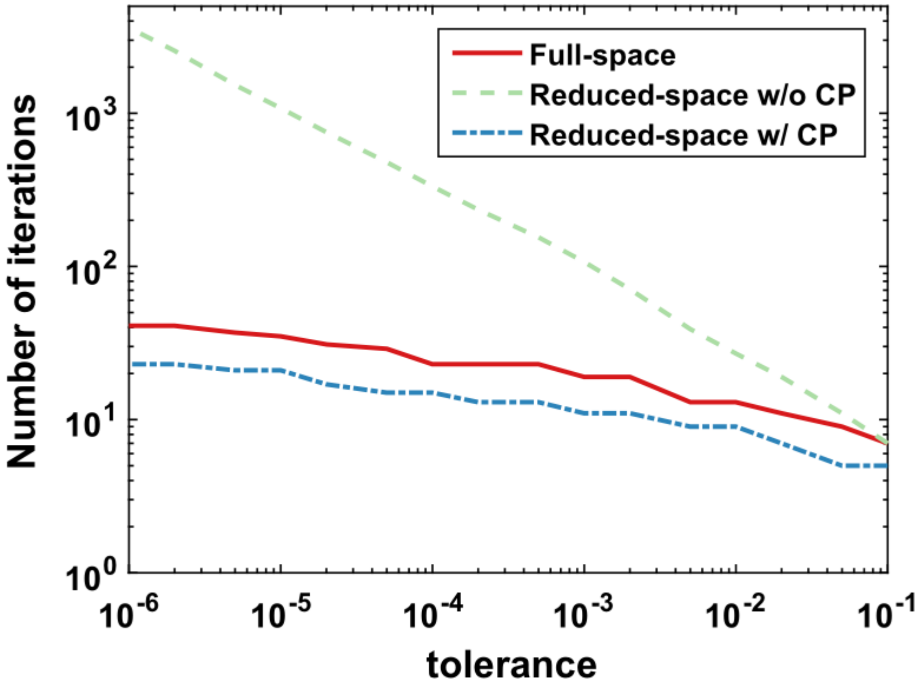
Epperly and Pistikopoulos, J. Global Optim., 1997.

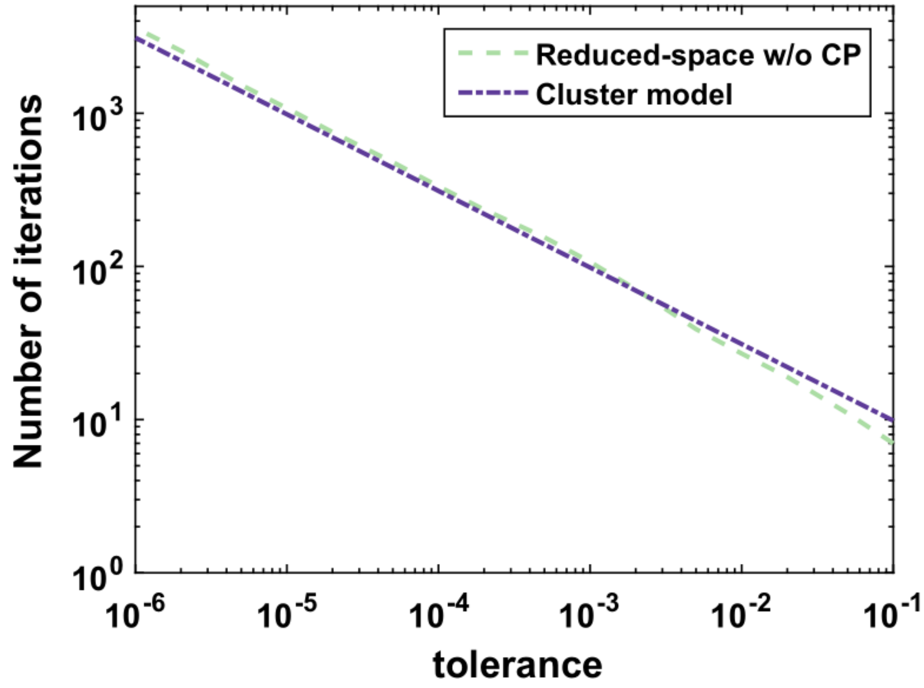
Consequences for Reduced-Space Branch-and-Bound Algorithms

$$\min_{x,y} \ \exp(x) - 4x + y$$

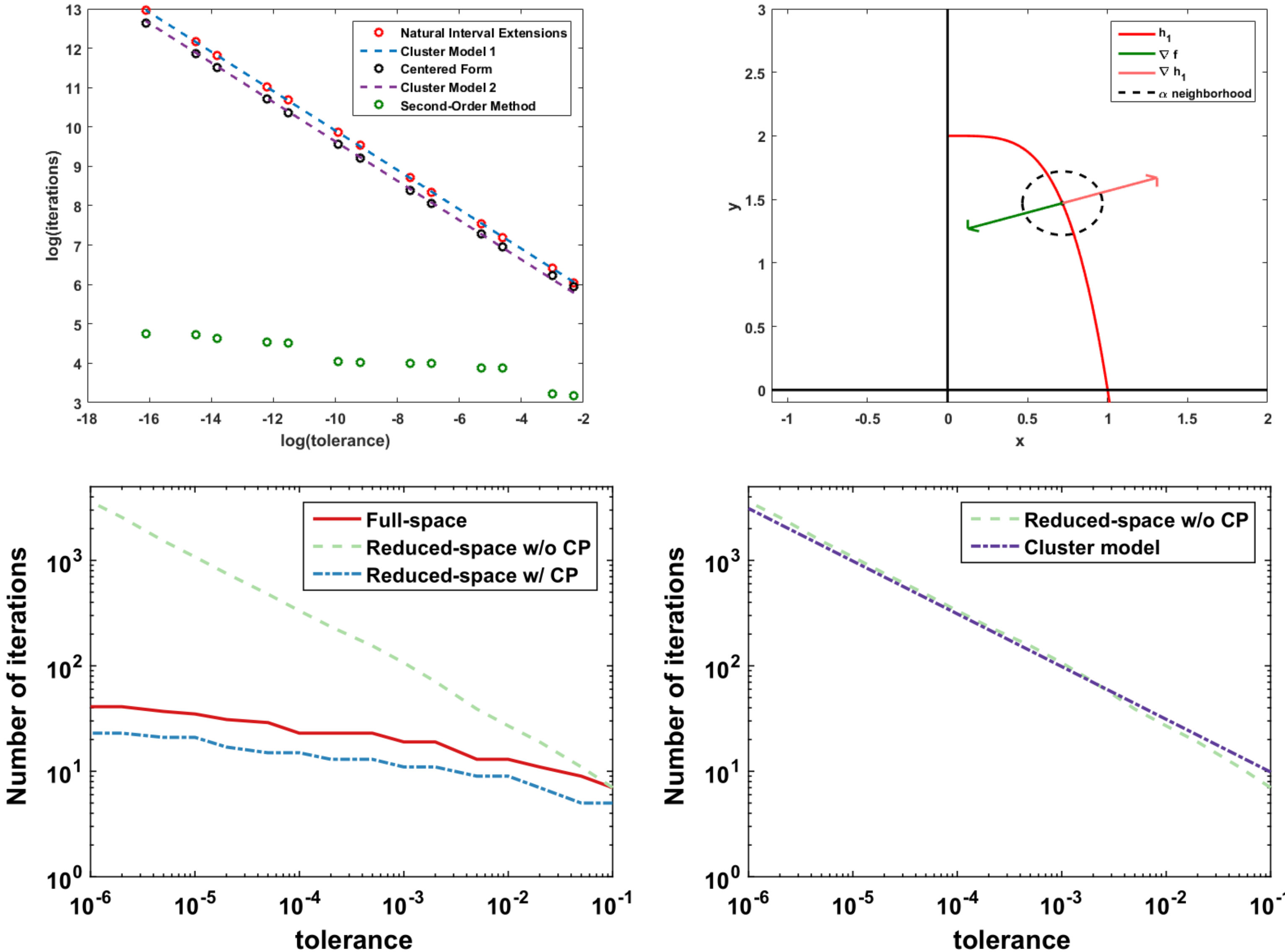
$$\text{s.t.} \ \ x^2 + x\exp(3-y) \le 10,$$

$$x \in [0.5, 2], \ \ y \in [-1, 1].$$





Summary of Part 2



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- Prof. Chris Floudas

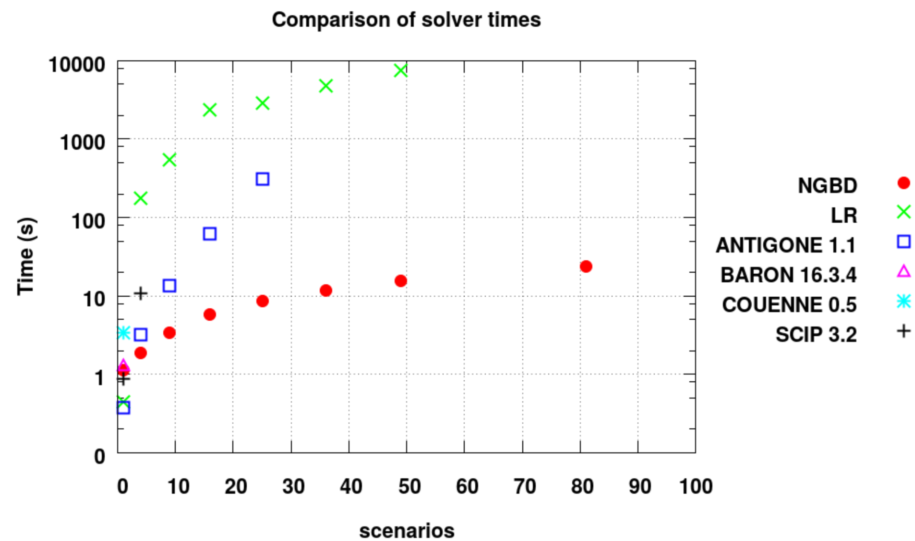
- Prof. Yu Yang
- Prof. Johannes Jäschke
- Adriaen Verheyleweghen

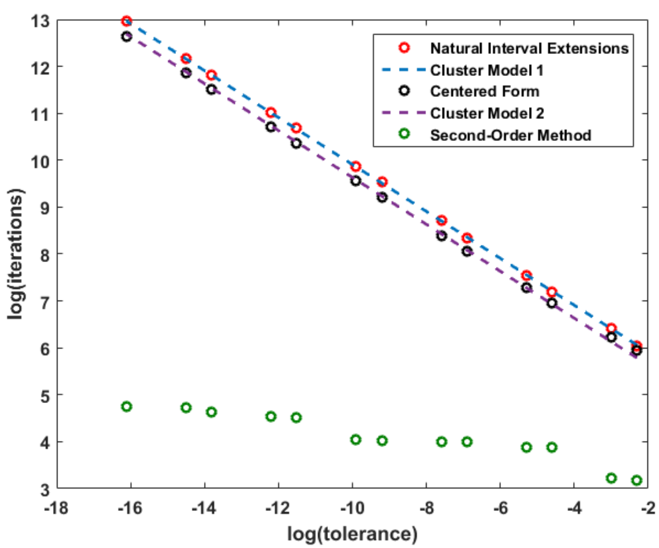
- Barton lab members

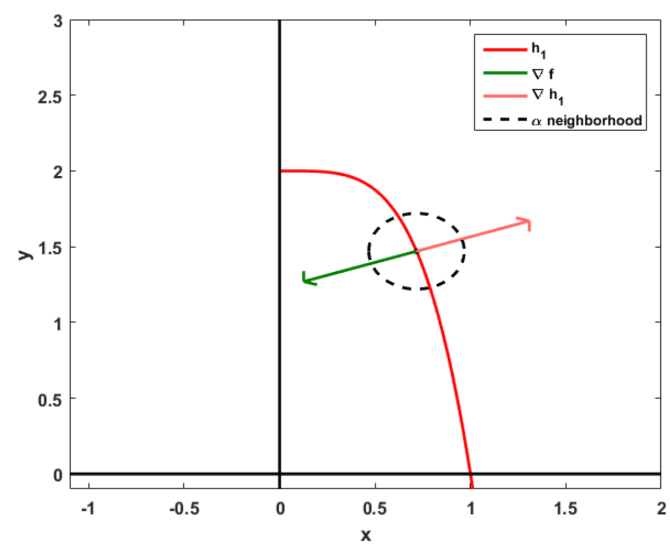
Summary

Inner minimization can be solved in a decomposable manner using NGBD

$$\sup_{\lambda_1,\cdots,\lambda_{s-1}} \boxed{\begin{aligned} \min_{\substack{x_1,\cdots,x_s,\\ y,z_1,\cdots,z_s}} \ & \sum_{h=1}^{s} p_h f_h(x_h, y, z_h) + \sum_{h=1}^{s-1} \lambda_h^T (z_h - z_{h+1}) \\ \text{s.t. } \ & g_h(x_h, y, z_h) \le 0, \ \forall h \in \{1,\cdots,s\}, \\ & x_h \in X_h, \ z_h \in Z, \ \forall h \in \{1,\cdots,s\}, \\ & y \in Y. \end{aligned}}$$







Backup Slides

Proposed Decomposition Approach
Modified Lagrangian Relaxation

- The B&B procedure can be accelerated using decomposable bounds tightening techniques

Continuous recourse variables

$$x_h^{i,\mathrm{lo}} = \min_{x_h, y, z} \; x_h^i$$
$$\text{s.t.} \;\; g_h^{\mathrm{cv}}(x_h, y, z) \le 0,$$
$$x_h \in \mathrm{conv}(X_h), \; y \in Y, \; z \in Z.$$

Continuous complicating variables

$$z^{j,\mathrm{lo}} = \max_{h \in \{1,\cdots,s\}} \; \min_{x_h, y, z_h} \; z_h^j$$
$$\text{s.t.} \; g_h^{\mathrm{cv}}(x_h, y, z_h) \le 0,$$
$$x_h \in \mathrm{conv}(X_h), \; y \in Y, \; z_h \in Z.$$

GOSSIP
Relaxation Strategies

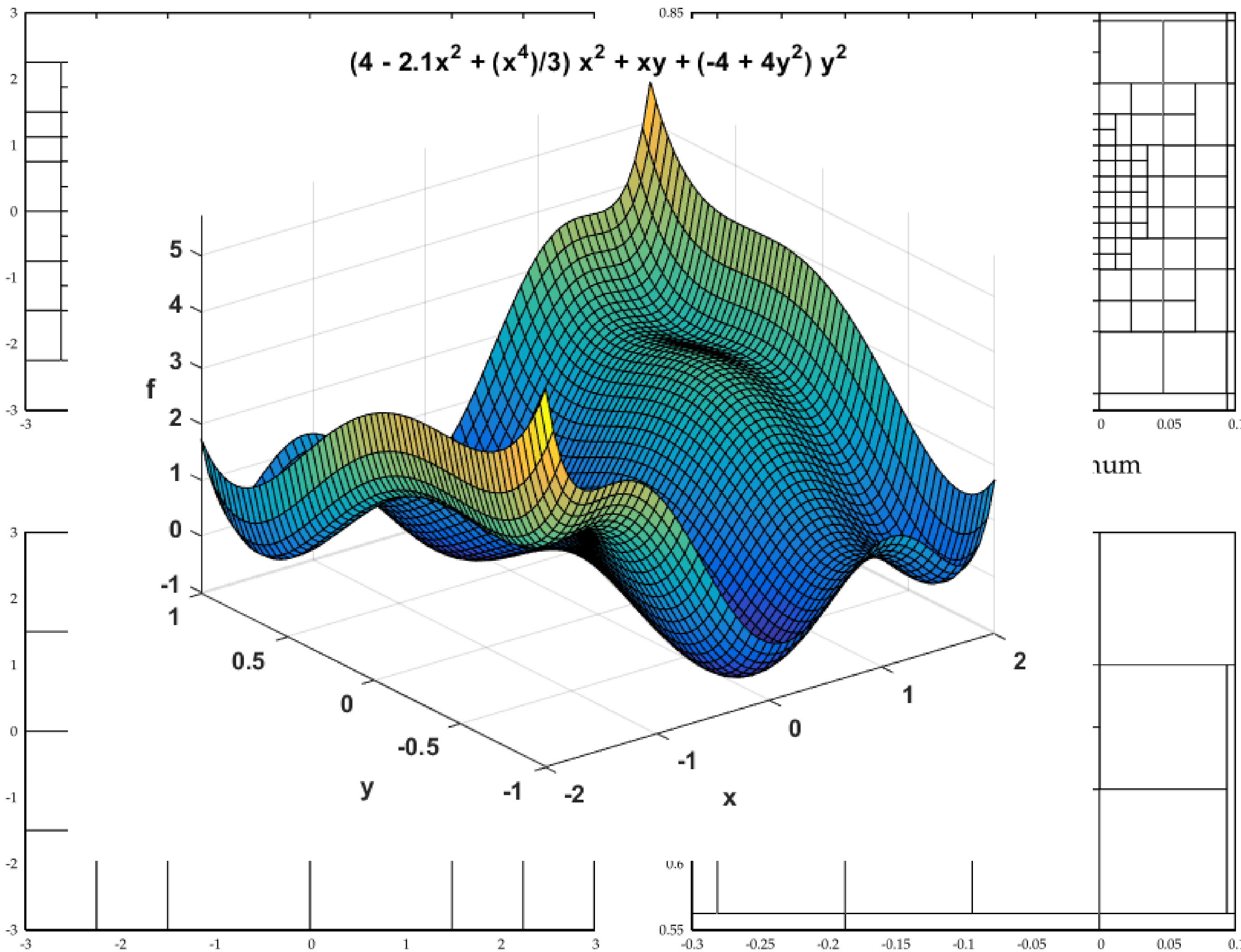
Term	Relaxation
xy	McCormick envelope
$\frac{x}{y}$	Bilinear reformulation, Quesada and Grossmann envelope
x^c	Secant, Liberti and Pantelides linearization
$\log(x)$	Secant
$\exp(x)$	Secant
x^y	Reformulate as $\exp(y \log(x))$
$\|x\|$	MIP reformulation
$\min(x, y)$	Reformulate as $\frac{1}{2}(x + y - \|x - y\|)$
$\max(x, y)$	Reformulate as $\frac{1}{2}(x + y + \|x - y\|)$
$x \log(x)$	Secant
$x \exp(x)$	Bilinear reformulation, Secant
xyz	Meyer and Floudas envelope
$xyzw$	Cafieri et al. relaxations
${x_1}^{c_1} \cdot {x_2}^{c_2} \cdots {x_n}^{c_n}$	Bilinear reformulation, Secant, Transformation-based relaxations

Motivation

Cluster Problem in Unconstrained Optimization

Natural Interval Extension

Centered Form



(c) Full domain

(d) Subset in vicinity of minimum