

# **Gossip: decomposition software for the Global Optimization of nonconvex two- Stage Stochastic mixed-Integer nonlinear Programs**

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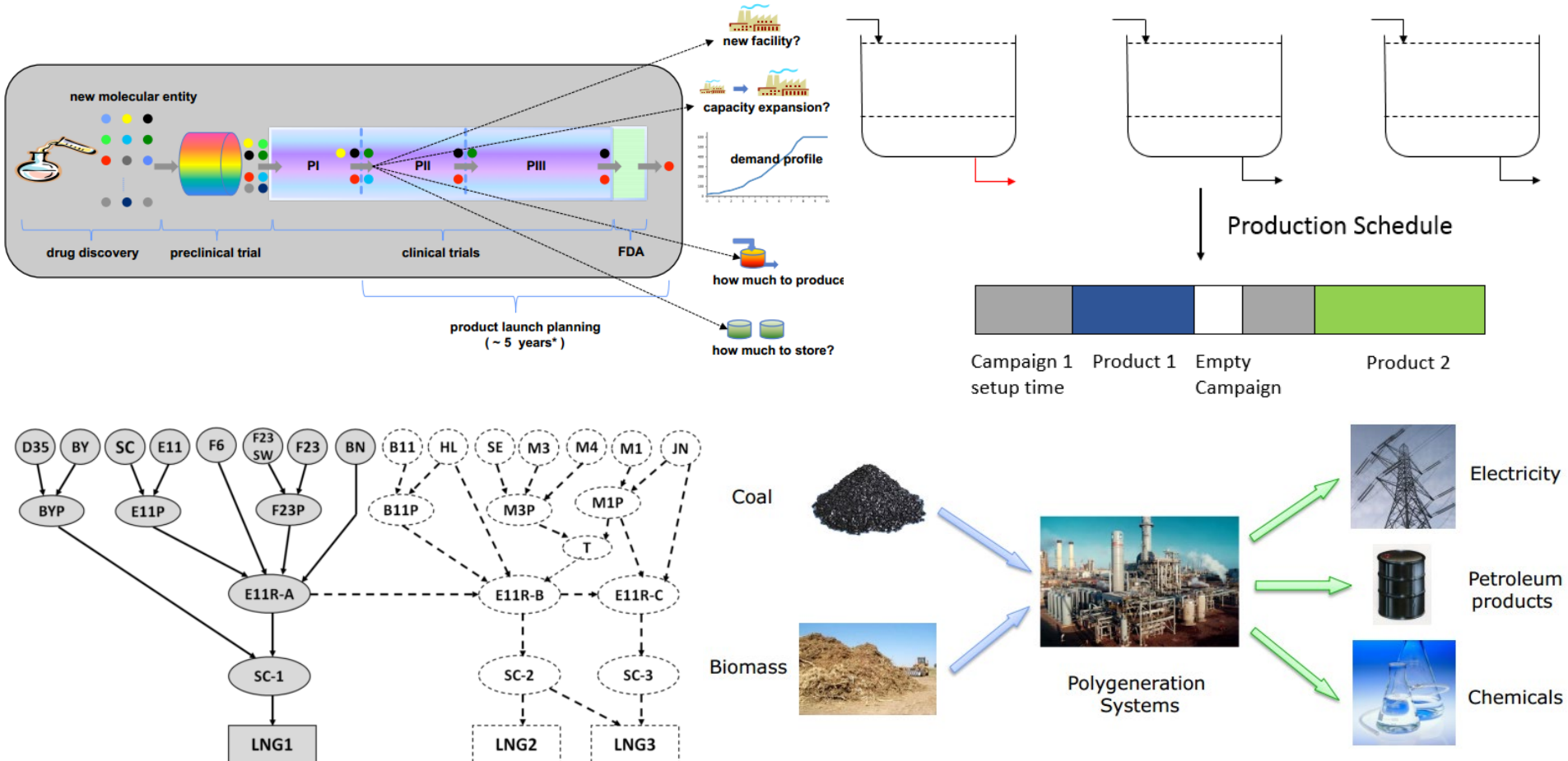
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**November 4, 2018**



# Motivation

## Engineering Applications



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

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

Sundaramoorthy, A. et al., Ind. Eng. Chem. Res., 2012.

Li, X. et al., Ind. Eng. Chem. Res., 2011.

# Two-Stage Stochastic MINLP Framework

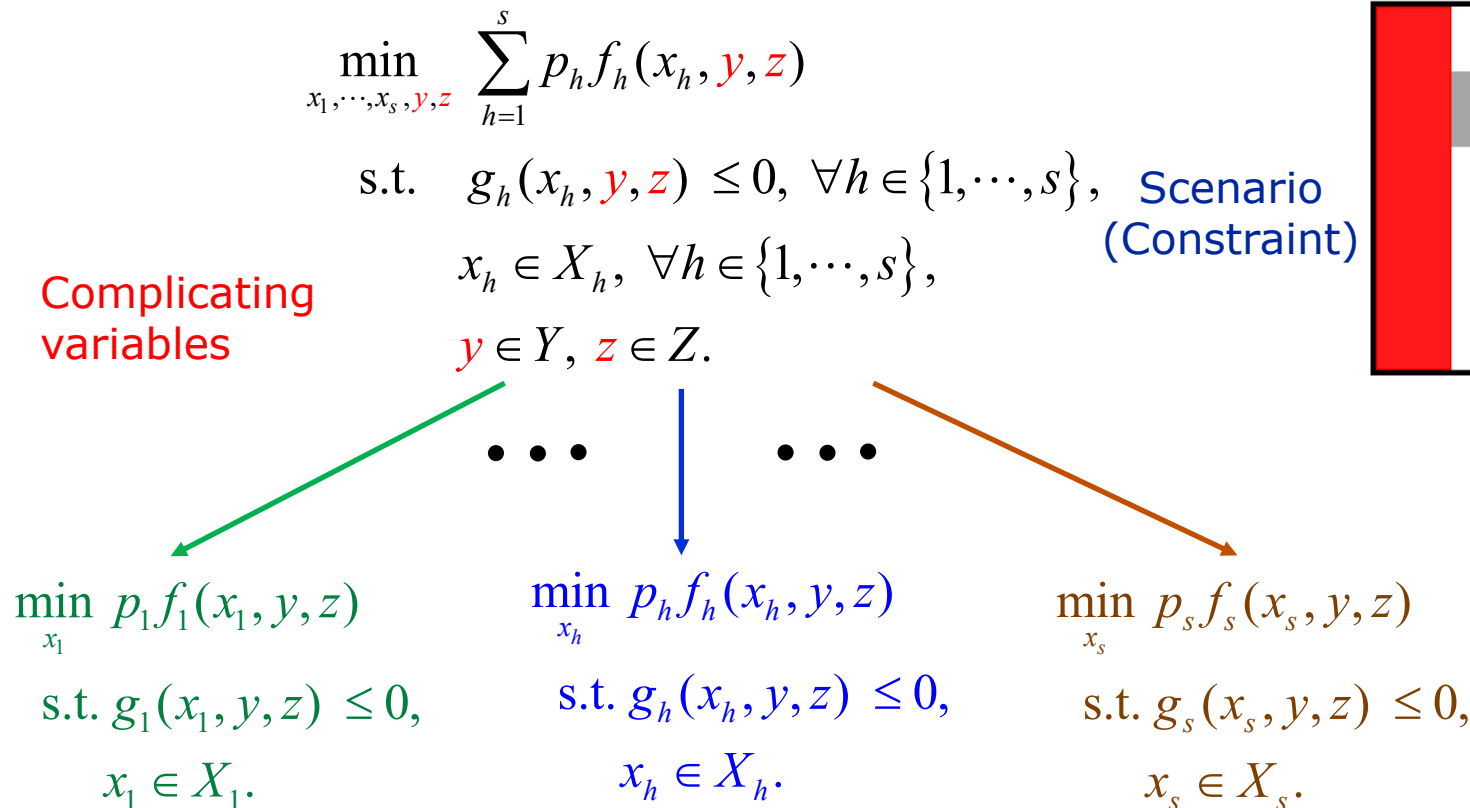
- Scenario-based formulation

$$\begin{aligned}
 & \min_{x_1, \dots, x_s, y, z} \sum_{h=1}^s p_h f_h(x_h, y, z) && \text{Minimize the expected cost} \\
 & \text{s.t. } g_h(x_h, y, z) \leq 0, \quad \forall h \in \{1, \dots, s\}, && \text{Constraints for all scenarios} \\
 & x_h \in X_h \subset \{0, 1\}^{n_{xb}} \times \mathbb{R}^{n_{xc}}, \quad \forall h \in \{1, \dots, s\}, && \text{Second-stage decisions for all scenarios} \\
 & y \in Y \subset \{0, 1\}^{n_y}, \quad z \in Z \subset \mathbb{R}^{n_z}. && \text{First-stage decisions}
 \end{aligned}$$

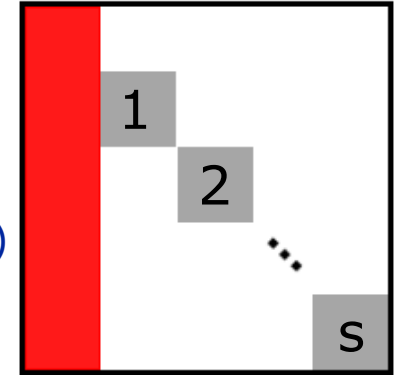
- The solution times of algorithms implemented in commercial general-purpose global optimization software are worst-case exponential in the number of scenarios

# Decomposition Strategy #1

## Complicating Variables Viewpoint

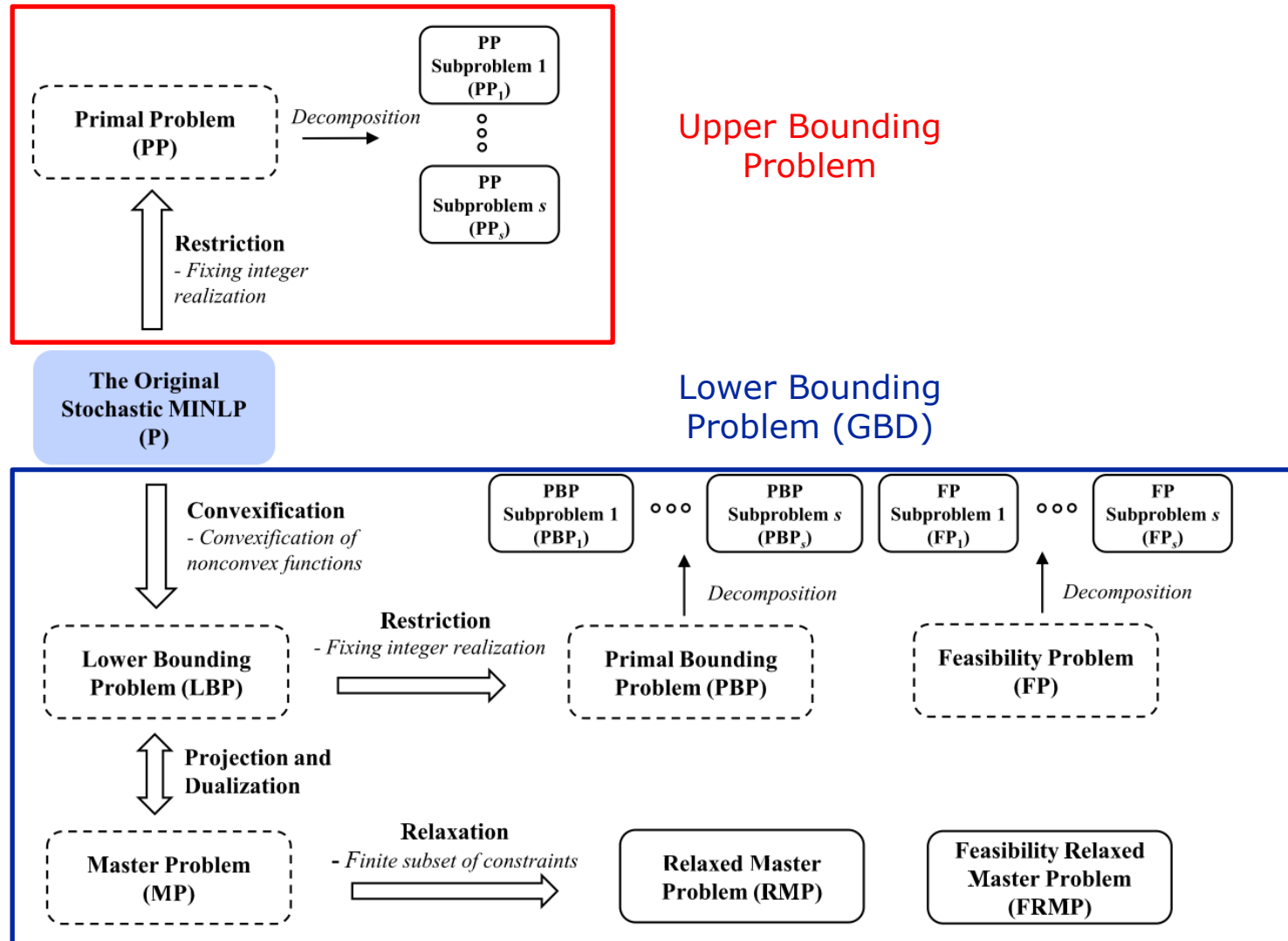


Variable



# Decomposition Algorithms

## Nonconvex Generalized Benders Decomposition (NGBD)



# Decomposition Algorithms

## Nonconvex Generalized Benders Decomposition (NGBD)

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

$$\text{s.t. } g_h(x_h, y) \leq 0, \forall h \in \{1, \dots, s\},$$

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

$$y \in Y \subset \{0,1\}^{n_y}.$$

Original Problem:  
Nonconvex MINLP

Convexification

$$\min_{\substack{x_1, \dots, x_s, \\ q_1, \dots, q_s, y}} \sum_{h=1}^s p_h \left[ f_h^{\text{cv}}(x_h, q_h) + c_{y,h}^T y \right]$$

$$\text{s.t. } g_h^{\text{cv}}(x_h, q_h) + B_{y,h} y \leq 0, \forall h \in \{1, \dots, s\},$$

$$(x_h, q_h) \in \text{conv}(X_h) \times Q_h, \forall h \in \{1, \dots, s\},$$

$$y \in \{0,1\}^{n_y}.$$

Lower Bounding  
Problem:  
MILP/Convex MINLP

Solve using GBD!

# Decomposition Strategy #2

## Complicating Constraints Viewpoint

Formulation

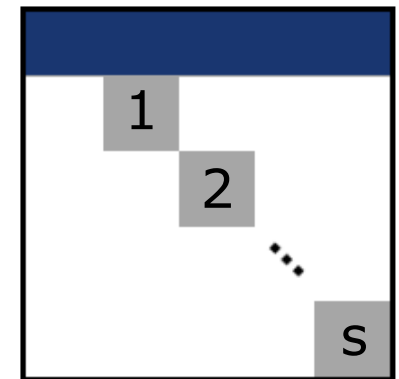
$$\begin{aligned}
 \min_{x_1, \dots, x_s, y, z} \quad & \sum_{h=1}^s p_h f_h(x_h, y, z) \\
 \text{s.t.} \quad & g_h(x_h, y, z) \leq 0, \quad \forall h \in \{1, \dots, s\}, \\
 & x_h \in X_h, \quad \forall h \in \{1, \dots, s\}, \\
 & y \in Y, \quad z \in Z.
 \end{aligned}$$

Equivalent Formulation

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

Complicating constraints

Scenario  
(Variable)



Constraint

# Decomposition Strategy #2

## Complicating Constraints Viewpoint

$$\min_{x_1, y_1, z_1} p_1 f_1(x_1, y_1, z_1)$$

$$\text{s.t. } g_1(x_1, y_1, z_1) \leq 0,$$

$$x_1 \in X_1, y_1 \in Y, z_1 \in Z.$$

$$\min_{x_h, y_h, z_h} p_h f_h(x_h, y_h, z_h)$$

$$\text{s.t. } g_h(x_h, y_h, z_h) \leq 0,$$

$$x_h \in X_h, y_h \in Y, z_h \in Z.$$

$$\min_{x_s, y_s, z_s} p_s f_s(x_s, y_s, z_s)$$

$$\text{s.t. } g_s(x_s, y_s, z_s) \leq 0,$$

$$x_s \in X_s, y_s \in Y, z_s \in Z.$$

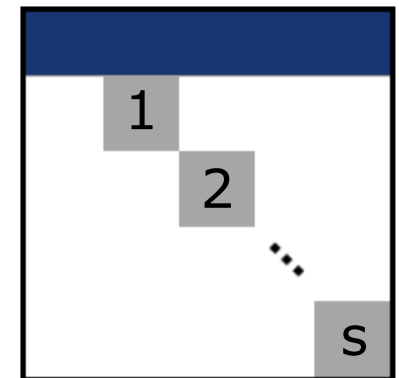
Equivalent  
Formulation

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

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

Constraint

Scenario  
(Variable)



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



# Decomposition Algorithms

## Lagrangian Relaxation (LR)


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

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

$$\begin{aligned} y_h - y_{h+1} &= 0, \quad \forall h \in \{1, \dots, s-1\}, \\ z_h - z_{h+1} &= 0, \quad \forall h \in \{1, \dots, s-1\}, \end{aligned} \quad \left. \vphantom{\begin{aligned} y_h - y_{h+1} \\ z_h - z_{h+1} \end{aligned}} \right\} \begin{array}{l} \text{Non-anticipativity} \\ \text{constraints} \end{array}$$

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

Dualize the  
nonanticipativity  
constraints



$$\begin{aligned} \sup_{\substack{\mu_1, \dots, \mu_{s-1}, \\ \lambda_1, \dots, \lambda_{s-1}}} \min_{\substack{x_1, \dots, x_s, \\ y_1, \dots, y_s, \\ z_1, \dots, z_s}} & \sum_{h=1}^s p_h f_h(x_h, y_h, z_h) + \sum_{h=1}^{s-1} \mu_h^T (y_h - y_{h+1}) + \sum_{h=1}^{s-1} \lambda_h^T (z_h - z_{h+1}) \\ \text{s.t.} & \quad g_h(x_h, y_h, z_h) \leq 0, \quad \forall h \in \{1, \dots, s\}, \\ & \quad x_h \in X_h, y_h \in Y, z_h \in Z, \quad \forall h \in \{1, \dots, s\}. \end{aligned}$$

The inner minimization  
can be decomposed  
into independent  
scenario problems

# Our proposed approach (MLR) aims to leverage the advantages of both NGBD and LR

- Upper bounds are generated using efficient local optimization techniques that exploit the near-decomposable structure
- Lower bounds are generated by relaxing the complicating constraints corresponding to the continuous first-stage variables  $z$

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

Inner minimization can be solved efficiently using NGBD

- Convergence is guaranteed by B&B, where it is sufficient to branch on the continuous first-stage variables  $z$  to converge
  - Convergence is accelerated potentially by using tailored decomposable bounds tightening techniques

# GOSSIP

## Overview and Motivation

- Software for the Global Optimization of nonconvex two-Stage Stochastic mixed-Integer nonlinear Programs
  - More than 100,000 lines of source code (primarily in C++)
  - Links to state-of-the-art solvers, e.g., CPLEX, IPOPT, ANTIGONE
  - Enables solution of large-scenario cases studies from the literature

### Motivation

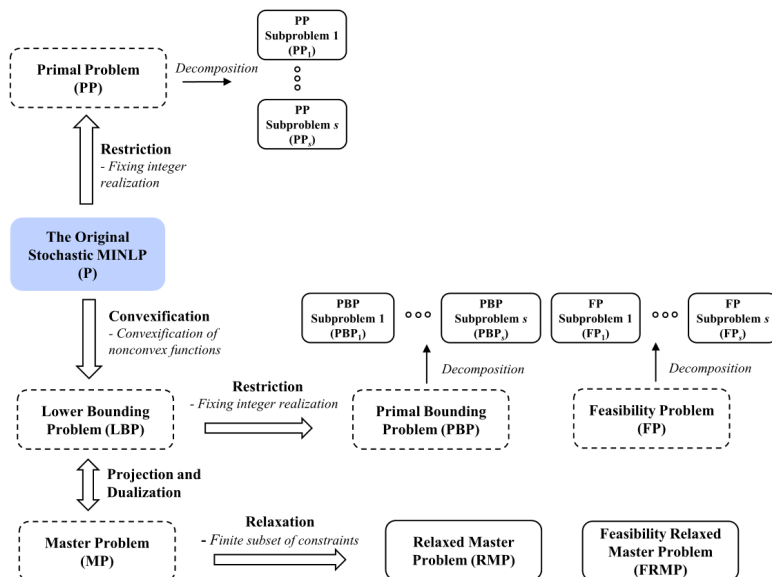
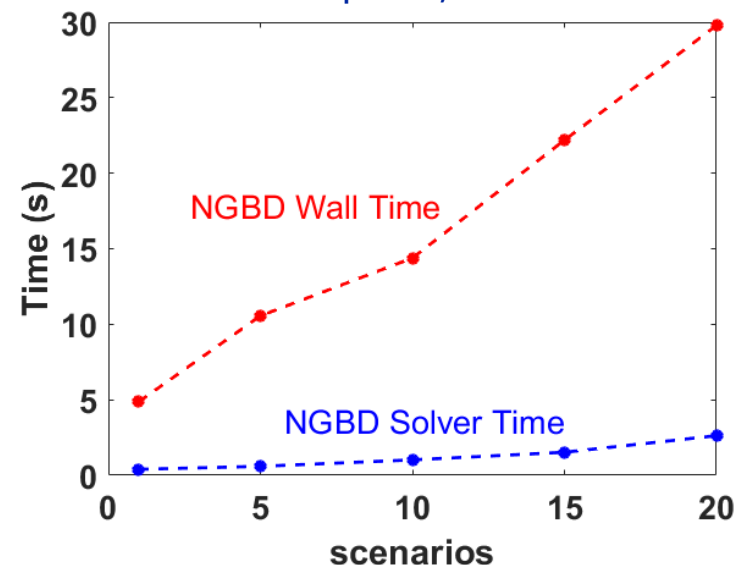


Image adapted from Li et al.,  
J. Global Optim., 2011

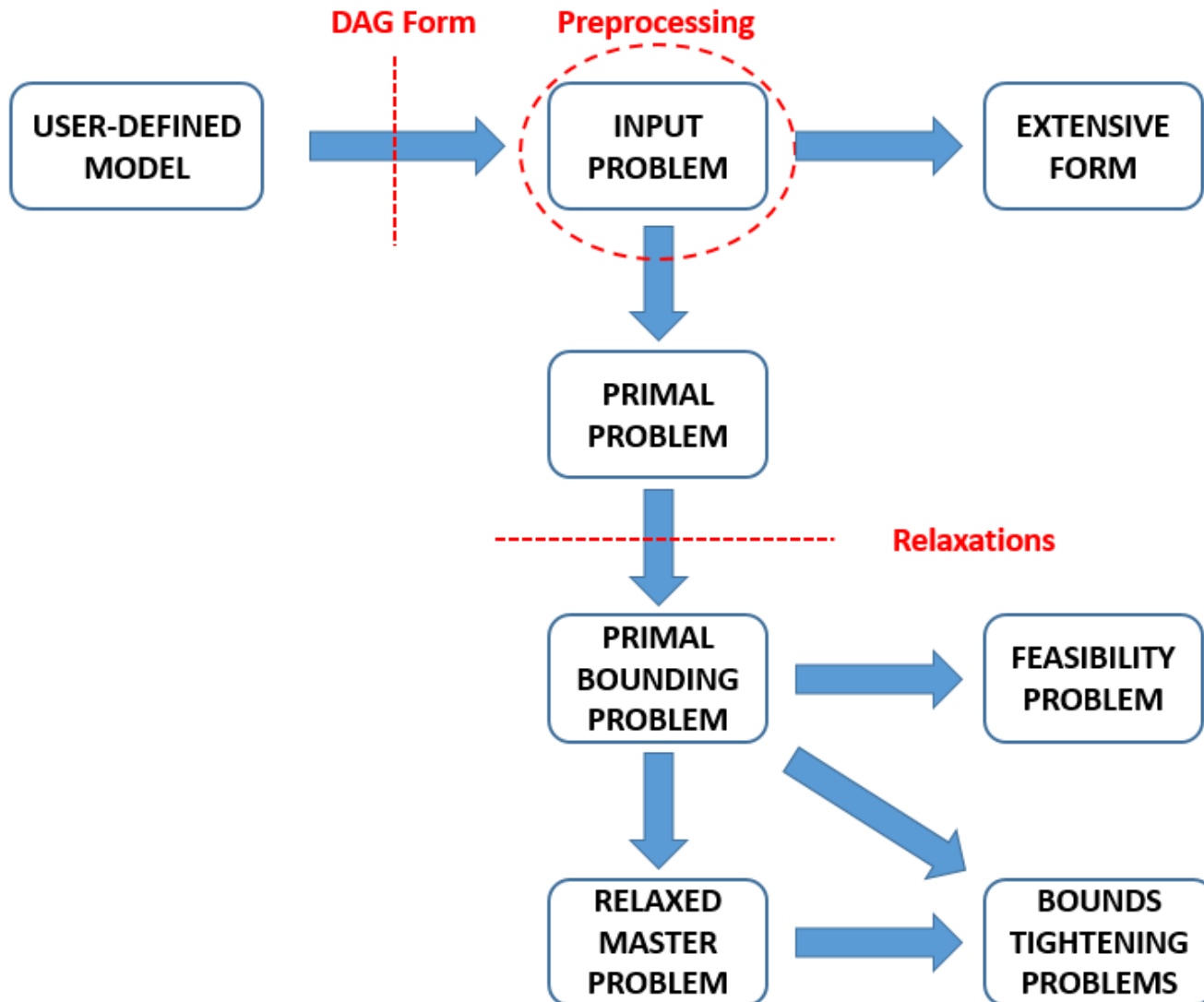


Implementing decomposition algorithms  
such as NGBD is a nontrivial task

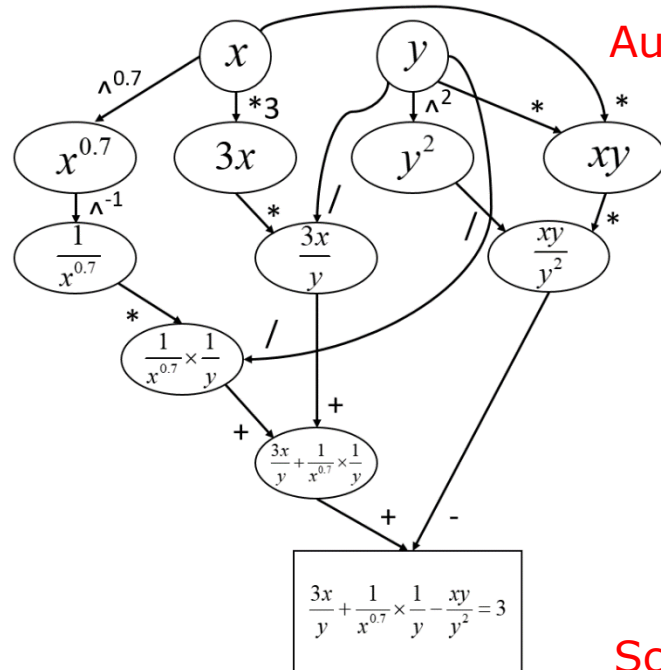
Naïve implementations may  
result in significant overhead

# GOSSIP

## Model Reformulation

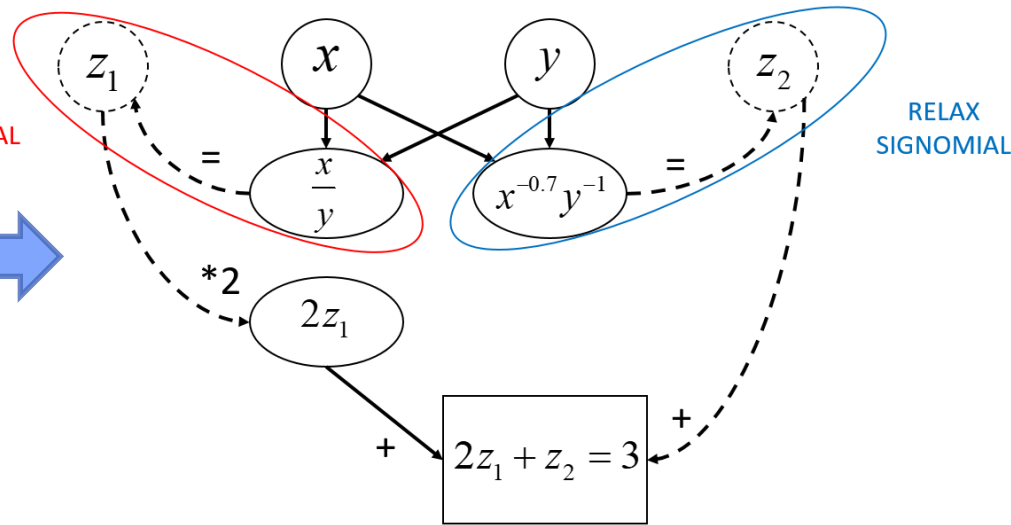


# Some of GOSSIP's features

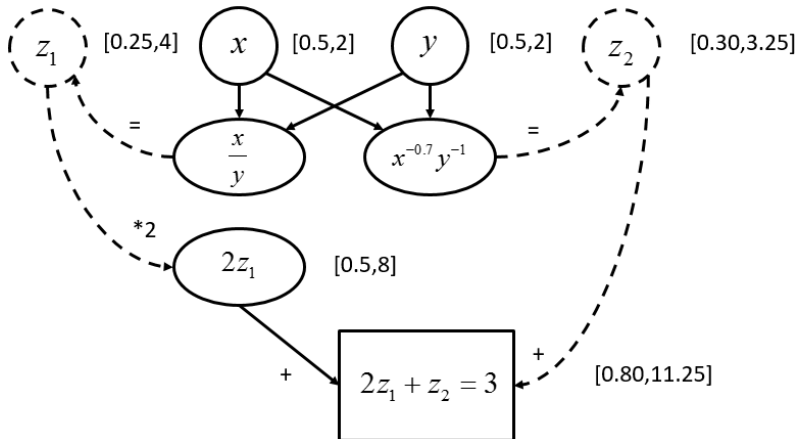


Automatic Structure Detection

RELAX  
FRACTIONAL



Scalable Bounds Tightening Techniques



$$z^{j,lo} = \max_{h \in \{1, \dots, s\}} \min_{x_h, y, z_h} z_h^j$$

s.t.  $g_h^{cv}(x_h, y, z_h) \leq 0,$   
 $x_h \in \text{conv}(X_h),$   
 $y \in Y, z_h \in Z.$

# Computational Studies

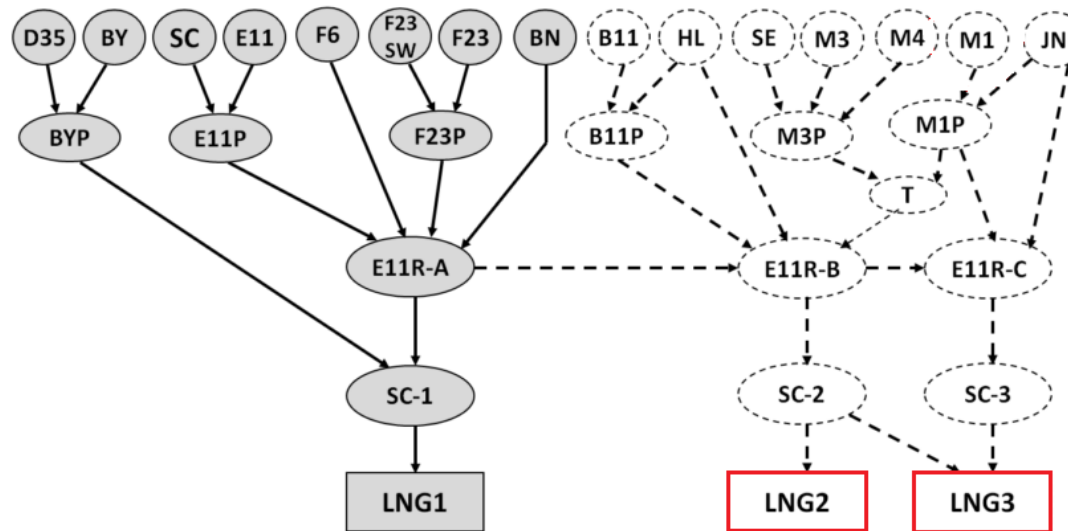
## Implementation Details

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- Platform
  - CPU 3.5 GHz, Memory 6.0 GB, VMWare Workstation, GAMS 24.7.1, GCC 4.8.1, GFortran 4.8.1
- GOSSIP Solvers
  - LP and MILP solver: CPLEX 12.6 (C library)
  - Global NLP solver: ANTIGONE 1.1 (C++ library)
  - Local NLP solver: IPOPT 3.12.8 (C++ library)
  - Bundle solver: MPBNGC 2.0 (Fortran library)
- Methods for comparison
  - ANTIGONE 1.1, BARON 16.3.4, COUENNE 0.5, SCIP 3.2
  - Nonconvex generalized Benders decomposition (NGBD)
  - Lagrangian relaxation (LR)
  - Modified Lagrangian relaxation (MLR)
- Relative tolerance:  $10^{-3}$ , Absolute tolerance:  $10^{-9}$
- Time Limit: 10,000 seconds

# Computational Study

## Design and Operation of a Natural Gas Network

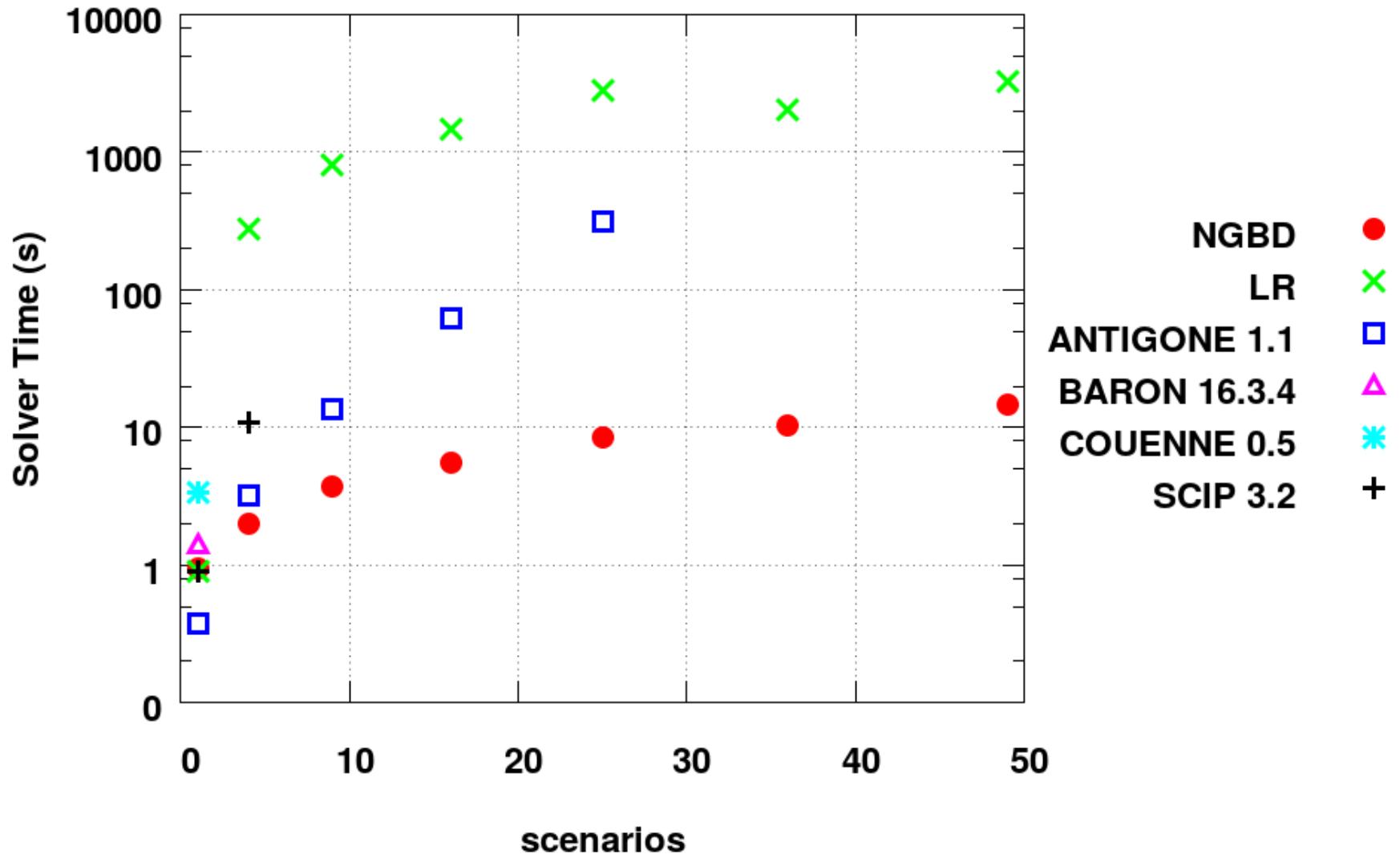


38 binary first-stage variables,  
 0 continuous first-stage variables,  
 93s continuous second-stage variables,  
 34s bilinear terms.

(s denotes the number of scenarios)

# Computational Study

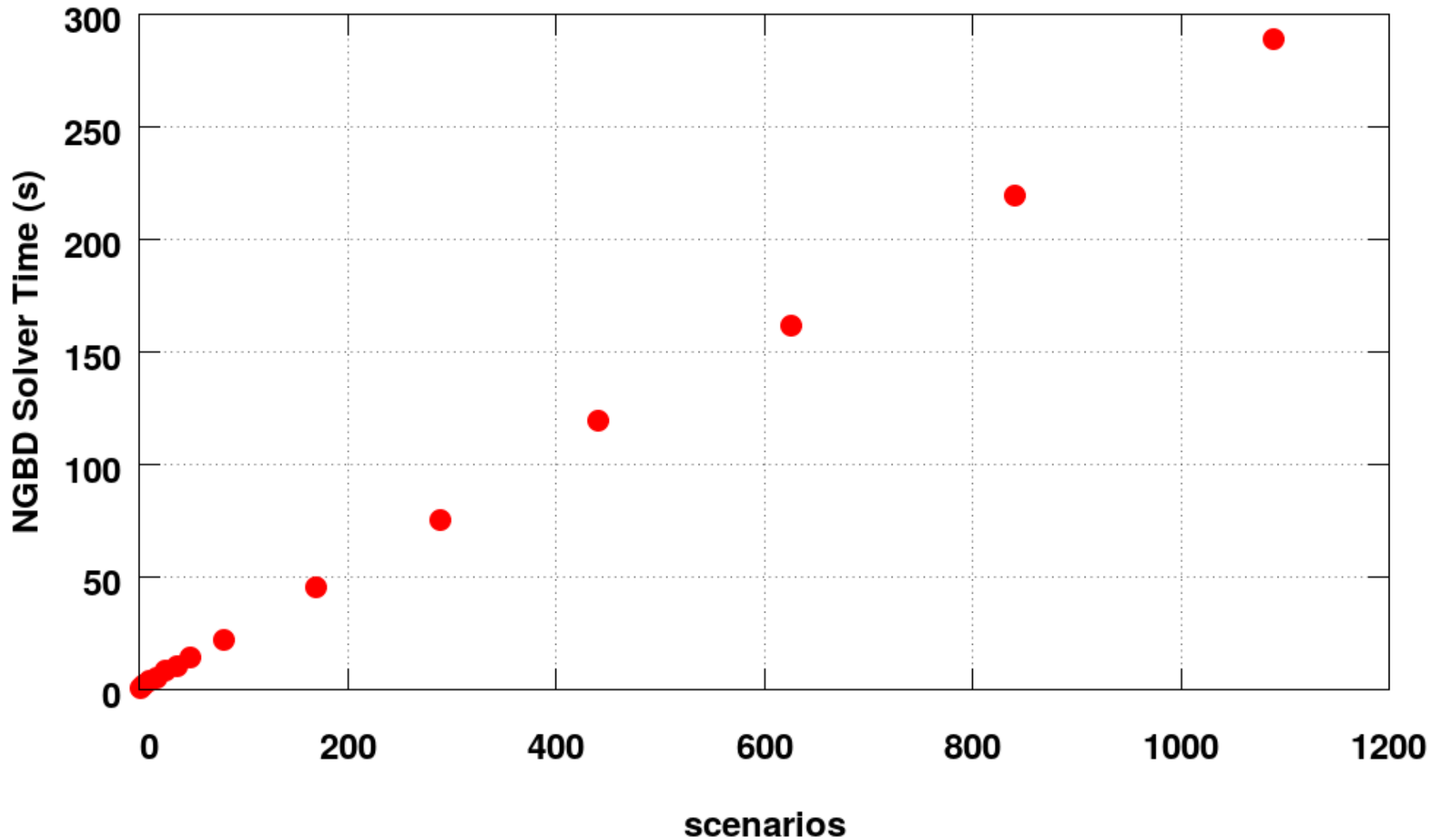
## Design and Operation of a Natural Gas Network





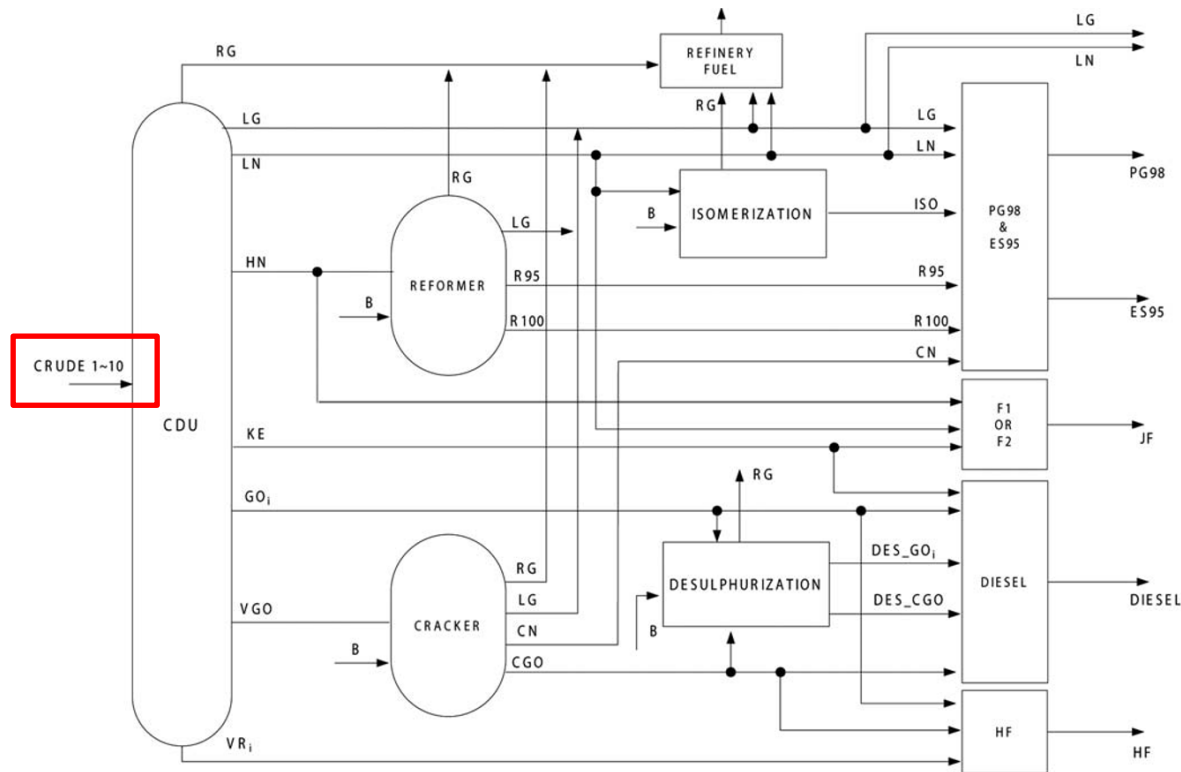
# Computational Study

## Design and Operation of a Natural Gas Network



# Computational Study

## Integrated Crude Selection and Refinery Operation

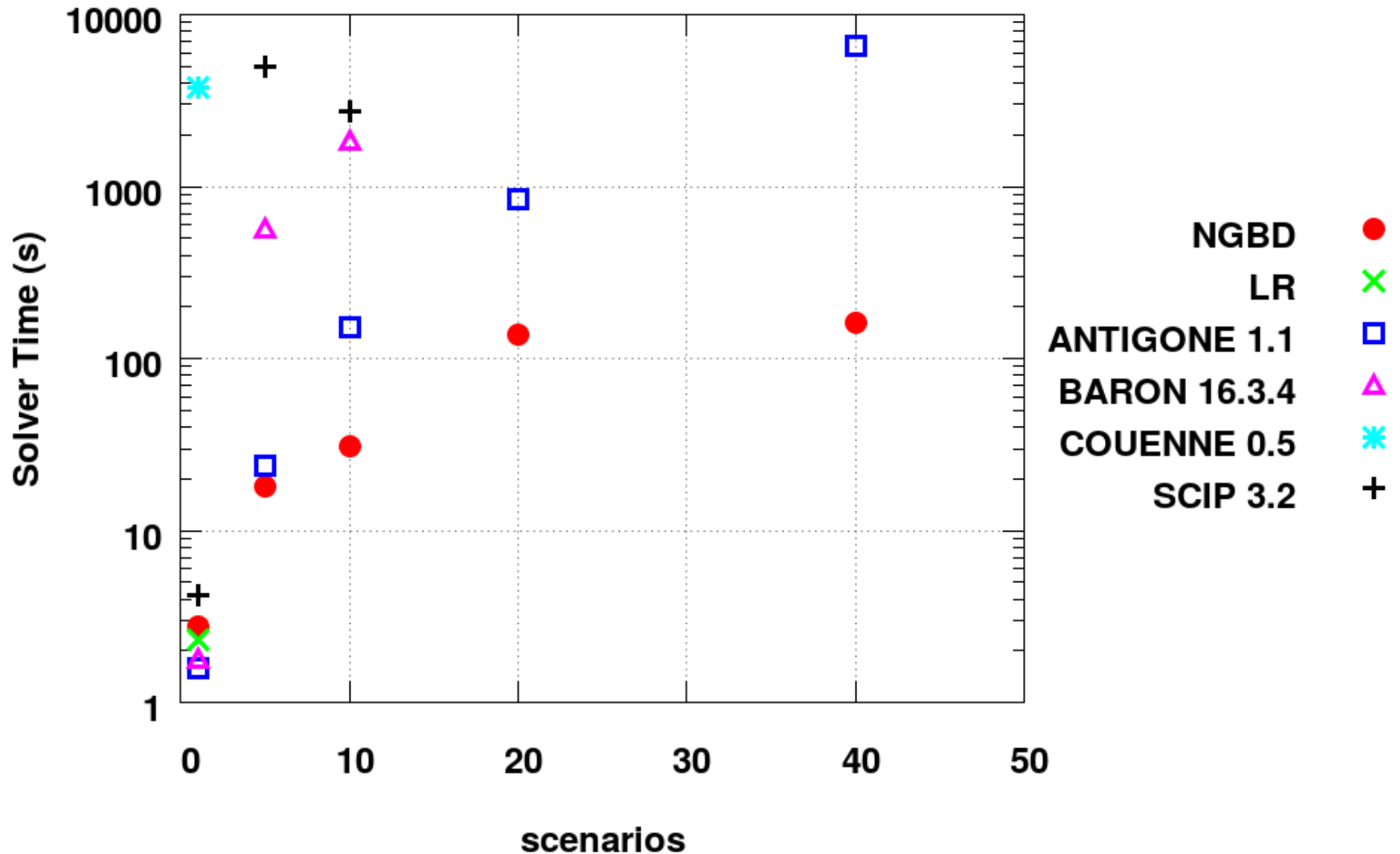


100 binary first-stage variables,  
 0 continuous first-stage variables,  
 122s continuous second-stage variables,  
 26s bilinear terms.

(s denotes the number of scenarios)

# Computational Study

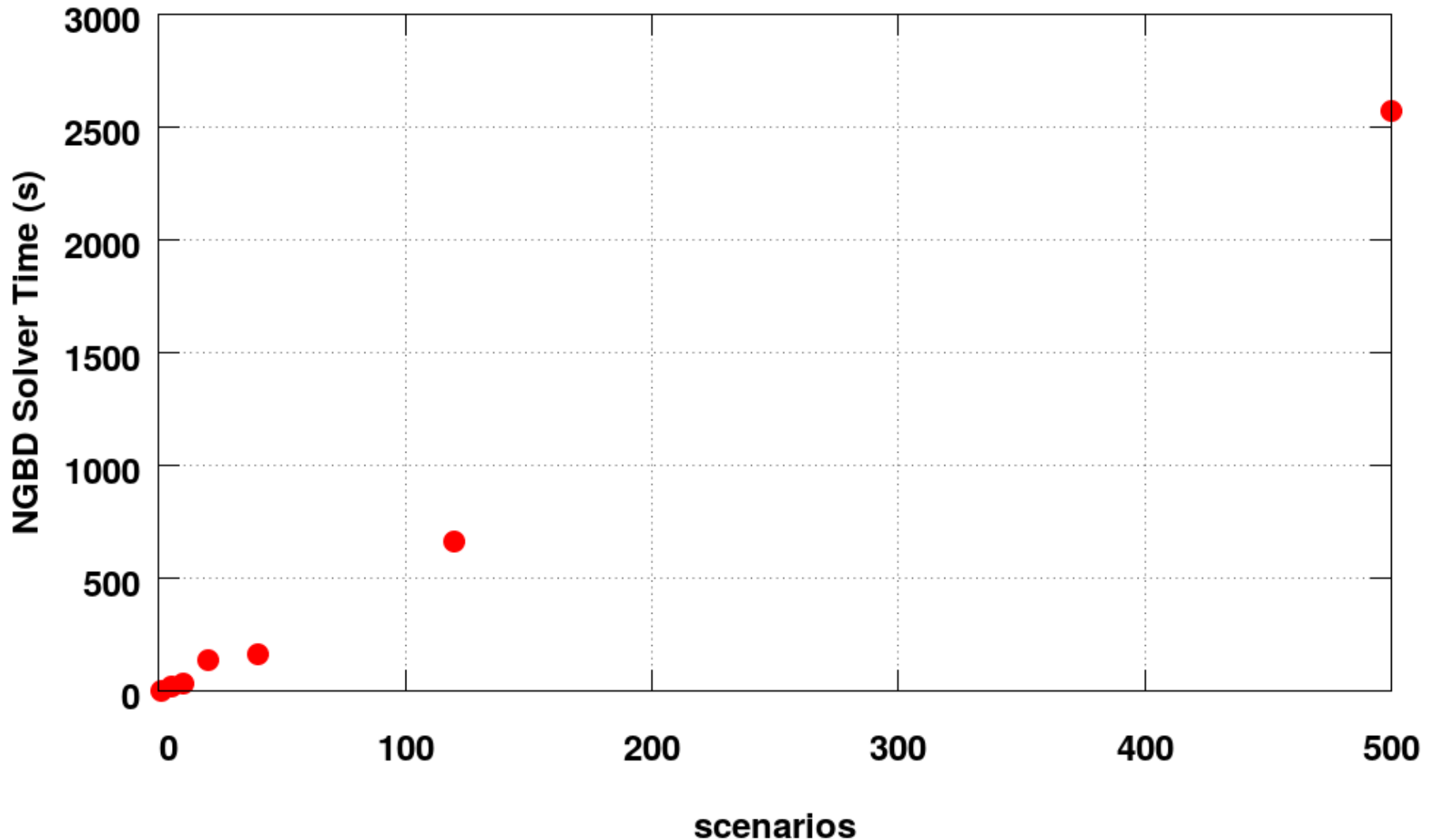
## Integrated Crude Selection and Refinery Operation



# Computational Study

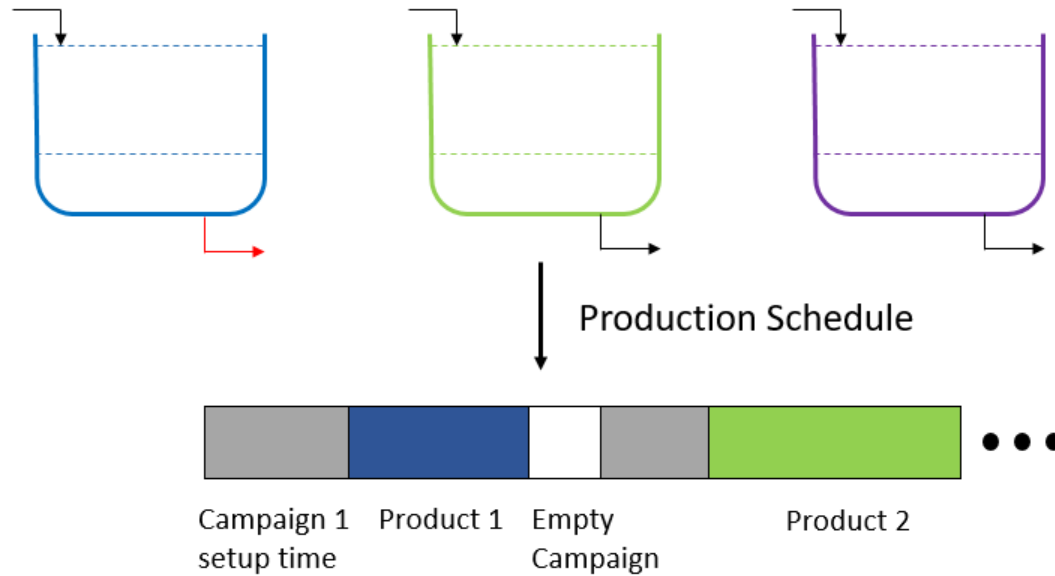
## Integrated Crude Selection and Refinery Operation

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# Computational Study

## Tank Sizing and Scheduling for a Chemical Plant

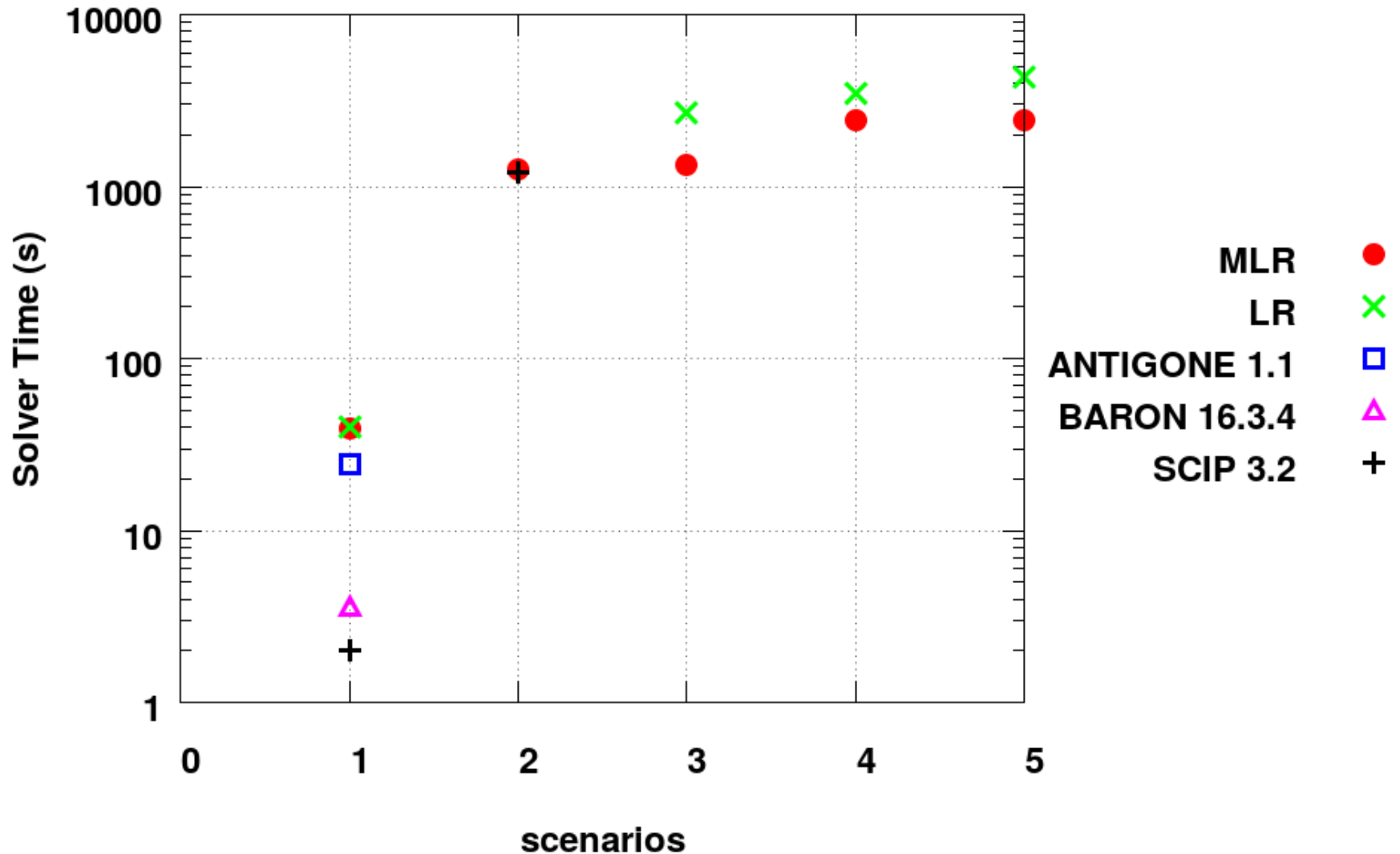


- 0 binary first-stage variables,
- 3 continuous first-stage variables,
- 9s binary second-stage variables,
- 38s continuous second-stage variables,
- 3 signomial terms,
- 47s bilinear terms.

(s denotes the number of scenarios)

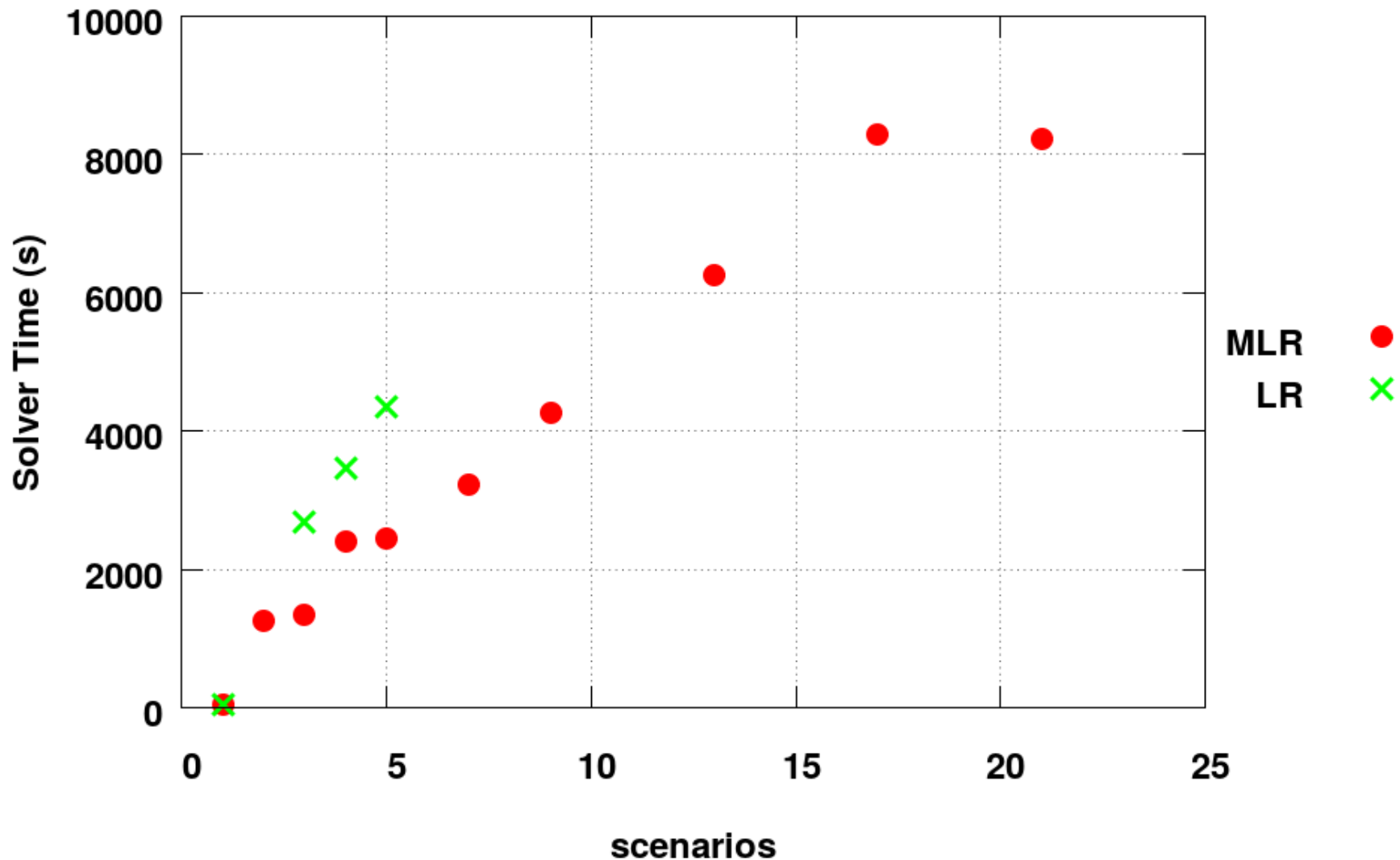
# Computational Study

## Tank Sizing and Scheduling for a Chemical Plant



# Computational Study

## Tank Sizing and Scheduling for a Chemical Plant



# Summary and Future Work

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- GOSSIP implements state-of-the-art decomposition techniques for nonconvex stochastic programs
- Case studies demonstrate the advantages of the software framework for solving large-scale problems
- Future work:
  - Additional features such as polyhedral relaxations, piecewise-convex relaxations, edge concave relaxations, RLT cuts
  - Incorporate alternate decomposition techniques such as nonconvex outer-approximation
- Please contribute to the test library ([rohitk@alum.mit.edu](mailto:rohitk@alum.mit.edu)). Contributions will be acknowledged



# Acknowledgements

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- Prof. Ruth Misener & Prof. Chris Floudas
- Prof. Yu Yang



# Decomposition Approaches

Formulation

$$\min_{x_1, \dots, x_s, \mathbf{y}, \mathbf{z}} \sum_{h=1}^s p_h \left[ f_h(x_h) + c_{y,h}^T \mathbf{y} + c_{z,h}^T \mathbf{z} \right]$$

s.t.

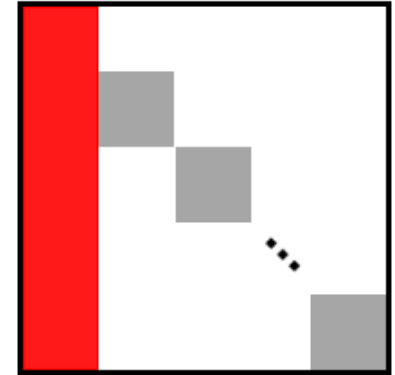
$$g_h(x_h) + B_{y,h} \mathbf{y} + B_{z,h} \mathbf{z} \leq 0, \quad \forall h \in \{1, \dots, s\},$$

$$A_y \mathbf{y} + A_z \mathbf{z} \leq d_{y,z},$$

$$x_h \in X_h, \quad \forall h \in \{1, \dots, s\},$$

$$\mathbf{y} \in Y, \quad \mathbf{z} \in Z.$$

Complicating variables



Equivalent Formulation

$$\min_{\substack{x_1, \dots, x_s, \\ y_1, \dots, y_s, \\ z_1, \dots, z_s}} \sum_{h=1}^s p_h \left[ f_h(x_h) + c_{y,h}^T y_h + c_{z,h}^T z_h \right]$$

s.t.

$$g_h(x_h) + B_{y,h} y_h + B_{z,h} z_h \leq 0, \quad \forall h \in \{1, \dots, s\},$$

$$A_y y_h + A_z z_h \leq d_{y,z}, \quad \forall h \in \{1, \dots, s\},$$

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

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

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

Complicating constraints



# Decomposition Algorithms

## Nonconvex Generalized Benders Decomposition

$$\begin{aligned}
 \min_{x_1, \dots, x_s, y} \quad & \sum_{h=1}^s p_h \left[ f_h(x_h) + c_{y,h}^T y \right] \\
 \text{s.t.} \quad & g_h(x_h) + B_{y,h} y \leq 0, \quad \forall h \in \{1, \dots, s\}, \\
 & A_y y \leq d_y, \\
 & x_h \in X_h \subset \{0,1\}^{n_{xb}} \times \mathbb{R}^{n_{xc}}, \quad \forall h \in \{1, \dots, s\}, \\
 & y \in Y \subset \{0,1\}^{n_y}.
 \end{aligned}$$

Original Problem:  
Nonconvex MINLP

Fix the first-stage  
variables

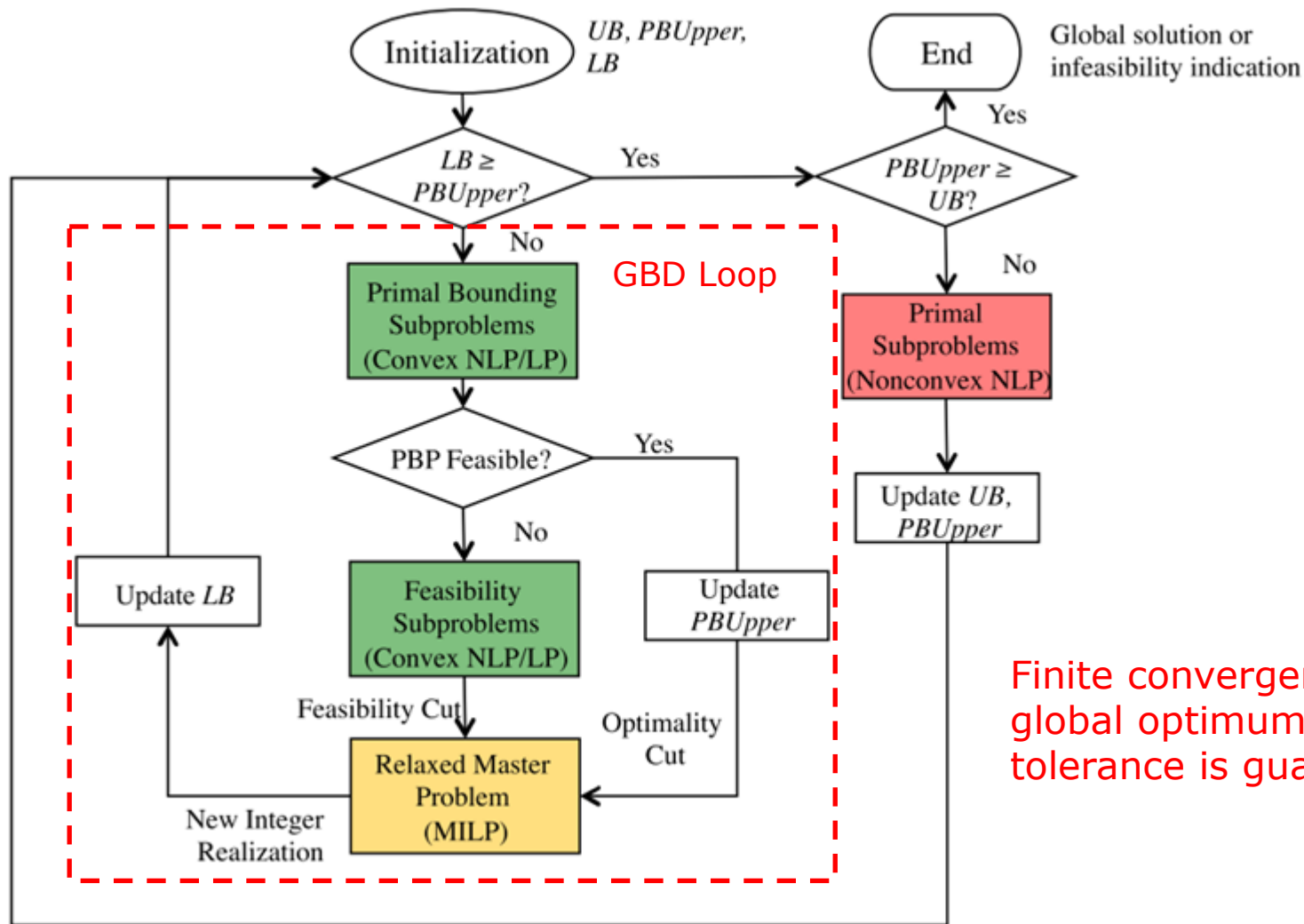
Solve the  
scenario primal  
problems  
independently

$$\begin{aligned}
 \min_{x_1, \dots, x_s} \quad & \sum_{h=1}^s p_h \left[ f_h(x_h) + c_{y,h}^T \bar{y} \right] \\
 \text{s.t.} \quad & g_h(x_h) + B_{y,h} \bar{y} \leq 0, \quad \forall h \in \{1, \dots, s\}, \\
 & x_h \in X_h \subset \{0,1\}^{n_{xb}} \times \mathbb{R}^{n_{xc}}, \quad \forall h \in \{1, \dots, s\}.
 \end{aligned}$$

Primal Problem:  
Nonconvex  
NLP/MINLP

# Decomposition Algorithms

## Nonconvex Generalized Benders Decomposition



# Decomposition Algorithms

## Modified Lagrangian Relaxation

$$\min_{\substack{x_1, \dots, x_s, y, \\ z_1, \dots, z_s}} \sum_{h=1}^s p_h \left[ f_h(x_h) + c_{y,h}^T y + c_{z,h}^T z_h \right]$$

$$\text{s.t.} \quad g_h(x_h) + B_{y,h} y + B_{z,h} z_h \leq 0, \quad \forall h \in \{1, \dots, s\},$$

$$A_y y + A_z z_h \leq d_{y,z}, \quad \forall h \in \{1, \dots, s\},$$

$$z_h = z_{h+1}, \quad \forall h \in \{1, \dots, s-1\}, \quad \longrightarrow \text{Non-anticipativity constraints}$$

$$x_h \in X_h, \quad z_h \in Z, \quad \forall h \in \{1, \dots, s\},$$

$$y \in Y \subset \{0,1\}^{n_y}.$$

Dualize the  
nonanticipativity  
constraints

$$\sup_{\lambda_1, \dots, \lambda_{s-1}} \min_{\substack{x_1, \dots, x_s, y, \\ z_1, \dots, z_s}} \sum_{h=1}^s \left( p_h \left[ f_h(x_h) + c_{y,h}^T y + c_{z,h}^T z_h \right] \right) + \sum_{h=1}^{s-1} \lambda_h^T (z_h - z_{h+1})$$

$$\text{s.t.} \quad g_h(x_h) + B_{y,h} y + B_{z,h} z_h \leq 0, \quad \forall h \in \{1, \dots, s\},$$

$$A_y y + A_z z_h \leq d_{y,z}, \quad \forall h \in \{1, \dots, s\},$$

$$x_h \in X_h, \quad z_h \in Z, \quad \forall h \in \{1, \dots, s\},$$

$$y \in Y.$$

The inner minimization can be solved in a decomposable manner using NGBD

# GOSSIP

## Model Formulation

```

for(int j=0;j<NUM_POOLS;++j)
  for(int j2=0;j2<NUM_POOLS;++j2)
    if(T_PP[j][j2])
      for(int h=0;h<NUM_SCEN;++h)
      {
        sprintf(clabel,"s_PP[%d][%d][%d]", j+1, j2+1, h+1);
        s_PP[j][j2][h].setIndependentVariable(
          ++varcount,
          compgraph::CONTINUOUS,
          I(0,1),
          0.,
          h+1,
          clabel);
      }

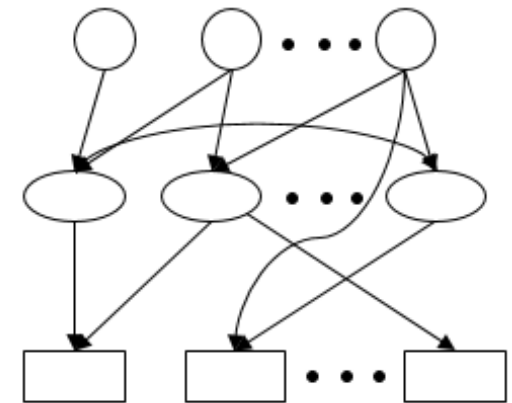
for(int j=0;j<NUM_POOLS;++j)
  for(int h=0;h<NUM_SCEN;++h)
  {
    split_bal[j][h] = 1;
    for(int j2=0;j2<NUM_POOLS;++j2)
      if(T_PP[j][j2])
        Split_bal[j][h] -= s_PP[j][j2][h];
    for(int k=0;k<NUM_TERMINALS;++k)
      if(T_PT[j][k])
        Split_bal[j][h] -= s_PT[j][k][h];
    Split_bal[j][h].setDependentVariable(++concount,compgraph::EQUALITY);
  }

```

Variables

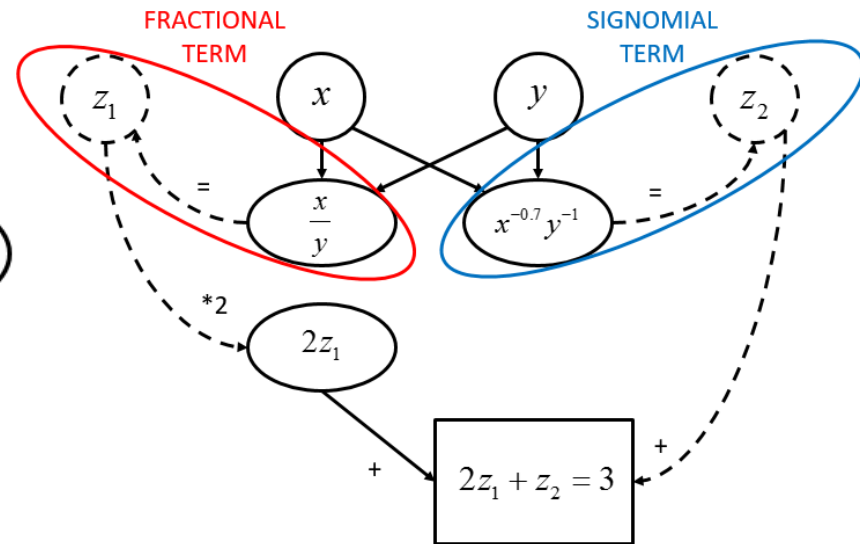
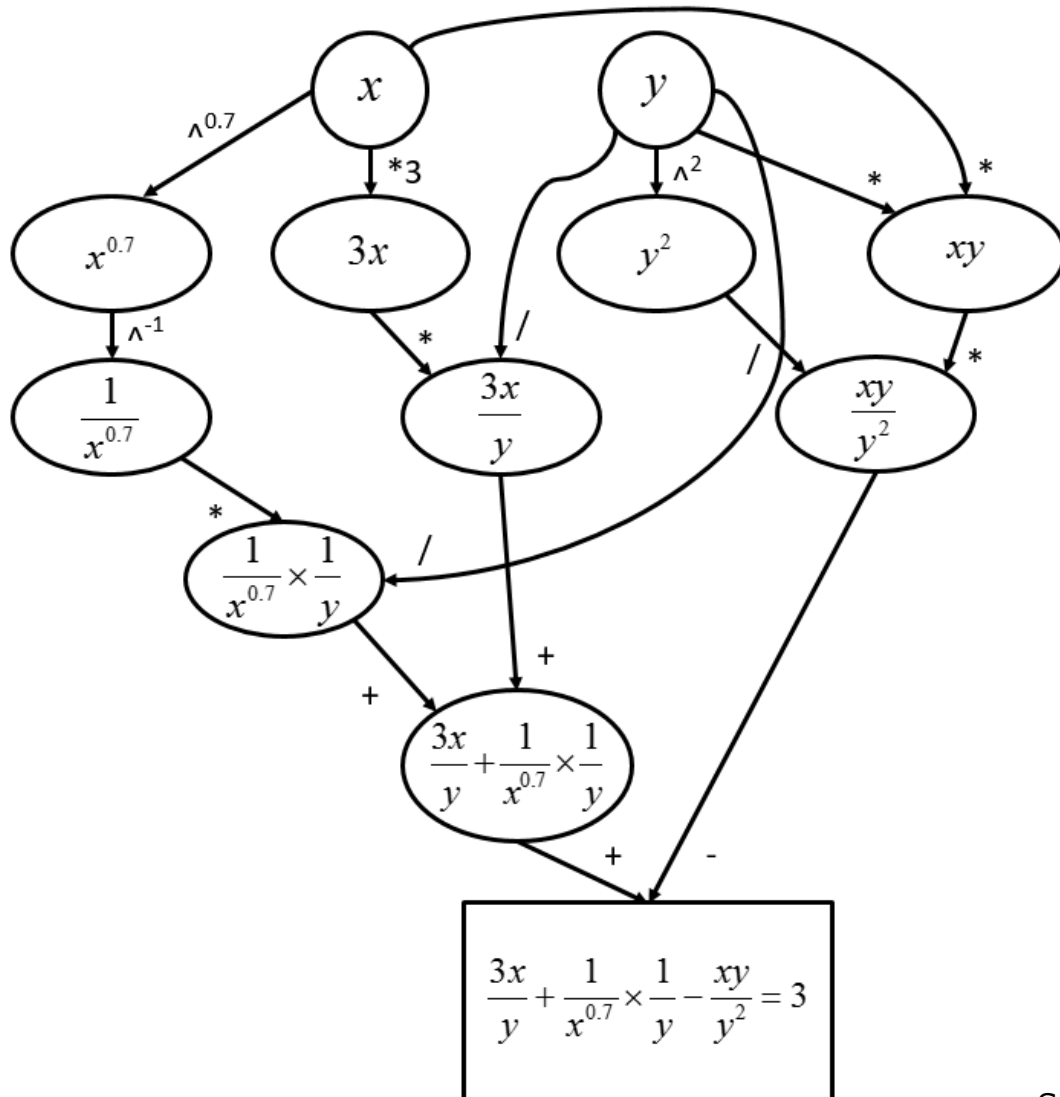
Constraints

DAG Representation



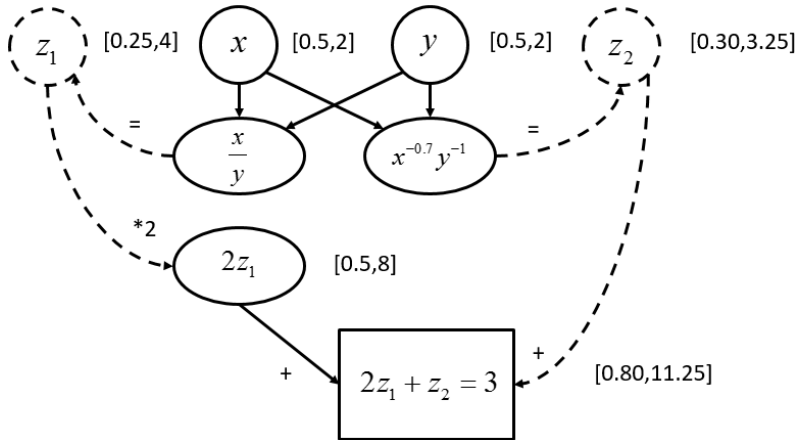
# GOSSIP

## Automatic Structure Detection



# GOSSIP

## Bounds Tightening Techniques



### Recourse Variables

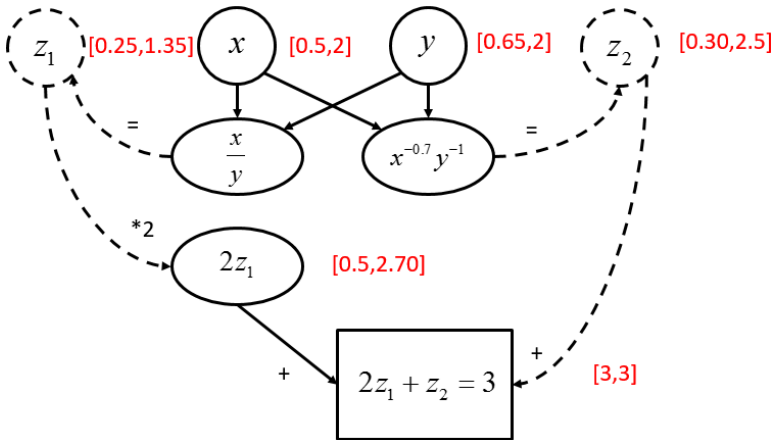
$$x_h^{i,L} = \min_{x_h, y, z} x_h^i$$

$$\text{s.t. } g_h^{\text{cv}}(x_h) + B_{y,h}y + B_{z,h}z \leq 0,$$

$$A_y y + A_z z \leq d_{y,z},$$

$$x_h \in \text{conv}(X_h),$$

$$y \in Y, z \in Z.$$



### Complicating Variables

$$z_h^{i,L} = \max_h \min_{x_h, y, z_h} z_h^i$$

$$\text{s.t. } g_h^{\text{cv}}(x_h) + B_{y,h}y + B_{z,h}z_h \leq 0,$$

$$A_y y + A_z z_h \leq d_{y,z},$$

$$x_h \in \text{conv}(X_h),$$

$$y \in Y, z_h \in Z.$$



# 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                                       |
| $x_1^{c_1} \cdot x_2^{c_2} \dots x_n^{c_n}$ | Bilinear reformulation, Secant, Transformation-based relaxations |

# GOSSIP

## Upper Bounding Techniques

### Lower Bounding Problem

$$\begin{aligned}
 & \sup_{\lambda_1, \dots, \lambda_{s-1}} \min_{\substack{x_1, \dots, x_s, y, \\ z_1, \dots, z_s}} \sum_{h=1}^s \left( p_h \left[ f_h(x_h) + c_{y,h}^T y + c_{z,h}^T z_h \right] \right) + \sum_{h=1}^{s-1} \lambda_h^T (z_h - z_{h+1}) \\
 & \text{s.t.} \quad g_h(x_h) + B_{y,h} y + B_{z,h} z_h \leq 0, \quad \forall h \in \{1, \dots, s\}, \\
 & \quad A_y y + A_z z_h \leq d_{y,z}, \quad \forall h \in \{1, \dots, s\}, \\
 & \quad x_h \in X_h, \quad z_h \in Z, \quad \forall h \in \{1, \dots, s\}, \\
 & \quad y \in Y.
 \end{aligned}$$

### Upper Bounding Problem

$$\begin{aligned}
 & \min_{\substack{x_1, \dots, x_s, y, \\ z_1, \dots, z_s}} \sum_{h=1}^s p_h \left[ f_h(x_h) + c_{y,h}^T y + c_{z,h}^T z_h \right] \\
 & \text{s.t.} \quad g_h(x_h) + B_{y,h} y + B_{z,h} z_h \leq 0, \quad \forall h \in \{1, \dots, s\}, \\
 & \quad A_y y + A_z z_h \leq d_{y,z}, \quad \forall h \in \{1, \dots, s\}, \\
 & \quad z_h = z_{h+1}, \quad \forall h \in \{1, \dots, s-1\}, \\
 & \quad x_h \in X_h, \quad z_h \in Z, \quad \forall h \in \{1, \dots, s\}, \\
 & \quad y \in Y.
 \end{aligned}$$

- Fix the binary variables in the upper bounding problem to the lower bounding solution
- Initialize the continuous second-stage variables to the lower bounding solution
- Initialize the continuous first-stage variables to the average lower bounding solution