A Decomposition Strategy for a Class of Nonconvex Two-Stage Stochastic Programs

Rohit Kannan and Paul I. Barton

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

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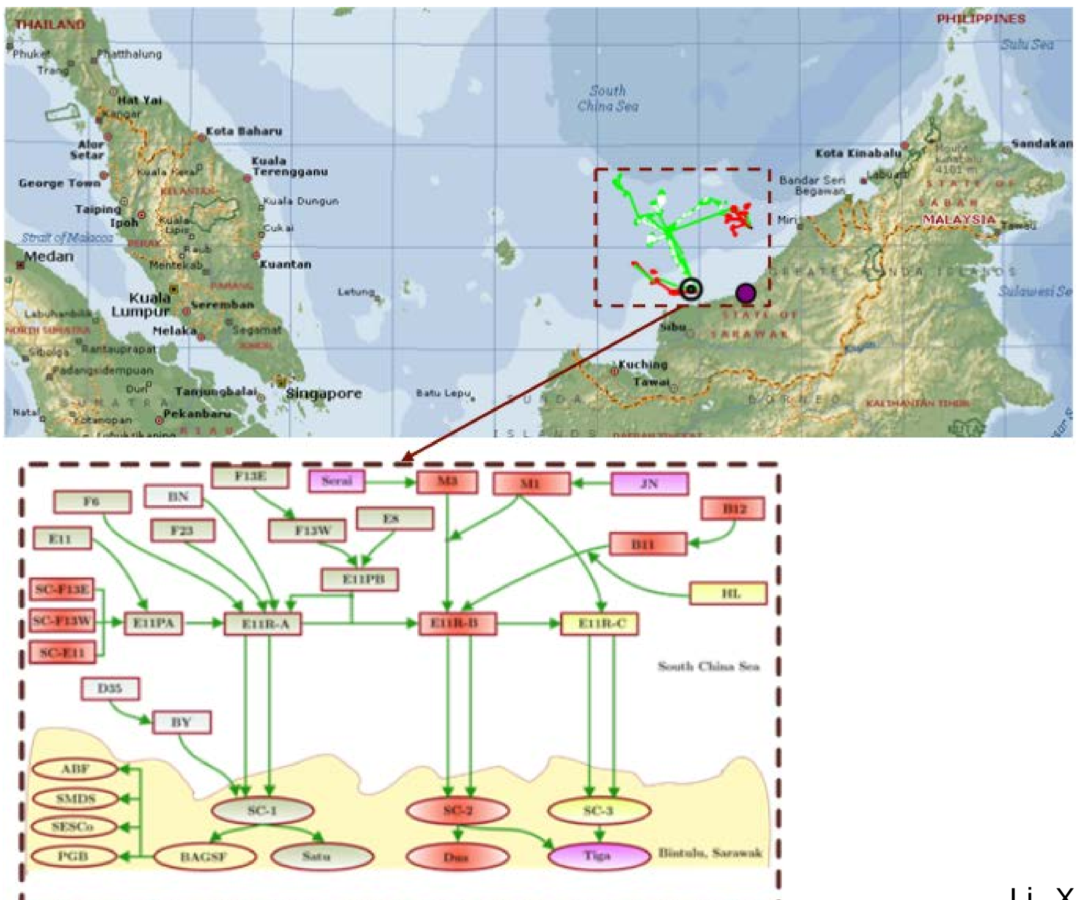
Motivation

- Uncertainty in problem data is a common feature of many real-life problems



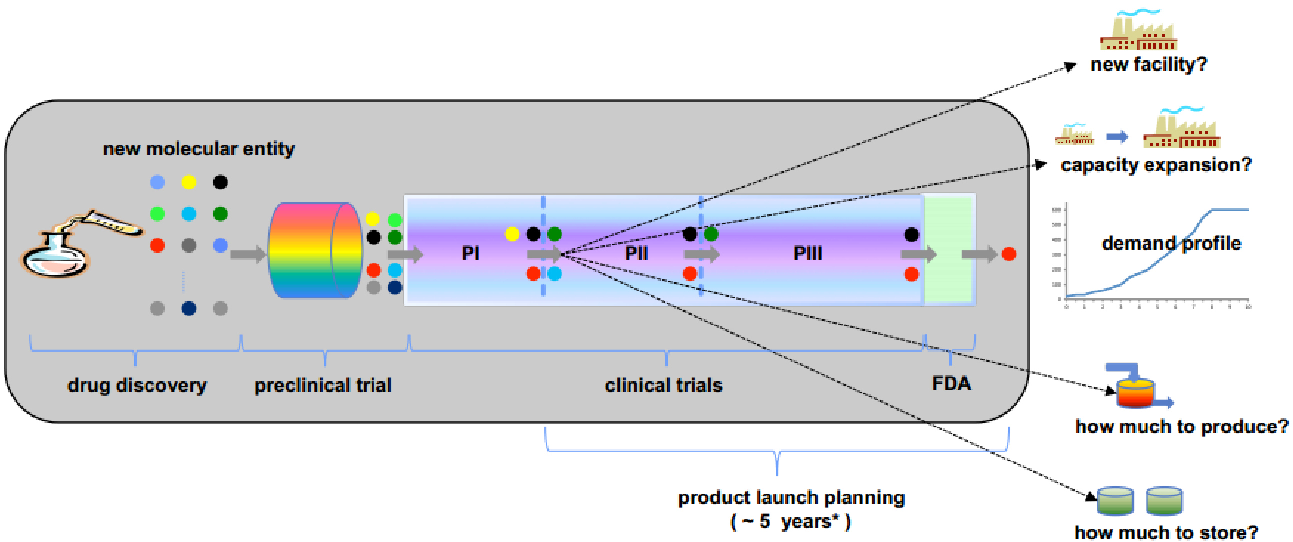
Sarawak Gas Production System

- Annual revenue of US $5 billion (4% of Malaysia's GDP)

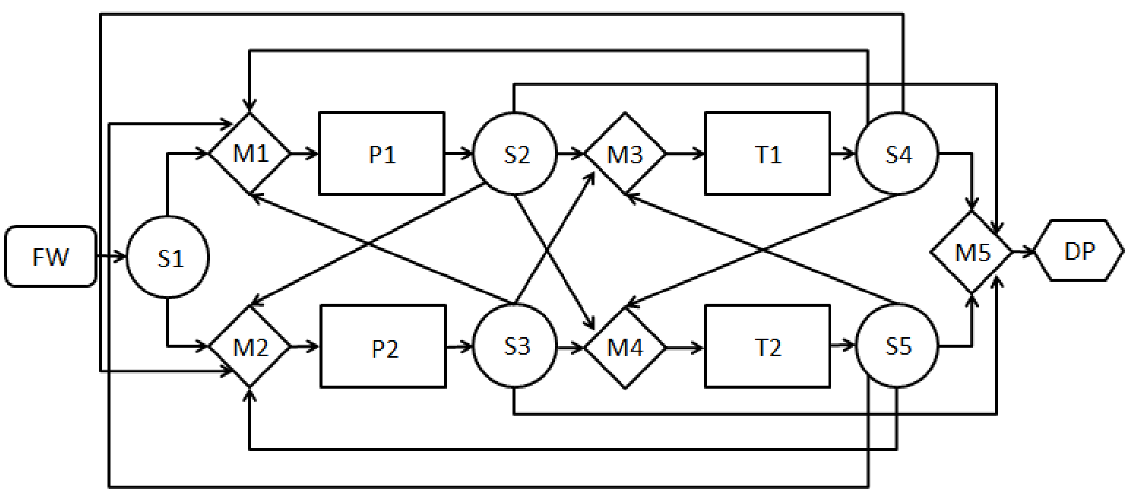
Li, X. et al., *AIChE J.*, 2011.

Motivation

More Chemical Engineering Applications



- Pharmaceutical capacity planning



- Integrated Water Networks

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

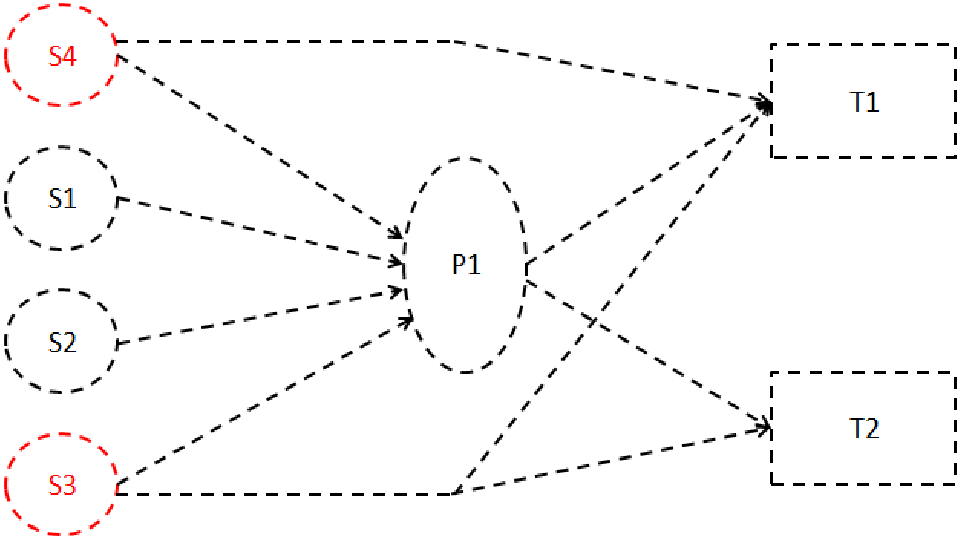
Karuppiah, R. et al., *Comput. Chem. Eng.*, 2008.

Motivation

Importance of Addressing Uncertainties

Stochastic pooling problem

Superstructure



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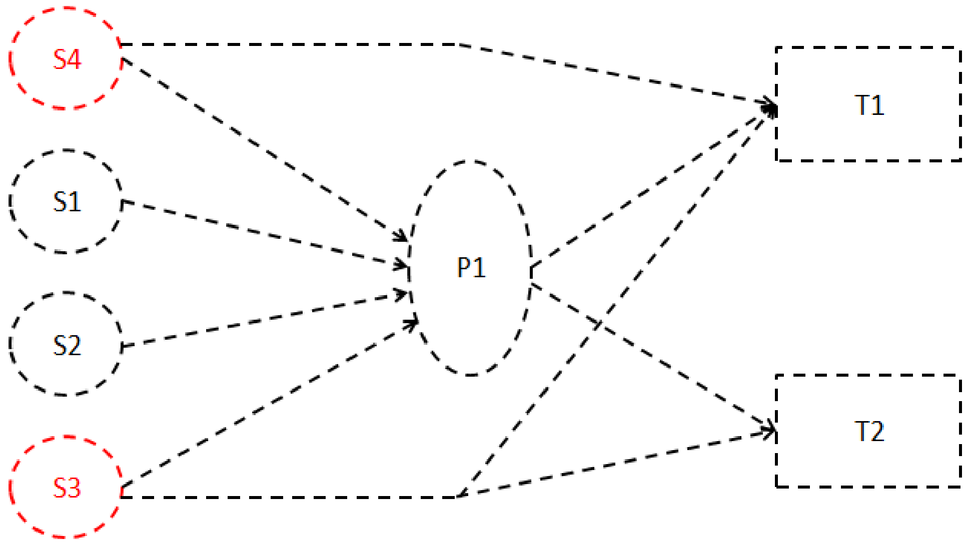
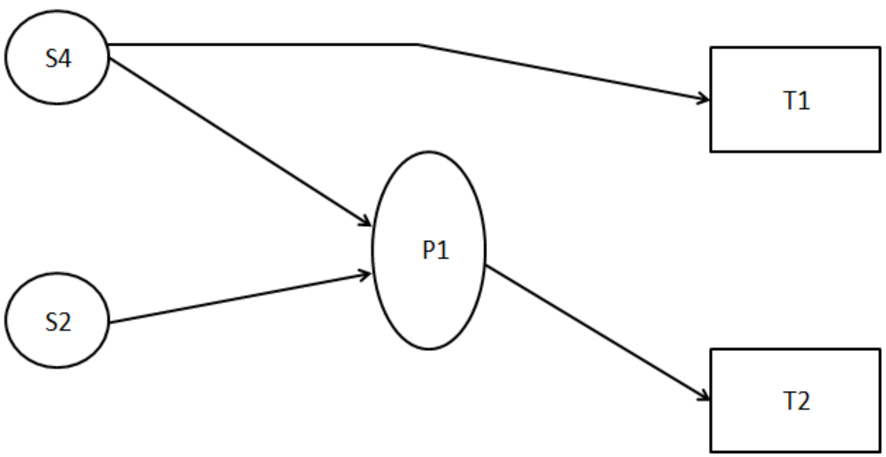
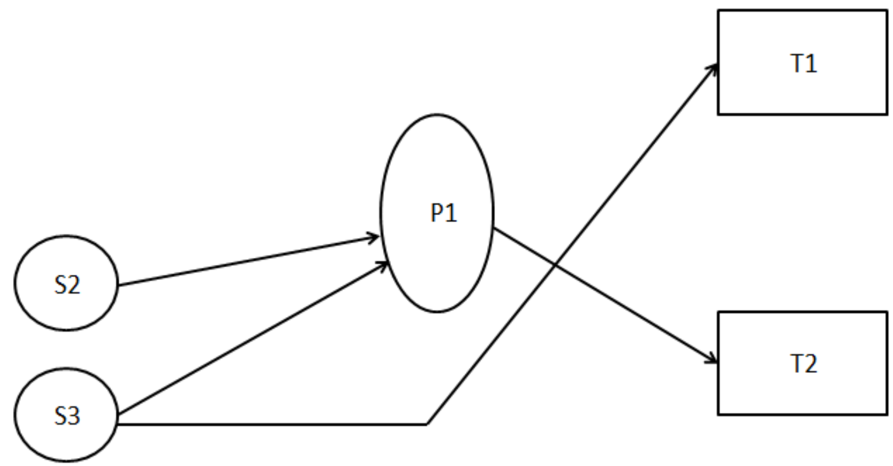


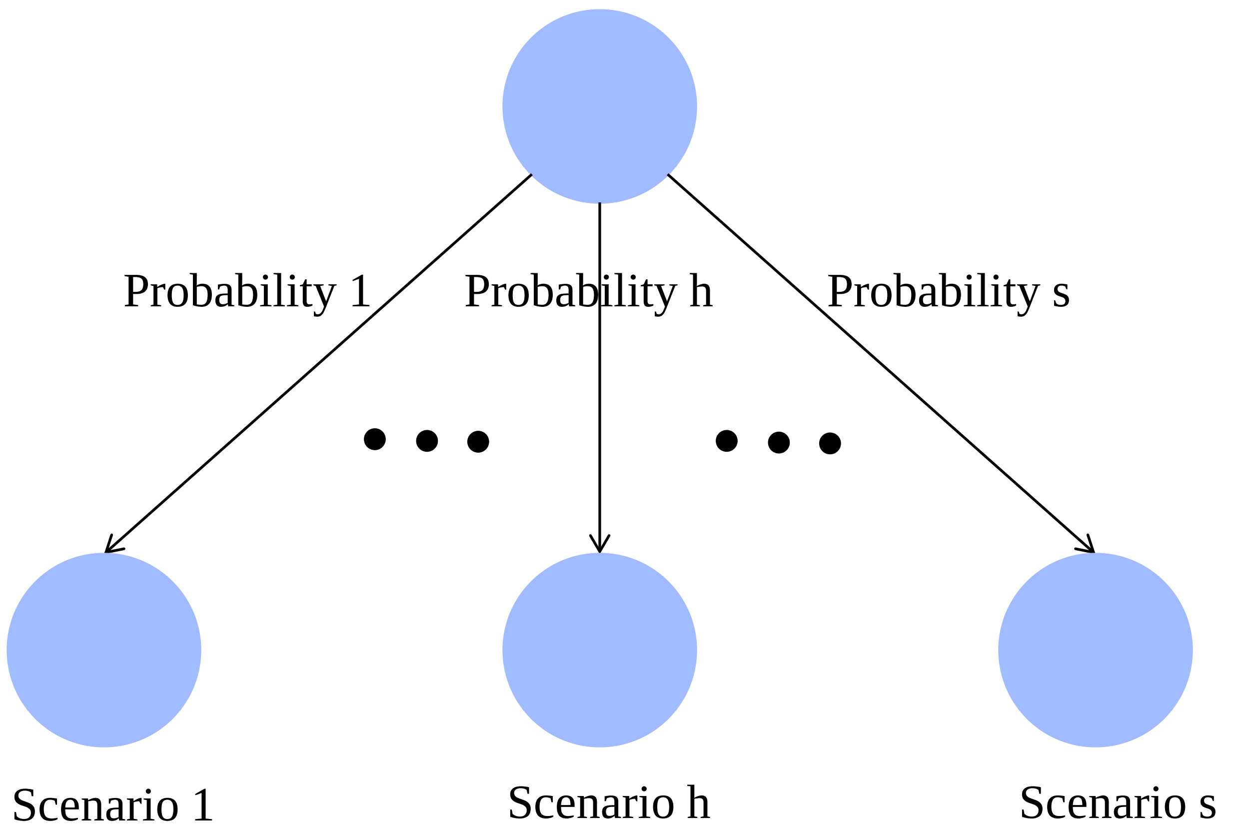


Deterministic solution



Stochastic solution

Two-Stage Stochastic Programming Framework



Stage 1 decisions
- made before the realization of the uncertainty
- e.g., design decisions

Realization of the uncertainty
- e.g., source qualities

Stage 2 decisions
- made after the realization of the uncertainty
- e.g., operational decisions

Nonconvex Two-Stage Stochastic Programs

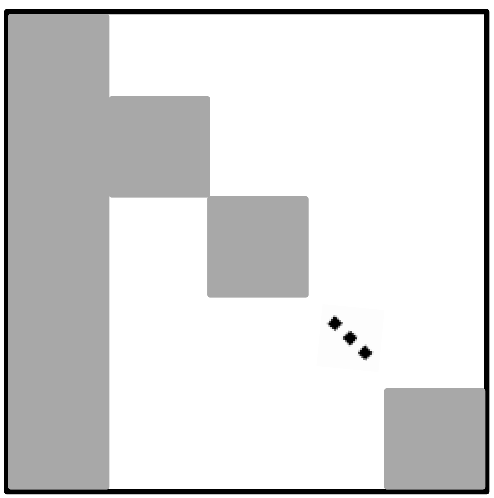
$$\begin{aligned} \min_{x_1,\cdots,x_s,y,z} \quad & \sum_{h=1}^{s} p_h f_h(x_h, y, z) && \text{(P)} \\ \text{s.t.} \quad & g_h(x_h, y, z) \leq 0, \ \forall h \in \{1,\cdots,s\}, \\ & x_h \in X_h \subset \{0,1\}^{n_{x_b}} \times \mathbb{R}^{n_{x_c}}, \ \forall h \in \{1,\cdots,s\}, \\ & y \in Y \subset \{0,1\}^{n_y}, \ z \in Z \subset \mathbb{R}^{n_z}. \end{aligned}$$

Assumptions: f_h, g_h, $\forall h \in \{1,\cdots,s\}$, continuous;
X_h, $\forall h \in \{1,\cdots,s\}$, Y, and Z nonempty; and
X_h, $\forall h \in \{1,\cdots,s\}$, and Z compact.

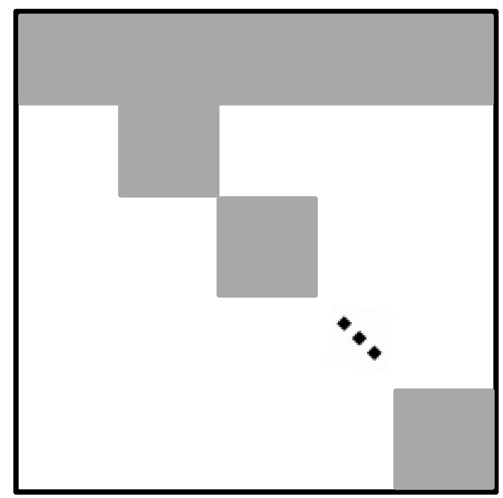
Existing Decomposition Approaches

$$
\begin{aligned}
\min_{x_1,\cdots,x_s,y} \quad & \sum_{h=1}^{s} p_h f_h(x_h, y) \\
\text{s.t.} \quad & g_h(x_h, y) \le 0, \ \forall h \in \{1,\cdots,s\}, \\
& x_h \in X_h \subset \{0,1\}^{n_{x_b}} \times \mathbb{R}^{n_{x_c}}, \ \forall h \in \{1,\cdots,s\}, \\
& y \in Y \subset \{0,1\}^{n_y}.
\end{aligned}
$$

$$
\begin{aligned}
\min_{\substack{x_1,\cdots,x_s,\\ y_1,\cdots,y_s,\\ z_1,\cdots,z_s}} \quad & \sum_{h=1}^{s} p_h f_h(x_h, y_h, z_h) \\
\text{s.t.} \quad & g_h(x_h, y_h, z_h) \le 0, \ \forall h \in \{1,\cdots,s\}, \\
& y_h - y_{h+1} = 0, \ \forall h \in \{1,\cdots,s-1\}, \\
& z_h - z_{h+1} = 0, \ \forall h \in \{1,\cdots,s-1\}, \\
& x_h \in X_h \subset \{0,1\}^{n_{x_b}} \times \mathbb{R}^{n_{x_c}}, \ \forall h \in \{1,\cdots,s\}, \\
& y_h \in Y \subset \{0,1\}^{n_y}, z_h \in Z \subset \mathbb{R}^{n_z}, \ \forall h \in \{1,\cdots,s\}.
\end{aligned}
$$

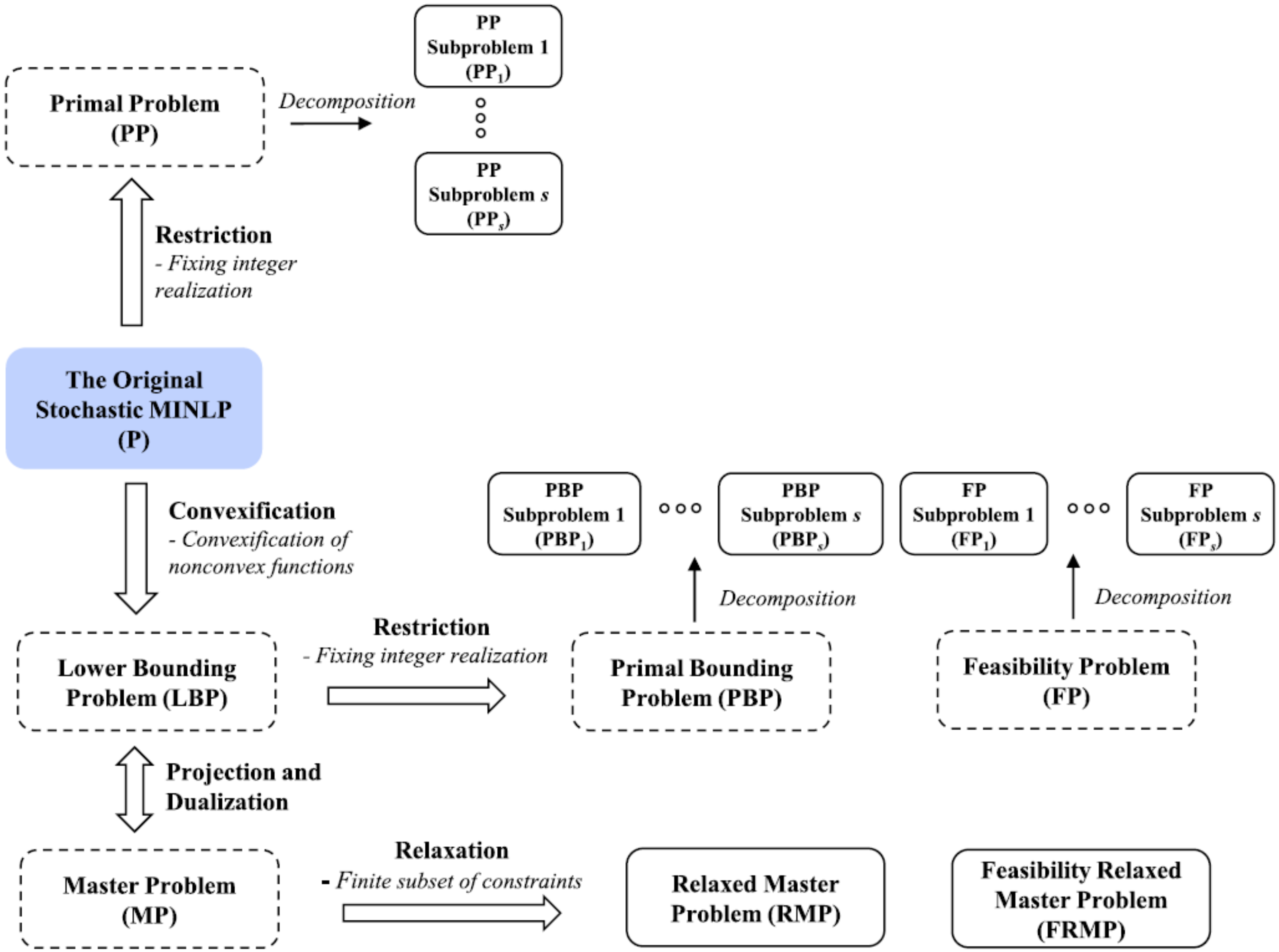


Nonconvex Generalized Benders Decomposition



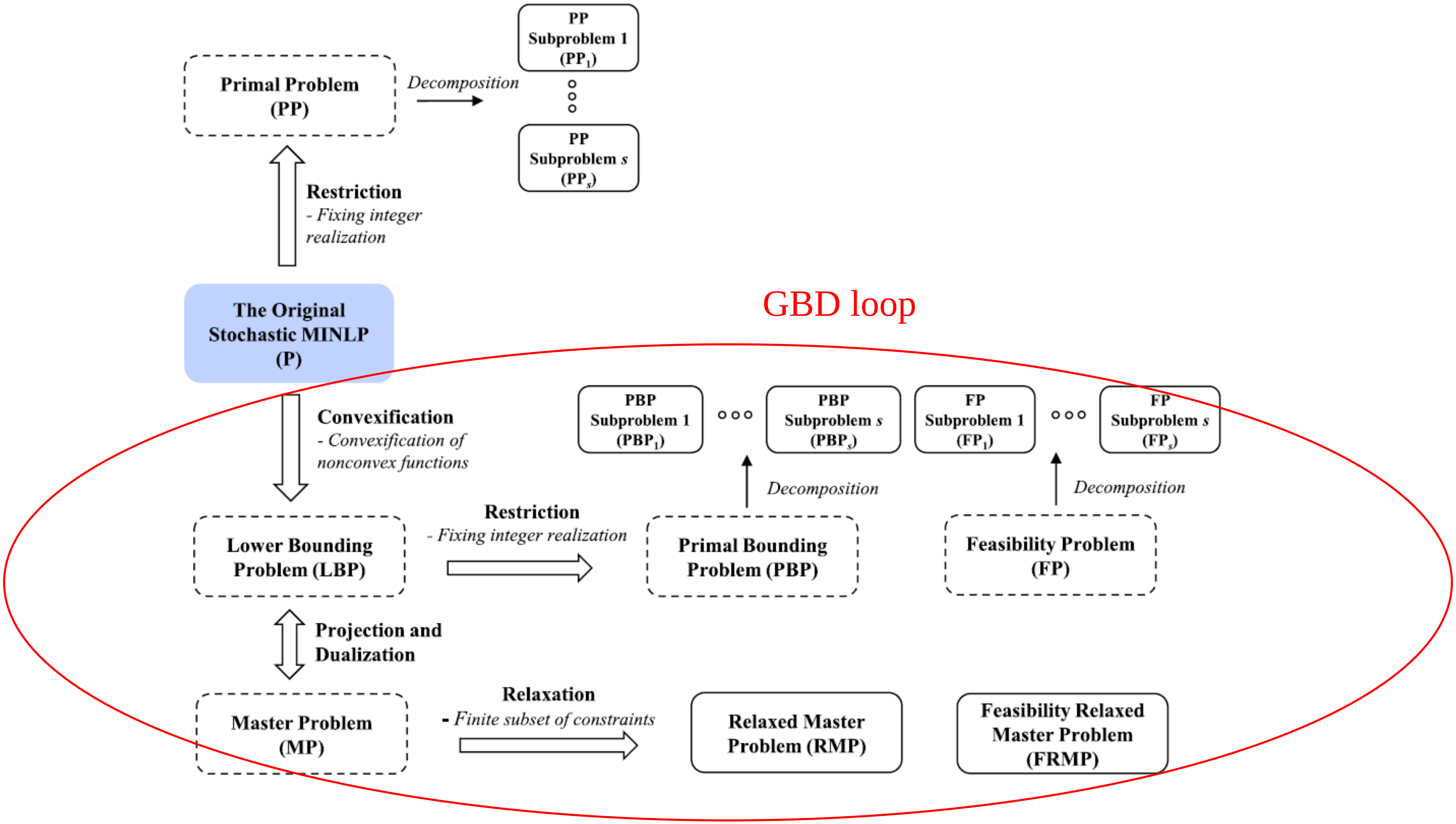
Lagrangian Relaxation

Nonconvex Generalized Benders Decomposition



Li, X. et al., *J. Optim. Theory Appl.*, 2011.

Nonconvex Generalized Benders Decomposition



Li, X. et al., *J. Optim. Theory Appl.*, 2011.

Nonconvex Generalized Benders Decomposition

Convergence

- At present, the NGBD algorithm only converges if the first-stage (complicating) decisions are integers
  - In this case, finite convergence to a solution within a given tolerance of a global minimum is guaranteed

Nonconvex Generalized Benders Decomposition
Convergence

- At present, the NGBD algorithm only converges if the first-stage (complicating) decisions are integers
  - In this case, finite convergence to a solution within a given tolerance of a global minimum is guaranteed

- In practice, only a small fraction of the integer realizations in the set Y are visited by the primal problem
  - Strength of relaxations of the nonconvex functions is important

Lagrangian Relaxation

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

$$\begin{aligned}
\text{s.t.}\quad & g_h(x_h, y_h, z_h) \le 0,\ \forall h \in \{1,\cdots,s\}, \\
& \left.\begin{aligned} & y_h - y_{h+1} = 0,\ \forall h \in \{1,\cdots,s-1\}, \\ & z_h - z_{h+1} = 0,\ \forall h \in \{1,\cdots,s-1\}, \end{aligned}\right\} \text{Non-anticipativity constraints} \\
& x_h \in X_h \subset \{0,1\}^{n_{x_b}} \times \mathbb{R}^{n_{x_c}},\ \forall h \in \{1,\cdots,s\}, \\
& y_h \in Y \subset \{0,1\}^{n_y},\ z_h \in Z \subset \mathbb{R}^{n_z},\ \forall h \in \{1,\cdots,s\}.
\end{aligned}$$

- The non-anticipativity constraints are hard constraints which link the different scenario problems

Lagrangian Relaxation
Lower Bounding Problem

$$\max_{\substack{\alpha_1,\cdots,\alpha_{s-1},\\ \beta_1,\cdots,\beta_{s-1}}} \quad \min_{\substack{x_1,\cdots,x_s,\\ y_1,\cdots,y_s,\\ z_1,\cdots,z_s}} \sum_{h=1}^{s} p_h f_h(x_h, y_h, z_h) + \sum_{h=1}^{s-1} \alpha_h^T (y_h - y_{h+1}) + \sum_{h=1}^{s-1} \beta_h^T (z_h - z_{h+1}) \qquad \text{(LRP)}$$

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

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

α_h, β_h are Lagrange multipliers

- Dualizing the non-anticipativity constraints provides a valid lower bounding problem ...

Lagrangian Relaxation

Lower Bounding Problem

$$\max_{\substack{\alpha_1,\cdots,\alpha_{s-1},\\ \beta_1,\cdots,\beta_{s-1}}} \min_{\substack{x_1,\cdots,x_s,\\ y_1,\cdots,y_s,\\ z_1,\cdots,z_s}} \sum_{h=1}^{s} p_h f_h(x_h, y_h, z_h) + \sum_{h=1}^{s-1} \alpha_h^T (y_h - y_{h+1}) + \sum_{h=1}^{s-1} \beta_h^T (z_h - z_{h+1}) \qquad \text{(LRP)}$$

$\alpha_h,\ \beta_h$ are Lagrange multipliers

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

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

- Dualizing the non-anticipativity constraints provides a valid lower bounding problem ...

... the inner minimization of which is decomposable

Lagrangian Relaxation
Convergence

- A branch and bound algorithm is employed to guarantee convergence
  - Sufficient to branch on the complicating variables (y, z) to converge

Lagrangian Relaxation
Convergence

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- Branching rule
  - Branch on the complicating variable with the maximum *dispersion*
  - An occasional bisection is performed to guarantee convergence

Lagrangian Relaxation
Convergence

- A branch and bound algorithm is employed to guarantee convergence
  - Sufficient to branch on the complicating variables (y, z) to converge
- Branching rule
  - Branch on the complicating variable with the maximum *dispersion*
  - An occasional bisection is performed to guarantee convergence
- The conventional Lagrangian relaxation algorithm may take a long time to converge
  - Requires the solution of several nonconvex MINLPs to obtain lower bounds
  - Multiple iterations of an algorithm applied to the dual may be required to generate tight lower bounds

Improved Lagrangian Relaxation

- Observation: The inner minimization of the dual problem can be solved using NGBD if the non-anticipativity constraints of only the continuous complicating variables are relaxed

$$\max_{\substack{\alpha_1,\cdots,\alpha_{s-1},\\ \beta_1,\cdots,\beta_{s-1}}} \min_{\substack{x_1,\cdots,x_s,\\ y_1,\cdots,y_s,\\ z_1,\cdots,z_s}} \sum_{h=1}^{s} p_h f_h(x_h, y_h, z_h) + \sum_{h=1}^{s-1} \alpha_h^T (y_h - y_{h+1}) + \sum_{h=1}^{s-1} \beta_h^T (z_h - z_{h+1}) \qquad \text{(LRP)}$$

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

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

Improved Lagrangian Relaxation

$$\max_{\beta_1,\cdots,\beta_{s-1}} \min_{\substack{x_1,\cdots,x_s,\\ y,z_1,\cdots,z_s}} \sum_{h=1}^{s} p_h f_h(x_h, y, z_h) + \sum_{h=1}^{s-1} \beta_h^T (z_h - z_{h+1}) \qquad \text{(LRP-NGBD)}$$

$$\begin{aligned} \text{s.t. } & g_h(x_h, y, z_h) \le 0, \ \forall h \in \{1,\cdots,s\}, \\ & x_h \in X_h, \ z_h \in Z, \ \forall h \in \{1,\cdots,s\}, \\ & y \in Y. \end{aligned}$$

Improved Lagrangian Relaxation

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

$$y \in Y.$$

- The inner minimization of Problem (LRP-NGBD) is not decomposable, but can be solved in a decomposable manner using NGBD

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$$\max_{\beta_1,\cdots,\beta_{s-1}} \min_{\substack{x_1,\cdots,x_s,\\ y,z_1,\cdots,z_s}} \sum_{h=1}^{s} p_h f_h(x_h,y,z_h) + \sum_{h=1}^{s-1} \beta_h^T (z_h - z_{h+1}) \qquad \text{(LRP-NGBD)}$$

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- The inner minimization of Problem (LRP-NGBD) is not decomposable, but can be solved in a decomposable manner using NGBD
- The above lower bounding problem provides tighter lower bounds than Problem (LRP)
- Sufficient to branch on the continuous complicating variables to converge

Improved Lagrangian Relaxation
Aggressive Bounds Tightening

- Tight bounds on the continuous complicating variables z may be required for good empirical convergence

Belotti, P. et al., *Optim. Method. Softw.*, 2009.

Improved Lagrangian Relaxation

Aggressive Bounds Tightening

- Tight bounds on the continuous complicating variables z may be required for good empirical convergence

- Suppose UBD is the current best upper bound for Problem (P), and $z^i \in [z^{i,lo}, z^{i,up}]$. If, for some $(\bar{z}^i, \bar{\beta})$, the optimal solution of the following lower bounding problem lies above UBD, then $z^i \in \left[\bar{z}^i, z^{i,up}\right]$ is a valid tightening

$$
\begin{aligned}
\min_{\substack{x_1,\cdots,x_s,\\ y,z_1,\cdots,z_s}} \quad & \sum_{h=1}^{s} p_h f_h(x_h, y, z_h) + \sum_{h=1}^{s-1} \bar{\beta}_h^T (z_h - z_{h+1}) \\
\text{s.t.} \quad & g_h(x_h, y, z_h) \le 0, \ \forall h \in \{1, \cdots, s\}, \\
& x_h \in X_h, \ z_h \in Z \cap \{z : z^i \le \bar{z}^i\}, \ \forall h \in \{1, \cdots, s\}, \\
& y \in Y.
\end{aligned}
$$

Nonconvex MINLP

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Improved Lagrangian Relaxation

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$$\min_{\substack{x_1,\cdots,x_s,\\ y,z_1,\cdots,z_s}} \sum_{h=1}^{s} p_h f_h(x_h, y, z_h) + \sum_{h=1}^{s-1} \bar{\beta}_h^T (z_h - z_{h+1})$$

Nonconvex MINLP

Can be solved using NGBD!

$$\begin{aligned}
\text{s.t. } & g_h(x_h, y, z_h) \le 0, \ \forall h \in \{1, \cdots, s\}, \\
& x_h \in X_h, \ z_h \in Z \cap \{z : z^i \le \bar{z}^i\}, \ \forall h \in \{1, \cdots, s\}, \\
& y \in Y.
\end{aligned}$$

Belotti, P. et al., *Optim. Method. Softw.*, 2009.

Improved Lagrangian Relaxation
Aggressive Bounds Tightening

- Multiple ABT iterations are carried out on a per-variable basis

- Solution of the lower bounding problem for ABT can be terminated if
  - the lower bound for the lower bounding problem, obtained during the NGBD algorithm, is larger than the current upper bound (fewer primal problems solved)
  - a feasible solution for the lower bounding problem which is smaller than the current upper bound is found

Improved Lagrangian Relaxation

Upper Bounds

- ABT requires a good upper bound to be able to effectively tighten the bounds of the continuous complicating variables

Improved Lagrangian Relaxation

Upper Bounds

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- Good upper bounds can be generated by solving Problem (P) using DICOPT, or by restricting the binary variables and solving the resulting problem using local solvers such as CONOPT
  - Local solvers which utilize the near-decomposable structure of Problem (P), through techniques such as Schur complements, can be employed

Improved Lagrangian Relaxation
Upper Bounds

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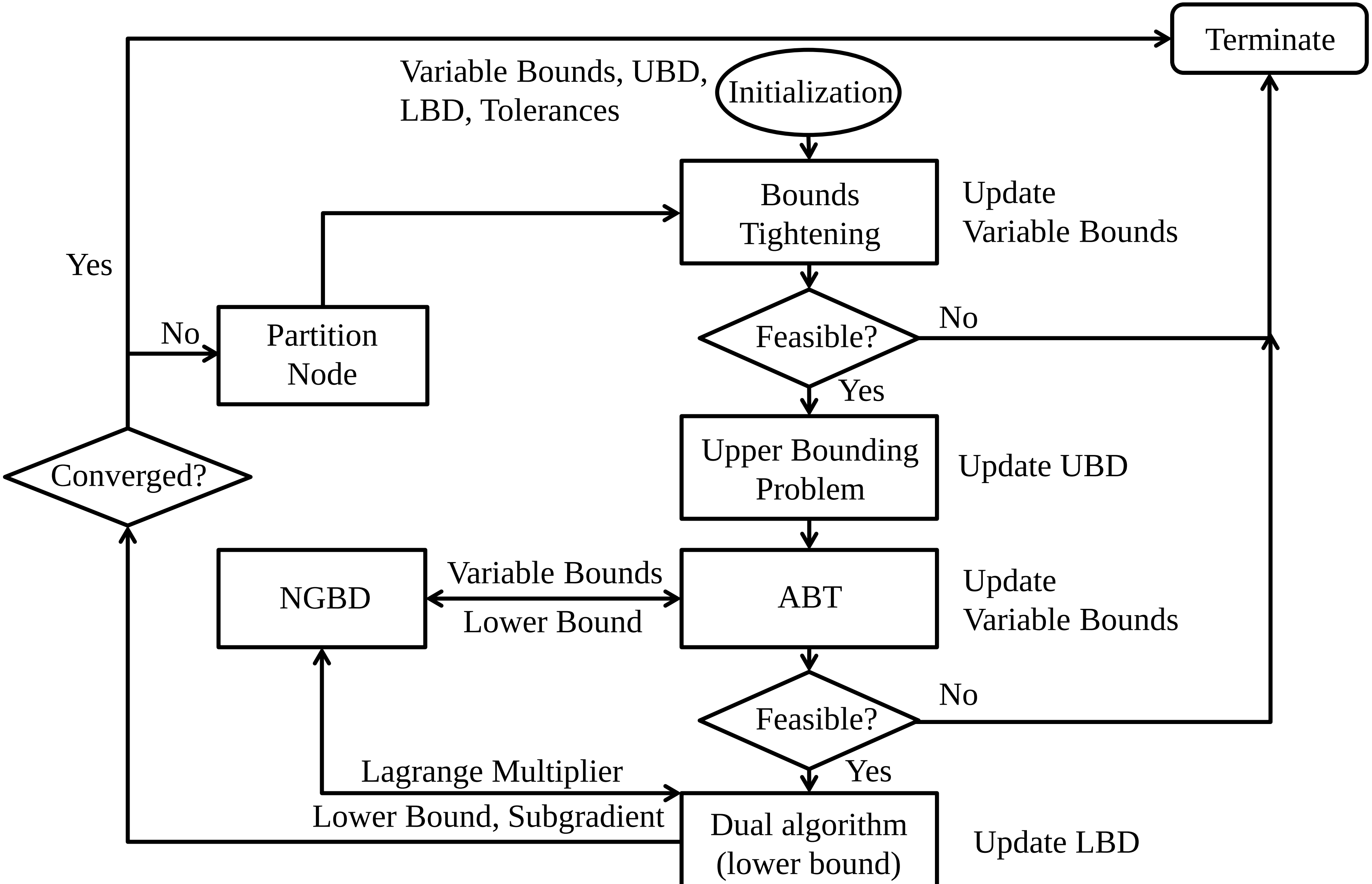
- Good upper bounds can be generated by solving Problem (P) using DICOPT, or by restricting the binary variables and solving the resulting problem using local solvers such as CONOPT
  - Local solvers which utilize the near-decomposable structure of Problem (P), through techniques such as Schur complements, can be employed

- Upper bounds can also be generated by attempting to solve Problem (P) using NGBD, or by restricting the continuous complicating variables and solving the resulting problem using NGBD

Improved Lagrangian Relaxation

Flowchart

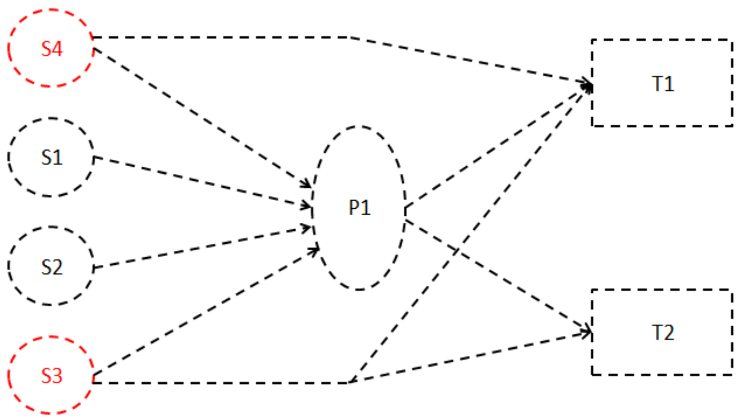


Computational Studies
Implementation Details

- **Platform**
  - CPU 3.07 GHz, Memory 12.0 GB, VMWare Linux Workstation on Windows 7 Desktop, GAMS 24.2, GCC 4.8.1, GFortran 4.8.1
- **Solvers**
  - LP and MILP solver: CPLEX
  - Global NLP solver: ANTIGONE
  - Local NLP solver: CONOPT
  - Upper bound solver: DICOPT
  - Bundle solver: MPBNGC 2.0
- **Methods for comparison**
  - ANTIGONE, BARON – State-of-the-art global optimization solvers
  - Conventional Lagrangian relaxation algorithm
  - Improved Lagrangian relaxation algorithm
- **Relative and absolute tolerance: 10^{-3}**

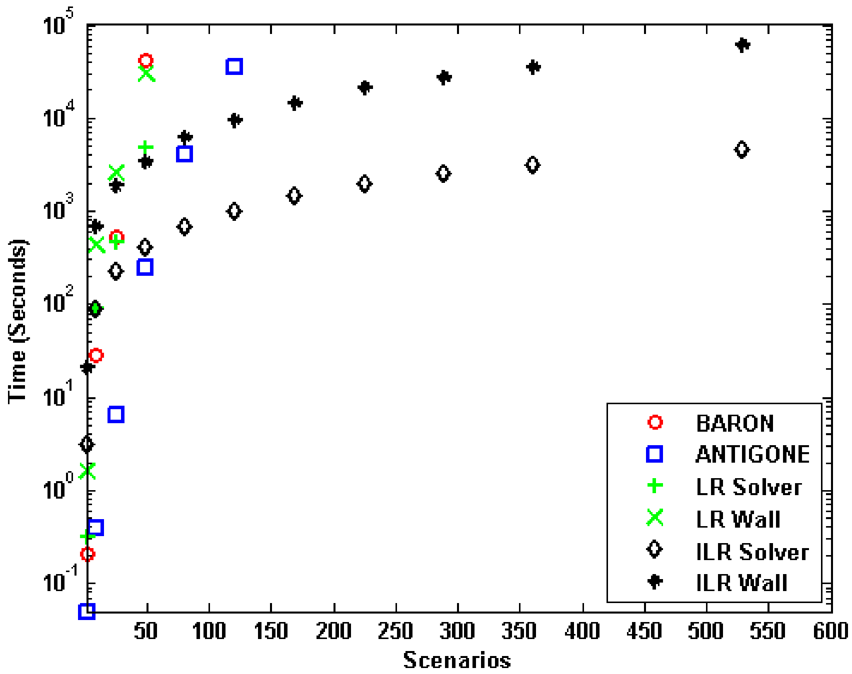
Computational Study

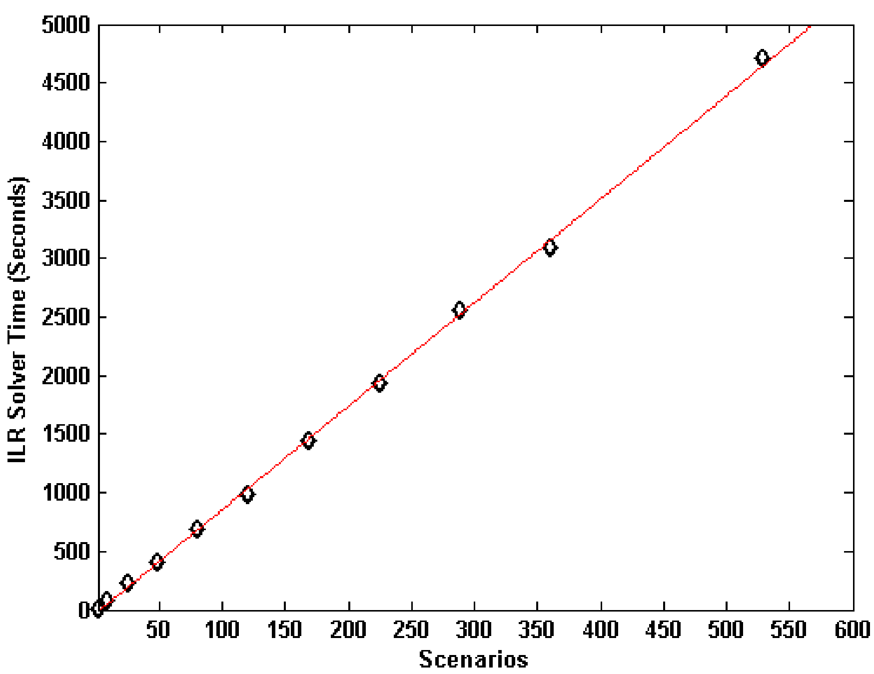
Case Study 1: Stochastic Pooling Problem



16 binary complicating variables,
4 continuous complicating variables,
13s continuous recourse variables
16s bilinear terms

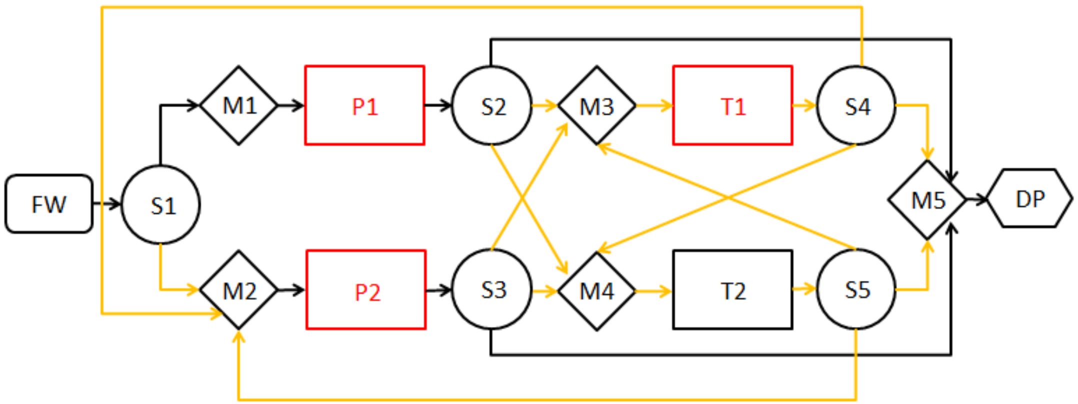
(s represents the number of scenarios).





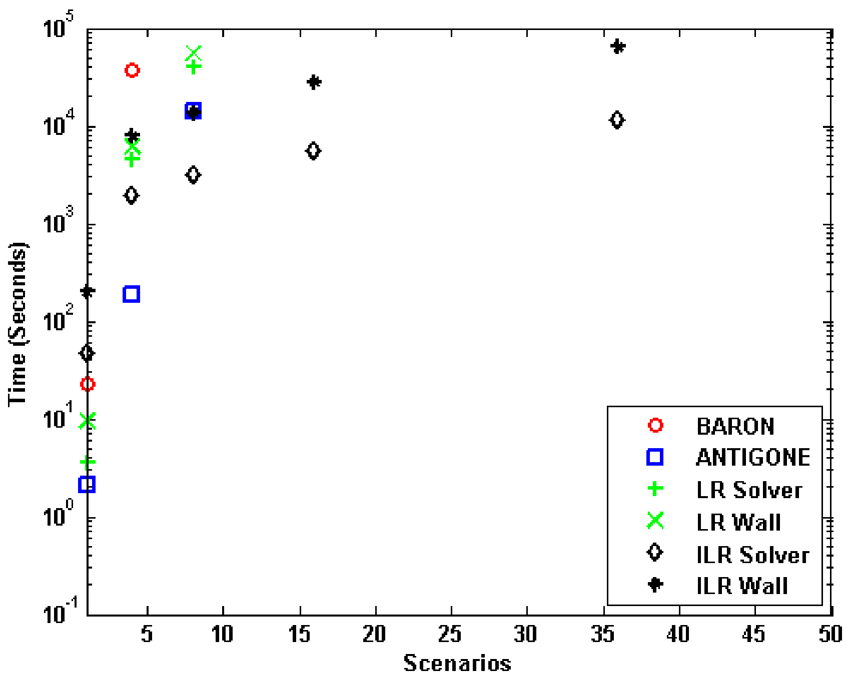
Computational Study

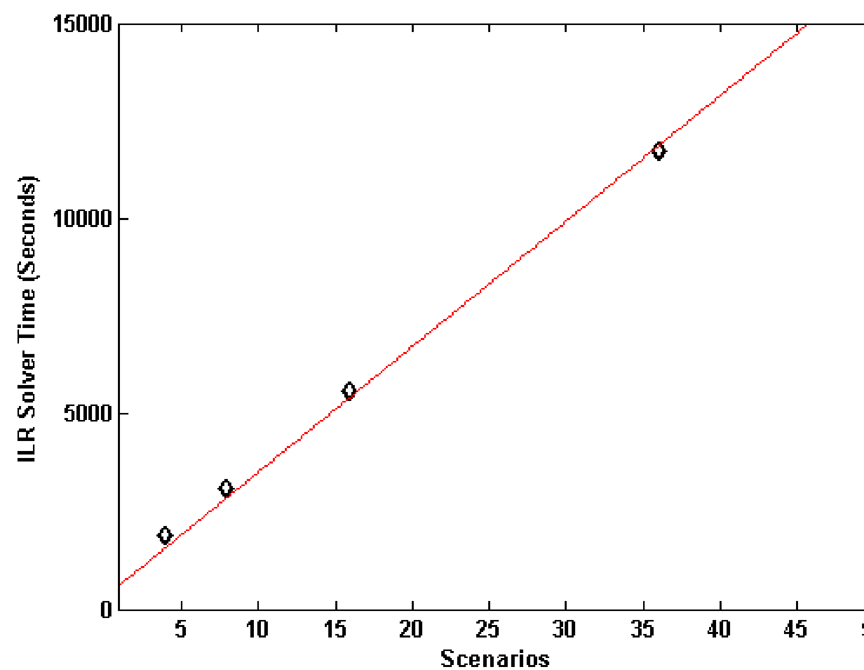
Case Study 2: Integrated Water Network



15 binary complicating variables,
20 continuous complicating variables,
94s continuous recourse variables
242s bilinear terms

(s represents the number of scenarios).





Conclusions and future work

- Nonconvex generalized Benders decomposition can be used in conjunction with bounds tightening techniques to improve the performance of the Lagrangian relaxation algorithm for general nonconvex two-stage stochastic programs

- Develop decomposition techniques to obtain good upper bounds

- Look at efficient ways to solve the dual problem

- Extend the algorithm to multi-stage problems

Acknowledgements

- The Barton group