Nonconvex Generalized Benders Decomposition

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Motivation

Two-stage Stochastic MINLPs & MILPs

$$\min_{x_1,\ldots,x_s,y} \quad \sum_{h=1}^{s} w_h f_h(x_h, y)$$

$$\text{s.t.} \quad g_h(x_h, y) \le 0, \qquad h = 1,\ldots,s$$

$$x_h \in X_h, \quad h = 1,\ldots,s$$

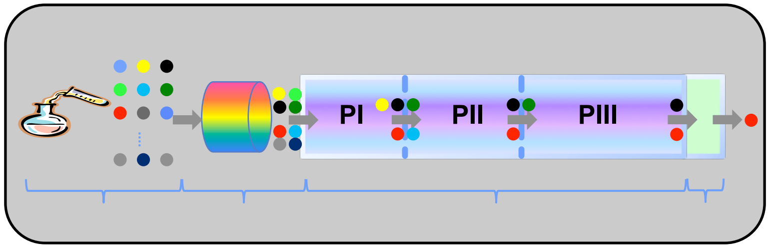
$$y \in Y \subset \{0,1\}^{n_y}$$

Natural Gas Production System

Energy Polygeneration Plant

Pump Network

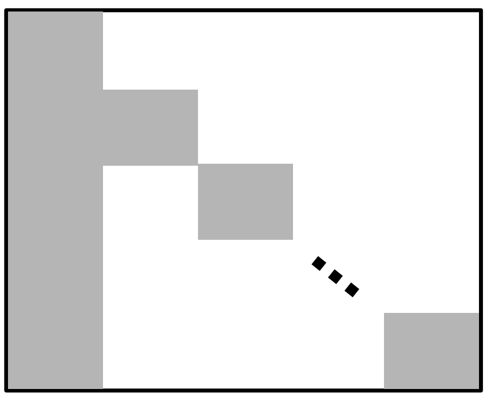
Oil Refinery



Pharmaceutical Product Launch

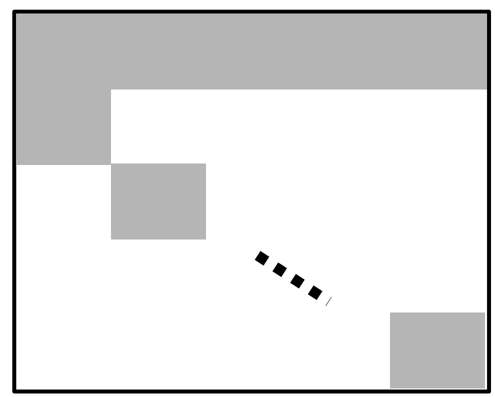
Two Different Decomposition Philosophies

$$\min_{x_1,\ldots,x_s,y} \sum_{h=1}^{s} w_h f_h(x_h, y)$$
$$\text{s.t.} \quad g_h(x_h, y) \le 0, \quad h = 1,\ldots,s$$
$$x_h \in X_h, \quad h = 1,\ldots,s$$
$$y \in Y \subset \{0,1\}^{n_y}$$



- Benders decomposition/L-shaped method
  - Linear duality
- Generalized Benders decomposition
  - Nonlinear duality
- **Nonconvex Generalized Benders decomposition**

$$\min_{x_1,\ldots,x_s,y_1,\ldots,y_s} \sum_{h=1}^{s} w_h f_h(x_h, y_h)$$
$$\text{s.t.} \quad g_h(x_h, y_h) \le 0, \quad h = 1,\ldots,s$$
$$y_h = y_{h+1}, \quad h = 1,\ldots,s-1$$
$$x_h \in X_h, \quad h = 1,\ldots,s$$
$$y_h \in Y \subset \{0,1\}^{n_y}$$



- Danzig-Wolfe decomposition
  - Linear duality
- Lagrangian relaxation
  - Nonlinear duality

Generalized Benders Decomposition

Master problem

$$\min_{x,y} \; f(x,y)$$
$$\text{s.t. } g(x,y) \le 0$$
$$x \in X, \; y \in Y$$

Master Problem

$$\min_{y,\eta} \; \eta$$
$$\text{s.t. } \eta \ge \inf_{x \in X} f(x,y) + \lambda^T g(x,y), \quad \forall \lambda \ge 0$$
$$0 \ge \inf_{x \in X} \mu^T g(x,y), \quad \forall \mu \in M$$

Optimality cuts

Feasibility cuts

$\Updownarrow$ **Projection**

$\Updownarrow$

$$\min_{y} \; \phi(y)$$
$$\text{s.t. } \phi(y) = \inf_{x \in X, g(x,y) \le 0} f(x,y)$$
$$y \in Y \cap V,$$
$$V = \{y : \exists x \in X, g\left(x,y\right) \le 0\}$$

Dualization $\Longleftrightarrow$

$$\min_{y \in Y} \; \phi(y)$$
$$\text{s.t. } \phi(y) = \sup_{\lambda \ge 0} \inf_{x \in X} f(x,y) + \lambda^T g(x,y)$$
$$0 \ge \inf_{x \in X} \mu^T g(x,y), \quad \forall \mu \in M$$

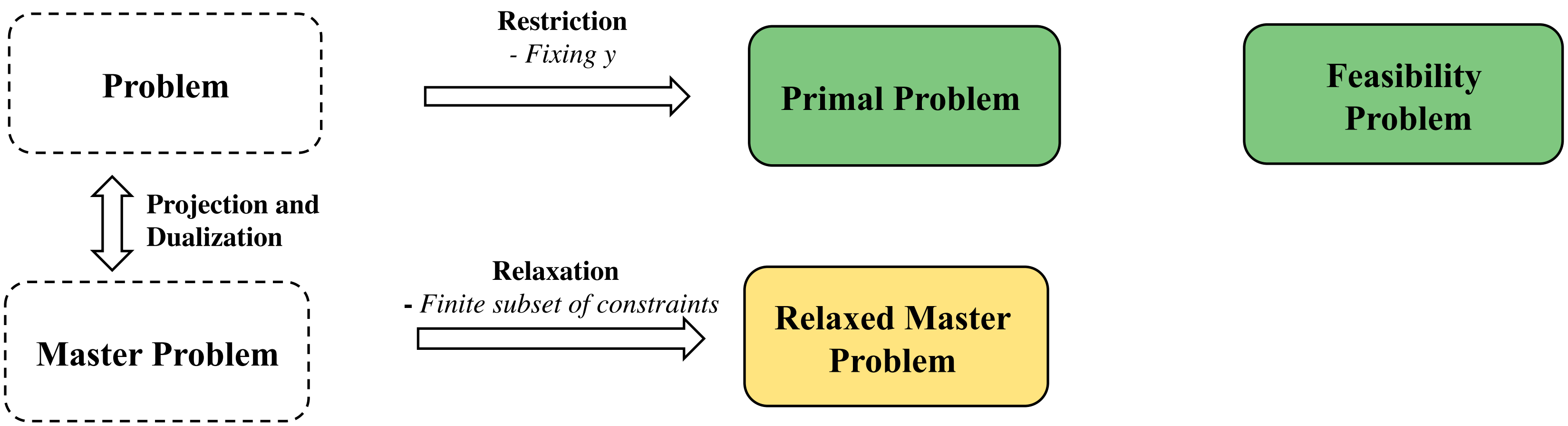
Generalized Benders Decomposition

Subproblems generated via restriction and relaxation

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

$$\begin{aligned}obj^{k}_{Primal} = \min_{x}\ & f(x,y^{(k)})\\ s.t.\ & g(x,y^{(k)})\le 0\\ & x\in X\end{aligned}$$

$$\begin{aligned}obj^{k}_{Feas} = \min_{x}\ & \lVert z\rVert\\ s.t.\ & g(x,y^{(k)})\le z,\\ & x\in X, z\in Z\subset\{z\in\mathbb{R}^m : z\ge 0\}\end{aligned}$$



$$\begin{aligned}\min_{y,\eta}\ & \eta\\ s.t.\ & \eta\ge\inf_{x\in X} f(x,y)+\lambda^T g(x,y),\quad \forall\lambda\ge 0\\ & 0\ge\inf_{x\in X}\mu^T g(x,y),\quad \forall\mu\in M\end{aligned}$$

$$\begin{aligned}\min_{y,\eta}\ & \eta\\ s.t.\ & \eta\ge\inf_{x\in X} f(x,y)+\left(\lambda^j\right)^T g(x,y),\quad \forall\lambda^j\in T^k\\ & 0\ge\inf_{x\in X}\left(\mu^i\right)^T g(x,y),\quad \forall\mu^i\in S^k\end{aligned}$$

Generalized Benders Decomposition

Relaxed master problem with separability in x and y

Relaxed Master Problem

$$\min_{y,\eta} \ \eta$$

$$s.t. \quad \eta \geq \inf_{x\in X} f(x,y) + \left(\lambda^j\right)^T g(x,y), \quad \forall \lambda^j \in T^k$$

$$0 \geq \inf_{x\in X} \left(\mu^i\right)^T g(x,y), \quad \forall \mu^i \in S^k$$

Property P!

$$f(x,y) \equiv f_1(x) + f_2(y), \ \ g(x,y) \equiv g_1(x) + g_2(y)\ *$$

$$\min_{y,\eta} \ \eta$$

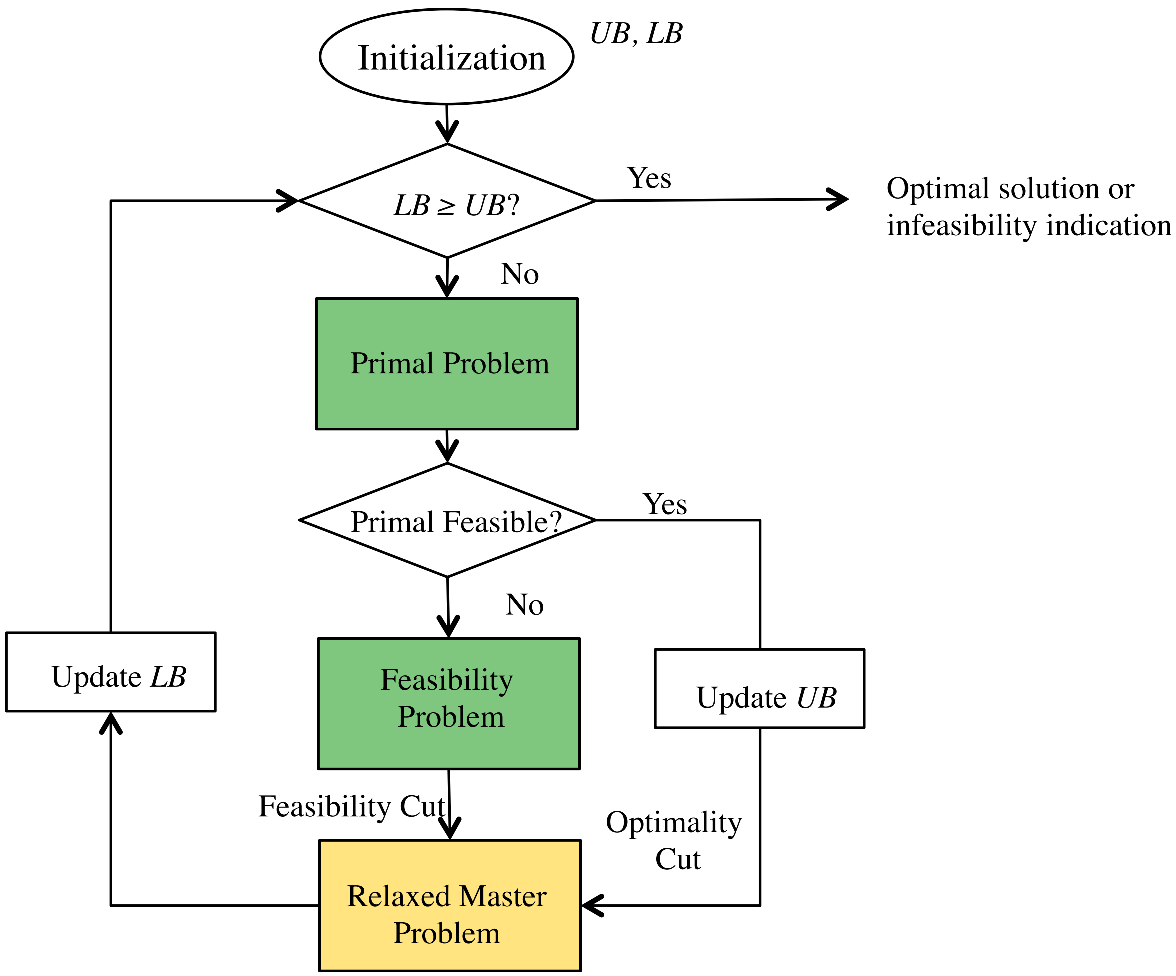
$$s.t. \quad \eta \geq obj^j_{\Pr imal} + f_2(y) - f_2(y^{(j)}) + \left(\lambda^j\right)^T \left[g_2(y) - g_2(y^{(j)})\right], \quad \forall \lambda^j \in T^k$$

$$0 \geq obj^i_{Feas} + \left(\mu^i\right)^T \left[g_2(y) - g_2(y^{(i)})\right], \quad \forall \mu^i \in S^k$$

* A.M. Geoffrion. Generalized Benders decomposition. *Journal of Optimization Theory and Applications*, 10(4):237–260, 1972.

Generalized Benders Decomposition

Algorithm flowchart

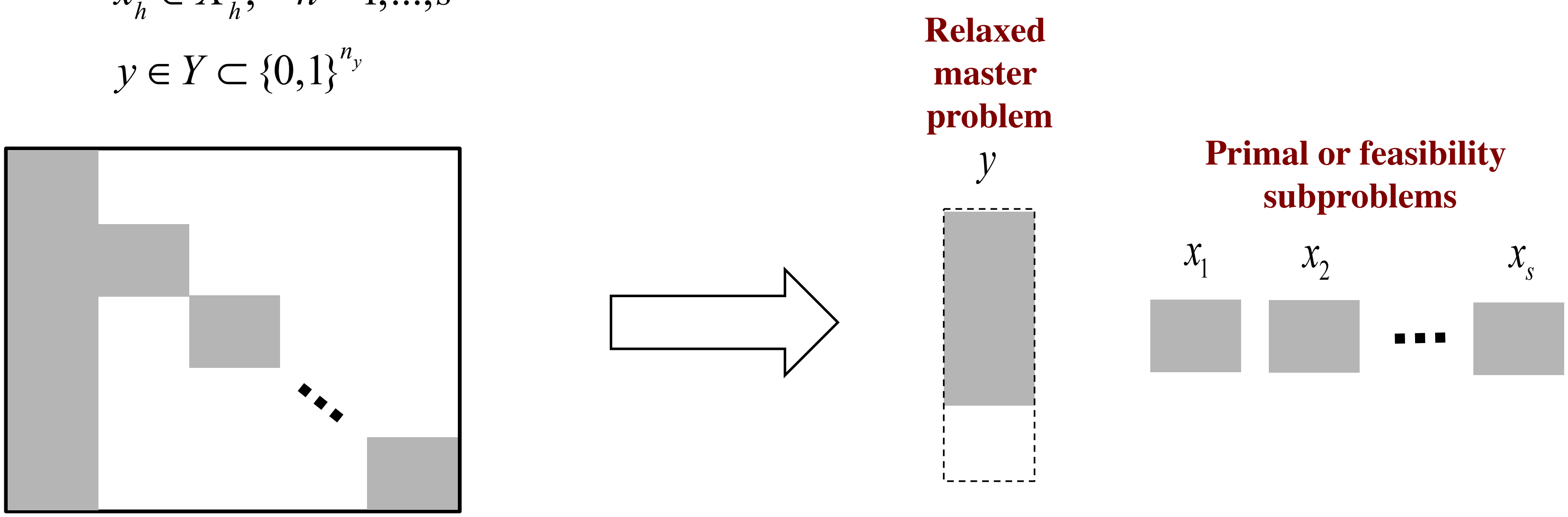


Generalized Benders Decomposition

GBD and scenario-based stochastic programs

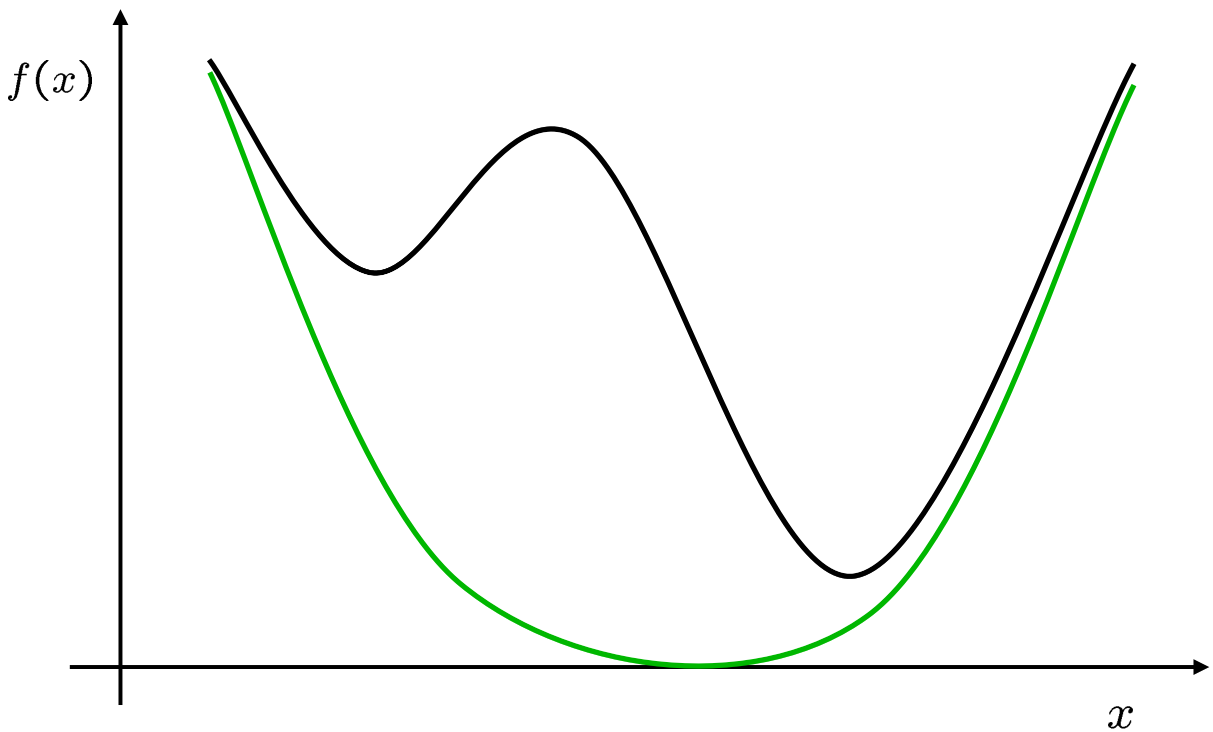
$$\min_{x_1,\ldots,x_s,y} \quad \sum_{h=1}^{s} w_h \left(f_h(x_h) + c_h^T y \right)$$

$$\begin{aligned} \text{s.t.} \quad & g_h(x_h) + B_h y \le 0, \quad h = 1,\ldots,s \\ & x_h \in X_h, \quad h = 1,\ldots,s \\ & y \in Y \subset \{0,1\}^{n_y} \end{aligned}$$



But, what if convexity assumption does not hold?

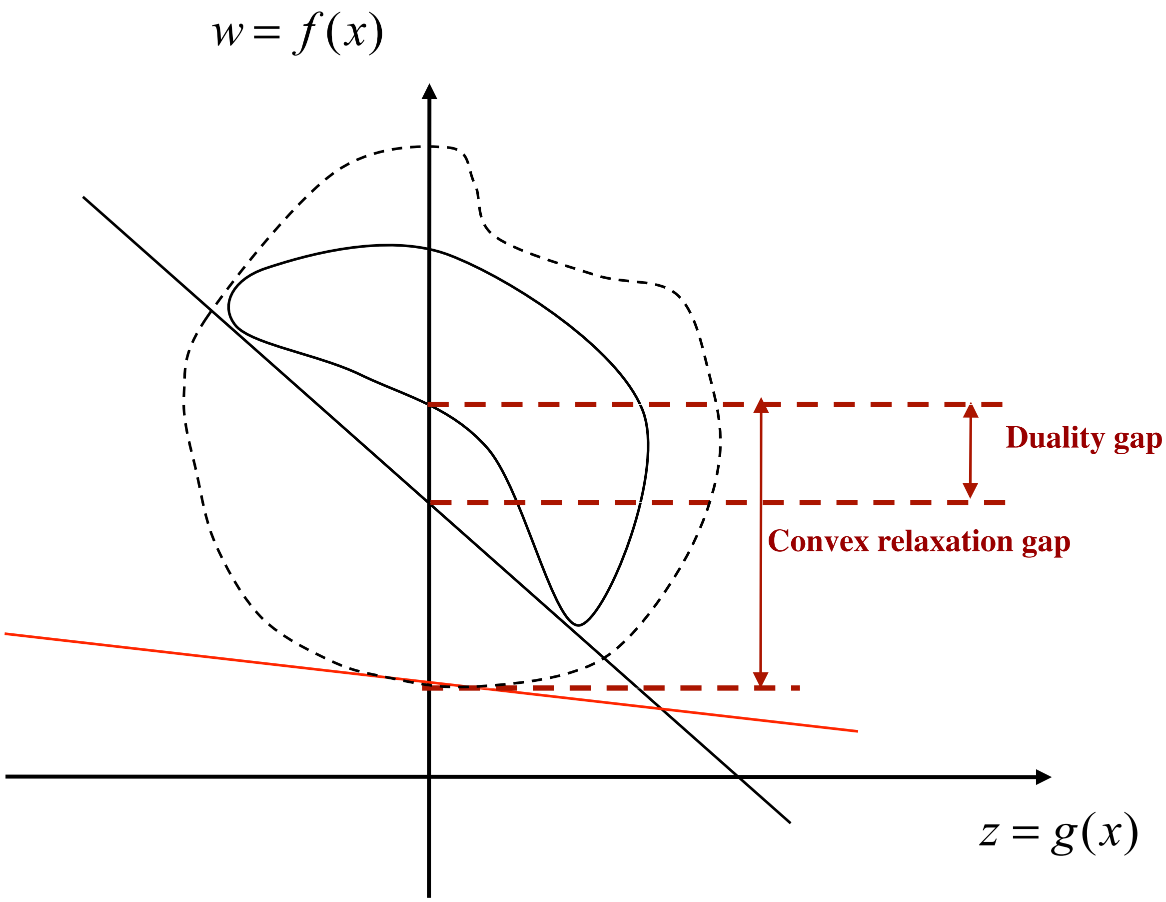
Convex Relaxations of Nonconvex Functions



- Convex Relaxation ≠ Convex Approximation
- Most practical problems can be relaxed via McCormick's approach

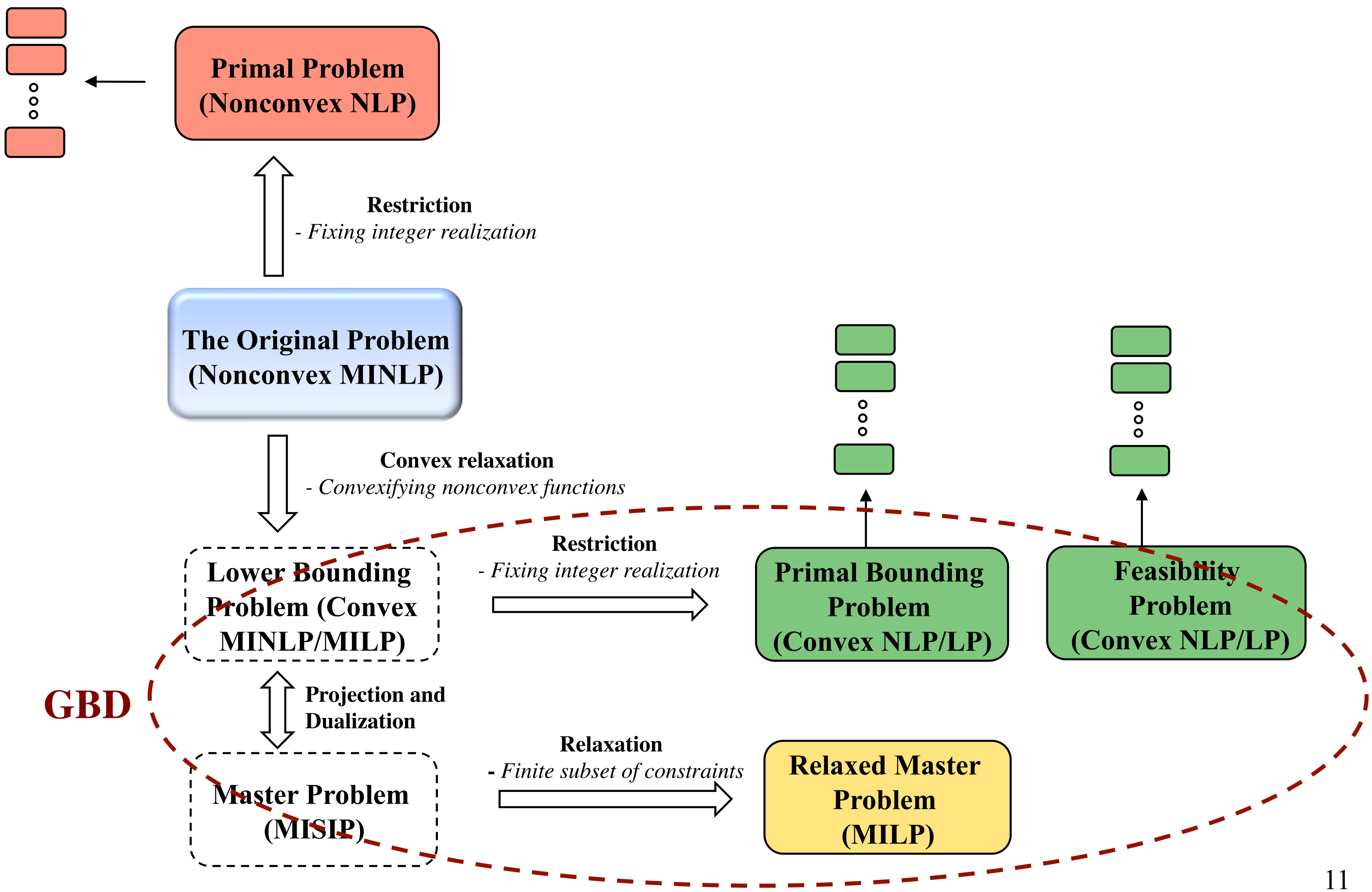
G. P. McCormick. Computability of global solutions to factorable nonconvex programs: Part I – Convex underestimating problems. *Mathematical Programming*, 10:147–175, 1976.

Gaps Due to Dual and Convex Relaxations



It is very difficult to obtain optimal dual solution for a nonconvex primal!

Nonconvex Generalized Benders Decomposition: Overview



Nonconvex Generalized Benders Decomposition

Lower bounding problem via convexification

The Original Problem (Nonconvex MINLP)

$$
\begin{aligned}
\min_{x_1,\dots,x_s,y} \quad & \sum_{h=1}^{s} w_h f_h(x_h, y) \\
\text{s.t.} \quad & g_h(x_h, y) \le 0, \quad h = 1,\dots,s \\
& x_h \in X_h, \quad h = 1,\dots,s \\
& y \in Y \subset \{0,1\}^{n_y}
\end{aligned}
$$

Lower Bounding Problem (Convex MINLP/MILP)

$$
\begin{aligned}
\min_{x_1,\dots,x_s,q_1,\dots,q_s,y} \quad & \sum_{h=1}^{s} w_h \left(u_{f,h}(x_h, q_h) + c_h^T y \right) \\
\text{s.t.} \quad & u_{g,h}(x_h, q_h) + B_h y \le 0, \quad h = 1,\dots,s \\
& (x_h, q_h) \in D_h, \quad h = 1,\dots,s \\
& y \in Y
\end{aligned}
$$

Desired separability can be induced by the process of convex relaxation

Nonconvex Generalized Benders Decomposition

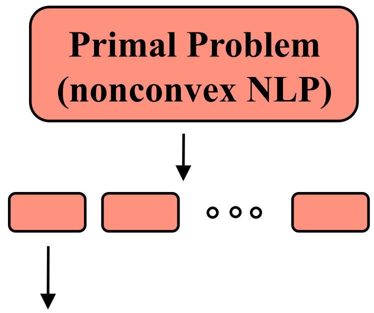
Relaxed master problem

Relaxed Master Problem (MILP)

$$
\begin{aligned}
\min_{\eta, y} \quad & \eta \\
s.t. \quad & \eta \geq obj_{PBP}^{(j)} + \left(\sum_{h=1}^{s} \left(w_h c_h^T + \left(\lambda_h^{(j)} \right)^T B_h \right) \right) \left(y - y^{(j)} \right), \quad \forall j \in T^k, \\
& 0 \geq obj_{FP}^{(i)} + \left(\sum_{h=1}^{s} \left(\mu_h^{(i)} \right)^T B_h \right) \left(y - y^{(i)} \right), \quad \forall i \in S^k, \\
& \sum_{r \in \Xi^{(1)}} y_r - \sum_{r \in \Xi^{(0)}} y_r \leq |\{ r : y_r^{(t)} = 1 \}| - 1, \quad \forall t \in T^k \bigcup S^k, \\
& y \in Y, \eta \in \mathbb{R}
\end{aligned}
$$

Nonconvex Generalized Benders Decomposition

Primal problem

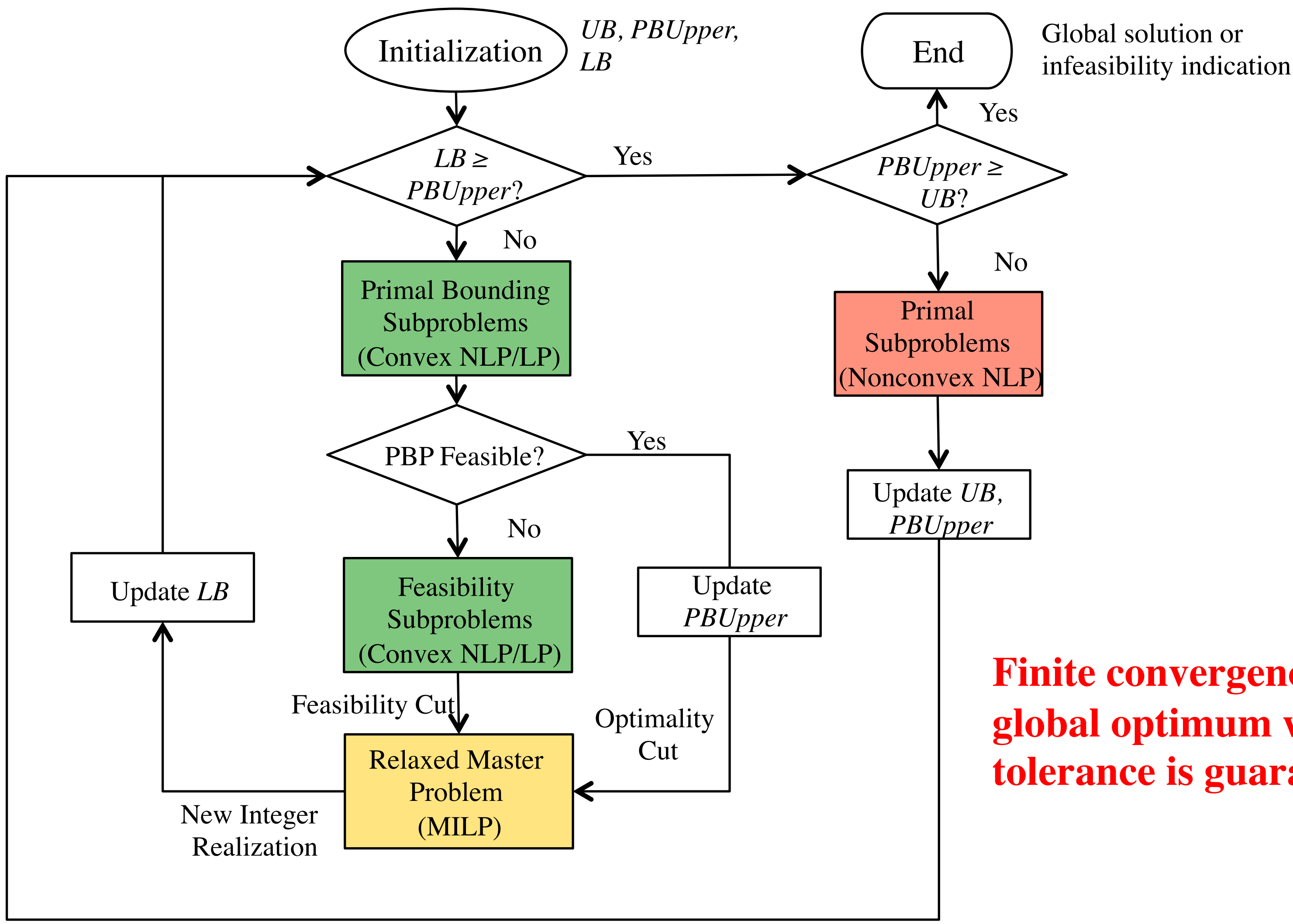


$$
\begin{aligned}
obj_{PP_h}^{(l)} = \min_{x_h} \quad & w_h f_h(x_h, y^{(l)}) \\
s.t. \quad & g_h(x_h, y^{(l)}) \leq 0, \\
& w_h f_h(x_h, y^{(l)}) \leq UBD_h^{(l)}, \\
& x_h \in X_h
\end{aligned}
$$

Deterministic global optimization solvers based on *continuous* branch-and-bound (e.g., BARON) can solve many nonconvex NLPs & MINLPs of small to medium size in reasonable times.

Nonconvex Generalized Benders Decomposition

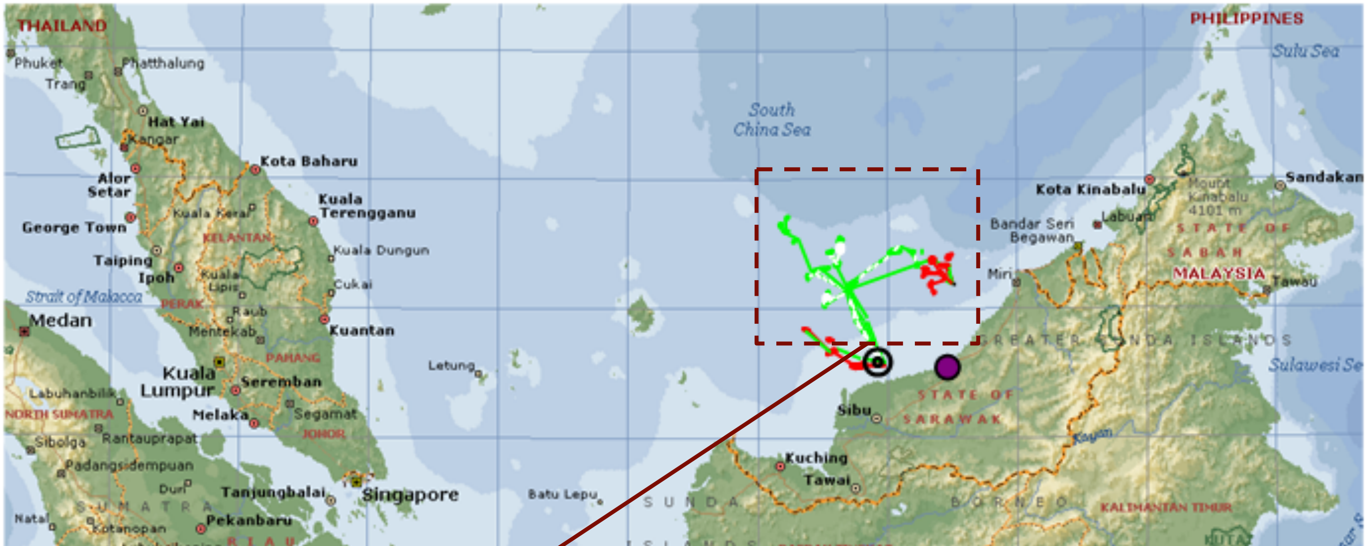
Algorithm flowchart

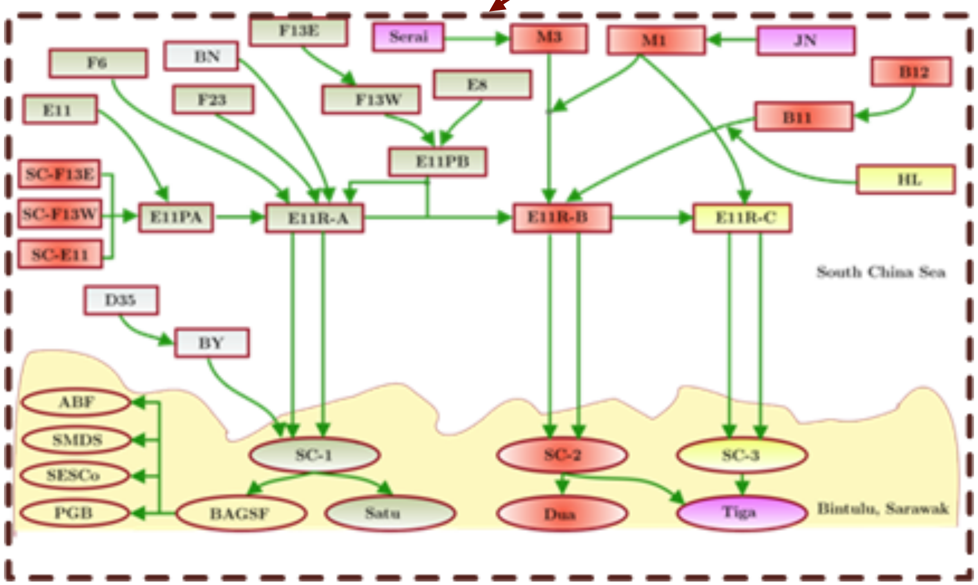


Finite convergence to a global optimum with a given tolerance is guaranteed.

Example

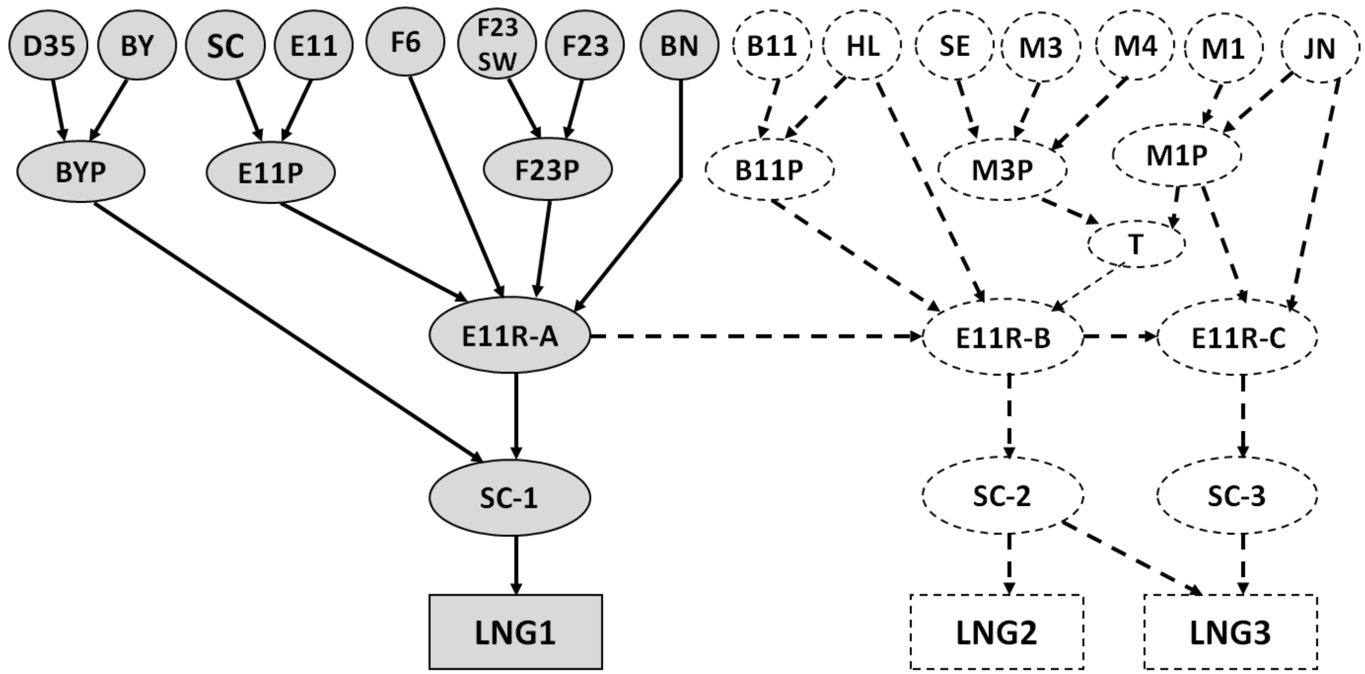
Sarawak Gas Production System (SGPS)





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

Infrastructure Expansion of SGPS Under Uncertainty



Goal

Optimal network design and long-term operation policy to

- maximize profitability
- satisfy product-specific constraints for all addressed uncertainty scenarios

Challenges and Novel Formulation

Challenges

- Strict specifications on gas products: H_2S, CO_2, GHV, etc.
- Large uncertainty in the system
  - quality and capacity of reservoirs
  - customer demands
  - etc.

Traditional deterministic linear model is not adequate

Novel Formulation

- Generalized pooling model to track gas flow qualities throughout the system
- Two-stage stochastic framework to address uncertainty explicitly

Stochastic pooling problem formulation combines

- generalized pooling model
- stochastic framework
- large-scale MINLP

Stochastic Pooling Problem

$$\min_{\substack{y,x_1,\ldots,x_s,\\ q_1,\ldots q_s,\\ u_1,\ldots u_s}} \quad c_1^T y + \sum_{h=1}^{s}\left(c_{2,h}^T x_h + c_{3,h}^T q_h + c_{4,h}^T u_h\right)$$

Economic objective

Nonconvex bilinear terms model gas qualities

$$\text{s.t.} \quad u_{h,l,t} = x_{h,l} q_{h,t}, \quad \forall (l,t)\in\Omega,\ \forall h\in\{1,\ldots,s\}$$

$$\tilde{A}_{2,h}^{(equ)} x_h + \tilde{A}_{3,h}^{(equ)} q_h + \tilde{A}_{4,h}^{(equ)} u_h = \tilde{b}_h^{(equ)},\ \forall h\in\{1,\ldots,s\}$$

Mass balances

$$A_{1,h} y + A_{2,h} x_h + A_{3,h} q_h + A_{4,h} u_h \le b_h,\ \forall h\in\{1,\ldots,s\}$$

$$\tilde{A}_{2,h} x_h + \tilde{A}_{3,h} q_h + \tilde{A}_{4,h} u_h \le \tilde{b}_h,\ \forall h\in\{1,\ldots,s\}$$

$$\mathrm{x}_h^L \le \mathrm{x}_h \le \mathrm{x}_h^U,\ q_h^L \le q_h \le q_h^U,\ \forall h\in\{1,\ldots,s\}$$

Flow constraints

$$\mathrm{B}y \le d,$$

Topology constraints

$$x_h \in \mathbb{R}^{n_x},\ q_h \in \mathbb{R}^{n_q},\ u_h \in \mathbb{R}^{n_u},\ \forall h\in\{1,\ldots,s\},\ y\in\{0,1\}^{n_y}$$

$$\Omega \subset \{1,\ldots,n_x\}\times\{1,\ldots,n_q\},\quad n_u = |\Omega|$$

Computational Study
Implementation Issues

Platform

- CPU 2.83 GHz, Memory 1 GB, Linux, GAMS 22.8.1

Solvers

- LP and MILP solver : CPLEX
- Global NLP solver: BARON
- Local NLP solver: SNOPT

Methods for Comparison

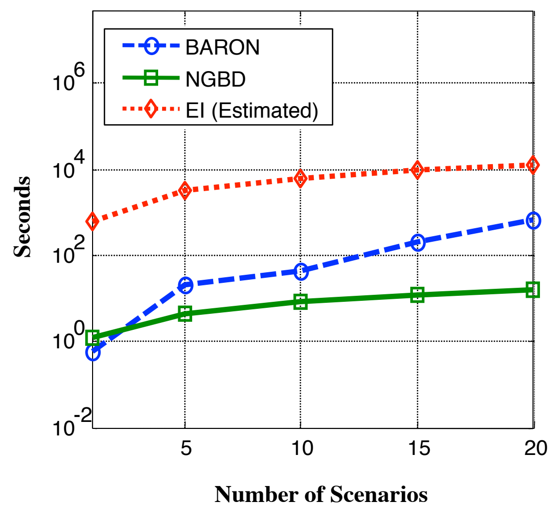
1. BARON – The state-of-the-art global optimization solver
2. NGBD – Nonconvex generalized Benders decomposition
3. EI – Naïve integer enumeration

Relative Tolerance for Global Optimization

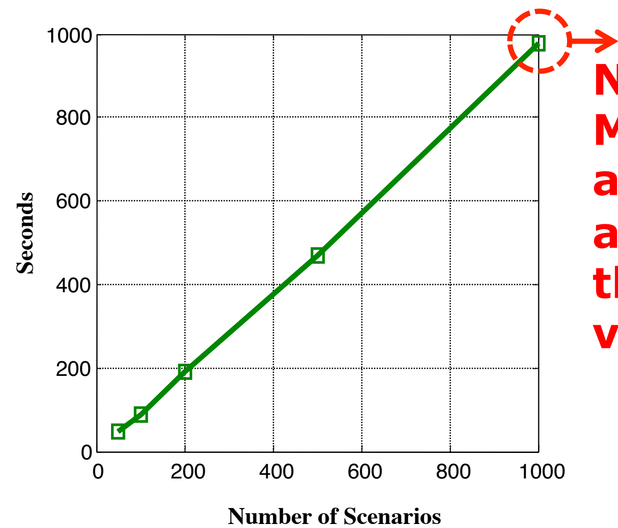
- 10^{-2}

Computational Study
SGPS design problem A

The stochastic problem contains 38 binary variables and 93s continuous variables (s represents total number of scenarios).



(a) Solver times with different methods



(b) Solver times with NGBD for more scenarios

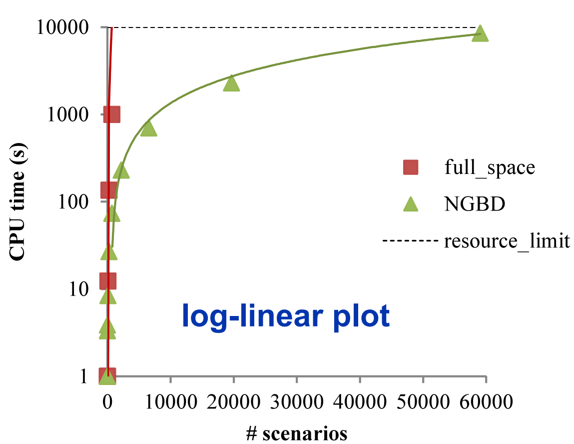
Nonconvex MINLP with almost a hundred thousand variables

Computational Results: MILP Recourse

	examples								
	Ex1	Ex2	Ex3	Ex4	Ex5	Ex6	Ex7	Ex8	Ex9
number of products	2	3	4	5	6	7	8	9	10
number of scenarios	9	27	81	243	729	2,187	6,561	19,683	59,049
number of 1st-stage binary variables	124	124	124	124	124	124	124	124	124
number of 2nd-stage binary variables (per scenario)	124	186	248	310	372	434	496	558	620
number of 2nd-stage continuous variables (per scenario)	744	1,023	1,302	1,581	1,860	2,139	2,418	2,697	2,976
number of constraints	7,382	27,749	100,568	354,179	1,220,474	4,135,745	13,830,716	45,763,103	150,102,686
time-fullmodel (s)	0.6	0.7	12.3	135.0	998.8	NA	NA	NA	NA
objective_fullmodel (Billion $)	17.525	25.573	32.176	41.929	49.452	NA	NA	NA	NA
relaxed objective* (Billion $)	17.550	25.613	32.227	41.940	49.466	55.276	63.840	NA	NA
time-NGBD (s)	3.3	3.9	8.4	26.7	73.5	229.1	697.9	2494.9	8488.9
UBD at termination (Billion $)	-17.523	-25.588	-32.198	-41.919	-49.435	-55.249	-63.801	-68.136	-72.482
LBD at termination (Billion $)	-17.533	-25.601	-32.216	-41.931	-49.449	-55.237	-63.789	-68.108	-72.437
integer realizations visited by PBP	17	5	5	2	2	2	2	2	2
integer realizations visited by PP	1	1	1	1	1	1	1	1	1

NA = No solution returned in 10,000 CPU seconds; *obtained by solving full-space MILP model as an LP.

36 million BVs!
176 million CVs!



Hardware: 3.2 GHz Intel Xeon CPU with 12 GB RAM on Windows
Software: GAMS 23.6 / CPLEX 12.2
Tolerance: 0.001 (relative) for both full model and NGBD

- With full model, the solution time increases **drastically** with # scenarios
- With NGBD, the solution time increases **linearly** with # scenarios

Computational Study
- Summary of studied nonconvex problems
(all solved to global optimality with given tolerances)

	Continuous variable /Integer variable	Time via NGBD (Second)	Nonconvexity	Implementation [1]
Haverly	21,000/16	93.4	Bilinear	(A)
Gas Network	68,000/19	15,610.7	Bilinear	(A)
SGPS A	93,000/38	978.2	Bilinear	(A)
SGPS B	93,000/38	977.1	Bilinear	(A)
SGPS C	146,410/20	4,234.8	Bilinear, quadratic, power	(B)
Software	10,648/8	260.7	Logarithmic	(B)
Pump	50,578/18	2,794.8	Bilinear, quadratic, cubic	(B)
Polygeneration	14,688/70	15,825.0 [2]	Bilinear	(C)

Note: [1] Problems were run with different CPUs, GAMS systems and relative termination tolerances ε:
(A) CPU 2.83 GHz , GAMS 28.1, $\varepsilon=10^{-2}$; (B) CPU 2.83 GHz, GAMS 23.4, $\varepsilon=10^{-3}$; (C) CPU 2.66 GHz, GAMS 23.5, $\varepsilon=10^{-2}$.
[2] Enhanced NGBD with tighter lower bounding problems employed.

Conclusions & Future Work

- Classical decomposition ideas (GBD) can be extended to certain problems with nonconvex recourse
  - Algorithm running time tends to grow linearly with no. scenarios
  - Applied to hard nonconvex optimization problems in optimal design & operation of energy systems under uncertainty
- Continuous complicating variables?
- Multi-stage problems?
- How to close the relaxation gap?

Acknowledgments

- Dr. Xiang Li, Dr. Arul Sundaramoorthy, MIT
- Prof. Asgeir Tomasgard, NTNU (Norway)
- Statoil (Norway)
- Novartis
- BP

Generalized Benders Decomposition

Principle of projection

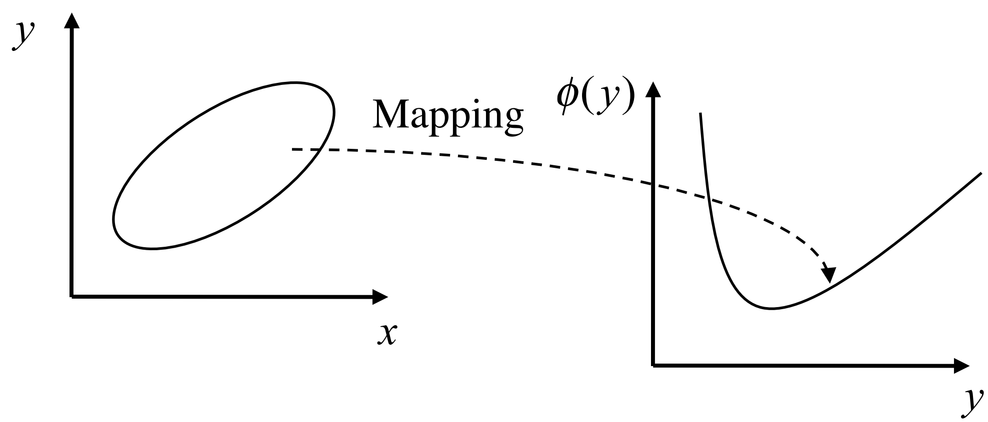
$$\min_{x,y} \; f(x,y)$$
$$\text{s.t. } g(x,y) \le 0$$
$$x \in X, \; y \in Y$$

$$\Longleftrightarrow$$

$$\min_{y} \; \phi(y)$$
$$\text{s.t. } \phi(y) = \inf_{x \in X, g(x,y) \le 0} f(x,y)$$
$$y \in Y \cap V,$$
$$V = \{y : \exists x \in X, g\left(x,y\right) \le 0\}$$

Optimality

Feasibility



* A.M. Geoffrion. Generalized Benders decomposition. *Journal of Optimization Theory and Applications*, 10(4):237–260, 1972.

Generalized Benders Decomposition

Optimality cuts

$$\min_{y} \ \phi(y)$$

$$s.t. \quad \phi(y) = \inf_{x\in X, g(x,y)\le 0} f(x,y) \qquad \text{Optimality}$$

$$y \in Y \cap V,$$

$$V = \{y : \exists x \in X, g(x,y) \le 0\} \qquad \text{Feasibility}$$

Generalized Benders Decomposition

Optimality

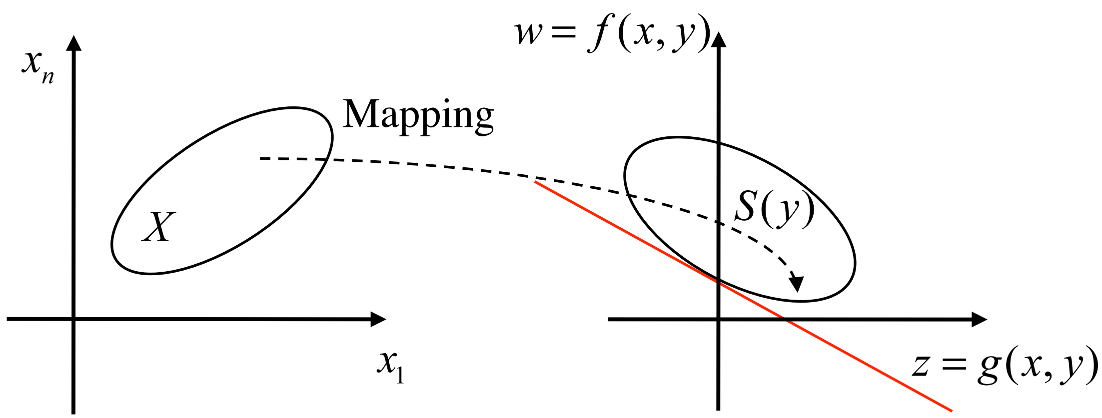
Convex recourse, Slater's condition holds

$$\min_y \ \phi(y)$$

$$s.t. \quad \phi(y) = \inf_{x \in X, g(x,y) \le 0} f(x,y) \qquad \text{Optimality} \qquad \Longleftrightarrow \qquad \phi(y) = \sup_{\lambda \ge 0} \inf_{x \in X} f(x,y) + \lambda^T g(x,y)$$

$$y \in Y \cap V,$$

$$V = \{y : \exists x \in X, g(x,y) \le 0\} \qquad \text{Feasibility}$$



Nonconvex Generalized Benders Decomposition

Primal bounding problem and feasibility problem

Primal Bounding Problem (convex NLP)

$$obj_{PBP_h}^{(k)} = \min_{x_h, q_h} \; w_h \left(u_{f,h}(x_h, q_h) + c_h^T y^{(k)} \right)$$
$$s.t. \; u_{g,h}(x_h, q_h) + B_h y^{(k)} \leq 0,$$
$$(x_h, q_h) \in X_h \times Q_h$$

Feasibility Problem (convex NLP)

$$obj_{FP_h}^{(k)} = \min_{x_h, q_h, z_h} \; w_h \, \| z_h \|$$
$$s.t. \; u_{g,h}(x_h, q_h) + B_h y^{(k)} \leq z_h,$$
$$(x_h, q_h) \in X_h \times Q_h,$$
$$z_h \in Z \subset \{ z \in \mathbb{R}^m : z \geq 0 \}$$

Nonconvex Generalized Benders Decomposition

Master problem

Master Problem (MISIP)

$$\min_{\eta,y} \quad \eta$$

$$s.t. \;\; \eta \geq \sum_{h=1}^{s}\left(w_h c_h^T + \lambda_h^T B_h\right) y + \sum_{h=1}^{s} \inf_{(x_h,q_h)\in X\times Q}\left[w_h u_{f,h}(x_h,q_h) + \lambda_h^T u_{g,h}(x_h,q_h)\right],$$

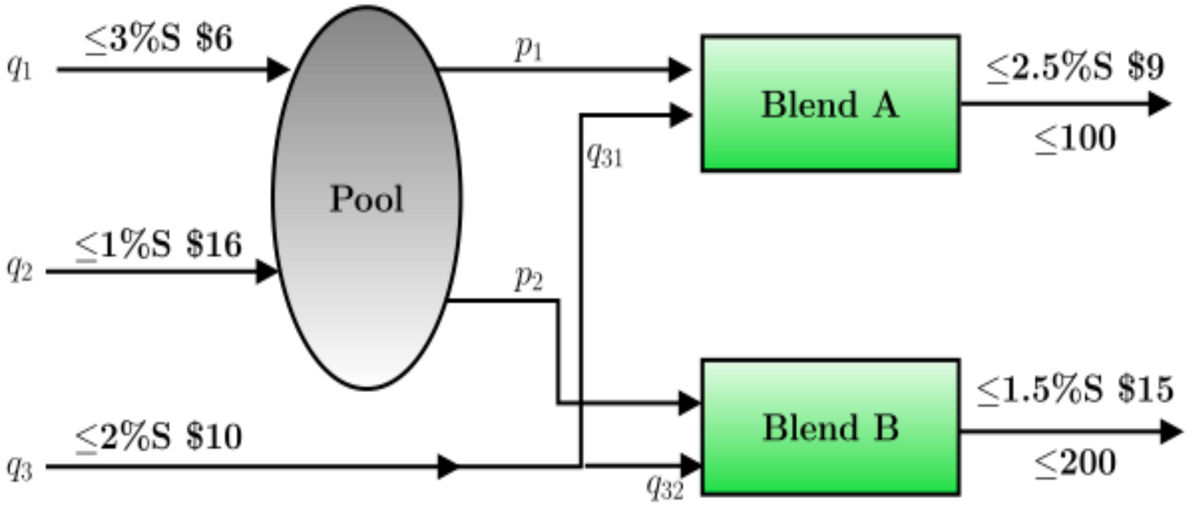
$$\forall \lambda_1,\ldots,\lambda_s \geq 0,$$

$$0 \geq \sum_{h=1}^{s} \mu_h^T B_h y + \sum_{h=1}^{s} \inf_{(x_h,q_h)\in X\times Q} \mu_h^T u_{g,h}(x_h,q_h),$$

$$\forall \mu_1,\ldots,\mu_s \in M,$$

$$y \in Y, \eta \in \mathbb{R}$$

Haverly's Pooling Problem



$$\max \quad 9(p_1 + q_{31}) + 15(p_2 + q_{32}) - (6q_1 + 16q_2 + 10q_3)$$

s.t.

$$q_1 + q_2 = p_1 + p_2$$

$$3q_1 + q_2 = x_s(p_1 + p_2)$$

$$q_{31} + q_{32} = q_3$$

+ linear inequalities

Haverly C. A., "Studies of the behaviour of recursion for the pooling problem", *ACM SIGMAP Bulletin, 25:29-32, 1978*.

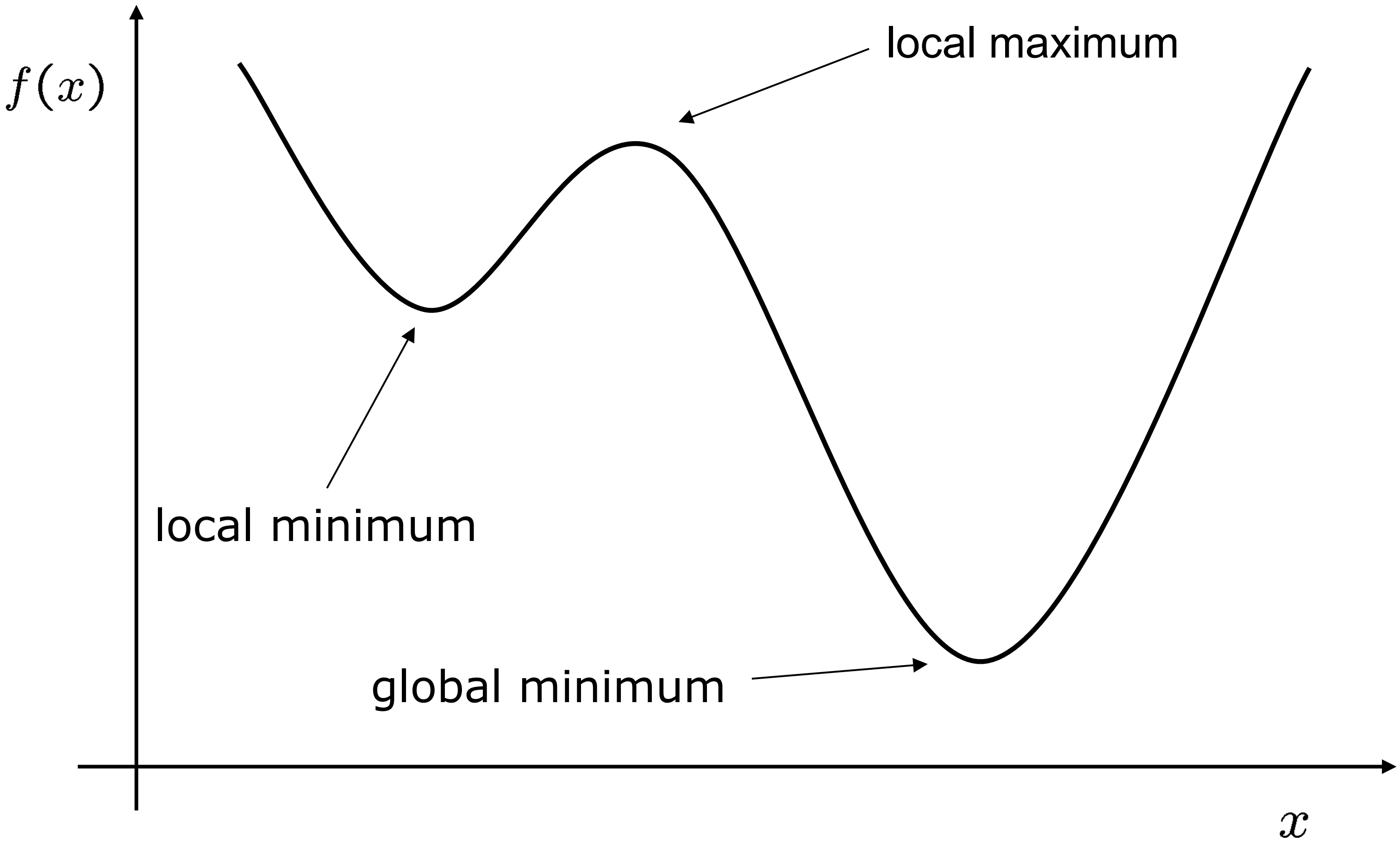
Need for *Global* Optimization

Solver	Type	Algorithm	Objective
BARON	Global	Branch-and-Reduce	400.0
SNOPT	Local	Sequential Quadratic Programming	0.0
MINOS	Local	Projected Lagrangian	0.0
CONOPT	Local	Generalized Reduced Gradient	0.0
KNITRO	Local	Interior Point	400.0

Deterministic global optimization solvers based on *continuous* branch-and-bound (e.g., BARON) can solve many nonconvex NLPs of small to medium size in reasonable times.

Global Optimization via Branch-and-Bound

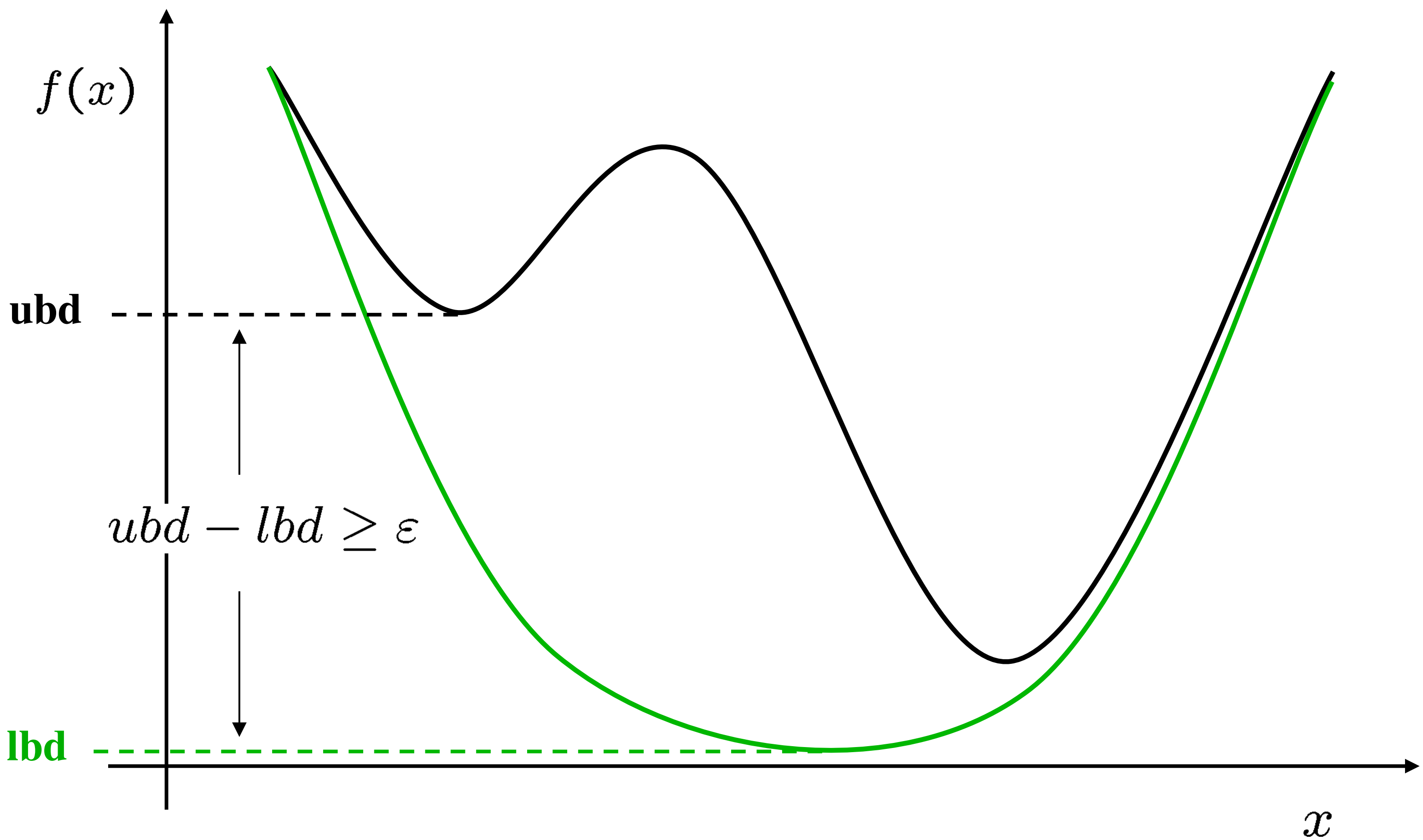
- Nonconvex optimization



Standard optimization techniques cannot distinguish between suboptimal local minima

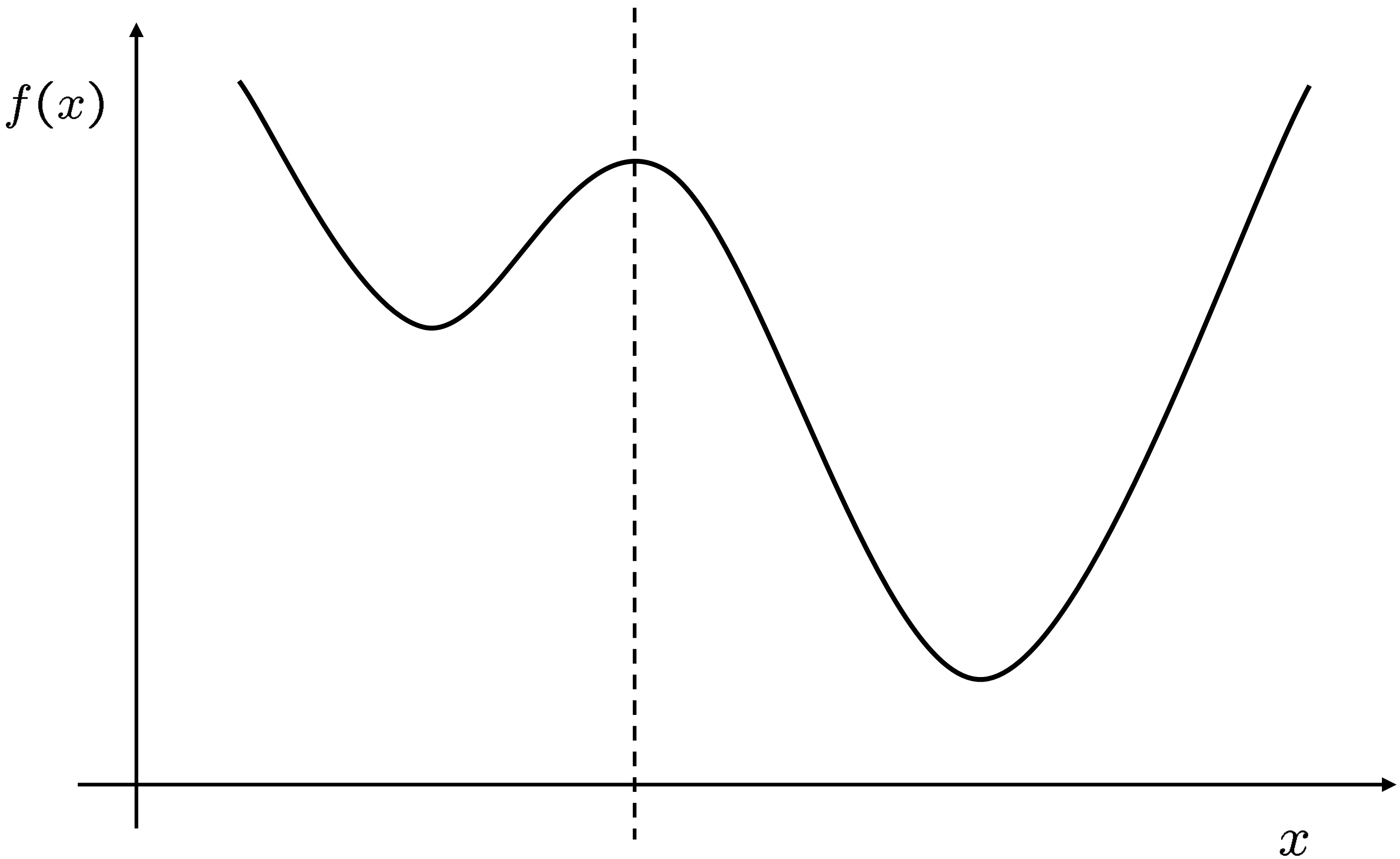
Global Optimization via Branch-and-Bound

- Convex Relaxation



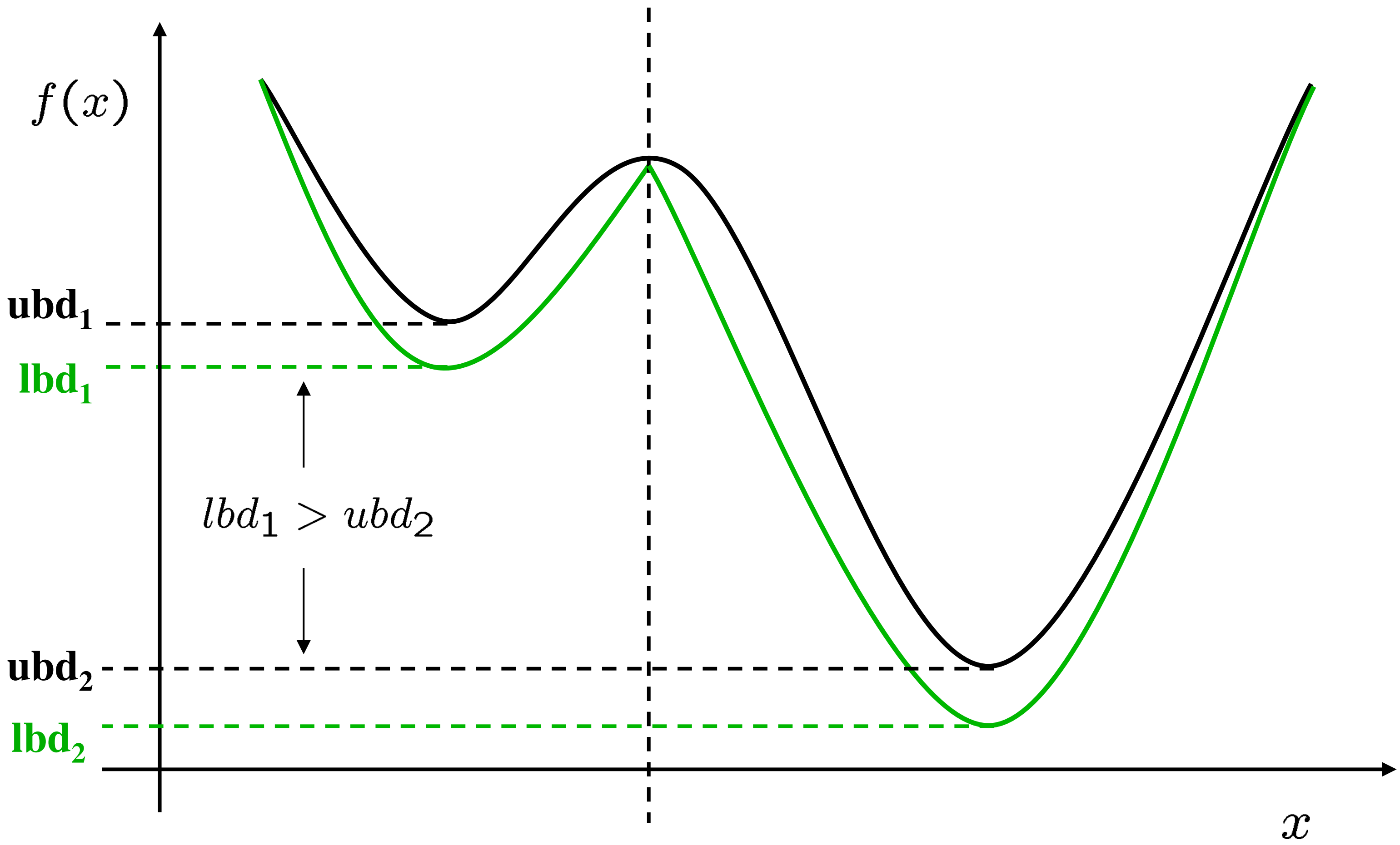
Global Optimization via Branch-and-Bound

- Branch



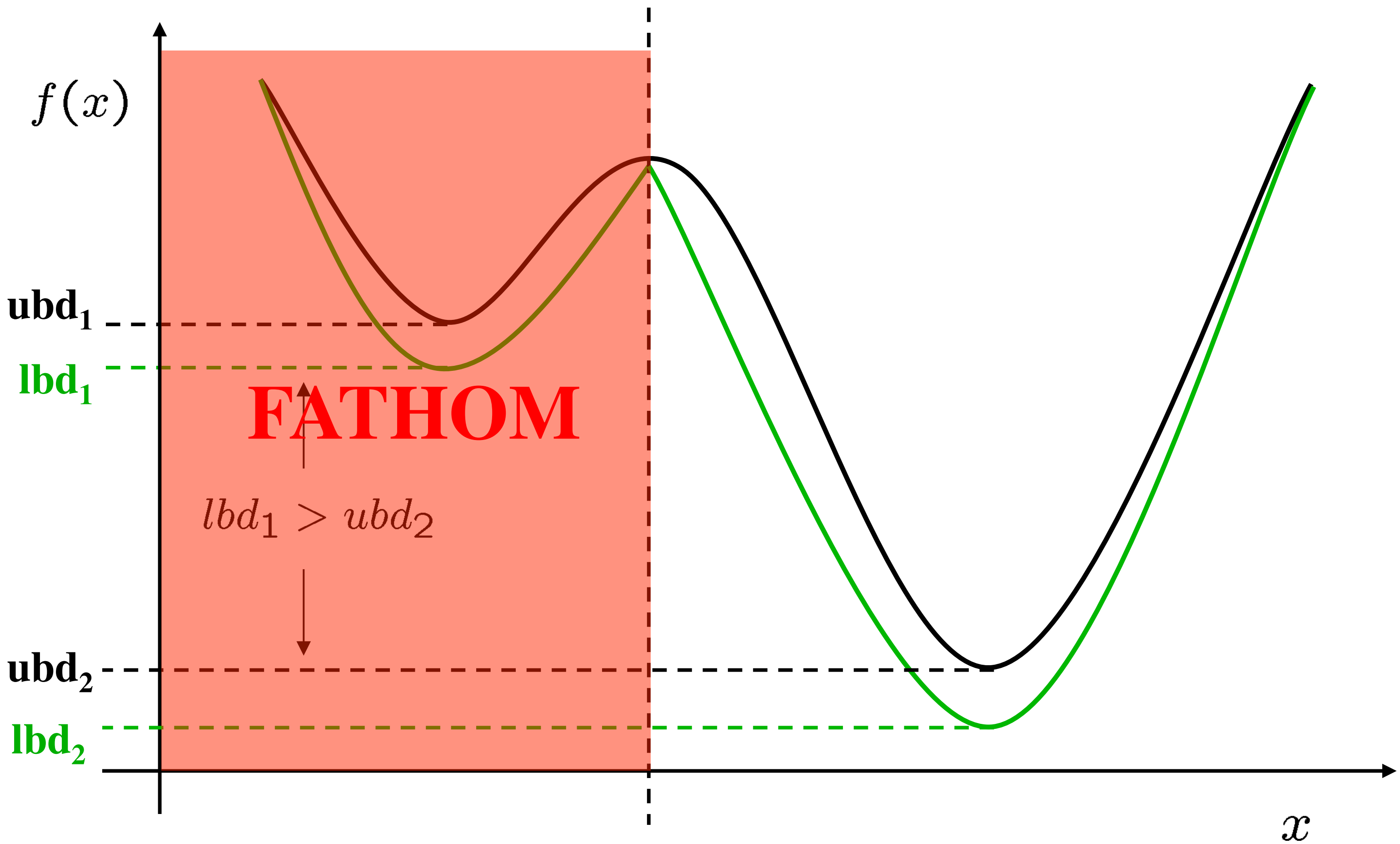
Global Optimization via Branch-and-Bound

- Branch, and bound

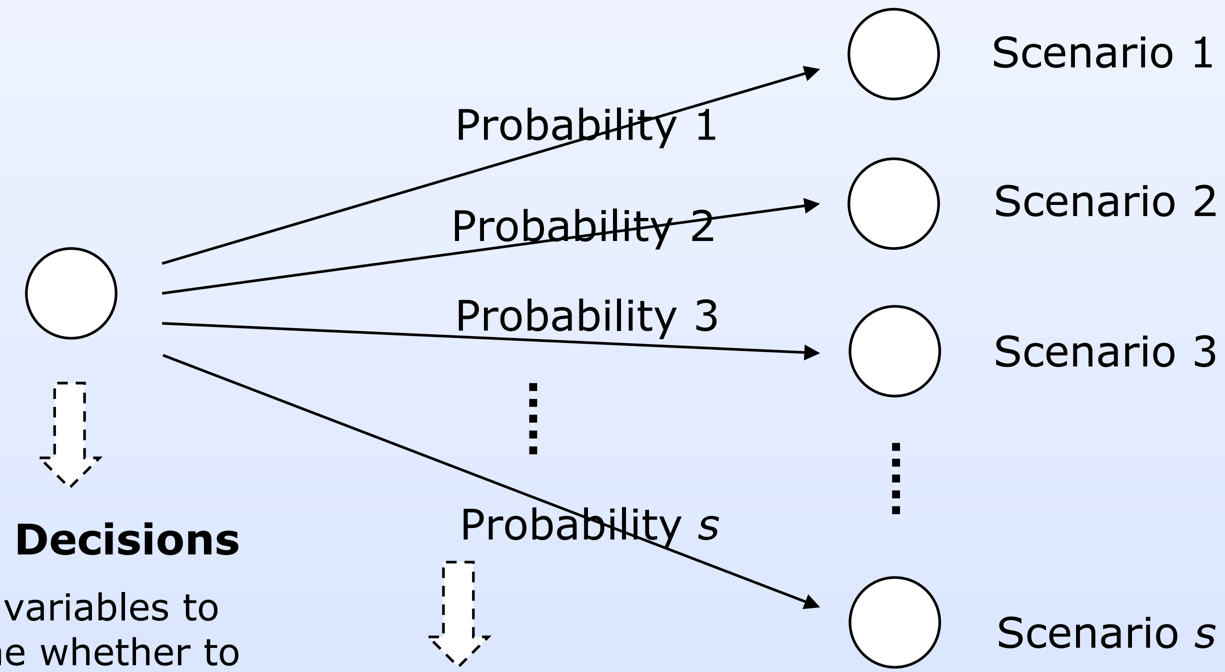


Global Optimization via Branch-and-Bound

- Branch, bound and fathom



Two-Stage Stochastic Programming Framework



Design Decisions

- Binary variables to determine whether to develop potential gas wells/fields, gas platforms and pipelines

Realization of uncertainty

- *Reservoir quality*
- *Customer demand*
- *Gas price*

Operational Decisions

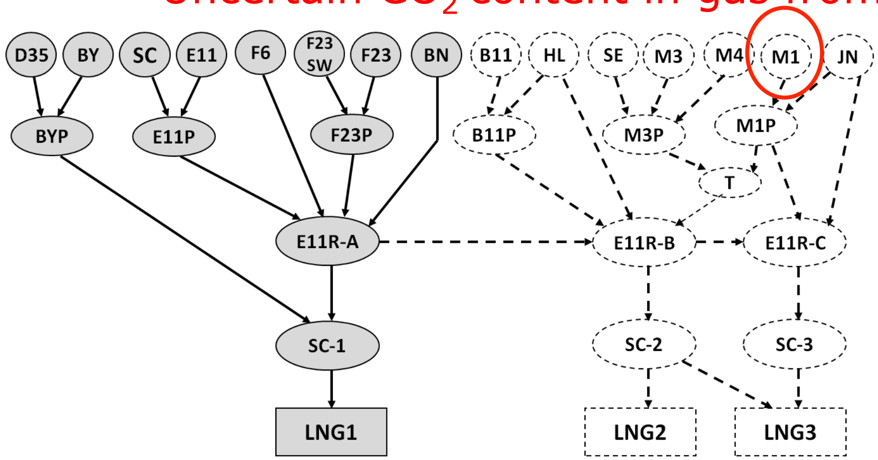
- Continuous variables to determine rates of the gas flows throughout the network in long-term operation

Goal

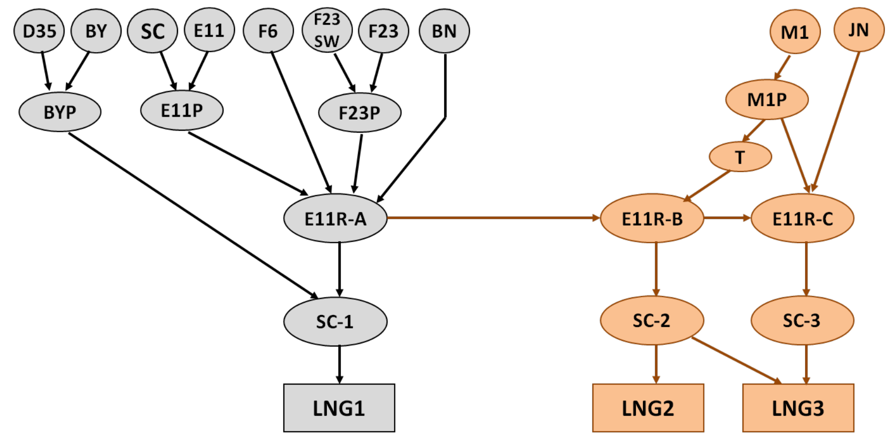
- Maximize expected net present value

The Different Design Results

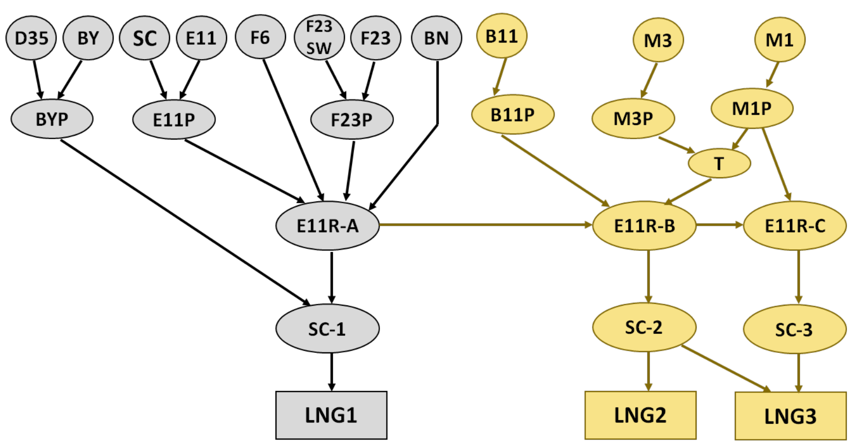
Uncertain CO_2 content in gas from M1



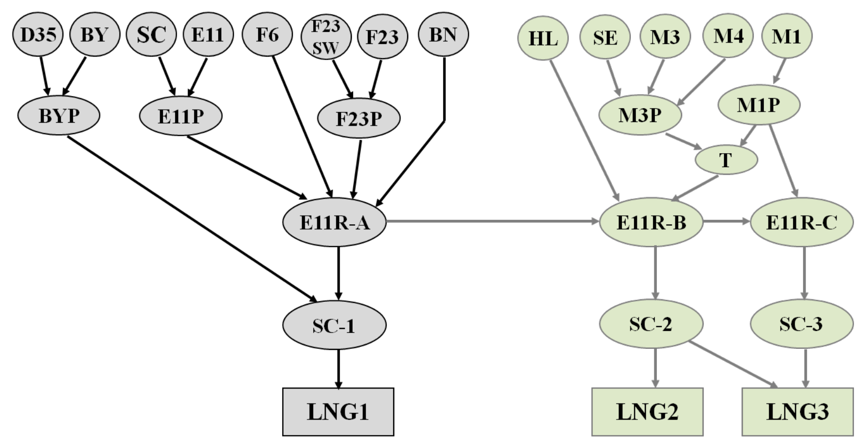
Superstructure of the problem



Formulation 1 – Uncertainty and quality not addressed



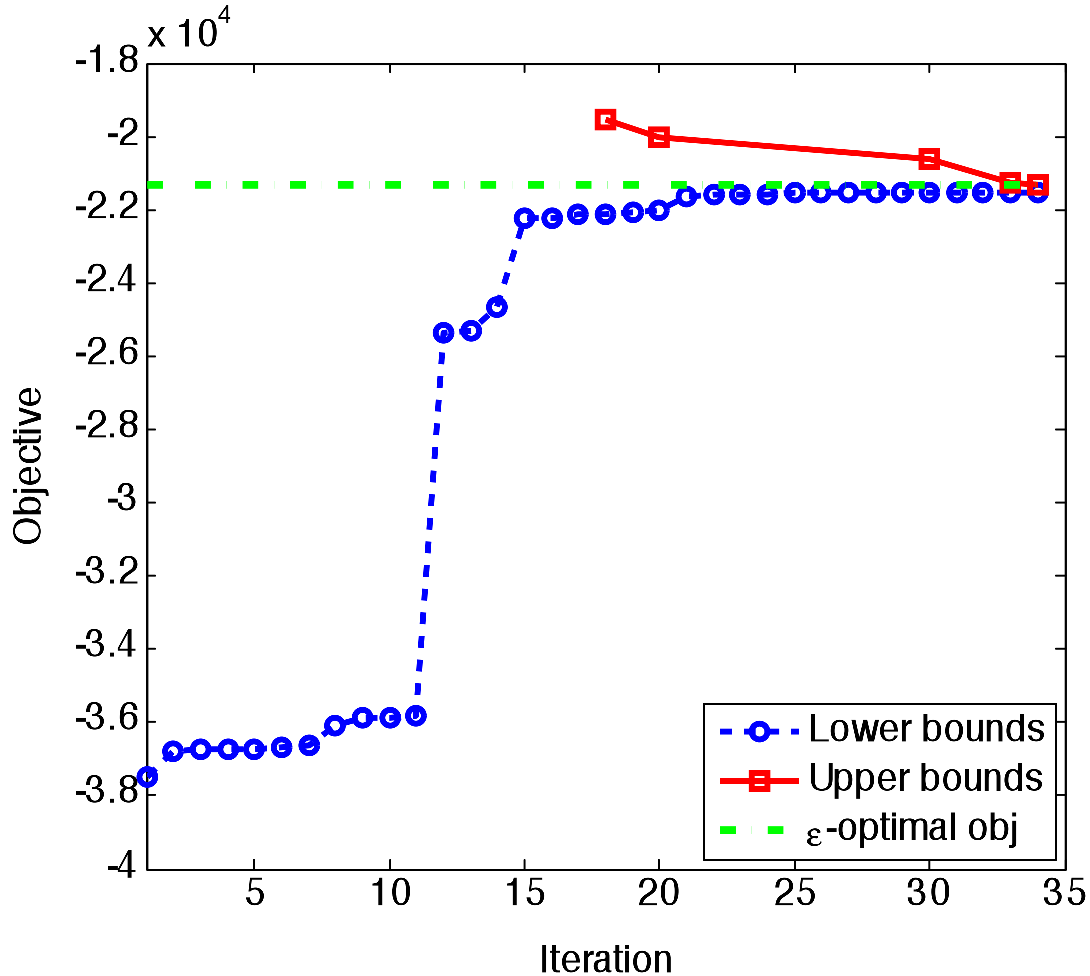
Formulation 2 – Only quality addressed



Formulation 3 – Both uncertainty and quality addressed

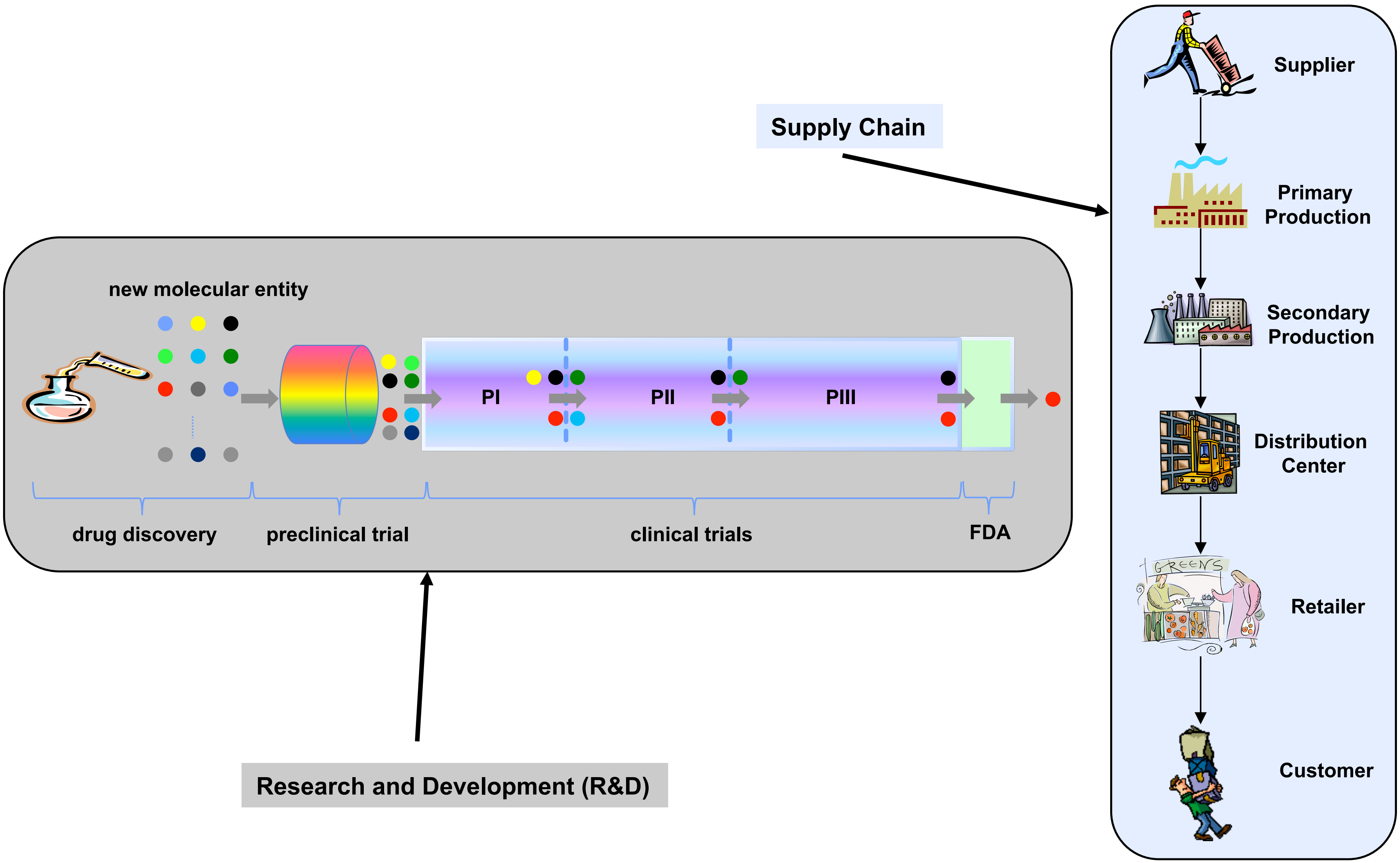
Computational Study

SGPS design problem A

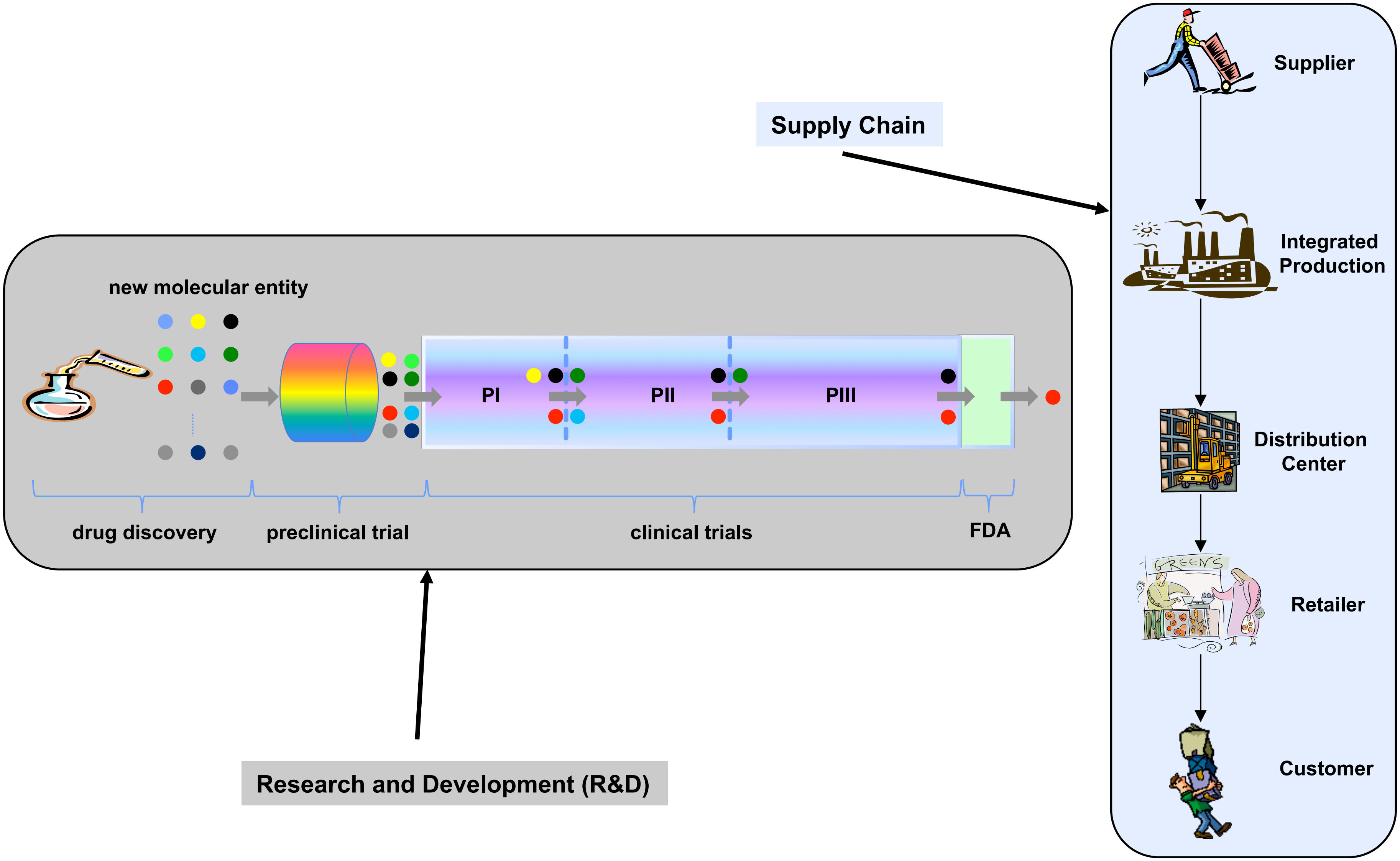


Convergence of the upper and lower bounds over the iterations

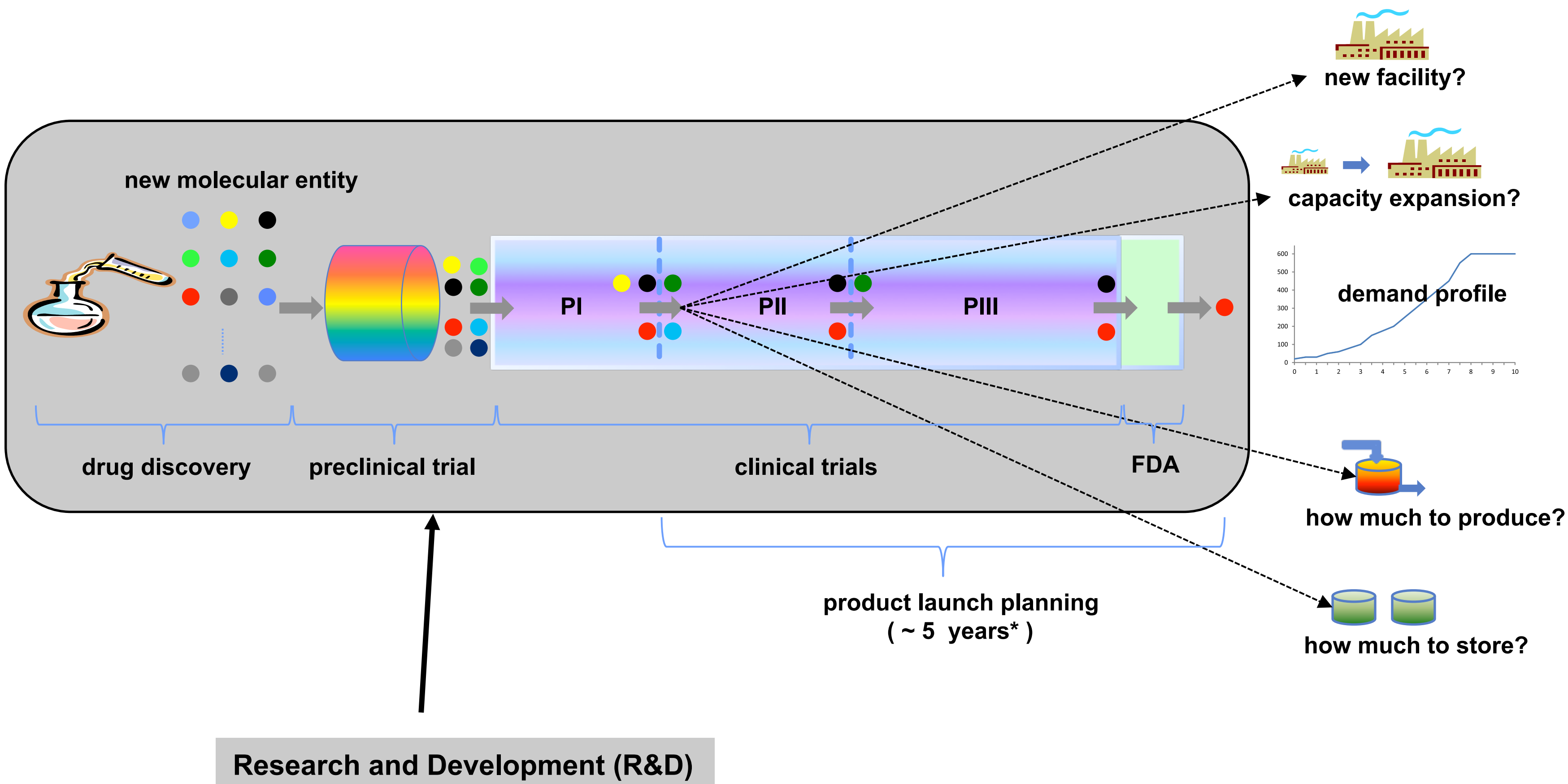
Pharmaceutical Business Processes



Pharmaceutical Business Processes



Pharmaceutical Business Processes



Product launch planning is made under clinical trial uncertainty!

*Stonebraker, J.S. How Bayer makes decisions to develop new drugs. *Interfaces*, 32, 77, 2002.

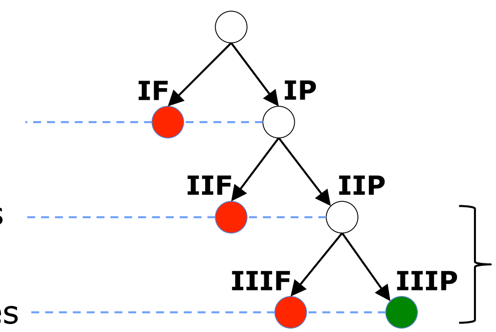
Uncertainty in the Problem

- The success of each clinical trial is uncertain
  - Each drug can have only 1 out of 4 possible outcomes*
    - For a drug i, Ω_i = {IF, IIF, IIIF, IIIP}; # scenarios = $4^{|\mathbf{I}|}$

PI outcomes

PII outcomes

PIII outcomes



IF/IP → PI fail/pass
IIF/IIP → PII fail/pass
IIIF/IIIP → PIII fail/pass

outcomes of interest in the product-launch planning

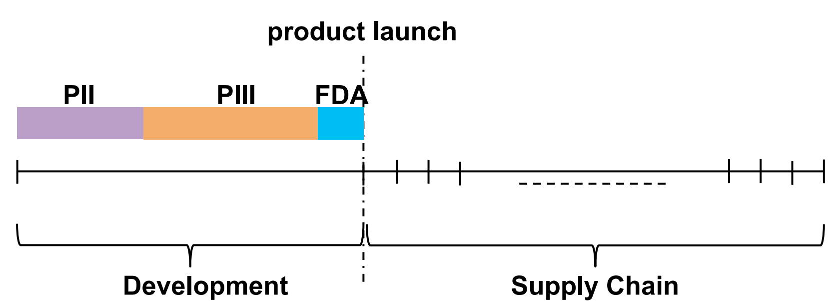
- We consider a subset of outcomes
  - PI outcomes are known a priori
    - For a drug i, Ω_i = {IIF, IIIF, IIIP}; # scenarios = $3^{|\mathbf{I}|}$

*Colvin, M; Maravelias, C.T. A Stochastic programming approach for clinical trial planning in new drug development. *Comput. Chem. Eng.*, 32, 2626-2642, 2008.

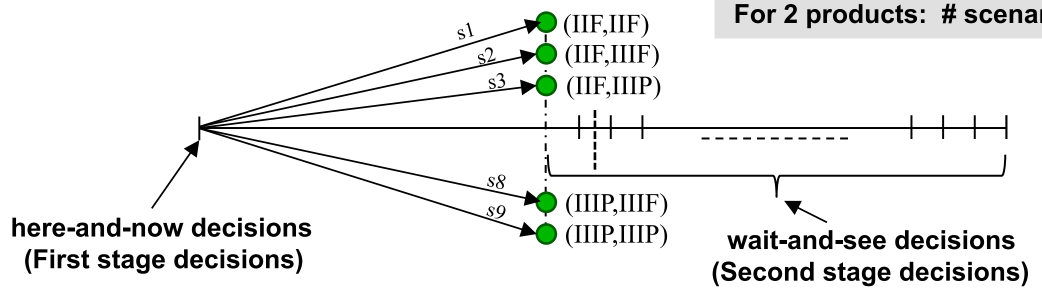
Proposed Approach

- Two-stage stochastic programming
  - First stage decisions
    - When to build a new facility
    - When to expand an existing facility
  - Second stage decisions
    - When, where, and how much to produce, store, and supply

Problem Description



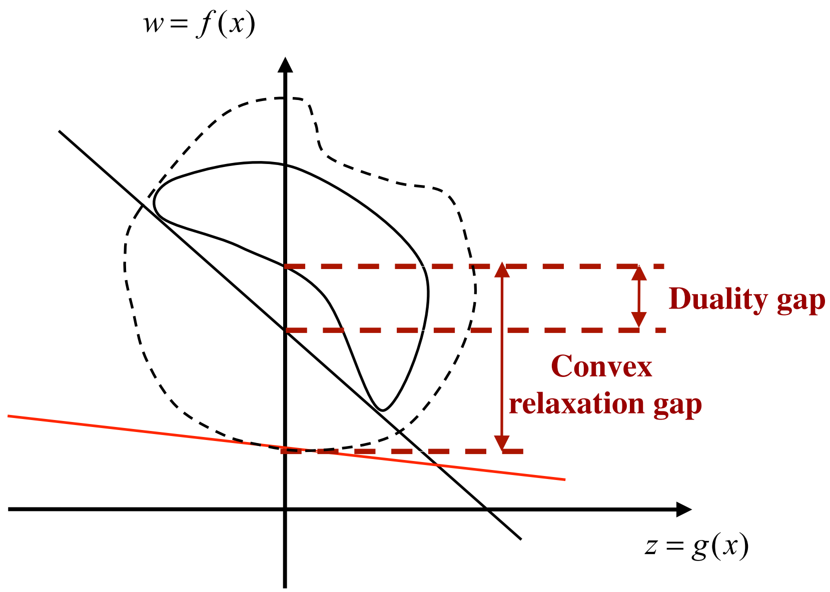
Decision Representation

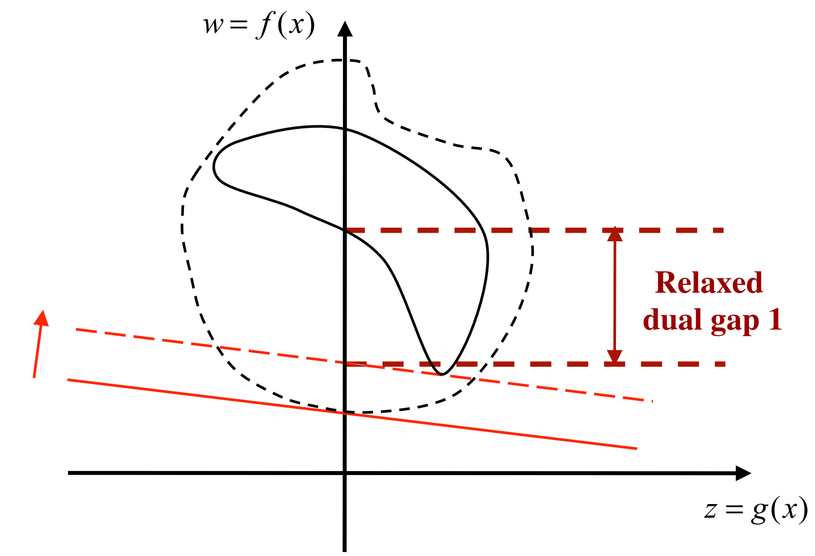


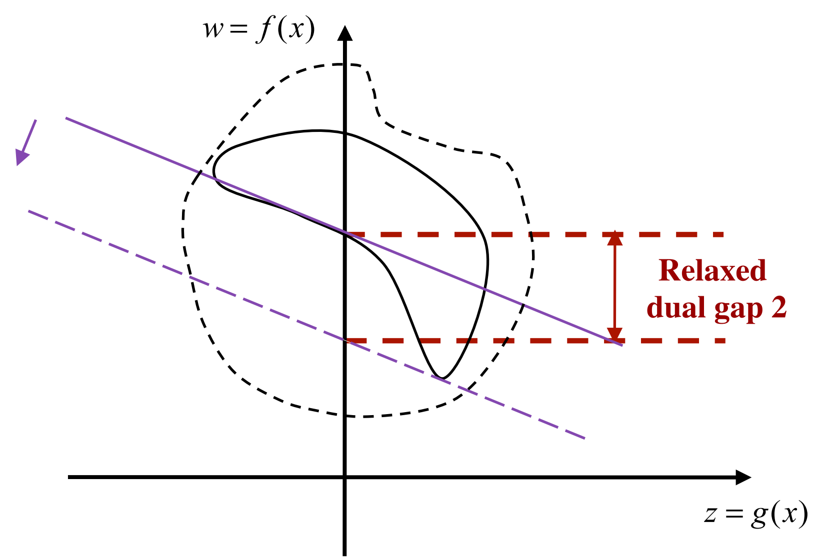
Model, Size, and Solution Method

- Mixed-integer linear programming (MILP) model
  - First-stage variables binary, recourse problem MILP
- The model size increases exponentially with the number of products
  - # scenarios = 3^n, where n is the total number of products
- When n = 10 products, the model size becomes prohibitively large
  - # binary variables > 35 million!
  - # cont. variables > 175 million!
  - # constraints > 150 million!
  - State-of-the-art commercial solvers cannot solve in reasonable time (eg. IBM / CPLEX)

Gaps Due to Dual and Convex Relaxations

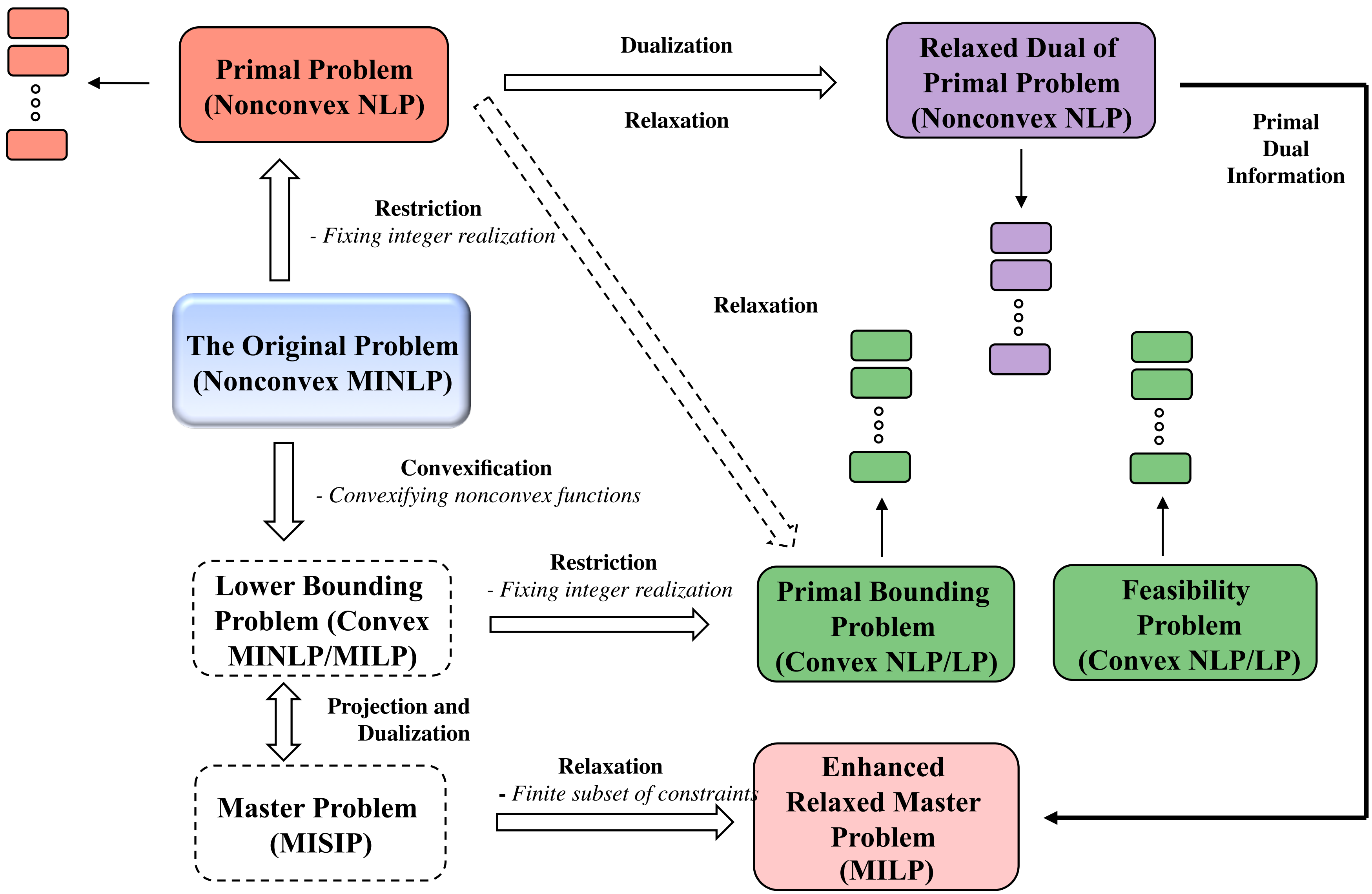






It is very difficult to obtain dual multipliers for a nonconvex problem!

Enhanced NGBD with More Dual Information



The Enhanced Decomposition Strategy
– Relaxed Dual of Primal Problem

Relaxed Dual of Primal Problem (NLP)

$$
\begin{cases}
obj_{DPP_h}(y^{(k)}) = \min\limits_{x_h, q_h, u_h} \quad c_{2,h}^T x_h + c_{3,h}^T q_h + c_{4,h}^T u_h + \left(\pi_h^{(k)}\right)\left(A_{1,h} y^{(k)} + A_{2,h} x_h + A_{3,h} q_h + A_{4,h} u_h - b_h\right) \\
s.t. \quad u_{h,l.t} = x_{h,l} q_{h,t}, \quad \forall (l,t) \in \Omega, \\
\qquad (x_h, q_h, u_h) \in \Pi_h
\end{cases}
$$

$$\pi_h^{(k)} = \lambda_h^{(k)} \quad \text{or} \quad \pi_h^{(k)} = \kappa_h^{(k)}$$

$\lambda_h^{(k)}$: Lagrange multipliers of Problem (PBP_h)

$\kappa_h^{(k)}$: Lagrange multipliers of Problem (PP_h)

The relaxed dual of the primal problem is usually much more difficult than the primal problem

The Enhanced Decomposition Strategy
–Enhanced Relaxed Master Problem

Enhanced Relaxed Master Problem (MILP)

$$
\begin{cases}
\min_{y,\eta} \ \eta \\
\text{s.t. } \eta \ge \tilde{\alpha}^{(r)} y + \tilde{\beta}^{(r)}, \quad \forall r \in U^k \subset T^k, \\
\eta \ge \breve{\alpha}^{(r)} y + \breve{\beta}^{(r)}, \quad \forall r \in U^k \subset T^k, \\
\eta \ge \alpha^{(j)} y + \beta^{(j)}, \quad \forall j \in T^k, \\
\gamma^{(i)} y + \theta^{(i)} \le 0, \quad \forall i \in S^k, \\
\sum_{l \in \{l : y_l^{(t)} = 1\}} y_l - \sum_{l \in \{l : y_l^{(t)} = 0\}} y_l \le \left| \{ l : y_l^{(t)} = 1 \} \right| - 1, \quad \forall t \in T^k \cup S^k, \\
y \in Y, \ \eta \in \mathbb{R}
\end{cases}
$$

$$\tilde{\alpha}^{(r)} = c_1^T + \sum_{h=1}^{s} \left(\lambda_h^{(r)}\right)^T A_{1,h}$$

$$\tilde{\beta}^{(r)} = \sum_{h=1}^{s} \left[c_{2,h}^T \tilde{x}_h^{(r)} + c_{3,h}^T \tilde{q}_h^{(r)} + c_{4,h}^T \tilde{u}_h^{(r)} \right] + \sum_{h=1}^{s} \left[\left(\lambda_h^{(r)}\right)^T \left(A_{2,h} \tilde{x}_h^{(r)} + A_{3,h} \tilde{q}_h^{(r)} + A_{4,h} \tilde{u}_h^{(r)} - b_h \right) \right]$$

$$\breve{\alpha}^{(r)} = c_1^T + \sum_{h=1}^{s} \left(\kappa_h^{(r)}\right)^T A_{1,h}$$

$$\breve{\beta}^{(r)} = \sum_{h=1}^{s} \left[c_{2,h}^T \breve{x}_h^{(r)} + c_{3,h}^T \breve{q}_h^{(r)} + c_{4,h}^T \breve{u}_h^{(r)} \right] + \sum_{h=1}^{s} \left[\left(\kappa_h^{(r)}\right)^T \left(A_{2,h} \breve{x}_h^{(r)} + A_{3,h} \breve{q}_h^{(r)} + A_{4,h} \breve{u}_h^{(r)} - b_h \right) \right]$$

$\left(\tilde{x}_h^{(j)}, \tilde{q}_h^{(j)}, \tilde{u}_h^{(j)}\right)$: Optimal solution of Problem (DPP$_h$) with $\lambda_h^{(k)}$

$\left(\breve{x}_h^{(j)}, \breve{q}_h^{(j)}, \breve{u}_h^{(j)}\right)$: Optimal solution of Problem (DPP$_h$) with $\kappa_h^{(k)}$

The Enhanced Decomposition Strategy
–Enhanced Relaxed Master Problem

Enhanced Relaxed Master Problem (MILP)

$$
\begin{aligned}
&\min_{y,\eta} \ \eta \\
\text{s.t. } &\eta \geq \tilde{\alpha}^{(r)} y + \tilde{\beta}^{(r)}, \quad \forall r \in U^k \subset T^k, \\
&\eta \geq \breve{\alpha}^{(r)} y + \breve{\beta}^{(r)}, \quad \forall r \in U^k \subset T^k, \\
&\eta \geq \alpha^{(j)} y + \beta^{(j)}, \quad \forall j \in T^k, \\
&\gamma^{(i)} y + \theta^{(i)} \leq 0, \quad \forall i \in S^k, \\
&\sum_{l \in \{l : y_l^{(t)} = 1\}} y_l - \sum_{l \in \{l : y_l^{(t)} = 0\}} y_l \leq \left| \{ l : y_l^{(t)} = 1 \} \right| - 1, \quad \forall t \in T^k \cup S^k, \\
&y \in Y, \ \eta \in \mathbb{R}
\end{aligned}
$$

Primal Dual Cuts

$$\tilde{\alpha}^{(r)} = c_1^T + \sum_{h=1}^{s} \left(\lambda_h^{(r)}\right)^T A_{1,h}$$

$$\tilde{\beta}^{(r)} = \sum_{h=1}^{s} \left[c_{2,h}^T \tilde{x}_h^{(r)} + c_{3,h}^T \tilde{q}_h^{(r)} + c_{4,h}^T \tilde{u}_h^{(r)} \right] + \sum_{h=1}^{s} \left[\left(\lambda_h^{(r)}\right)^T \left(A_{2,h} \tilde{x}_h^{(r)} + A_{3,h} \tilde{q}_h^{(r)} + A_{4,h} \tilde{u}_h^{(r)} - b_h \right) \right]$$

$$\breve{\alpha}^{(r)} = c_1^T + \sum_{h=1}^{s} \left(\kappa_h^{(r)}\right)^T A_{1,h}$$

$$\breve{\beta}^{(r)} = \sum_{h=1}^{s} \left[c_{2,h}^T \breve{x}_h^{(r)} + c_{3,h}^T \breve{q}_h^{(r)} + c_{4,h}^T \breve{u}_h^{(r)} \right] + \sum_{h=1}^{s} \left[\left(\kappa_h^{(r)}\right)^T \left(A_{2,h} \breve{x}_h^{(r)} + A_{3,h} \breve{q}_h^{(r)} + A_{4,h} \breve{u}_h^{(r)} - b_h \right) \right]$$

$\left(\tilde{x}_h^{(j)}, \tilde{q}_h^{(j)}, \tilde{u}_h^{(j)}\right)$: Optimal solution of Problem (DPP$_h$) with $\lambda_h^{(k)}$

$\left(\breve{x}_h^{(j)}, \breve{q}_h^{(j)}, \breve{u}_h^{(j)}\right)$: Optimal solution of Problem (DPP$_h$) with $\kappa_h^{(k)}$

The Enhanced Decomposition Strategy
–Enhanced Relaxed Master Problem with Primal Dual Multicuts

Multicut Enhanced Relaxed Master Problem (MILP)

$$
\begin{cases}
\min\limits_{\substack{y,\eta,\\ \eta_1,\dots,\eta_s,}} \ \eta \\
\text{s.t. } \ \eta \ge c_1^T y + \sum_{h=1}^{s} \eta_h, \\
\qquad \eta_h \ge \tilde{\alpha}_h^{(r)} y + \tilde{\beta}_h^{(r)}, \quad \forall h \in \{1,\dots,s\},\ \forall r \in U^k \subset T^k, \\
\qquad \eta_h \ge \breve{\alpha}_h^{(r)} y + \breve{\beta}_h^{(r)}, \quad \forall h \in \{1,\dots,s\},\ \forall r \in U^k \subset T^k, \\
\qquad \eta \ge \alpha^{(j)} y + \beta^{(j)}, \quad \forall j \in T^k, \\
\qquad \gamma^{(i)} y + \theta^{(i)} \le 0, \quad \forall i \in S^k, \\
\qquad \sum_{l \in \left\{l : y_l^{(t)} = 1\right\}} y_l - \sum_{l \in \left\{l : y_l^{(t)} = 0\right\}} y_l \le \left| \left\{ l : y_l^{(t)} = 1 \right\} \right| - 1, \quad \forall t \in T^k \cup S^k, \\
\qquad y \in Y,\ \eta \in \mathbb{R}
\end{cases}
$$

$$\tilde{\alpha}_h^{(r)} = \left(\lambda_h^{(r)}\right)^T A_{1,h}$$

$$\tilde{\beta}_h^{(r)} = c_{2,h}^T \tilde{x}_h^{(r)} + c_{3,h}^T \tilde{q}_h^{(r)} + c_{4,h}^T \tilde{u}_h^{(r)} + \left(\lambda_h^{(r)}\right)^T \left(A_{2,h}\tilde{x}_h^{(r)} + A_{3,h}\tilde{q}_h^{(r)} + A_{4,h}\tilde{u}_h^{(r)} - b_h\right)$$

$$\breve{\alpha}_h^{(r)} = \left(\kappa_h^{(r)}\right)^T A_{1,h}$$

$$\breve{\beta}_h^{(r)} = c_{2,h}^T \breve{x}_h^{(r)} + c_{3,h}^T \breve{q}_h^{(r)} + c_{4,h}^T \breve{u}_h^{(r)} + \left(\kappa_h^{(r)}\right)^T \left(A_{2,h}\breve{x}_h^{(r)} + A_{3,h}\breve{q}_h^{(r)} + A_{4,h}\breve{u}_h^{(r)} - b_h\right)$$

The Enhanced Decomposition Strategy
–Enhanced Relaxed Master Problem with Primal Dual Multicuts

Multicut Enhanced Relaxed Master Problem (MILP)

$$
\left\{
\begin{aligned}
& \min_{\substack{y,\eta,\\ \eta_1,\dots,\eta_s,}} \quad \eta \\
\text{s.t.} \quad & \eta \geq c_1^T y + \sum_{h=1}^{s} \eta_h, \\
& \eta_h \geq \tilde{\alpha}_h^{(r)} y + \tilde{\beta}_h^{(r)}, \quad \forall h \in \{1,\dots,s\}, \ \forall r \in U^k \subset T^k, \\
& \eta_h \geq \breve{\alpha}_h^{(r)} y + \breve{\beta}_h^{(r)}, \quad \forall h \in \{1,\dots,s\}, \ \forall r \in U^k \subset T^k, \\
& \eta \geq \alpha^{(j)} y + \beta^{(j)}, \quad \forall j \in T^k, \\
& \gamma^{(i)} y + \theta^{(i)} \leq 0, \quad \forall i \in S^k, \\
& \sum_{l \in \{l : y_l^{(t)} = 1\}} y_l - \sum_{l \in \{l : y_l^{(t)} = 0\}} y_l \leq \left| \{ l : y_l^{(t)} = 1 \} \right| - 1, \quad \forall t \in T^k \cup S^k, \\
& y \in Y, \ \eta \in \mathbb{R}
\end{aligned}
\right.
$$

Primal Dual Multicuts

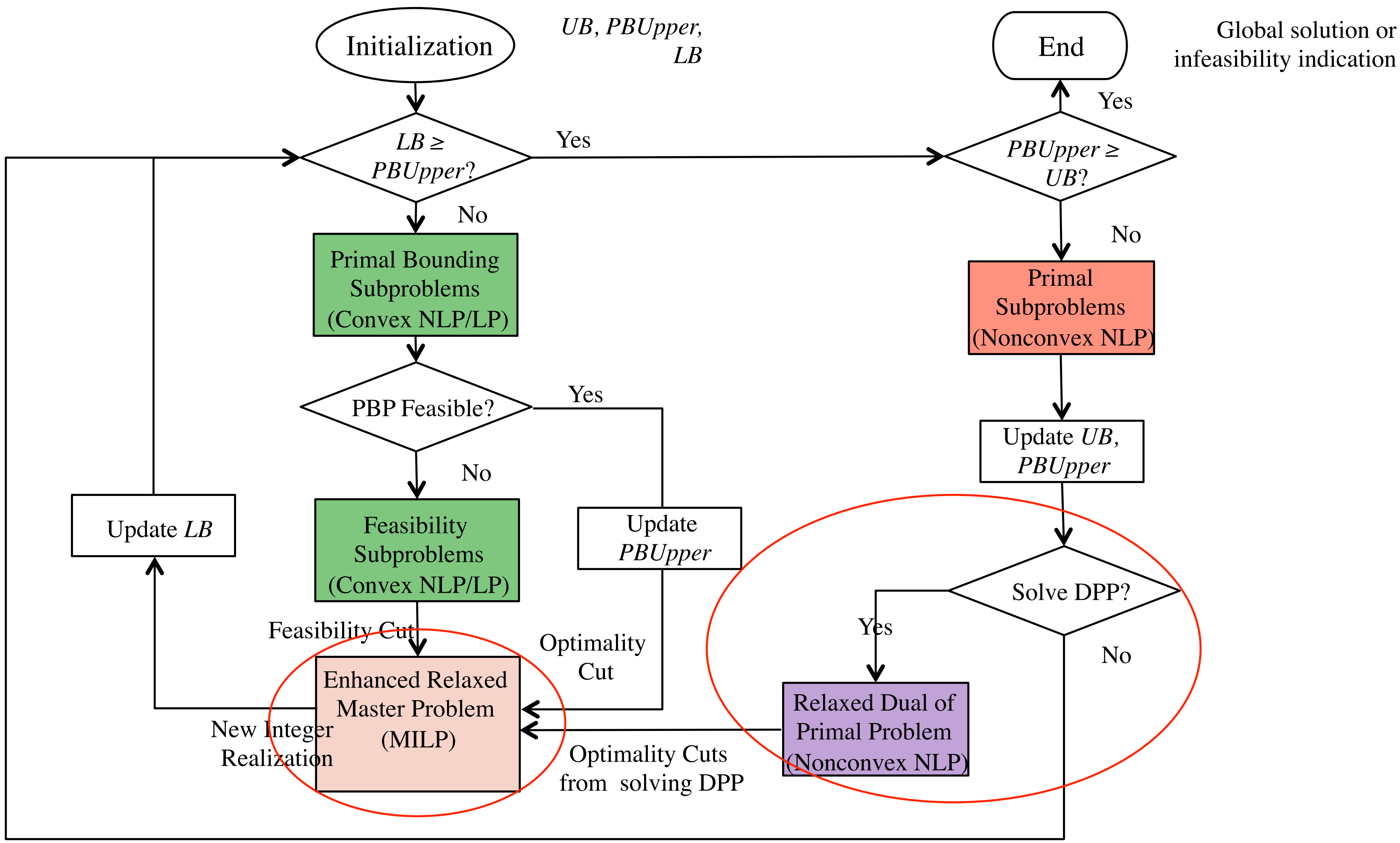
$$\tilde{\alpha}_h^{(r)} = \left(\lambda_h^{(r)}\right)^T A_{1,h}$$

$$\tilde{\beta}_h^{(r)} = c_{2,h}^T \tilde{x}_h^{(r)} + c_{3,h}^T \tilde{q}_h^{(r)} + c_{4,h}^T \tilde{u}_h^{(r)} + \left(\lambda_h^{(r)}\right)^T \left(A_{2,h} \tilde{x}_h^{(r)} + A_{3,h} \tilde{q}_h^{(r)} + A_{4,h} \tilde{u}_h^{(r)} - b_h\right)$$

$$\breve{\alpha}_h^{(r)} = \left(\kappa_h^{(r)}\right)^T A_{1,h}$$

$$\breve{\beta}_h^{(r)} = c_{2,h}^T \breve{x}_h^{(r)} + c_{3,h}^T \breve{q}_h^{(r)} + c_{4,h}^T \breve{u}_h^{(r)} + \left(\kappa_h^{(r)}\right)^T \left(A_{2,h} \breve{x}_h^{(r)} + A_{3,h} \breve{q}_h^{(r)} + A_{4,h} \breve{u}_h^{(r)} - b_h\right)$$

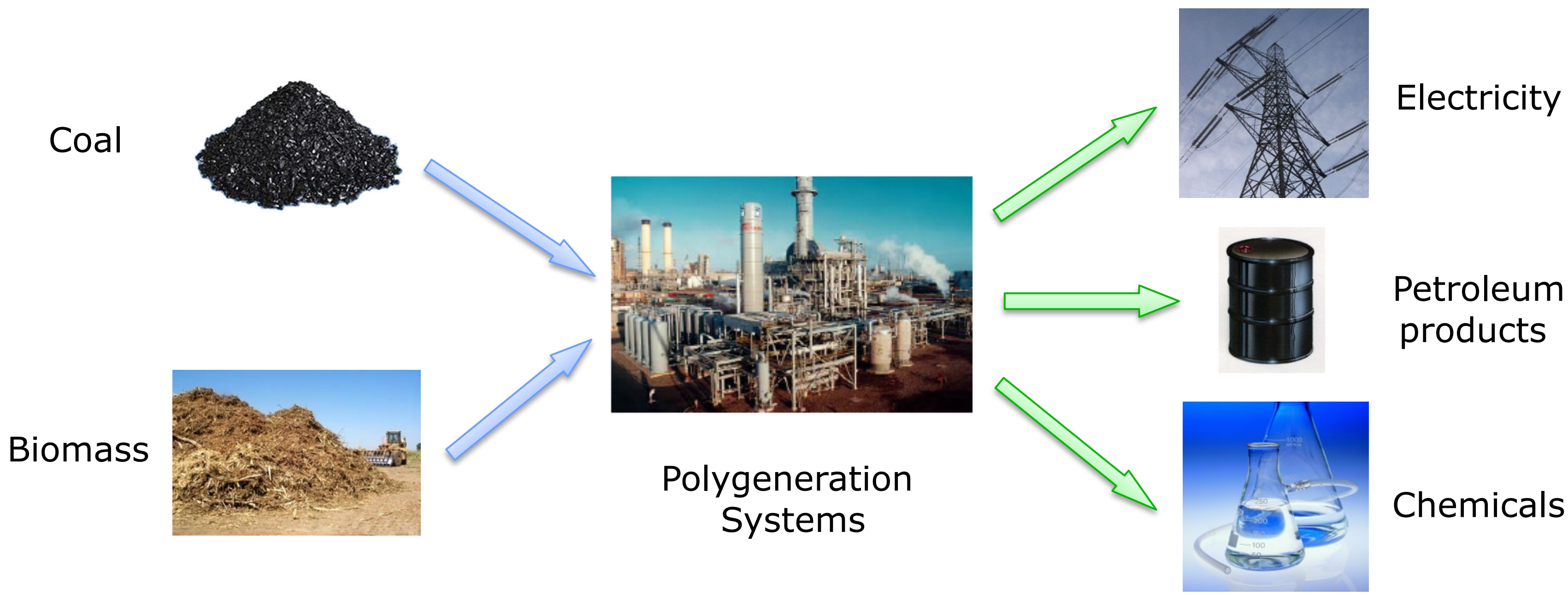
Enhanced NGBD Algorithm Flowchart

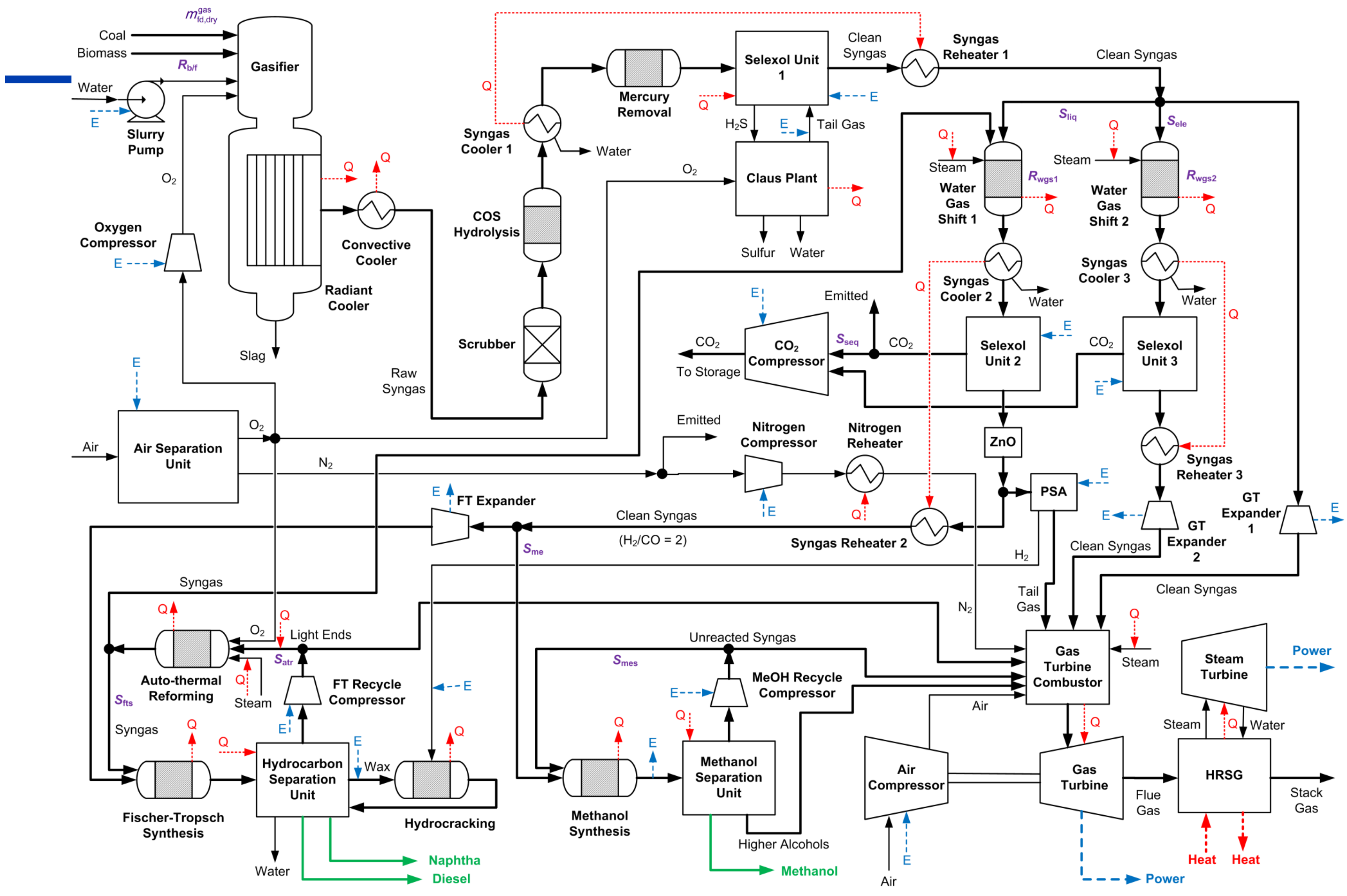


What is polygeneration?

Polygeneration is a novel conversion process

- Multiple feedstocks and multiple products
- Multiple processes with strong synergy in a single plant
- Flexible product portfolios in response to market conditions





Coal
Biomass
Water
E
Slurry Pump
Gasifier
$m^{gas}_{fd,dry}$
$R_{b/f}$
O_2
Oxygen Compressor
Radiant Cooler
Convective Cooler
Slag
Raw Syngas
Scrubber
COS Hydrolysis
Syngas Cooler 1
Mercury Removal
Selexol Unit 1
Clean Syngas
Syngas Reheater 1
H_2S
Tail Gas
Claus Plant
Sulfur
Water
Steam
Water Gas Shift 1
Water Gas Shift 2
R_{wgs1}
R_{wgs2}
S_{liq}
S_{ele}
Syngas Cooler 2
Syngas Cooler 3
Selexol Unit 2
Selexol Unit 3
CO_2 Compressor
CO_2
To Storage
Emitted
S_{seq}
ZnO
PSA
Syngas Reheater 3
GT Expander 1
GT Expander 2
Air Separation Unit
Air
N_2
Nitrogen Compressor
Nitrogen Reheater
FT Expander
Clean Syngas
(H_2/CO = 2)
Syngas Reheater 2
S_{me}
H_2
Tail Gas
Syngas
Auto-thermal Reforming
Light Ends
S_{atr}
S_{fts}
FT Recycle Compressor
Fischer-Tropsch Synthesis
Hydrocarbon Separation Unit
Wax
Hydrocracking
Naphtha
Diesel
Unreacted Syngas
S_{mes}
MeOH Recycle Compressor
Methanol Synthesis
Methanol Separation Unit
Higher Alcohols
Methanol
Air Compressor
Gas Turbine Combustor
Gas Turbine
Flue Gas
Steam Turbine
HRSG
Stack Gas
Power
Heat
Q

Case Study

Problem Sizes and Optimization Results

	Case 1	Case 2
Case Study	Middle Oil Price Middle Carbon Tax 100% Flexibility	Middle Oil Price Middle Carbon Tax 100% Flexibility
Number of Scenarios	**8**	**24**
Explanation of Scenarios	Daytime and nighttime in 4 seasons	Daytime and nighttime in 12 months
Number of Binary Variables	70	70
Number of Continuous Variables	4896	14688
Optimization Results ($MM)	1122.95	1124.31

Case 1 Results

	BARON	NGBD	Enhanced NGBD	Multicut Enhanced NGBD
Total Time	--- [1]	73004.91	11985.4	3065.11
Time for PBP		3.02	1.24	0.41
Time for FP		0.42	0.49	0.23
Time for RM		87.42	7.6	4.43
Time for PP		72914.05	9403.55	1299.12
Time for DPP			2572.52	1760.92
Integers Visited [2]		347/292	108/58	46/9

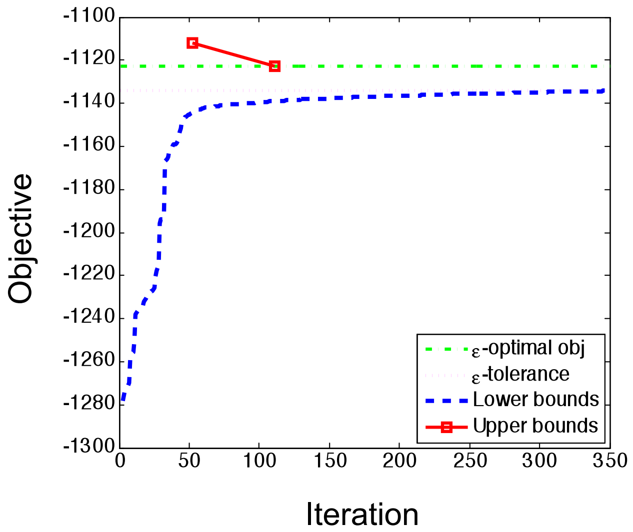
Tolerance: 10^{-2}

[1] No global solution returned within 48 hours.

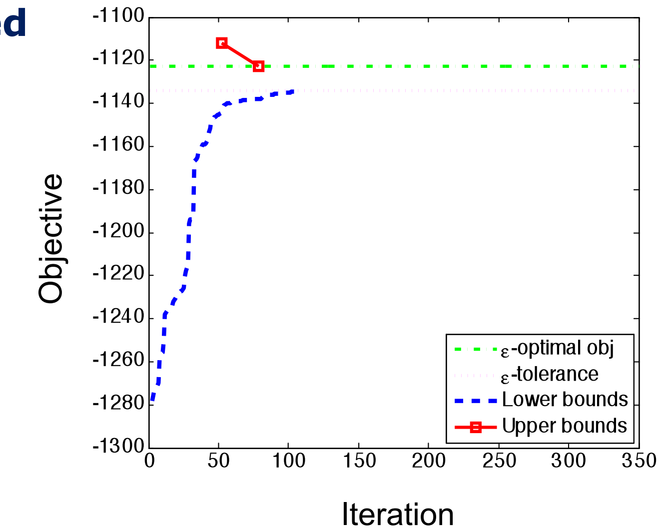
[2] Total number of integers visited / Number of integers visited by the primal problem

Case 1 Results

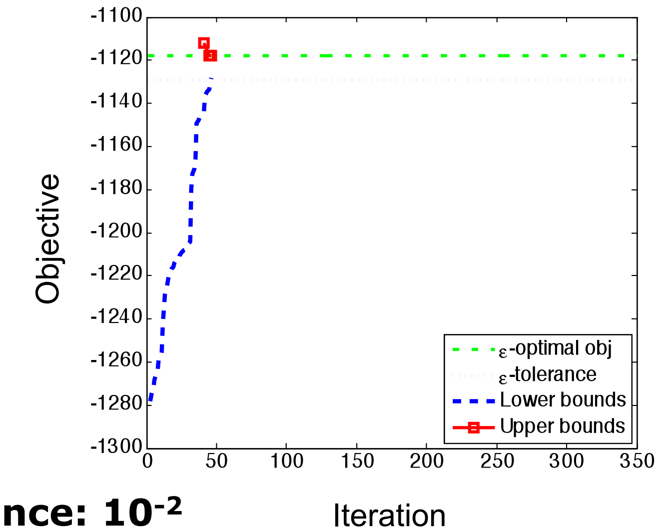
NGBD



Enhanced NGBD



Multicut Enhanced NGBD



Tolerance: 10^{-2}

Case 2 Results

	BARON	NGBD	Enhanced NGBD	Multicut Enhanced NGBD
Total Time	--- [1]	---	48430.99	15824.95
Time for PBP			3.1	1.01
Time for FP			0.77	0.47
Time for RM			8.65	10.38
Time for PP			37571.26	6770.02
Time for DPP			10847.21	9043.07
Integers Visited [2]			106/55	44/10

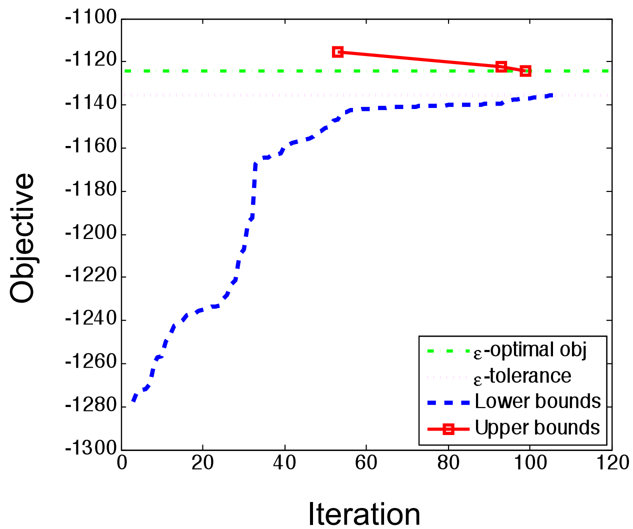
Tolerance: 10^{-2}

[1] No global solution returned within 48 hours.

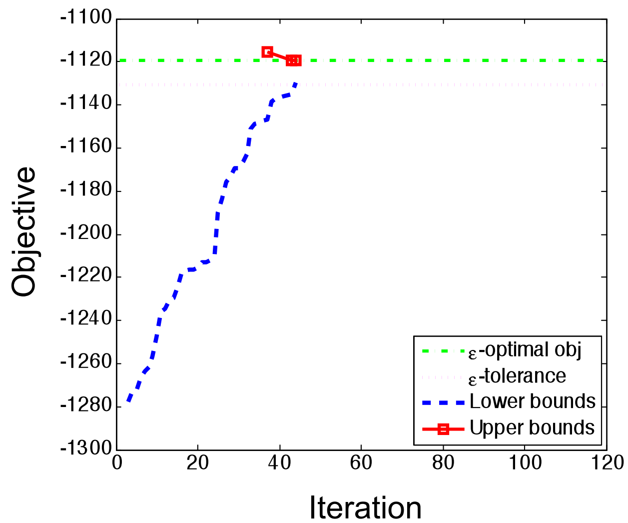
[2] Total number of integers visited / Number of integers visited by the primal problem

Case 2 Results

Enhanced NGBD



Multicut Enhanced NGBD



Tolerance: 10^{-2}

Case 1 Results

	BARON	NGBD	Enhanced NGBD	Multicut Enhanced NGBD
Total Time	--- [1]	---	21323.92	16447.34
Time for PBP			16.6	4.57
Time for FP			1.91	2.84
Time for RM			22.37	7.16
Time for PP			12853.22	9214.1
Time for DPP			8429.82	7218.67
Integers Visited [2]			133/87	50/14

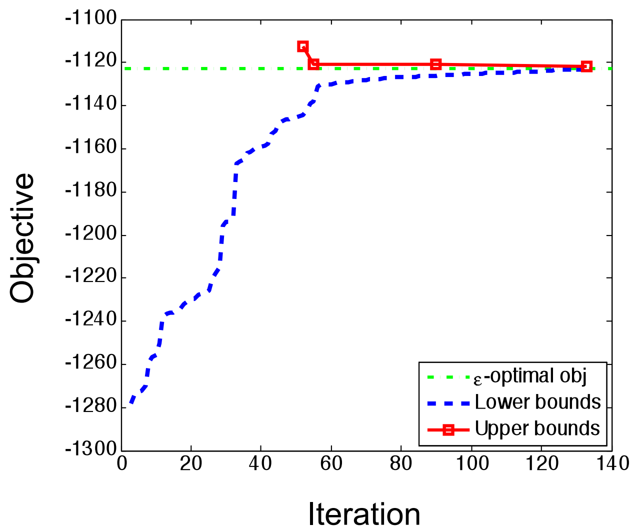
Tolerance: 10^{-3}

[1] No global solution returned within 48 hours.

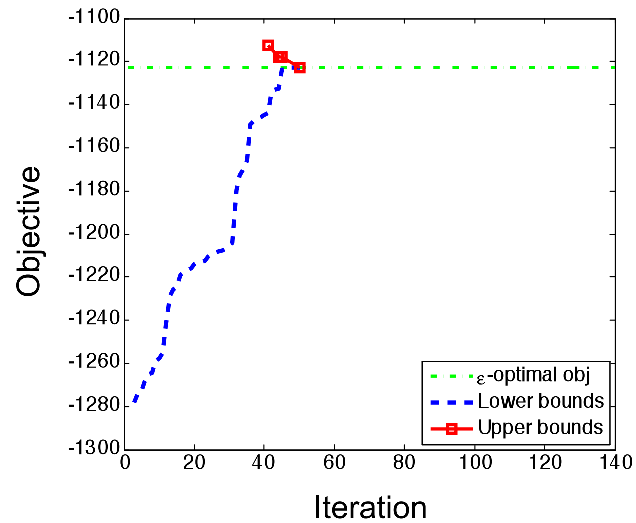
[2] Total number of integers visited / Number of integers visited by the primal problem

Case 1 Results

Enhanced NGBD



Multicut Enhanced NGBD



Tolerance: 10^{-3}

More Case Study Results

Scenarios Addressed in the Stochastic Formulation

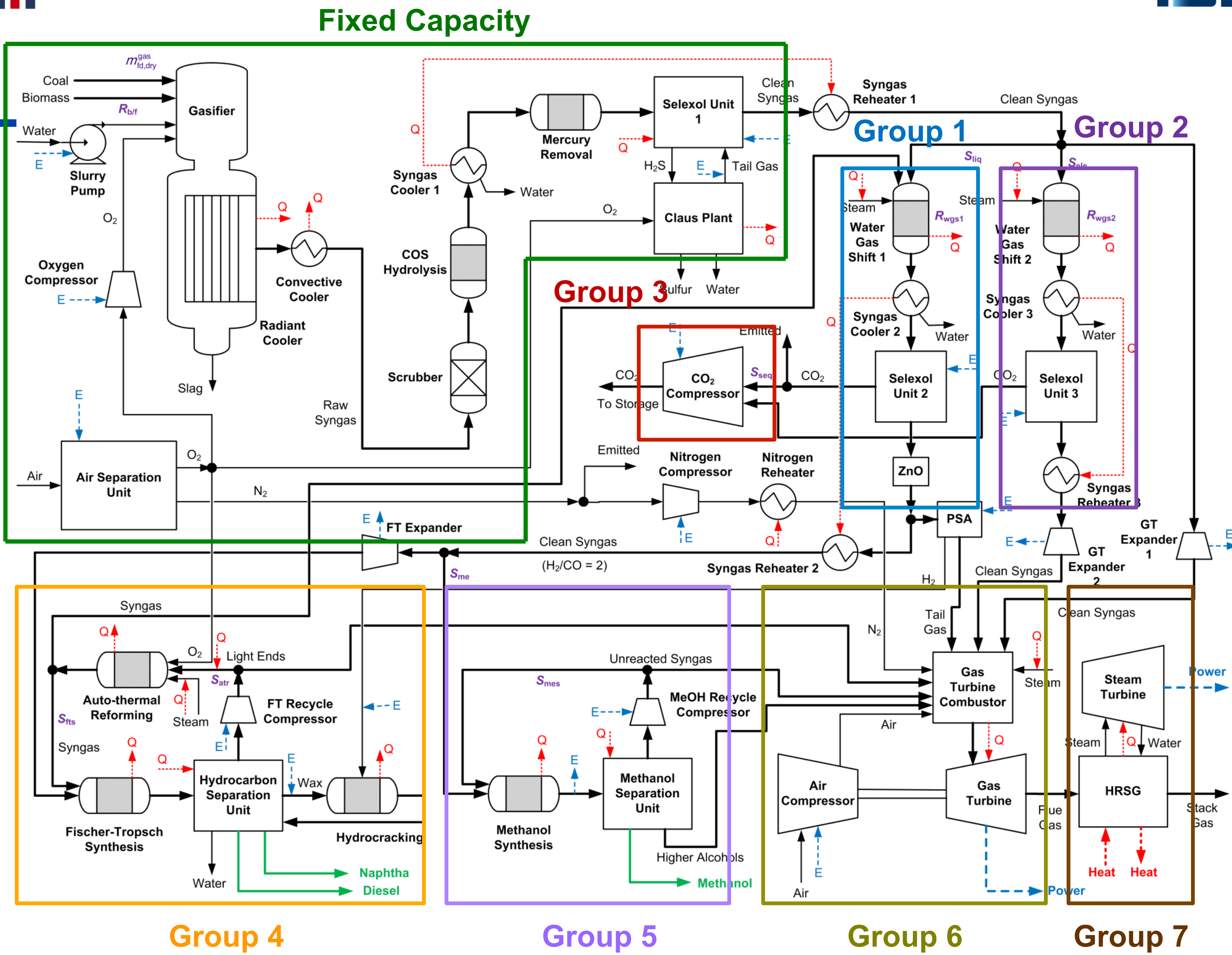
Scenario	No. 1	No. 2	No. 3	No. 4	No. 5
Probability	0.036	0.238	0.451	0.238	0.036
M1 quality[1]	1.90	2.62	3.34	4.06	4.78

[1] *Quality means the CO_2 mole percentage in gas.*

More Results With the Three Formulations

	Average NPV ($B)	Satisfaction of the CO_2 specification for the five scenarios			Capital Cost ($B)
		LNG 1	LNG 2	LNG 3	
1	34.4[1]	Y/Y/Y/Y/Y[2]	Y/N/N/N/N	Y/N/N/N/N	20.8
2	29.5	Y/Y/Y/Y/Y	Y/Y/Y/Y/Y	Y/Y/Y/Y/Y	21.5
3	32.3	Y/Y/Y/Y/Y	Y/Y/Y/Y/Y	Y/Y/Y/Y/Y	21.5

[1] *This NPV cannot be achieved in reality because of the violation of the CO_2 specification .*
[2] *'Y' indicates that the CO_2 specification is satisfied in one of the five scenarios and 'N' otherwise.*


Fixed Capacity
Coal
Biomass
Water
E
Slurry Pump
Gasifier
O2
Oxygen Compressor
Convective Cooler
Radiant Cooler
Slag
Air
Air Separation Unit
O2
N2
Raw Syngas
Scrubber
COS Hydrolysis
Syngas Cooler 1
Water
Mercury Removal
Selexol Unit 1
Clean Syngas
H2S
Tail Gas
Claus Plant
Sulfur
Water
Syngas Reheater 1
Clean Syngas
Group 1
Group 2
Group 3
Steam
Water Gas Shift 1
Water Gas Shift 2
Syngas Cooler 2
Syngas Cooler 3
Selexol Unit 2
Selexol Unit 3
CO2
CO2 Compressor
To Storage
Emitted
ZnO
PSA
Syngas Reheater 3
Nitrogen Compressor
Nitrogen Reheater
FT Expander
Clean Syngas
(H2/CO = 2)
Syngas Reheater 2
GT Expander 1
GT Expander 2
H2
Tail Gas
N2
Syngas
Auto-thermal Reforming
Light Ends
FT Recycle Compressor
Fischer-Tropsch Synthesis
Hydrocarbon Separation Unit
Wax
Hydrocracking
Naphtha
Diesel
Unreacted Syngas
MeOH Recycle Compressor
Methanol Synthesis
Methanol Separation Unit
Higher Alcohols
Methanol
Gas Turbine Combustor
Air Compressor
Gas Turbine
Flue Gas
Power
Steam Turbine
HRSG
Stack Gas
Heat
Group 4
Group 5
Group 6
Group 7