A Lagrangean Based Branch-and-Cut Algorithm for Global Optimization of Nonconvex Mixed-Integer Nonlinear Programs with Decomposable Structures

Ramkumar Karuppiah and Ignacio E. Grossmann

Department of Chemical Engineering
Carnegie Mellon University

Workshop on Global Optimization:
Methods and Applications
Fields Institute

May 2007

Introduction

- Many real-world optimization problems are nonconvex
  - Have multiple local optima
  - Hard to converge to global optimum

Examples: Water Networks and Crude Oil Scheduling

- Many of these models have decomposable structures
  - 2-stage stochastic programming problems
  - Planning and Scheduling models
  - Engineering design models

- Models are large in size and hard to solve to global optimality

  scaling issue

GOAL: Develop an algorithm to globally optimize large-scale models by exploiting decomposable structure

Problem Description

MINLP

Non-convex model

$$
\begin{aligned}
\min \quad & z = s(x,y) + \sum_{n=1}^{N} r_n(u_n, v_n) \\
s.t. \quad & h_n(u_n, v_n) = 0 \qquad n = 1,\dots,N \\
& g_n(u_n, v_n) \le 0 \qquad n = 1,\dots,N \\
& h'_n(x, y, u_n, v_n) = 0 \qquad n = 1,\dots,N \\
& g'_n(x, y, u_n, v_n) \le 0 \qquad n = 1,\dots,N \\
& x^L \le x \le x^U \\
& y \in \{0,1\}^J \\
& u_n^L \le u_n \le u_n^U \qquad n = 1,\dots,N \\
& v_n \in \{0,1\}^{m_{v_n}} \qquad n = 1,\dots,N \\
& x \in R^I,\ u_n \in R^{m_{u_n}}
\end{aligned}
\qquad \textbf{(P)}
$$

Linking constraints

$$\left.\begin{aligned} g'_n &: R^{I+J+m_{u_n}+m_{v_n}} \to R^{q_{g'_n}} \\ h'_n &: R^{I+J+m_{u_n}+m_{v_n}} \to R^{q_{h'_n}} \end{aligned}\right\}$$

Link together sub-models

Non-Linking Constraints

$$\left.\begin{aligned} g_n &: R^{m_{u_n}+m_{v_n}} \to R^{q_{g_n}} \\ h_n &: R^{m_{u_n}+m_{v_n}} \to R^{q_{h_n}} \end{aligned}\right\}$$

Constraints for separate sub-models

Linking Variables

$$\boxed{\begin{aligned} x &= [x_i] \qquad i = 1,\dots,I \\ y &= [y_j] \qquad j = 1,\dots,J \end{aligned}}$$

Binary variables

Non-Linking Variables

$$\boxed{\begin{aligned} &\{u_n\}_{n=1,\dots,N} \\ &\{v_n\}_{n=1,\dots,N} \end{aligned}}$$

Optimization of MINLP model

Models are large and often difficult to solve to global optimality

Direct application of deterministic global optimization algorithms (*spatial branch and bound*) not effective

Computationally inefficient

Major reason:

Weak lower bounds from MI(N)LP relaxation of (P) constructed with convex envelopes

Alternative approach: Lagrangean Decomposition

- Exploit decomposable structure of the large-scale model

Model Reformulation

How to bring (P) to decomposable form ?

- Create N identical copies of the linking variables

$$\{x^1, x^2, \ldots, x^N\}$$
$$\{y^1, y^2, \ldots, y^N\}$$

Duplicate variables

- Write linking constraints in (P) in terms of **Duplicate Variables**
- Introduce Coupling constraints into model (P)

$$x^1 = x^2 = \ldots = x^N$$

$$y^1 = y^2 = \ldots = y^N$$

$$\begin{array}{lll}
\min & z^{RP} = \sum_{n=1}^{N} w_n s(x^n, y^n) + \sum_{n=1}^{N} r_n(u_n, v_n) & \\
s.t. & h_n(u_n, v_n) = 0 & n = 1, \ldots, N \\
& g_n(u_n, v_n) \le 0 & n = 1, \ldots, N \\
& h'_n(x^n, y^n, u_n, v_n) = 0 & n = 1, \ldots, N \\
& g'_n(x^n, y^n, u_n, v_n) \le 0 & n = 1, \ldots, N \\
& x^n - x^{n+1} = 0 & n = 1, \ldots, N-1 \\
& y^n - y^{n+1} = 0 & n = 1, \ldots, N-1 \\
& x^L \le x^n \le x^U & n = 1, \ldots, N \\
& y^n \in \{0,1\}^J & n = 1, \ldots, N \\
& u_n^L \le u_n \le u_n^U & n = 1, \ldots, N \\
& v_n \in \{0,1\}^{m_{v_n}} & n = 1, \ldots, N \\
& x^n \in R^I, \; u_n \in R^{m_{u_n}} & \sum_{n=1}^{N} w_n = 1 \qquad 0 \le w_n \le 1
\end{array}$$

New coupling constraints

(RP)

Lagrangean Decomposition

- Dualize Coupling constraints
  - **Multiply coupling constraints with Lagrange multipliers, transfer them to objective function**

$$\min \ z^{LRP} = \sum_{n=1}^{N} w_n s(x^n, y^n) + \sum_{n=1}^{N} r_n(u_n, v_n) + \sum_{n=1}^{N-1} (\bar{\lambda}_n^x)^T (x^n - x^{n+1}) + \sum_{n=1}^{N-1} (\bar{\lambda}_n^y)^T (y^n - y^{n+1})$$

Lagrange Multipliers

- Obtain decomposable Lagrangean relaxation

$$\begin{aligned}
\min \ z^{LRP} = & \sum_{n=1}^{N} w_n s(x^n, y^n) + \sum_{n=1}^{N} r_n(u_n, v_n) + \sum_{n=1}^{N-1} (\bar{\lambda}_n^x)^T (x^n - x^{n+1}) + \sum_{n=1}^{N-1} (\bar{\lambda}_n^y)^T (y^n - y^{n+1}) \\
s.t. \quad & h_n(u_n, v_n) = 0 \qquad n = 1, \dots, N \\
& g_n(u_n, v_n) \le 0 \qquad n = 1, \dots, N \\
& h_n'(x^n, y^n, u_n, v_n) = 0 \qquad n = 1, \dots, N \\
& g_n'(x^n, y^n, u_n, v_n) \le 0 \qquad n = 1, \dots, N \\
& x^L \le x^n \le x^U \qquad n = 1, \dots, N \\
& y^n \in \{0,1\}^J \qquad n = 1, \dots, N \\
& u_n^L \le u_n \le u_n^U \qquad n = 1, \dots, N \\
& v_n \in \{0,1\}^{m_{v_n}} \qquad n = 1, \dots, N \\
& x^n \in R^I, u_n \in R^{m_{u_n}}
\end{aligned}$$

(LRP)

Model Decomposition

- Decomposed sub-problems (fixed multipliers) ⇨ Smaller and easier to solve

$$
\left.
\begin{aligned}
\min\ & z_n = w_n s(x^n, y^n) + r_n(u_n, v_n) + (\overline{\lambda}_n^x - \overline{\lambda}_{n-1}^x)^T (x^n) + (\overline{\lambda}_n^y - \overline{\lambda}_{n-1}^y)^T (y^n) \\
s.t.\ & h_n(u_n, v_n) = 0 \\
& g_n(u_n, v_n) \le 0 \\
& h_n'(x^n, y^n, u_n, v_n) = 0 \\
& g_n'(x^n, y^n, u_n, v_n) \le 0 \\
& x^L \le x^n \le x^U \\
& y^n \in \{0,1\}^J \\
& u_n^L \le u_n \le u_n^U \\
& v_n \in \{0,1\}^{m_{v_n}} \\
& x^n \in R^I, u_n \in R^{m_{u_n}}
\end{aligned}
\right\} \quad n = 1, \ldots, N
$$

⇨ Globally Optimize each sub-model to get solution z_n^*

$$\overline{\lambda}_0^x = 0 \quad \overline{\lambda}_0^y = 0 \quad \overline{\lambda}_N^x = 0 \quad \overline{\lambda}_N^y = 0$$

$(\mathbf{SP_n})$

Lower bound (Lagrangean Decomposition) : $\sum_{n=1}^{N} z_n^* = z^{LB}$

Could use as a basis for B&B (Caroe and Schultz, 99)

Basic Ideas of Proposed Algorithm

- Combine ***Spatial branch and bound*** with Lagrangean decomposition

- Strengthen MI(N)LP relaxation of (P) with Lagrangean cuts

Branch and Cut Algorithm

At each node of search tree:

Cut Generation : Solve to global optimality dual subproblems for one or more sets of multiplier values

Lower Bound : Solve MIL(N)P relaxation with convexified Lagrangean cuts

Upper Bound : Feasible solution to nonconvex model which is obtained by globally solving NLP with fixed integer variables

→ ***Guaranteed to converge*** to global optimum given a tolerance ε between lower and upper bounds

Optimality based Cutting Planes

- Combine convex relaxations and Lagrangean decomposition

- Using solution z_n^* (Globally optimal solution of subproblem (SP_n)) derive cuts:

$$\boxed{z_n^* \le w_n s(x,y) + r_n(u_n,v_n) + (\bar{\lambda}_n^x - \bar{\lambda}_{n-1}^x)^T (x) + (\bar{\lambda}_n^y - \bar{\lambda}_{n-1}^y)^T (y)} \qquad (C_n)$$

Note: nonconvex cut written in terms of original coupling variables

- Update Lagrange multipliers (Fisher, 1981) and generate more cuts

Incorporation of Cutting Planes

- Add bound strengthening cuts to (P) and convexify resulting problem to get MI(N)LP relaxation (R)

$$
\begin{aligned}
\min\ & z^R = \bar{s}(x,y) + \sum_{n=1}^{N} \bar{r}_n(u_n,v_n) \\
s.t.\ & \bar{h}_n(u_n,v_n) = 0 \qquad n=1,\ldots,N \\
& \bar{g}_n(u_n,v_n) \le 0 \qquad n=1,\ldots,N \\
& \bar{h}'_n(x,y,u_n,v_n) = 0 \qquad n=1,\ldots,N \\
& \bar{g}'_n(x,y,u_n,v_n) \le 0 \qquad n=1,\ldots,N \\
& z_n^* \le w_n \bar{s}(x,y) + \bar{r}_n(u_n,v_n) + (\bar{\lambda}_n^x - \bar{\lambda}_{n-1}^x)^T(x) + (\bar{\lambda}_n^y - \bar{\lambda}_{n-1}^y)^T(y) \qquad n=1,\ldots,N \\
& x^L \le x \le x^U \\
& y \in \{0,1\}^J \\
& u_n^L \le u_n \le u_n^U \quad n=1,\ldots,N \\
& v_n \in \{0,1\}^{m_{v_n}} \qquad n=1,\ldots,N \\
& x \in R^I, u_n \in R^{m_{u_n}}
\end{aligned}
\qquad \textbf{(R)}
$$

$\bar{h}_n(.)=0 \quad \bar{g}_n(.)\le 0 \quad \bar{h}'_n(.)=0 \quad \bar{g}'_n(.)\le 0 \quad \bar{s}(.) \quad \bar{r}_n(.)$ ⇐ Convexified functions

- Solve model (R) to get a **valid lower bound** on the global optimum of (P)

Properties of Lagrangean Cuts

Theorem 1. The Lagrangean cuts

$$z_n^* \le w_n s(x,y) + r_n(u_n, v_n) + (\overline{\lambda}_n^x - \overline{\lambda}_{n-1}^x)^T(x) + (\overline{\lambda}_n^y - \overline{\lambda}_{n-1}^y)^T(y) \qquad \mathbf{(C_n)}$$

are valid, and do not cut off any portion of the MIP feasible region of MINLP model (P)

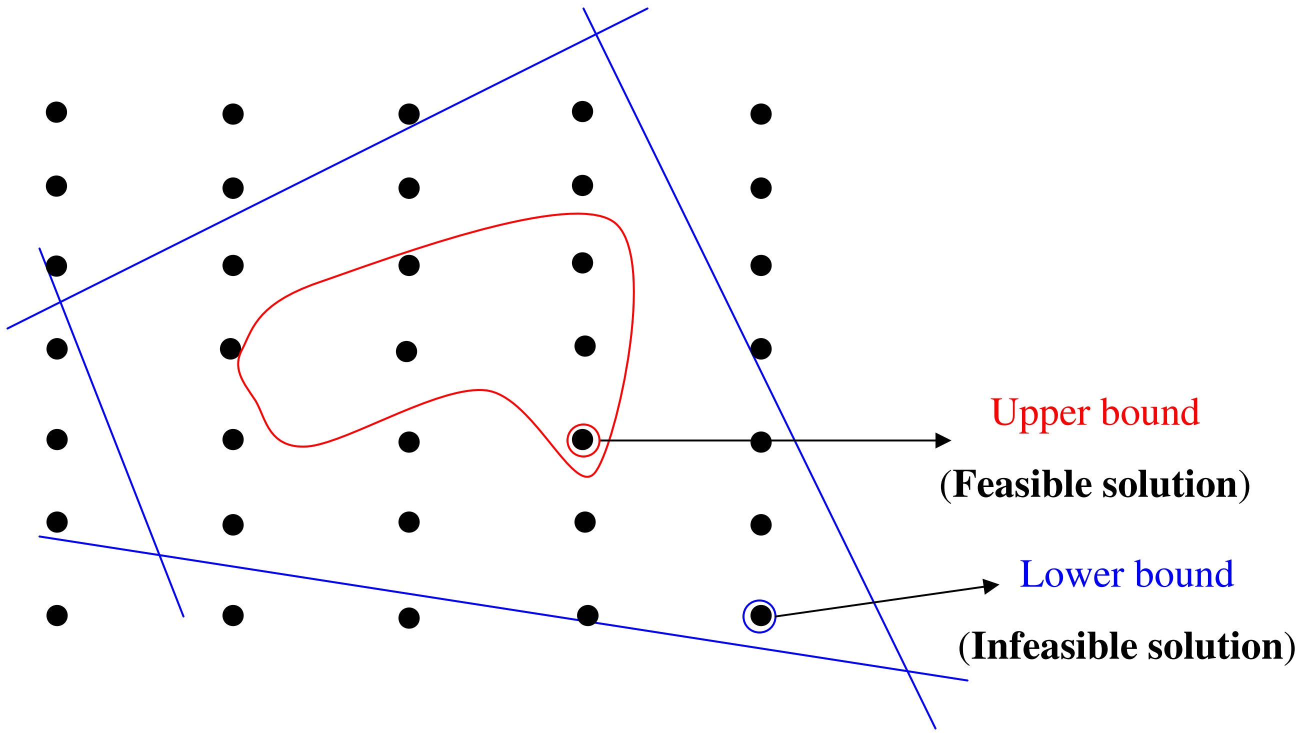
Proposition 1. The lower bound obtained by solving MI(N)LP with cuts is at least as strong as the one obtained by solving the MILP relaxation (CR) obtained by convexifying the nonconvex terms

Proposition 2. The lower bound obtained by solving MI(N)LP with cuts is at least as strong as the lower bound obtained from Lagrangean decomposition when all *N* sub-models are solved to global optimality.

Remarks

1. Cuts can be generated by solving subproblems in parallel
2. Update Lagrange multipliers: extension of method by Fisher (1981)
3. Global solution of subproblems can be obtained with standard solvers (BARON)

Constructing a Relaxation



- Linearize nonlinear terms and use **convex envelopes**

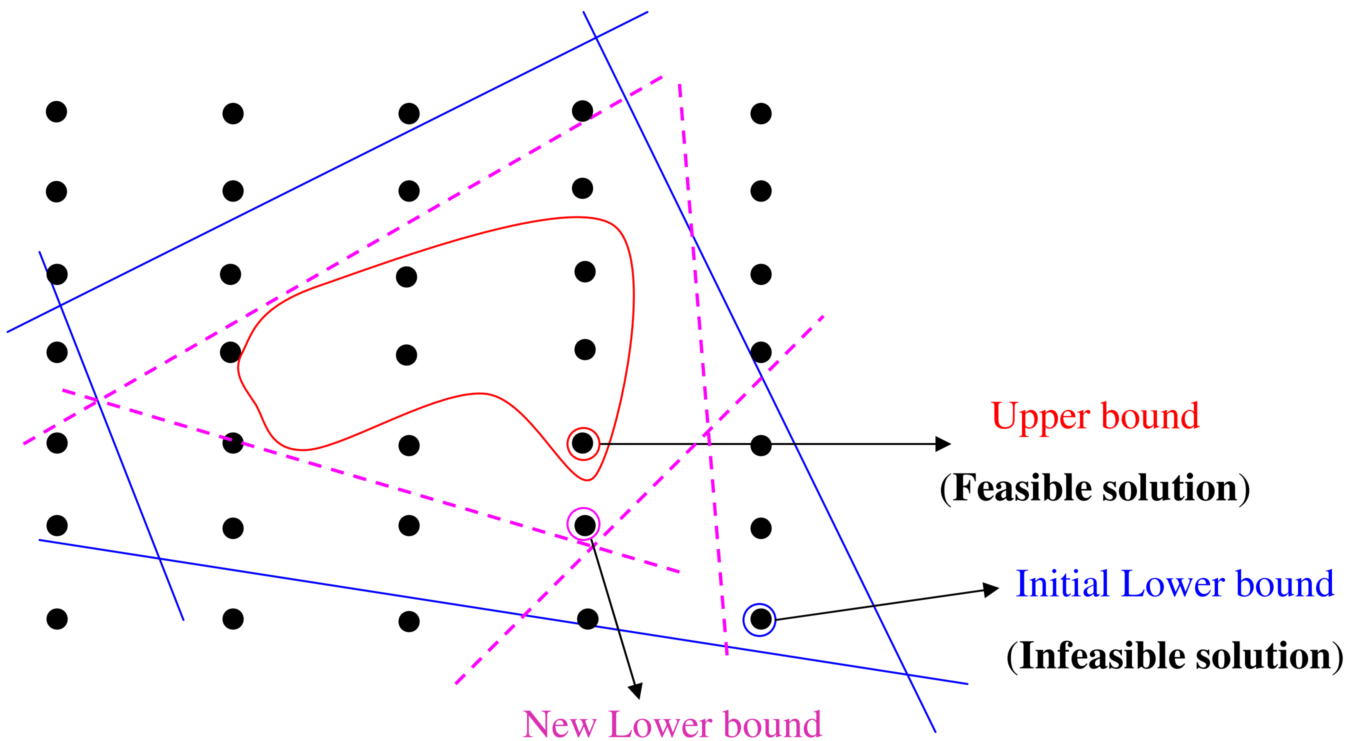
McCormick, 1976
Tawarmalani and Sahinidis, 2002

MINLP model relaxation → **MI(N)LP**

- Usually weak relaxations → Upper and Lower bounds are far apart

Geometric Interpretation

Incorporate cutting planes to tighten relaxation



Branch and Cut Algorithm

At each node of the branch and bound tree

Step 1. Initialization: Setting of variable bounds

Step 2. Bound contraction (*Optional*)

Step 3. Formulation of Lagrangean relaxation and decomposition:

a. *Derive model (LRP) and decompose into separate sub-problems*

b. *Solve each smaller sub-problem to global optimality*

c. *Generate cutting planes and add to (P) to get model (P')*

Step 4. Lower bound: Convexify model (P') to get model (R) and solve (R) to obtain a lower bound on the solution

Branch and Cut Algorithm

At each node of the branch and bound tree

Step 5. Upper bound: Fix binary variables in (P) to the values obtained by solving (R) and globally optimize the resulting nonconvex NLP

Step 6. Termination: Fathom node –

a. *If* $LB \geq UB$

b. *Optimality gap* $\leq \varepsilon$

c. *Solution of sub-problems is feasible for model (RP) i.e. non-anticipativity constraints hold in relaxation (LRP)*

Step 7. Branching: Similar to technique by Caroe and Schultz (1999)

- Branch on linking variables following heuristics

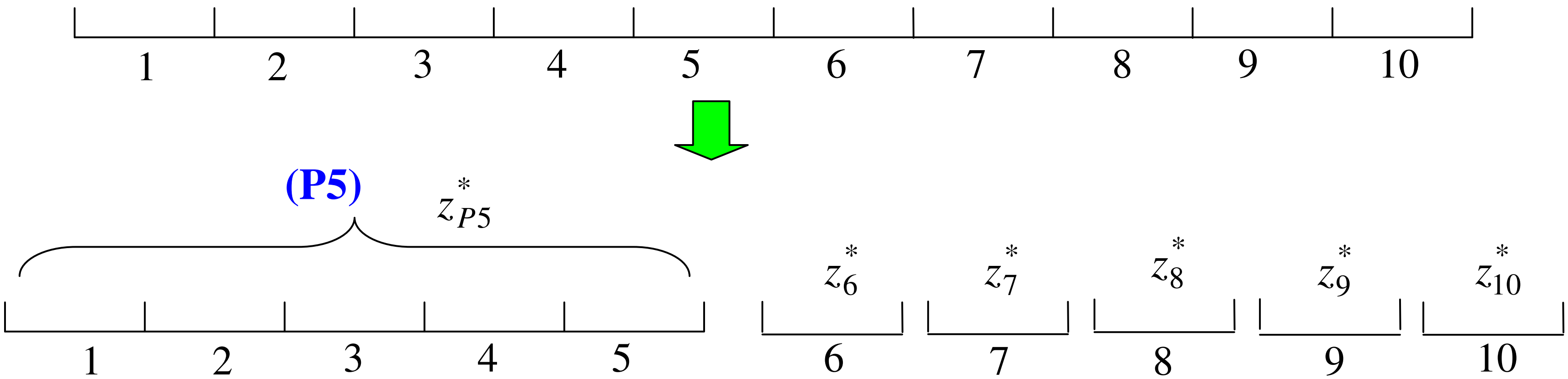
Convergence: Guaranteed for ε - convergence

Feasible region is continuously partitioned into sub-regions with non-decreasing lower bounds obtained over each sub-region

Remark: Lower Bounding Problem in Reduced Space

- Combine **proposed algorithm** (involving cutting planes) with conventional **Lagrangean decomposition**

Example : Problem (P) contains 10 sub-models



1. Decompose (P) into only **6 sub-problems** as opposed to 10 sub-problems
   - Sub-problem **(P5) (collection of 5 sub-problems)** , and 6, 7, 8, 9, 10
2. Solve (P5) using proposed algorithm (cutting plane technique) and 6, 7, 8, 9, 10 using BARON
3. Add global optima of sub-problems to obtain valid lower bound on solution

$$Lower \quad bound \; = z^*_{P5} + z^*_6 + z^*_7 + z^*_8 + z^*_9 + z^*_{10}$$

- In this way **lower bounding problem** at any node does not have to be solved in full space

Illustrative Problem

$$\min \quad z^{EP} = 5x + 7y + 2u_{11} + 6u_{14} + 5u_{21} + 9u_{24} + 3u_{31} + 11u_{34}$$

$$s.t. \quad \left.\begin{array}{l} u_{11}u_{14} - 3u_{12}u_{15} + 4u_{13}u_{16} + 4 = 0 \\ u_{11}u_{13} - 5 = 0 \\ 5u_{21}u_{24} - u_{22}u_{25} - u_{23}u_{26} + 5 = 0 \\ u_{21}u_{23} + u_{22}u_{24} - 2u_{25}u_{26} - 5 = 0 \\ 3u_{31}u_{34} + 4u_{32}u_{35} - u_{33}u_{36} + 3 = 0 \\ u_{31}u_{33} + u_{32}u_{34} - 4 = 0 \end{array}\right\} \text{Non-linking equations}$$

Bilinear

$$\left.\begin{array}{l} x \ge u_{11} \\ x \ge u_{21} \\ x \ge u_{31} \\ 3y \le x \le 5y \end{array}\right\} \text{Linking constraints}$$

$$0 \le x \le 5$$

$$y \in \{0,1\}$$

$$\begin{array}{lll} 1.5 \le u_{11} \le 3 & 0.5 \le u_{21} \le 4.5 & 1.5 \le u_{31} \le 3.5 \\ 1.3 \le u_{12} \le 11 & 0.2 \le u_{22} \le 0.5 & 0.5 \le u_{32} \le 13 \\ 1 \le u_{13} \le 2.5 & 0 \le u_{23} \le 5 & 1 \le u_{33} \le 1.9 \\ 2 \le u_{14} \le 4 & 0.25 \le u_{24} \le 5 & 0.5 \le u_{34} \le 2.5 \\ 0 \le u_{15} \le 3 & 3.2 \le u_{25} \le 8.7 & 2 \le u_{35} \le 7.2 \\ 0 \le u_{16} \le 10 & 0.15 \le u_{26} \le 7.8 & 1.5 \le u_{36} \le 9 \end{array}$$

(EP)

Linking variables $\Rightarrow$ x, y

Non-linking variables $\Rightarrow$ u_{11}, u_{21}, u_{31} u_{14}, u_{24}, u_{34} u_{12}, u_{22}, u_{32} u_{15}, u_{25}, u_{35} u_{13}, u_{23}, u_{33} u_{16}, u_{26}, u_{36}

1 binary variable, 19 continuous variables, 10 constraints, 15 nonconvex terms

Numerical Results

- Formulate Lagrangean relaxation and decompose into 3 sub-models and solve each sub-model with 2 sets of Lagrange multipliers
  - *Generate 6 cutting planes*

Root node results

Lower bound (LB) using algorithm = **64.01**

Upper bound (UB) obtained = **64.499**

Lower and Upper bounds converge within 1 % tolerance at root node of Branch and Bound tree

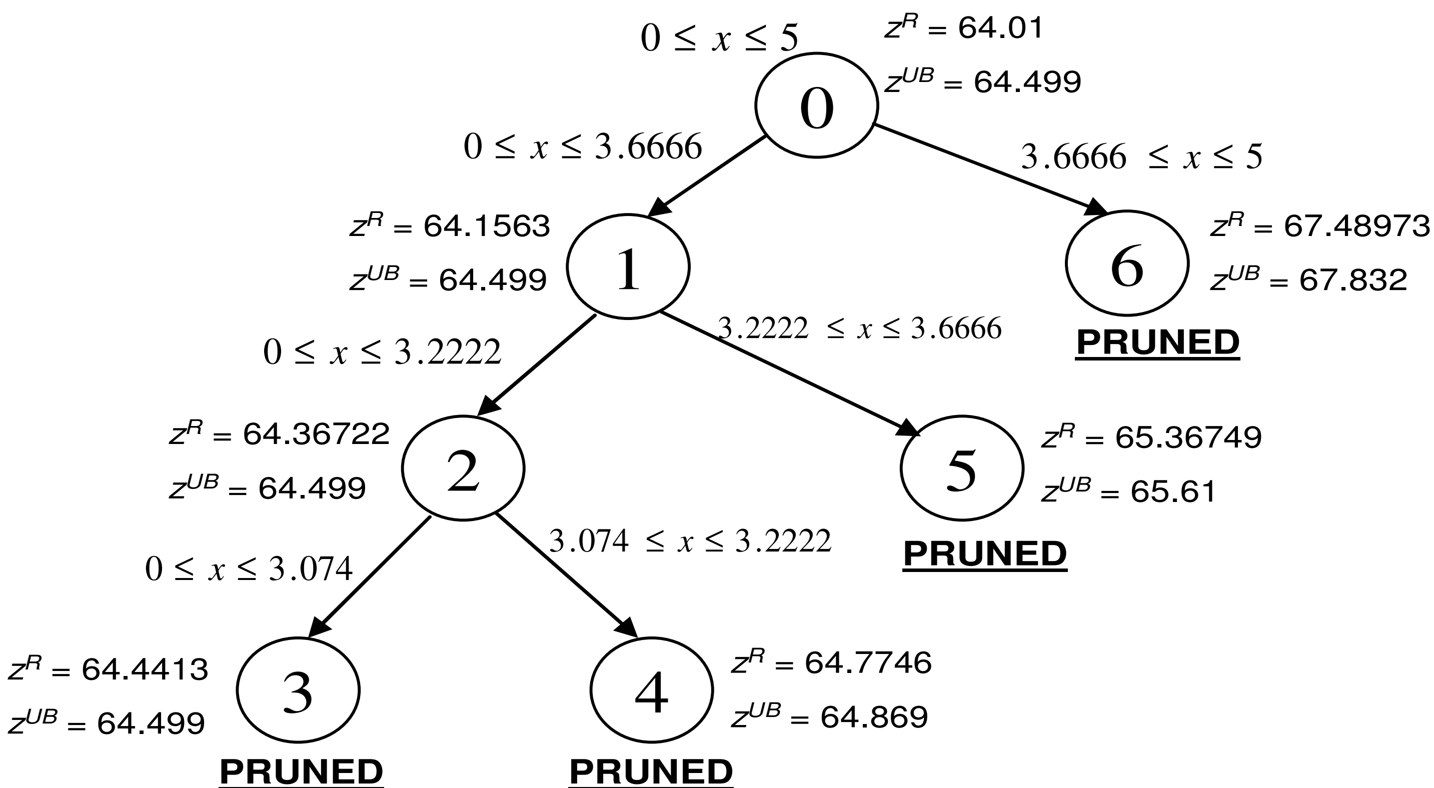
Comparison with standard relaxations

LB (using cutting planes) = **64.01** **vs** LB (using Lagrangean decomposition) = **63.33**

LB (from MI(N)LP relaxation) = **61.63**

Branch and Bound Tree

Relaxation gap reduced to 0.1 %



Test Examples

6 test examples

Example	Original MINLP model (P)		
	Number of Binary Variables	Number of Continuous Variables	Number of Constraints
1	**1**	**19**	**10**
2	**48**	**300**	**946**
3	**42**	**330**	**994**
4	**57**	**381**	**1167**
5	**24**	**764**	**928**
6	**77**	**1222**	**1377**

Illustrative problem

Scheduling problems

Process synthesis problems

Comparison of relaxations

Example	Global optimum	Relaxation at root node (with proposed cuts)	Relaxation at root node (without proposed cuts)
1	64.499	**64.01**	61.63
2	281.14	**68.45**	55.24
3	351.32	**133.80**	113.35
4	383.69	**189.19**	147.24
5	651,653.65	**645,951.64**	610,092.61
6	1,369,067.5	**1,347,297.36**	1,319,882.36

MILP

2 cuts

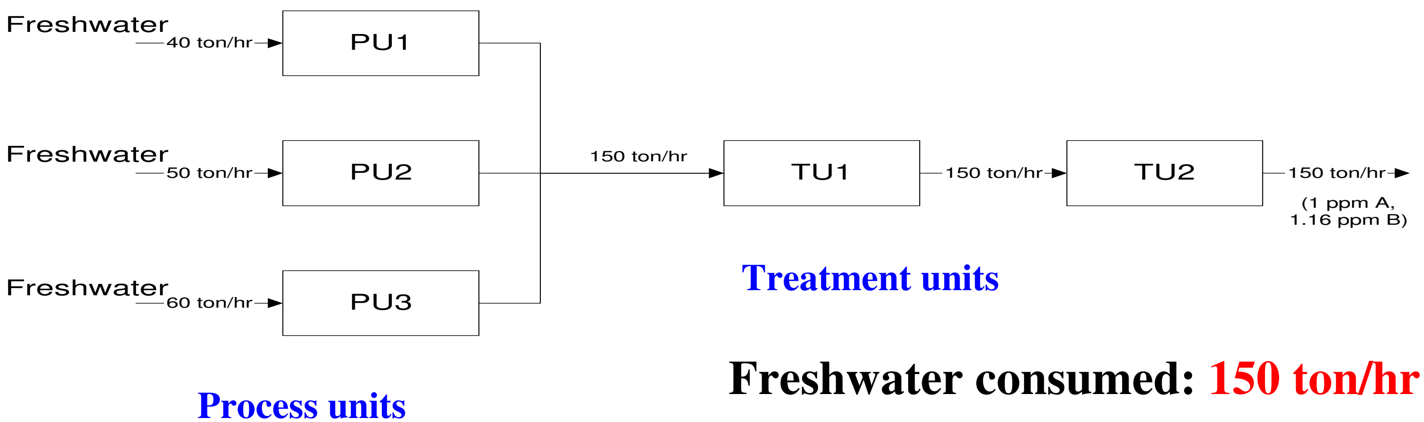
10 cuts

Synthesis of Integrated Process Water Systems

Karuppiah, Grossmann (2006)

WATER → One of MOST IMPORTANT resources used in process industry

Conventional water network: centralized



Freshwater consumed: 150 ton/hr

How to synthesize a network involving water reuse and decentralized water treatment that will:

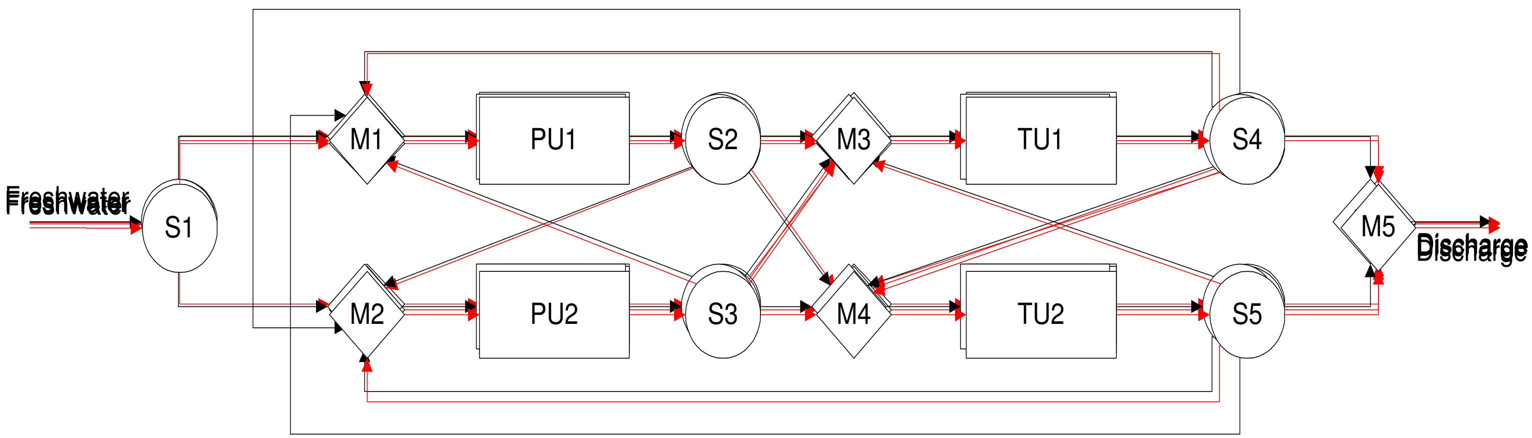
a) Reduce consumption of freshwater

b) Minimize cost

=> Global Optimization Problem

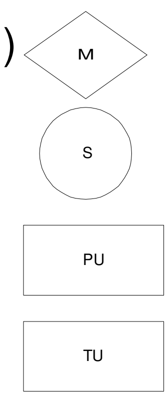
Superstructure for integrating Water Using/Treating Units

Integrated Water Network with reuse and recycle flows is proposed



- Superstructure consists of

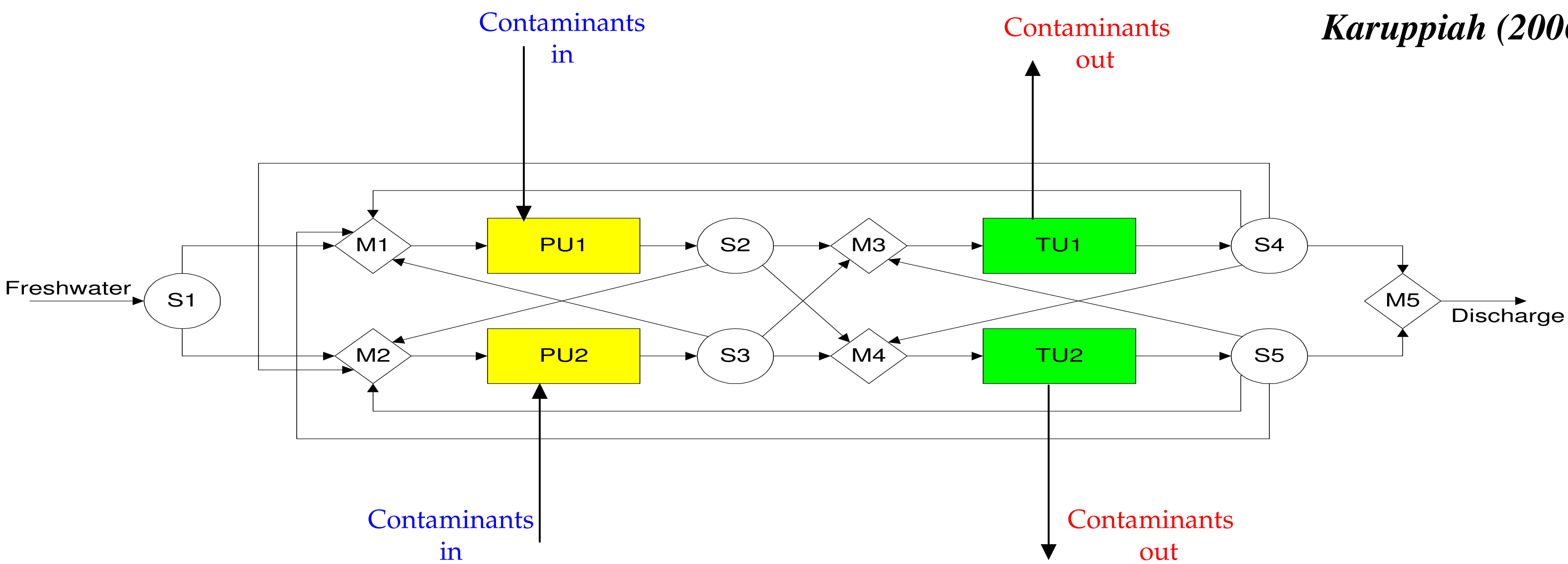
1. Mixers (MU)
2. Splitters (SU)
3. Process Units (PU)
4. Treatment Units (TU)



Design under Uncertainty

Superstructure of an Integrated Water Network

Karuppiah (2006)



- Uncertain Parameters (i) Contaminant loads in each Process unit

  (ii) Contaminant removal ratios in each Treatment unit

  Take on different values at different points of time

- Uncertainty has to be handled at the Design Stage

Superstructure optimization is formulated as an Mixed Integer Non-linear Programming Problem

Multiscenario MINLP Model

- Uncertainty in the system modeled using a finite set of scenarios denoted by N
  - Uncertain parameters assume different values in each scenario n ∈ N

Objective Function

Concave

$$\text{Min} \quad \underbrace{AR\left[\sum_i \left(C_p^i y^i + IP^i\left(\hat{F}^i\right)^{\delta}\right)\right] + AR\sum_{\substack{t\in TU\\ i\in t_{out}}} IC^t\left(\hat{F}^i\right)^{\alpha}}_{1^{st}\text{ stage costs}} + \underbrace{H\sum_n p_n \sum_i PM^i F_n^i + H\sum_n p_n C_{FW} FW_n + H\sum_n p_n \sum_{\substack{t\in TU\\ i\in t_{out}}} OC^t F_n^i}_{2^{nd}\text{ stage costs}} \qquad (1)$$

$\hat{F}^i$	= First stage design variable pertaining to maximum flow in the pipe *i*
y^i	= Design variable pertaining to existence of pipe *i*
F_n^i	= Second stage state variable corresponding to flow in pipe *i* in scenario *n*
C_p^i	= Cost coefficient corresponding to existence of pipe *i*
$IP^i\left(\hat{F}^i\right)^{\delta}$	= Investment cost of pipe *i* ($)
$PM^i F_n^i$	= Cost of pumping water in pipe *i* in scenario *n* ($)
H	= Hours of operation of plant per annum (hrs)
C_{FW}	= Cost of freshwater ($/ ton)
$IC^t\left(\hat{F}^i\right)^{\alpha}$	= Investment cost of a treatment unit *t* ($)
$OC^t F_n^i$	= Operating cost of a treatment unit *t* in scenario *n* ($)
AR	= Annualized factor for investment

MINLP Model

Mixer Units

Overall Material Balance

$$F_n^k = \sum_{i \in m_{in}} F_n^i \qquad \forall m \in MU,\ k \in m_{out}, \forall n \in N \tag{2}$$

Contaminant Balance

$$F_n^k C_{jn}^k = \sum_{i \in m_{in}} F_n^i C_{jn}^i \qquad \forall j, \forall m \in MU,\ k \in m_{out}, \forall n \in N \tag{3}$$

Bilinear

Splitter Units

Overall Material Balance

$$F_n^k = \sum_{i \in s_{out}} F_n^i \qquad \forall s \in SU,\ k \in s_{in}, \forall n \in N \tag{4}$$

Contaminant Balance

$$C_{jn}^i = C_{jn}^k \qquad \forall j, \forall s \in SU, \forall i \in s_{out}, k \in s_{in}, \forall n \in N \tag{5}$$

Process Units

Flow Balance

$$F_n^k = F_n^i = P^p \qquad \forall p \in PU,\ i \in p_{in},\ k \in p_{out}, \forall n \in N \tag{6}$$

Contaminant Balance

$$P^p C_{jn}^i + L_{jn}^p \times 10^3 = P^p C_{jn}^k \qquad \forall j, \forall p \in PU,\ i \in p_{in}, k \in p_{out}, \forall n \in N \tag{7}$$

Treatment Units

Total Flow Balance

$$F_n^k = F_n^i \qquad \forall t \in TU,\ i \in t_{out},\ k \in t_{in}, \forall n \in N \tag{8}$$

Contaminant Balance

$$C_{jn}^i = \beta_{jn}^t C_{jn}^k \qquad \forall j, \forall t \in TU,\ i \in t_{out},\ k \in t_{in}, \forall n \in N \tag{9}$$

MINLP Model (cont.)

Bound Strengthening Cuts

$$\sum_{p \in PU} L^p_{jn} \times 10^3 = \sum_{\substack{t \in TU \\ k \in t_{in}}} \left(1 - \beta^t_{jn}\right) F^k_n C^k_{jn} + F^{out}_n C^{out}_{jn} \quad \forall j, \forall n \in N \qquad (10)$$

Redundant overall mass balance each component

Design Constraints

$$\hat{F}^{iL} y^i \le \hat{F}^i \le \hat{F}^{iU} y^i \qquad \forall i \qquad (11)$$

If $y^i = 0$, then stream i does not exist and so $\hat{F}^i$ is 0

Linking Constraints ("Hard Constraints")

$$\hat{F}^i \ge F^i_n \qquad \forall i, \forall n \in N \qquad (12)$$

Design Variable

Flow variable in scenario n

Relaxation of Nonconvex NLP

- Bilinear terms $F^i C_j^i$ (in contaminant balance for mixers) are replaced by another variable f_j^i

$$f_j^k = \sum_{i \in m_{in}} f_j^i \quad \forall j, \forall m \in MU, \forall k \in m_{out} \qquad (10)$$

- Concave cost functions $(F^i)^\alpha$ (in the objective function) are replaced by another variable $(\overline{F}^i)$ to get a relaxed objective function

$$\Phi_{\text{relax}} = HC_{FW} FW + AR \sum_{\substack{t \in TU \\ i \in t_{out}}} IC^t \left(\overline{F}^i\right) + H \sum_{\substack{t \in TU \\ i \in t_{out}}} OC^t F^i \qquad (11)$$

- We construct Convex and Concave Envelopes for the Bilinear terms and the Concave functions

$\Downarrow$

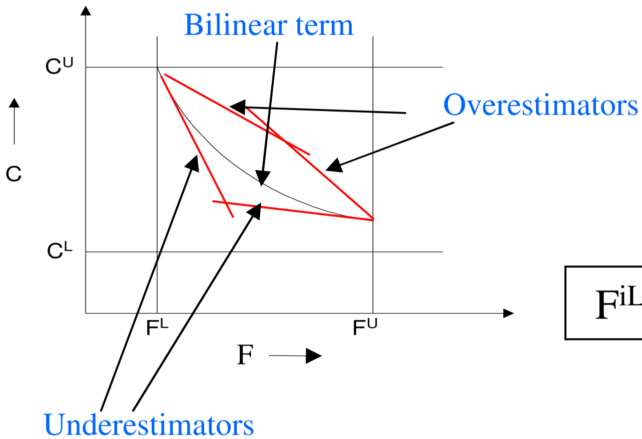
Linear Programming Relaxation

$\Downarrow$

Very large gap between the Lower and Upper bounds

Convexification of Nonconvex Functions

Concave and Convex Envelopes for Bilinear Terms



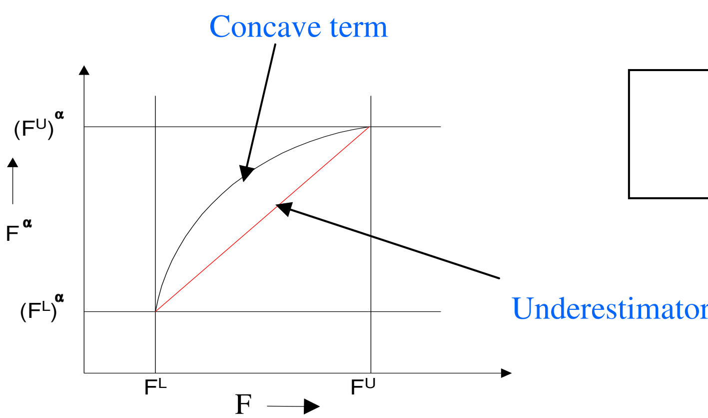
$$
\begin{aligned}
f_j^i &\ge F^{iL} C_j^i + C_j^{iL} F^i - F^{iL} C_j^{iL} \\
f_j^i &\ge F^{iU} C_j^i + C_j^{iU} F^i - F^{iU} C_j^{iU} \\
f_j^i &\le F^{iL} C_j^i + C_j^{iU} F^i - F^{iL} C_j^{iU} \\
f_j^i &\le F^{iU} C_j^i + C_j^{iL} F^i - F^{iU} C_j^{iL}
\end{aligned} \qquad (12)
$$

McCormick (1976)

Under- and over-estimators
(Linear Inequalities)

$$F^{iL} \le F^i \le F^{iU} \qquad C_j^{iL} \le C_j^i \le C_j^{iU}$$

Underestimation of Concave functions



$$\left(\overline{F}^i\right) \ge \left(F^{iL}\right)^\alpha + \left(\frac{\left(F^{iU}\right)^\alpha - \left(F^{iL}\right)^\alpha}{F^{iU} - F^{iL}}\right) \times \left(F^i - F^{iL}\right)$$

(Secant line)

$$F^{iL} \le F^i \le F^{iU}$$

Illustrative Example

Optimization of 2 Process Unit - 2 Treatment Unit network operating under uncertainty

Process Unit data

Unit	Flow (ton/hr)	Discharge load (Kg/hr)	n1	n2	n3	n4	n5	n6	n7	n8	n9	n10	Maximum Inlet Conc. (ppm) A	B
PU1	40	A	2	1	0.5	1	1	2	0.5	1	0.5	2	0	0
		B	2.5	1.5	1	1.5	1.5	2.5	1	1.5	1	2.5		
PU2	50	A	2	1	0.5	2	1	1	1	0.5	2	0.5	50	50
		B	2	1	0.5	2	1	1	1	0.5	2	0.5		

Treatment Unit data

Unit	Removal ratio (%)	n1	n2	n3	n4	n5	n6	n7	n8	n9	n10	IC	OC	α
TU1	A	90	95	99	95	99	95	95	99	95	90	16800	1	0.7
	B	0	0	0	0	0	0	0	0	0	0			
TU2	A	0	0	0	0	0	0	0	0	0	0	12600	0.0067	0.7
	B	90	95	99	95	95	95	90	90	95	95			

Scenario Probabilities

Scenario	Probablity (p_n)
n1	0.2
n2	0.3
n3	0.15
n4	0.1
n5	0.05
n6	0.05
n7	0.03
n8	0.02
n9	0.05
n10	0.05

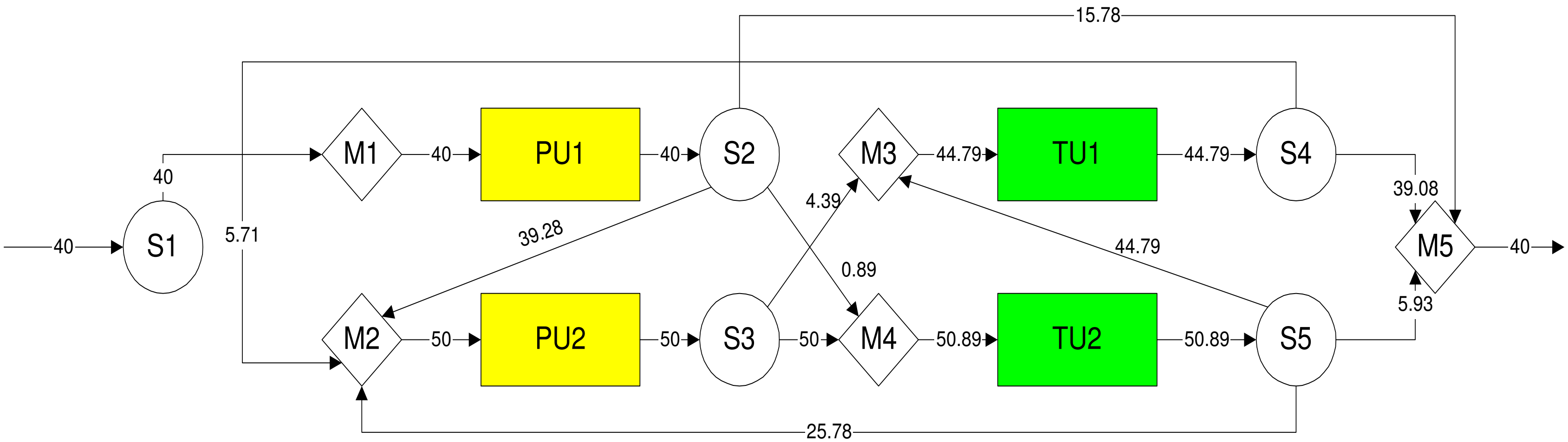
Environmental discharge limit for both contaminants = 10 ppm

Cost coefficient for pipe connection (C_p) = 6
Investment cost coefficient for pipe (IP) = 100
Operating cost coefficient for pumping water (PM) = 0.006

Annualized factor for investment (AR) = 0.1
Hours of operation of plant per annum (H) = 8000 hrs
Cost of Freshwater (C_{FW}) = 1 $ / ton

Optimal Network Topology

10 scenarios for uncertain contaminant loads (A,B) in process units, and uncertain recovery in treatment units



(Maximum flows to be handled in the pipes are shown)

Freshwater use reduced from 90 ton/h to 40 ton/h

MINLP 24 0-1 var
764 cont. var
928 constr.

Global minimum of Network Capital Cost and Expected Operating Cost = $651,653.1/yr

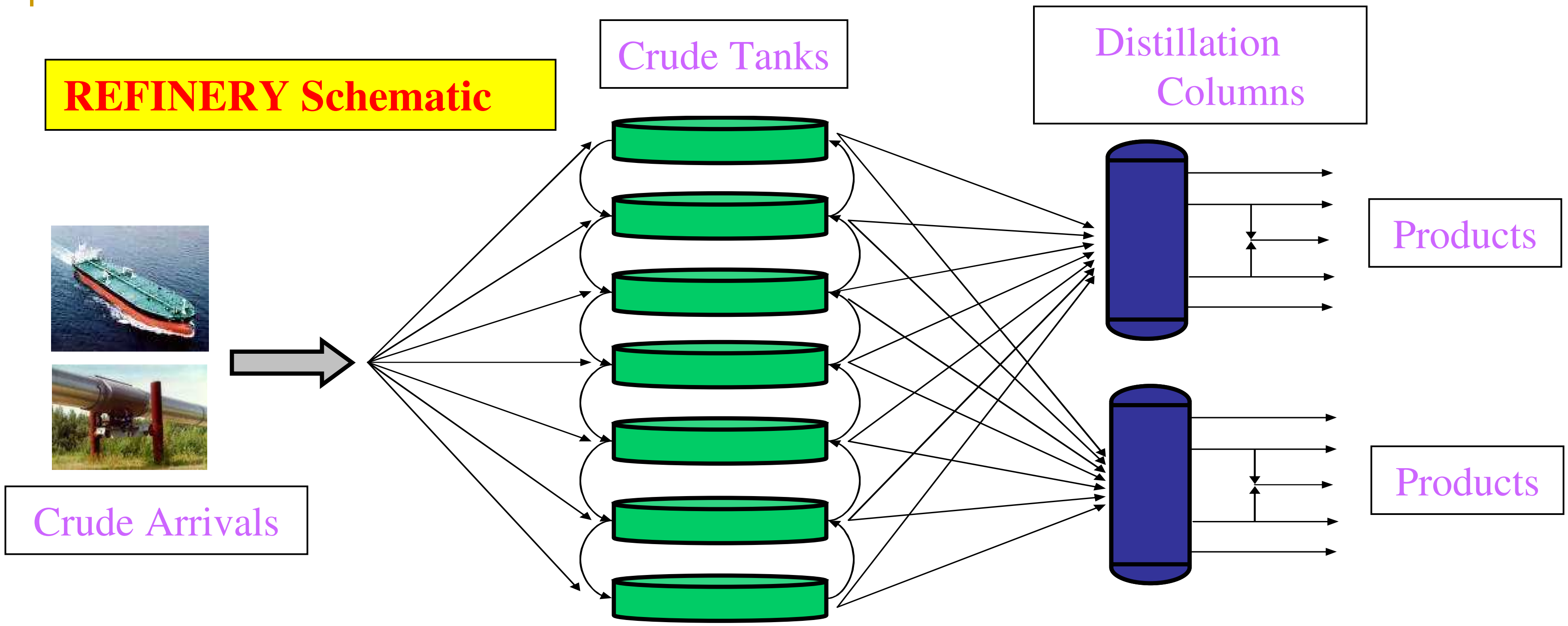
– Lower bound (LB) generated using proposed algorithm = $645,951.64/yr

– Upper bound (UB) obtained = $651,653.1/yr

Lower and Upper bounds converge **within 1 % tolerance at root node** of Branch and Bound tree

– Total time = **62.8** secs (GAMS/CPLEX, CONOPT, BARON)

Scheduling Problem



Given:

1. Scheduling Horizon
2. Tank inventory (min, max, initial levels)
3. Available crude types and their properties
4. Product property specifications and demands
5. Bounds on crude and product flows

Optimization

Determine:

1. When to order crudes
2. How much of each crude to order
3. Operating flows of crude between tanks
4. Charges to Pipestills
5. How much of each product to produce

Scheduling Model

- Continuous time formulation by Furman et al. (2006)

- Scheduling problem modeled as a Mixed Integer Nonlinear Program (MINLP)
  - Discrete variables used to determine which flows should exist and when
  - Model is non-linear and non-convex

Optimization model

Minimize *total cost* = *waiting cost for supply streams*
+ *unloading cost of supply streams*
+ *inventory cost for each tank over scheduling horizon*
+ *setup cost for charging CDUs with different charging tanks*

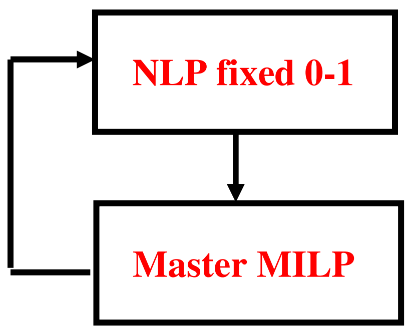
s.t. Tank constraints (Bilinear)
Distillation unit (CDU) constraints
Supply stream constraints
Variable bounds

(P)

Global Optimization of MINLP

- Large-scale non-convex MINLPs such as (P) are very difficult to solve
    - Commercial global optimization solvers *fail to converge to solution* in tractable computational times

- Special Outer-Approximation algorithm proposed to solve problem to global optimality



Upper Bound

Lower Bound

Solving this convex relaxation is time consuming!

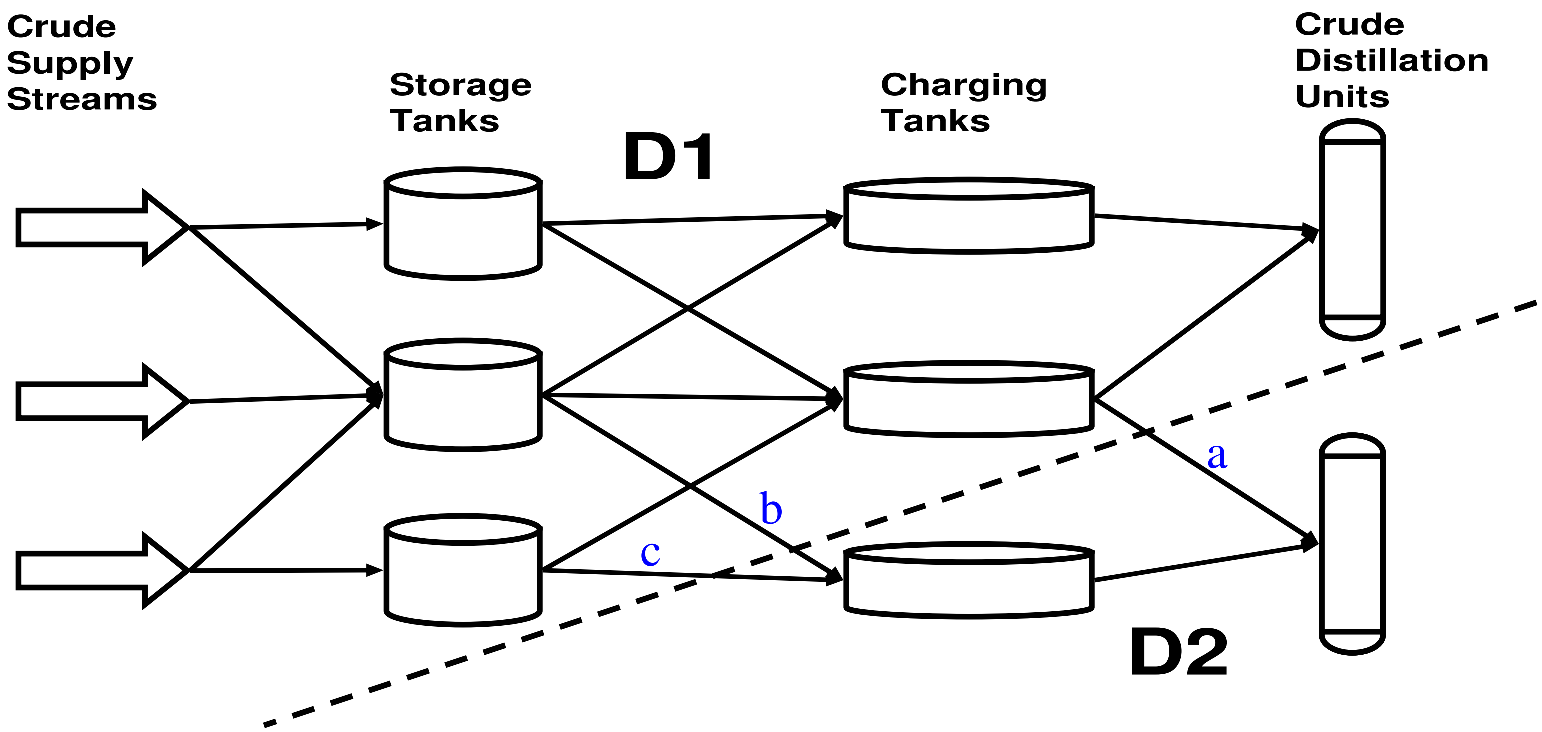
- ***Guaranteed to converge*** to global optimum given certain tolerance between lower and upper bounds

Upper Bound : Feasible solution of (P)

Lower Bound : Obtained by solving a MILP relaxation (R) of the non-convex MINLP model with Lagrangean Decomposition based cuts added to it

Spatial Decomposition of the Network

How to derive the Lagrangean cuts ?



- Network is split into two decoupled sub-structures D1 and D2
    - Physically interpreted as cutting some pipelines (Here ***a***, ***b*** **and** ***c***)
    - Set of split streams denoted by $p \in \{a, b, c\}$

Decomposed Sub-models

Sub-problem corresponding to sub-structure D1

min z_1 = *waiting cost for supply streams + unloading cost of supply streams + inventory cost for tanks in D1 over scheduling horizon + setup costs for charging CDUs in D1 with different charging tanks +*

$$\sum_p\sum_t \lambda^{Vtot}_{p,t} V^{tot,1}_{p,t} + \sum_j\sum_p\sum_t \lambda^{V}_{j,p,t} V^{j,1}_{p,t} + \sum_p\sum_t \lambda^{T1}_{p,t} T^{1,1}_{p,t} + \sum_p\sum_t \lambda^{T2}_{p,t} T^{2,1}_{p,t} + \sum_p\sum_t \lambda^{w}_{p,t} w^{1}_{p,t}$$

s.t. Tank constraints
Distillation unit constraints
Supply stream constraints
Variable bounds

(LD1)

Optimize to get solution z_1^*

Sub-problem corresponding to sub-structure D2

min z_2 = *inventory cost for tanks in D2 over scheduling horizon + setup costs for charging CDUs in D2 with different charging tanks +*

$$-\sum_p\sum_t \lambda^{Vtot}_{p,t} V^{tot,2}_{p,t} - \sum_j\sum_p\sum_t \lambda^{V}_{j,p,t} V^{j,2}_{p,t} - \sum_p\sum_t \lambda^{T1}_{p,t} T^{1,2}_{p,t} - \sum_p\sum_t \lambda^{T2}_{p,t} T^{2,2}_{p,t} - \sum_p\sum_t \lambda^{w}_{p,t} w^{2}_{p,t}$$

s.t. Tank constraints
Distillation unit constraints
Variable bounds

(LD2)

Optimize to get solution z_2^*

Cut Generation

- Using solutions z_1^* and z_2^* we develop the following cuts :

$z_1^* \leq$ *waiting cost for supply streams + unloading cost of supply streams + inventory cost for tanks in D1 over scheduling horizon + setup costs for charging CDUs in D1 with different charging tanks +*

$$\sum_p \sum_t \lambda_{p,t}^{Vtot} V_{p,t}^{tot} + \sum_j \sum_p \sum_t \lambda_{j,p,t}^{V} V_{p,t}^{j} + \sum_p \sum_t \lambda_{p,t}^{T1} T_{p,t}^{1} + \sum_p \sum_t \lambda_{p,t}^{T2} T_{p,t}^{2} + \sum_p \sum_t \lambda_{p,t}^{w} w_{p,t}$$

Lagrange Multipliers

$z_2^* \leq$ *inventory cost for tanks in D2 over scheduling horizon + setup costs for charging CDUs in D2 with different charging tanks +*

$$-\sum_p \sum_t \lambda_{p,t}^{Vtot} V_{p,t}^{tot} - \sum_j \sum_p \sum_t \lambda_{j,p,t}^{V} V_{p,t}^{j} - \sum_p \sum_t \lambda_{p,t}^{T1} T_{p,t}^{1} - \sum_p \sum_t \lambda_{p,t}^{T2} T_{p,t}^{2} - \sum_p \sum_t \lambda_{p,t}^{w} w_{p,t}$$

- Add above cuts to (R) to get (RP) which is solved to obtain a valid lower bound on global optimum of (P)

Remark: Update Lagrange multipliers and generate more cuts to add to (R)

Computational Results

	Example	Original MINLP model (P)		
		Number of Binary Variables	Number of Continuous Variables	Number of Constraints
3 Supply streams – 3 Storage tanks – 3 Charging tanks – 2 Distillation units	1	**48**	**300**	**946**
3 Supply streams – 3 Storage tanks – 3 Charging tanks – 2 Distillation units	2	**42**	**330**	**994**
3 Supply streams – 6 Storage tanks – 4 Charging tanks – 3 Distillation units	3	**57**	**381**	**1167**

Solvers : **MILP** ⇨ CPLEX 9.0, **NLP** ⇨ BARON 7.2.5 (Sahinidis, 1996)

Example	Lower bound [obtained by solving relaxation (RP)] (z^{RP})	Upper bound [on solving (P-NLP) using BARON] ($z^{P\text{-}NLP}$)	Relaxation gap (%)	Total time taken for one iteration of algorithm* (CPUsecs)	Local optimum (using DICOPT)
1	281.14	282.19	0.37	827.7	291.93
2	351.32	359.48	2.27	6913.9	361.63
3	383.69	383.69	0	8928.6	383.69

BARON could not guarantee global optimality in more than 10 hours*

Example	Solving MILP model (R)				Solving MILP model (RP) (including proposed cuts)			
	Solution (z^R)	LP relaxation at root node	No. of nodes	Time taken to solve (R)* (CPUsecs)	Solution (z^{RP})	LP relaxation at root node	No. of nodes	Time taken to solve (RP)* (CPUsecs)
1	281.14	-55.24	940800	1953.3	281.14	68.45	334300	758.8
2	351.32	113.35	931700	14481.7	351.32	133.80	310600	5873.2
3	383.69	147.24	3029600	15874.8	383.69	189.19	1258100	8025.9

* Pentium IV, 2.8 GHz , 512 MB RAM

Summary

1. Proposed a novel branch-and-cut algorithm for global optimization of large-scale nonconvex MINLP models with decomposable structures

   - **Orders of magnitude reduction in solution time can be obtained compared to standard solvers**

2. Presented a technique to combine the concepts of Lagrangean decomposition and convex relaxations to generate tight relaxations of nonconvex models

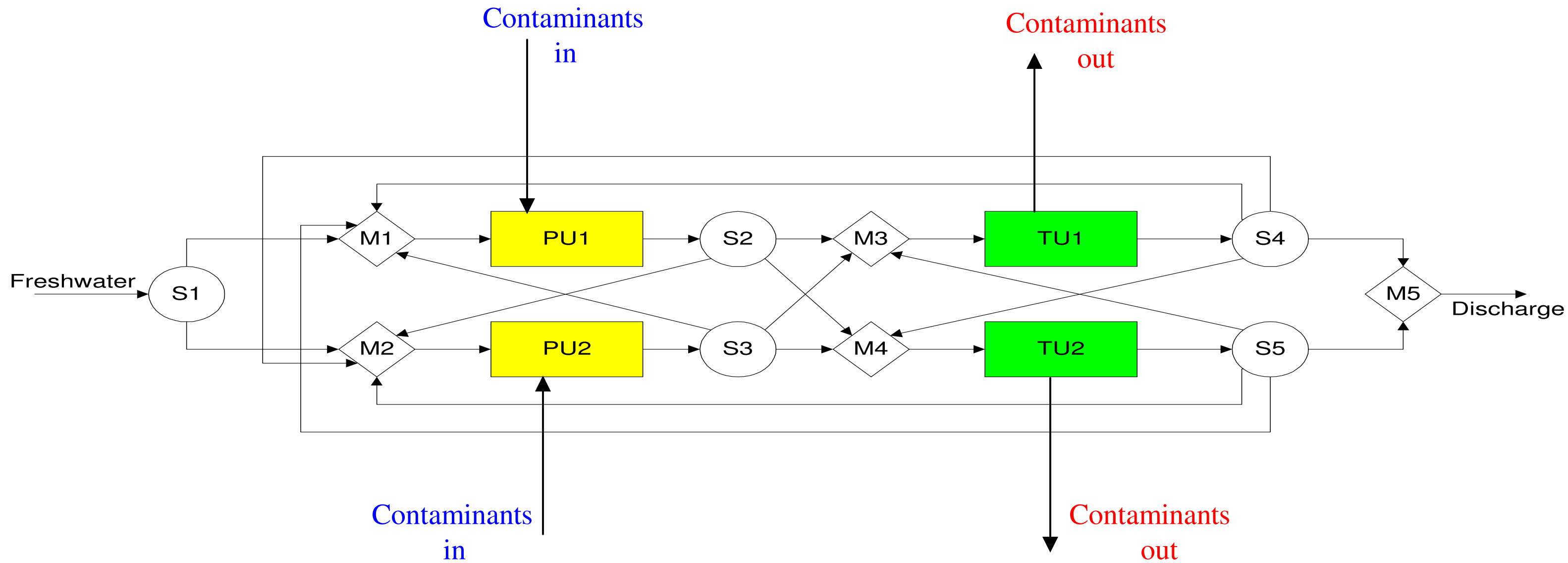
3. Successful applications in integrated water systems and crude oil scheduling

THANK YOU !!

¿QUESTIONS ?

Illustrative Example

Superstructure optimization problem



- Uncertain Parameters (i) Contaminant loads in each Process unit
  (ii) Contaminant removals in each Treatment unit

Take on different values at different points of time

Design problem formulated using a ***two-stage stochastic programming framework***

Objective: minimize 1st stage capital costs **+** 2nd stage expected operating costs

Numerical Data

Optimization of 2 Process Unit - 2 Treatment Unit network operating under uncertainty

Process Unit data

Unit	Flowrate (ton/hr)	Discharge load (Kg/hr)	n1	n2	n3	n4	n5	n6	n7	n8	n9	n10	Maximum Inlet Conc. (ppm) A	B
PU1	40	A	2	1	0.5	1	1	2	0.5	1	0.5	2	0	0
		B	2.5	1.5	1	1.5	1.5	2.5	1	1.5	1	2.5		
PU2	50	A	2	1	0.5	2	1	1	1	0.5	2	0.5	50	50
		B	2	1	0.5	2	1	1	1	0.5	2	0.5		

Treatment Unit data

Unit	Removal ratio (%)	n1	n2	n3	n4	n5	n6	n7	n8	n9	n10	IC	OC	α
TU1	A	90	95	99	95	99	95	95	99	95	90	16800	1	0.7
	B	0	0	0	0	0	0	0	0	0	0			
TU2	A	0	0	0	0	0	0	0	0	0	0	12600	0.0067	0.7
	B	90	95	99	95	95	95	90	90	95	95			

Scenario Probabilities

Scenario	Probablity (p_n)
n1	0.2
n2	0.3
n3	0.15
n4	0.1
n5	0.05
n6	0.05
n7	0.03
n8	0.02
n9	0.05
n10	0.05

Environmental discharge limit for both contaminants = 10 ppm

Cost coefficient for pipe connection (C_p) = 6

Investment cost coefficient for pipe (IP) = 100

Operating cost coefficient for pumping water (PM) = 0.006

Annualized factor for investment (AR) = 0.1

Hours of operation of plant per annum (H) = 8000 hrs

Cost of Freshwater (C_{FW}) = 1 $ / ton

Computational Results

MINLP Model :

- Number of Binary Variables = 24
- Number of Continuous Variables = 764
- Number of Constraints = 928
- Number of Non-convexities = 406

- Proposed Algorithm

Solvers Used : **LP / MILP** ⇒ CPLEX 9.0, **NLP** ⇒ CONOPT3

20 cutting planes used at each node

Node #	Lower bound using proposed algorithm (z^R)	Best bound from Lagrangean Decomposition (z^{LB})	Lower bound from MILP Relaxation (z^{CR})	Upper Bound (z^{UB})	Total time taken at node (CPUsecs*)
0 (root node)	**645,951.64**	644,856.82	610,092.61	651,653.65	19.33
1	**648,566.716**	647,496.24	610,115.37	672,971.83	4.1
2	**648,828.60**	648,073.24	610,109.06	661,439.35	61.83

Lower and Upper bounds converge within 1 % tolerance at root node of Branch and Bound tree

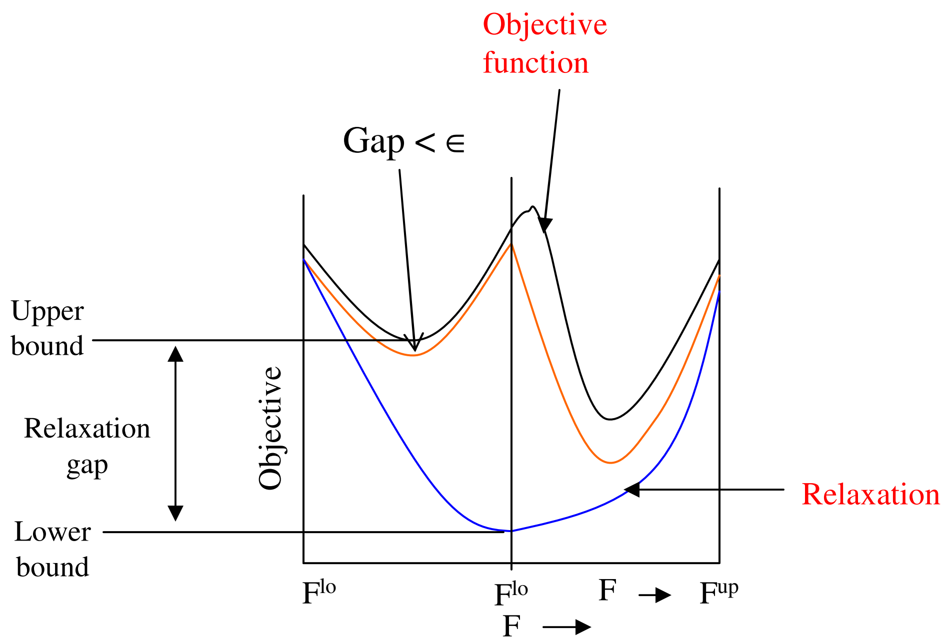
Total time taken in solving problem to global optimality = **85.6** sec*

- BARON (Global Optimization MINLP Solver, Sahinidis (1996))

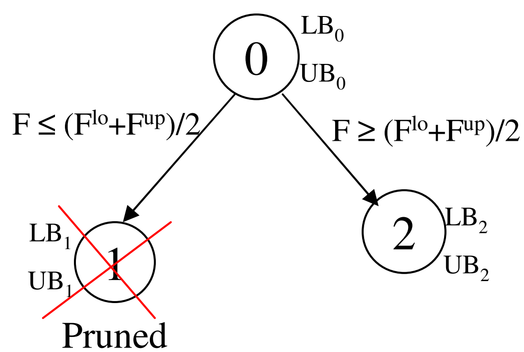
  – Could not guarantee global optimality in more than **10** hours*

* Pentium IV, 3.2 GHz , 1024 MB RAM

Geometric Interpretation



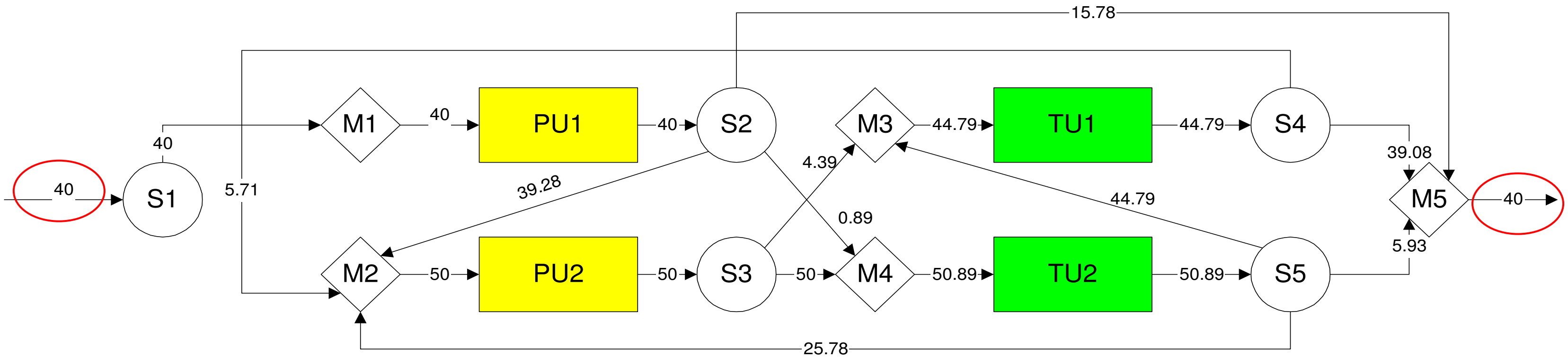
Tree Representation



Optimal Network Topology

Integrated network operating under uncertainty

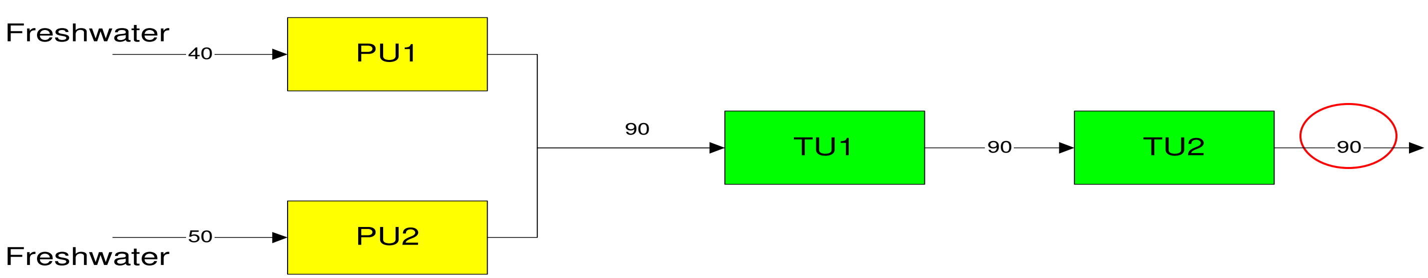
Global minimum sum of Network Design Cost and Expected Operating Cost = **$ 651,653.1**



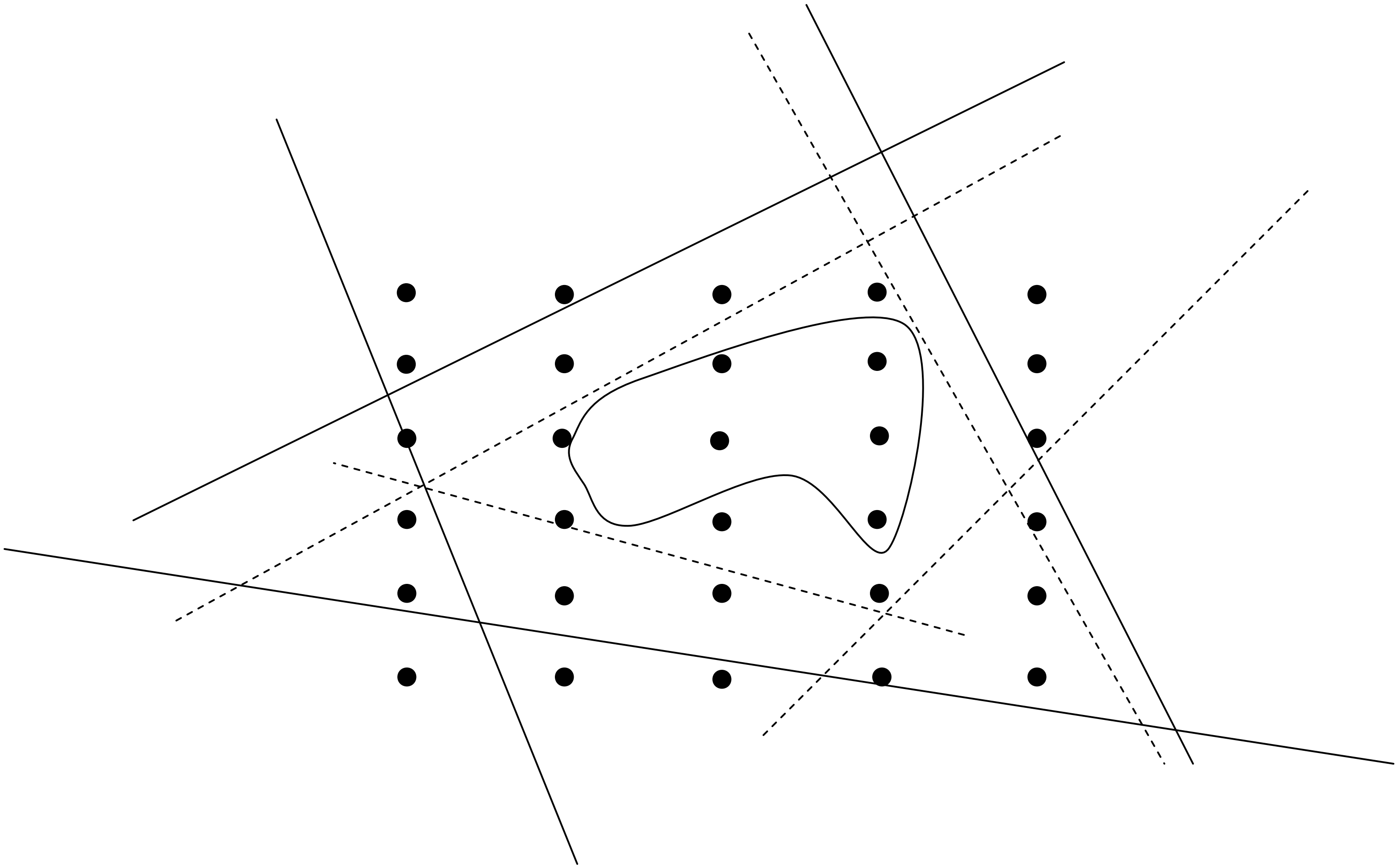
(Maximum flows to be handled in the pipes are shown)

Vs

Conventional Network

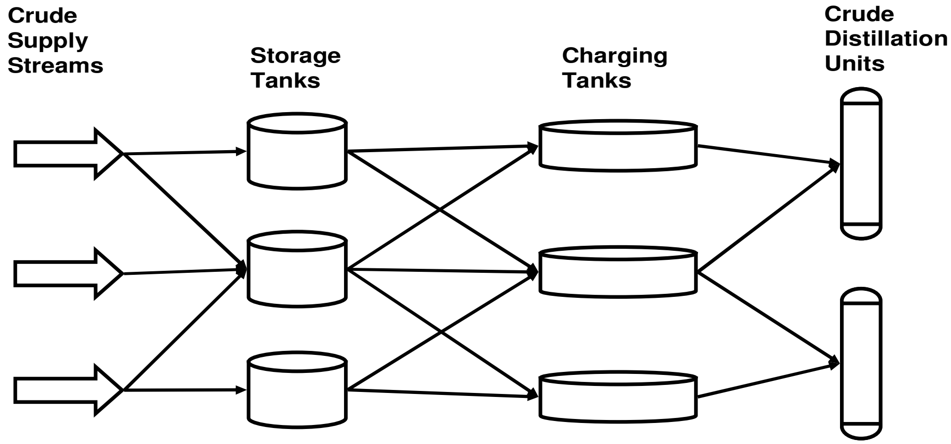


Objective Function value for the Conventional Network = **$ 1,568,286.7**



Example	Global optimum	Relaxation (using proposed algorithm)	Convex Relaxation at root node	Lagrangean decomposition at root node
1				
2	281.14	68.45	-55.24	201.335
3	351.32	133.80	113.35	276.582
4	383.69	189.19	147.24	344.267
5				
6				

Problem Statement



Given:

(a) Maximum and minimum inventory levels for a tank
(b) Initial total and component inventories in a tank
(c) Upper and lower bounds on the fraction of key components in the crude inside a tank
(d) Times of arrival of crude oil in the supply streams
(e) Amount of crude arriving in the supply streams
(f) Fractions of various components in the supply streams
(g) Bounds on the flowrates of the streams in the network
(h) Time horizon for scheduling

Determine:

(i) Inventory levels in the tanks at various points of time
(ii) Flow volumes from one unit to another in a certain time interval
(iii) Start and end times of the flows in the network

Objective: Minimize Cost