ϵ-OA for the solution of bi-objective generalized disjunctive programming problems in the synthesis of nonlinear process networks

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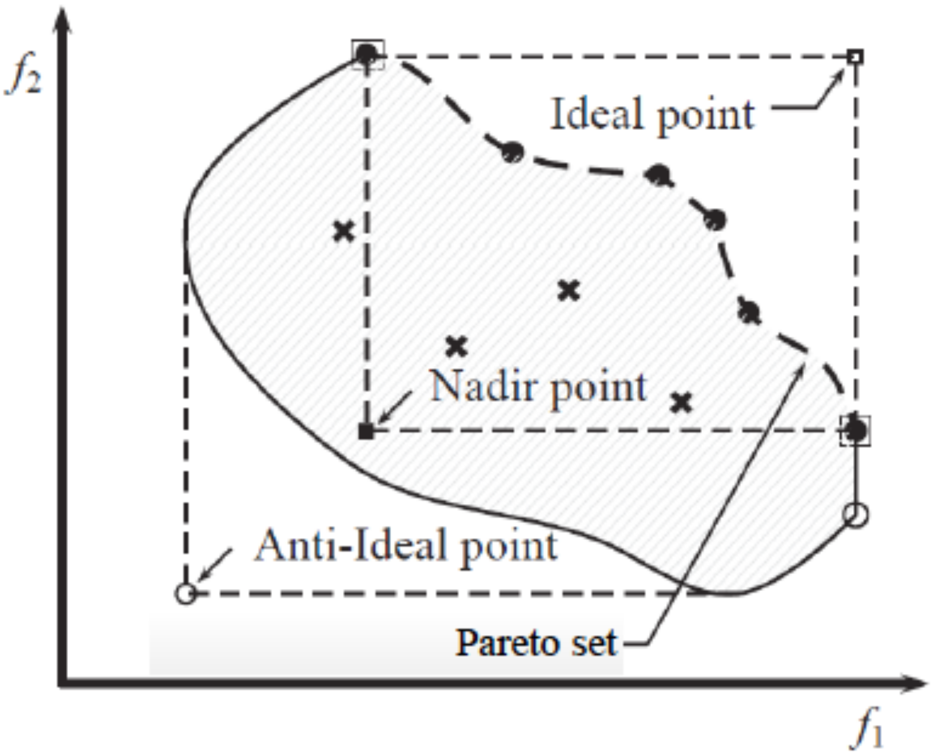
MULTI-OBJECTIVE OPTIMIZATION

- Multi-objective optimization problems (MOOP) involve optimizing simultaneously N objective functions $f_1, f_2, \ldots, f_N$ over a feasible set X.

$$\max \; F(x) = \left(f_1(x), \ldots, f_N(x) \right)$$
$$s.t. \qquad x \in X$$

- Many survey papers were published (Ulungu&Teghem, 1994; Ehrgott&Gandibleux, 2000; Ehrgott, 2005)
- Research on solution algorithms:
  - Continuous and convex: a variety of algorithms – maturing
  - Continuous and nonconvex: a few algorithms
  - Combinatorial: a number of papers in the last 5 years
  - Discrete-continuous – linear: a handful of papers in the last 3 years
  - Discrete-continuous – nonlinear: only 5 papers straighforward use of algorithms developed for continuous and convex problems

TERMINOLOGY



- Let $x, x' \in X$
- x dominates x'
  $f_n(x) \geq f_n(x') \quad \forall n = 1,\dots,N$ and $\exists \tilde{n} \in \{1,\dots,N\}$
  with $f_{\tilde{n}}(x) > f_{\tilde{n}}(x')$
- x strictly dominates x'
  $f_n(x) > f_n(x') \quad \forall n = 1,\dots,N$
- x weakly dominates x'
  $f_n(x) \geq f_n(x') \quad \forall n = 1,\dots,N$
- x is Pareto optimal or efficient
  $\forall x' \in X$ that does not dominate x

- *Ideal Point (Utopia Point):* all objectives are optimized simultaneously
- *Anti-Ideal Point:* all objectives are at their worst
- *Pareto set:* entire set of non-dominated solutions
- *Nadir Point:* lower bound of each objective in the Pareto set

ϵ-CONSTRAINT APPROACH

- Haimes et al., 1971
  - ✓ Presented the ϵ-constraint approach to solving MOOP.
  - ✓ The maximum and minimum values for all objectives are found separately
  - ✓ One of the objectives is retained and the rest of the objectives are converted into constraints
  - ✓ A virtual grid is constructed to include all N-1 objective functions.
  - ✓ Then the following sub-problem is solved iteratively for each i_j

$$
\begin{aligned}
&\max\ f_1(x)\\
&s.t.\\
&f_j(x) \geq Lb_j + i_j \epsilon_j \quad \forall j = 2,\ldots,N\\
&\qquad x \in X
\end{aligned}
$$

Lb_j: the lower bound on the objective j

ϵ_j: range of the objective j in the iteration i_j

AUGMENTED ϵ-CONSTRAINT APPROACH

- The ϵ-constraint approach may find weakly efficient solutions.
- Mavrotas, 2009
  - ✓ Modified the ϵ-constraint method by introducing a slack variable to the each objective that is converted into a constraint.
  - ✓ A penalty term with scalar μ (10^{-3}-10^{-6}) is added to the objective

$$\max \; f_1(x) + \mu \sum_{j=2}^{N} \frac{s_j}{r_j}$$

$$s.t.$$

$$f_j(x) - s_j = Lb_j + i_j \epsilon_j \quad \forall j = 2,\dots,N$$

$$s_j \geq 0 \quad \forall j = 2,\dots,N$$

$$x \in X$$

s_j: slack variable for each objective j that is converted into a constraint

r_j: the range of objective j

Lb_j: the lower bound on the objective j

ϵ_j: range of the objective j in the iteration i_j

LITERATURE ON MOMINLP

- **T-ϵ-con**: Straightforward extension of ϵ-constraint approach

  - Chakraborty&Linninger (2002), Plant-wide waste management. 1. Synthesis and multi-objective design
  - Cucek, P.S. Varbanov, J.J. Klemes, Z. Kravanja (2012), Total footprints-based multi-criteria optimisation of regional biomass energy supply chains
  - Cucek, J.J. Klemes, P.S. Varbanov, Z. Kravanja (2102), Reducing the dimensionality of criteria in multi-objective optimisation of biomass energy supply chains
  - Martinez, A.M. Eliceche (2008), Minimization of life cycle greenhouse emissions and cost in the operation of steam and power plants
  - Martinez, A.M. Eliceche (2011), Bi-objective minimization of environmental impact and cost in utility plants

- Theoretical analysis of the problem (MOMINLP) and computational issues with the striaghtforward extension of ϵ-constraint approach are missing

LOGIC-BASED OA

$$\min \quad Z = (z_1, z_2) = \left(\sum_i c_i + f_1(x), \sum_i p_i + f_2(x) \right)$$

$$\text{s.t.} \quad g(x) \le 0,$$

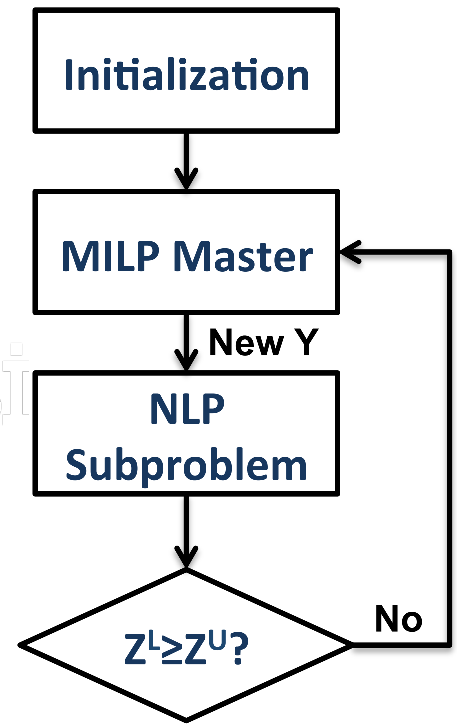
$$\begin{bmatrix} Y_i \\ h_i(x) \le 0 \\ c_i = \gamma_i \\ p_i = \eta_i \end{bmatrix} \vee \begin{bmatrix} \neg Y_i \\ B^i x = 0 \\ c_i = 0 \\ p_i = 0 \end{bmatrix} \quad \forall i \in D,$$

$$\Omega(Y) = True,$$

$$x \in \mathbb{R}^n,\ c \ge 0,\ p \ge 0,\ Y \in \{True, False\}^m.$$

Turkay&Grossmann, 1996

- Logic-Based OA
- Logic-Based Benders Decomposition



NLP SUBPROMLEMS & MILP MASTER

NLP Subproblems

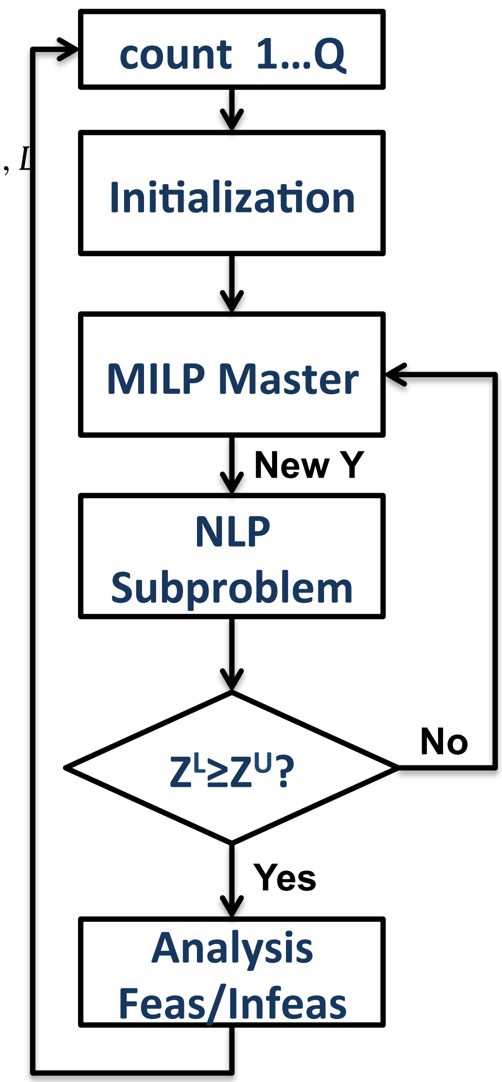
$$
\begin{aligned}
\min \quad & Z_U^{aug} = \sum_i c_i + f_1(x) - \frac{\mu}{r} s \\
\text{s.t.} \quad & \sum_i p_i + f_2(x) + s = z_2^U - j\epsilon, \\
& g(x) \le 0, \\
& \left.\begin{aligned} h_i(x) &\le 0 \\ c_i &= \gamma_i \\ p_i &= \eta_i \end{aligned}\right\} \forall \overline{Y_i} = True, \\
& \left.\begin{aligned} B^i x &= 0 \\ c_i &= 0 \\ p_i &= 0 \end{aligned}\right\} \forall \overline{Y_i} = False, \\
& x \in \mathbb{R}^n,\ c \ge 0,\ p \ge 0.
\end{aligned}
$$

MILP Master

$$
\begin{aligned}
\min \quad & Z_L^{aug} = \sum_i \gamma_i y_i + \alpha_{oa} - \frac{\mu}{r} s \\
\text{s.t.} \quad & \alpha_{oa} \ge f_1(x^l) + \nabla f_1(x^l)^T (x - x^l) \quad \forall l = 1, \ldots, L \\
& g(x^l) + \nabla g(x^l)^T (x - x^l) \le 0 \quad \forall l = 1, \ldots, L \\
& \sum_i \eta_i y_i + f_2(x^l) + \nabla f_2(x^l)^T (x - x^l) + s \\
& \quad = z_2^U - j\epsilon \quad \forall l = 1, \ldots, L \\
& \nabla h_i(x^l)^T x \le \left(-h_i(x^l) + \nabla h_i(x^l)^T x^l \right) y_i \\
& \quad \forall l = 1, \ldots, L,\ i \in D \\
& B^i x \le M_i y_i \quad \forall i \in D \\
& Ay \le a \\
& \alpha_{oa} \in \mathbb{R}^1,\ x \in \mathbb{R}^n,\ y \in \{0, 1\}^m.
\end{aligned}
$$

+ No good cuts

ϵ-OA



SOLUTIONS FOR SUB-PROBLEMS

- **Theorem 1:** The optimal solution found by the sub-problem in the augmented ϵ-constraint method is efficient within the search region of the sub-problem.
- **Proof:**

$$Z_A = f_1(x_A) + \mu \sum_{j=2}^{N} \frac{f_j(x_A) - Lb_j - i_j\epsilon_j}{r_j}$$

$$Z_B = f_1(x_B) + \mu \sum_{j=2}^{N} \frac{f_j(x_B) - Lb_j - i_j\epsilon_j}{r_j}$$

$$\Rightarrow Z_A - Z_B = f_1(x_A) - f_1(x_B) + \mu \sum_{j=2}^{N} \frac{f_j(x_A) - f_j(x_B)}{r_j}$$

2 cases are possible:

1. $f_1(x_A) \geq f_1(x_B)$ and $\sum_{j=2}^{N} \frac{f_j(x_A)}{r_j} > \sum_{j=2}^{N} \frac{f_j(x_B)}{r_j}$,so $Z_A > Z_B$
2. $f_1(x_A) > f_1(x_B)$ and $\sum_{j=2}^{N} \frac{f_j(x_A)}{r_j} = \sum_{j=2}^{N} \frac{f_j(x_B)}{r_j}$,so $Z_A - Z_B > 0$

EFFICIENT SOLUTIONS

- **Theorem 2:** The efficient solution found by the sub-problem in the augmented ϵ-constraint method is also efficient for the original MOMINLP.
- **Proof by contradiction:**

✓ Consider x_A as the optimal solution for a particular sub-problem. Theorem 1 proves that it is efficient the same sub-problem. $\hat{i}_2, \cdots, \hat{i}_N$

✓ Assume that x_C is feasible for the original MOOP but not the feasible for the particular sub-problem where x_A is optimal.

✓ Therefore, $x_C \in X$ but $f_j(x_C) \geq Lb_j + \hat{i}_j \epsilon_j, \quad j = 2, \cdots, N$

✓ Suppose that x_C dominates x_A meaning that $f_j(x_C) \geq f_j(x_A)$ with at least one strict inequality

✓ Since $f_j(x_A) \geq Lb_j + \hat{i}_j \epsilon_j$,then $f_j(x_C) \geq f_j(x_A) \geq Lb_j + \hat{i}_j \epsilon_j$

✓ Therefore, x_C must be feasible for the same sub-problem which contradicts with

  ✓ assumption of x_C being not feasible for the particular sub-problem

  ✓ x_A being the optimal solution for the particular sub-problem

THEORETICAL ANALYSIS-BRIEF

- Theorem1 and Theorem 2 proves that as long as each sub-problem is solved to optimality, then the augmented ϵ-constraint method guarantees that every solution generated is contained in the Pareto set.
- These theorems are valid for all deterministic optimization problems.

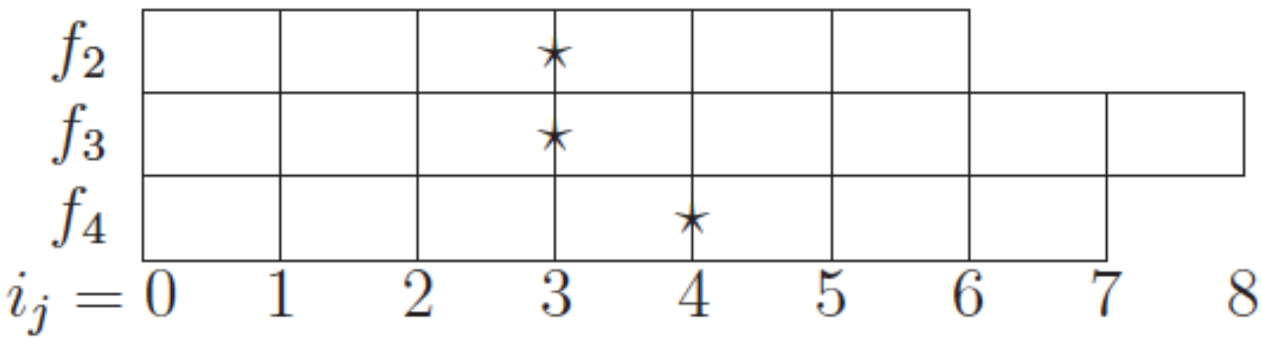
- Computational Issues:
  - Infeasible Subproblems
  - Feasible Subproblems

INFEASIBLE SUB-PROBLEMS

- If there is sub-problem, $\hat{i}_2, \cdots, \hat{i}_N$, that is infeasible;

$$\nexists x \in X \text{ such that } f_j(x) \geq Lb_j + \hat{i}_j \epsilon_j, \ \ \forall j = 2, \cdots, N$$

- Then, increasing the iteration count ($\hat{i}_j$) would make the problem more restrictive. So, the next iteration will be infeasible for all possible combinations of these indices.
- Ex: Sub-problem for $i_2=3$, $i_3=3$ and $i_4=4$ is infeasible.



- Any sub-problem generated such that $i_2 \geq 3$, $i_3 \geq 3$ and $i_4 \geq 4$ is also infeasible.

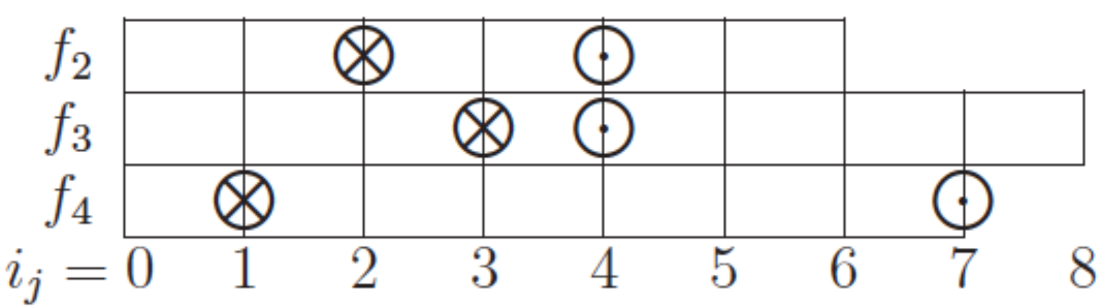
FEASIBLE SUB-PROBLEMS

- If the sub-problem, $\hat{i}_2, \cdots, \hat{i}_N$, is optimal;

$$f_j(\hat{x}) \geq Lb_j + \hat{i}_j \epsilon_j, \ \ \forall j = 2, \cdots, N$$

- Then, $\tilde{i}_j = \max_{i_j = \hat{i}_j, \hat{i}_j+1, \cdots, q_j} \{f_j(\hat{x}) \geq Lb_j + i_j \epsilon_j\}, \forall j = 2, \cdots, N$

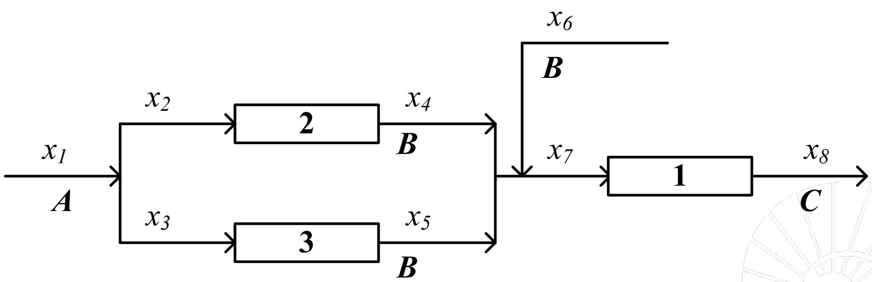
  satisfies the same inequality.
- For any set of indices, $i_2, \cdots, i_N$, such that $\hat{i}_j \leq i_j \leq \tilde{i}_j, \ \ \forall j = 2, \cdots, N$ the optimal solution is the same and we do not need to solve them again.
- Ex: Sub-problem for i_2=2, i_3=3 and i_4=1 is optimal and each ϵ-constraint until i_2=4, i_3=4 and i_4=7 is feasible.



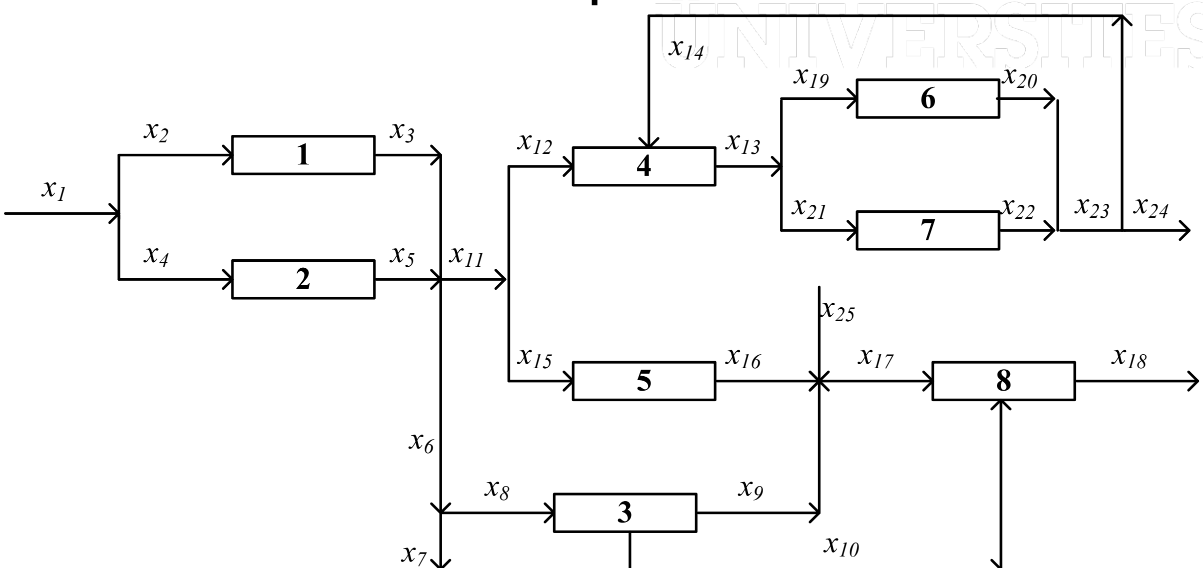
- Any sub-problem generated such that $2 \geq i_2 \geq 4$, $3 \geq i_3 \geq 4$ and $1 \geq i_4 \geq 7$ have the same optimal solution.

EXAMPLES

➢ 3 Process Example



➢ 8 Process Example



$$\min \quad Z=(z_1,z_2)$$

$$z_1=c_1+c_2+c_3+x_4+1.8x_1+1.2x_5+7x_6-11x_8$$

$$z_2=p_1+p_2+p_3$$

$$+1.8x_1+2x_2+3x_3+x_4+1.2x_5+7x_6-5x_7-11x_8$$

$$x_1-x_2-x_3=0,$$

$$x_7-x_4-x_5-x_6=0,$$

$$x_5\le 5,$$

$$x_8\le 1$$

$$\begin{bmatrix} Y_1 \\ x_8=0.9x_7 \\ c_1=3.5 \\ p_1=3.5 \end{bmatrix} \vee \begin{bmatrix} \neg Y_1 \\ x_7=x_8=0 \\ c_1=0 \\ p_1=0 \end{bmatrix},$$

$$\begin{bmatrix} Y_2 \\ x_4=\ln(1+x_2) \\ c_2=1 \\ p_2=1 \end{bmatrix} \vee \begin{bmatrix} \neg Y_2 \\ x_2=x_4=0 \\ c_2=0 \\ p_2=0 \end{bmatrix},$$

$$\begin{bmatrix} Y_3 \\ x_5=1.2\ln(1+x_3) \\ c_3=1.5 \\ p_3=12 \end{bmatrix} \vee \begin{bmatrix} \neg Y_3 \\ x_3=x_5=0 \\ c_3=0 \\ p_3=0 \end{bmatrix}$$

$$Y_1 \Rightarrow Y_2 \vee Y_3 \vee (\neg Y_2 \wedge \neg Y_3),$$

$$Y_2 \Rightarrow Y_1,$$

$$Y_3 \Rightarrow Y_1,$$

$$\neg Y_2 \vee \neg Y_3$$

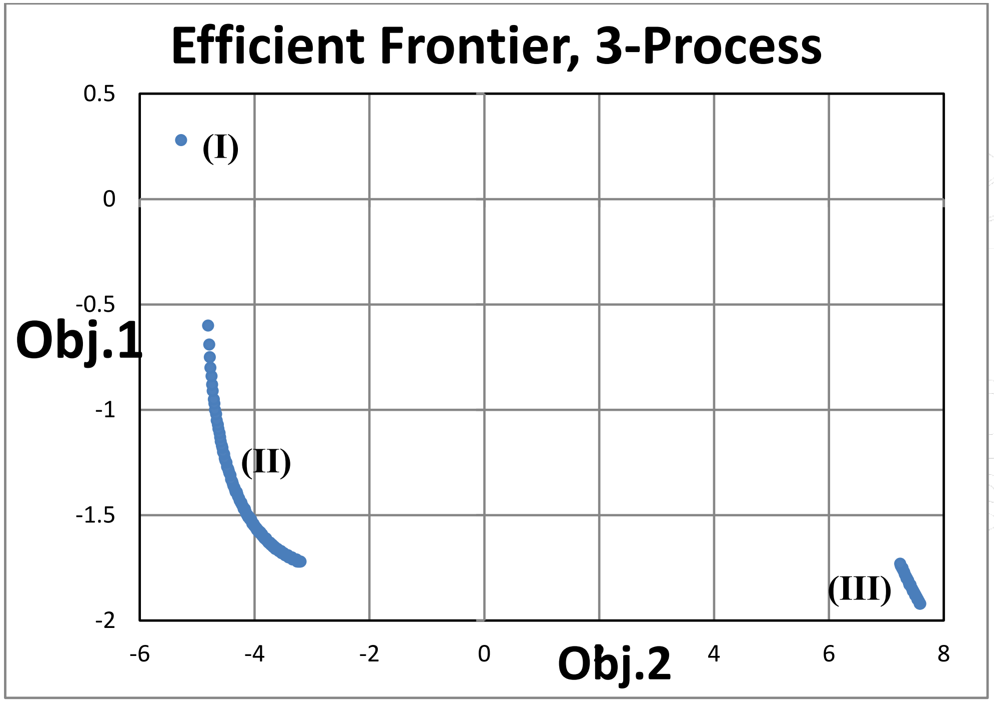
$$x_k \ge 0 \quad \forall k=1,\dots,8,$$

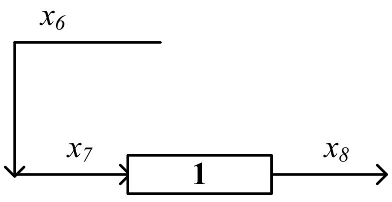
$$c_i,p_i \ge 0 \quad \forall i=1,2,3,$$

$$Y_i \in \{True, False\} \quad \forall i=1,2,3$$

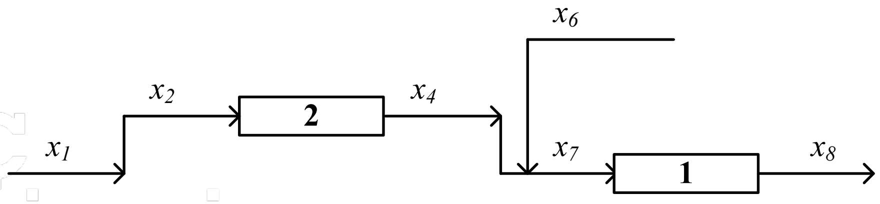
PARETO SOLUTIONS-1

- Example 1: 3 process

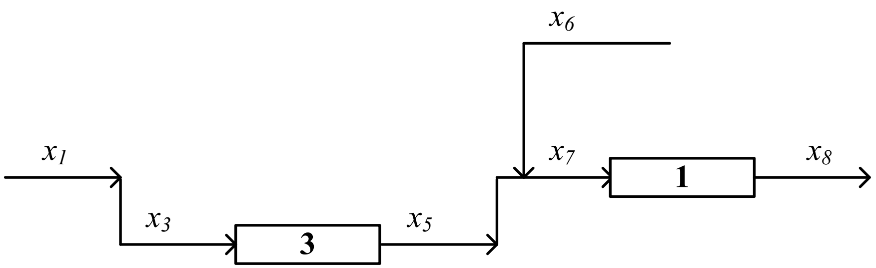




a) Topology for section (I)



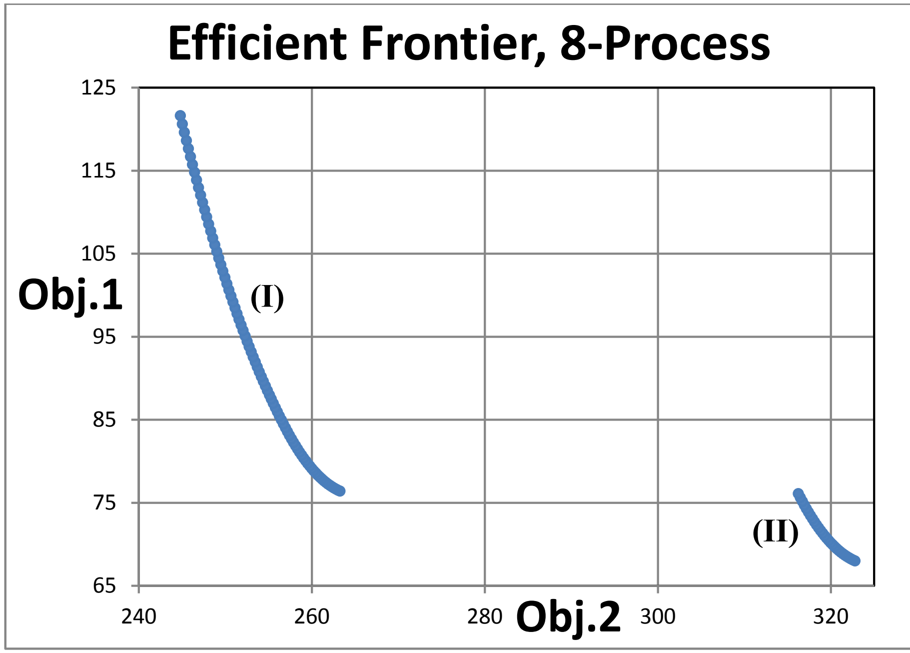
b) Topology for section (II)

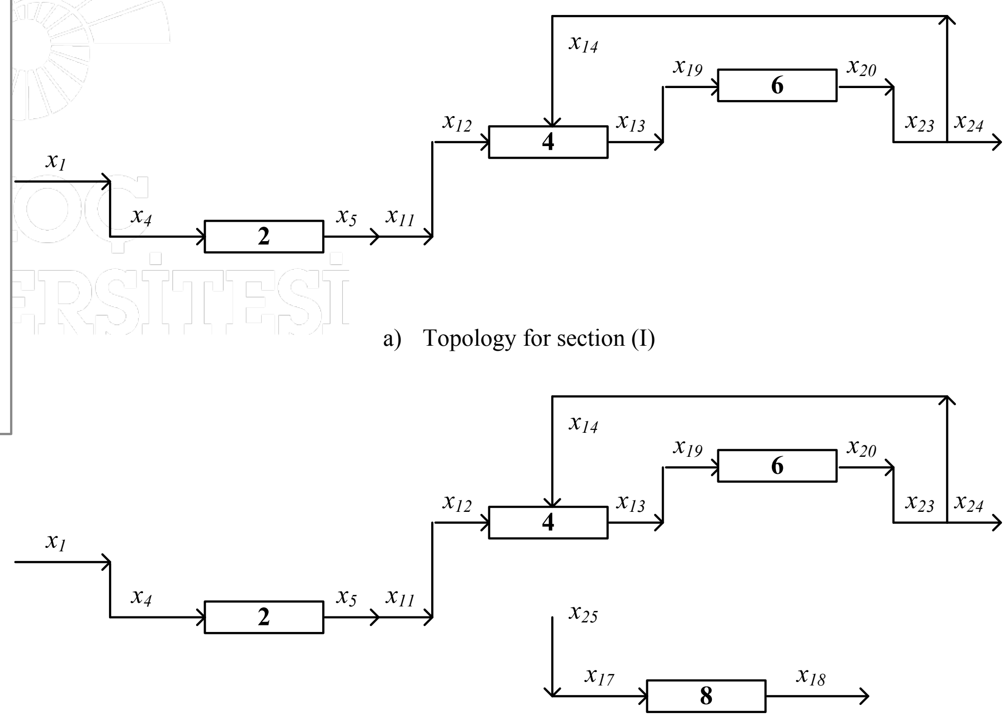


c) Topology for section (III)

PARETO SOLUTIONS-2

- Example 1: 8 process



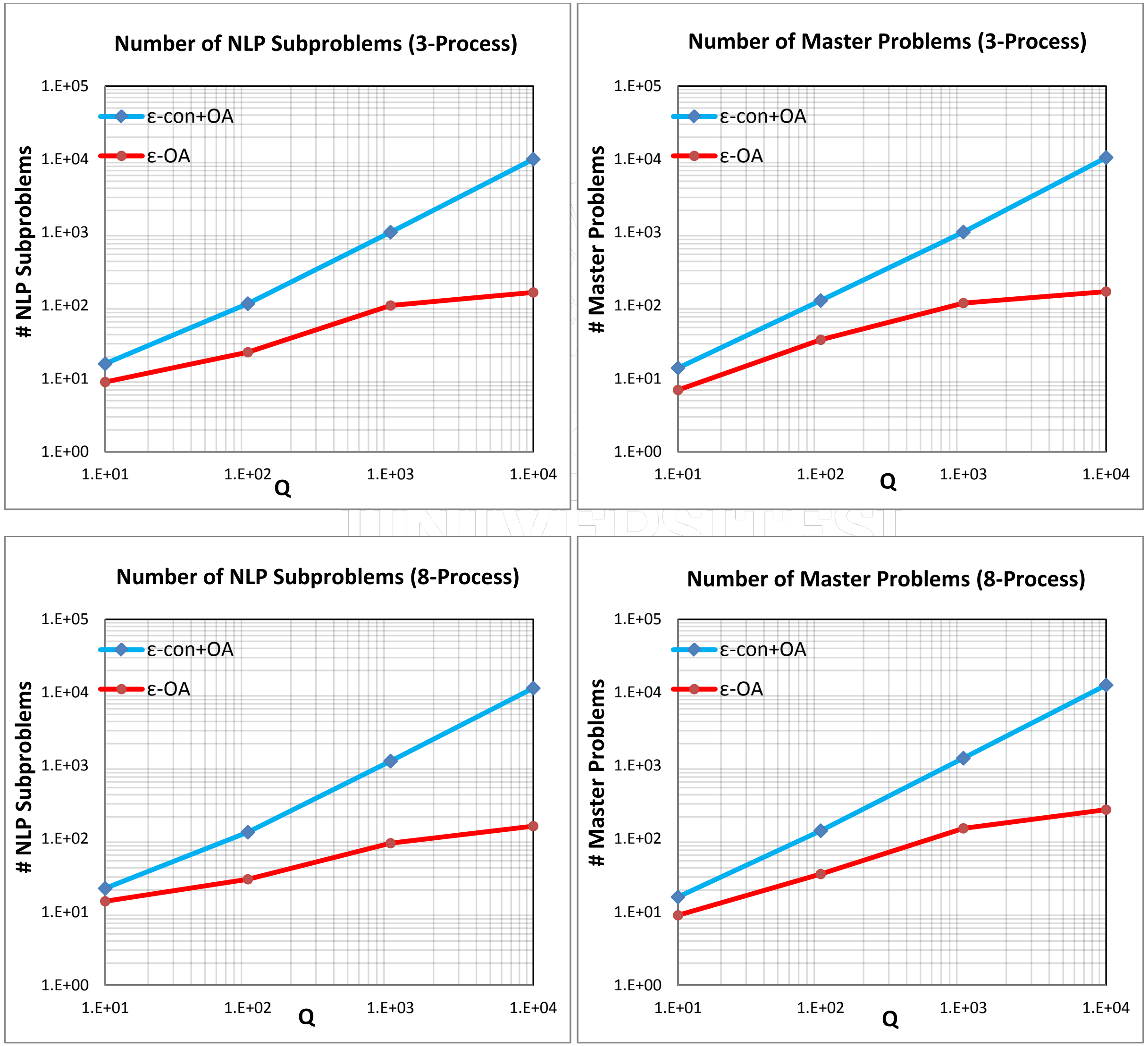


a) Topology for section (I)

b) Topology for section (II)

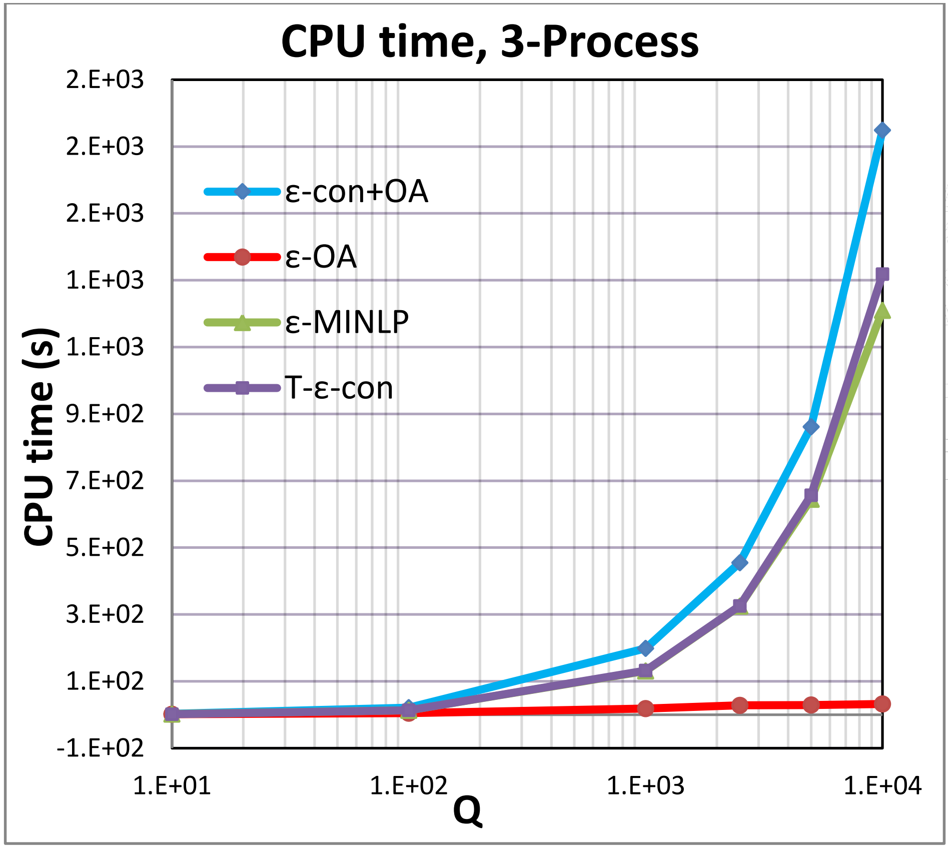
ITERATIONS

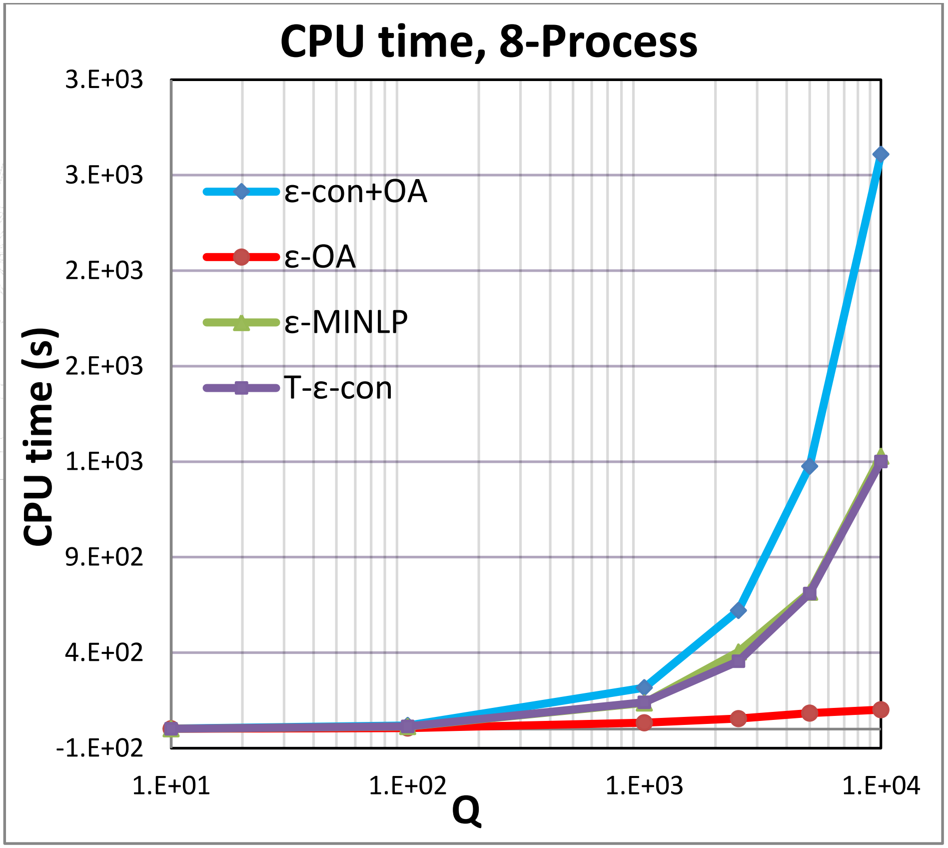
➢ The number of NLP subproblems and MILP master problems



CPU TIMES

- CPU time comparison





SUMMARY

- Generation of the Pareto set for MOMINLP is challenging
- The augmented ϵ-constraint method for nonlinear process network synthesis
  - Theoretical analysis
    - The solution of each sub-problem is theoretically guaranteed to be efficient provided that it is optimal
    - Augmented penalty value is critical
  - Algorithmic improvements
    - Infeasible solutions
    - Feasible solutions
  - Computational performance on two benchmark problems

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