Comparing Inclusion Techniques on Chemical Engineering Problems

Ali Baharev, Endre Rév

Dep. of Chemical and Environmental Process Engineering,

Budapest University of Technology and Economics; Hungary

Outline

- Affine arithmetic
- Root-finding procedure
- Numerical examples
  - affine vs. interval arithmetic
  - convex envelopes
- Conclusions

Affine arithmetic

Dependency problem

- The simple example

  $X - X \neq [\,0, 0]$ (diameter: double of X)

- Affine arithmetic keeps track of first-order correlation between computed and input quantities

- For example, with affine arithmetic (Figueiredo'97)

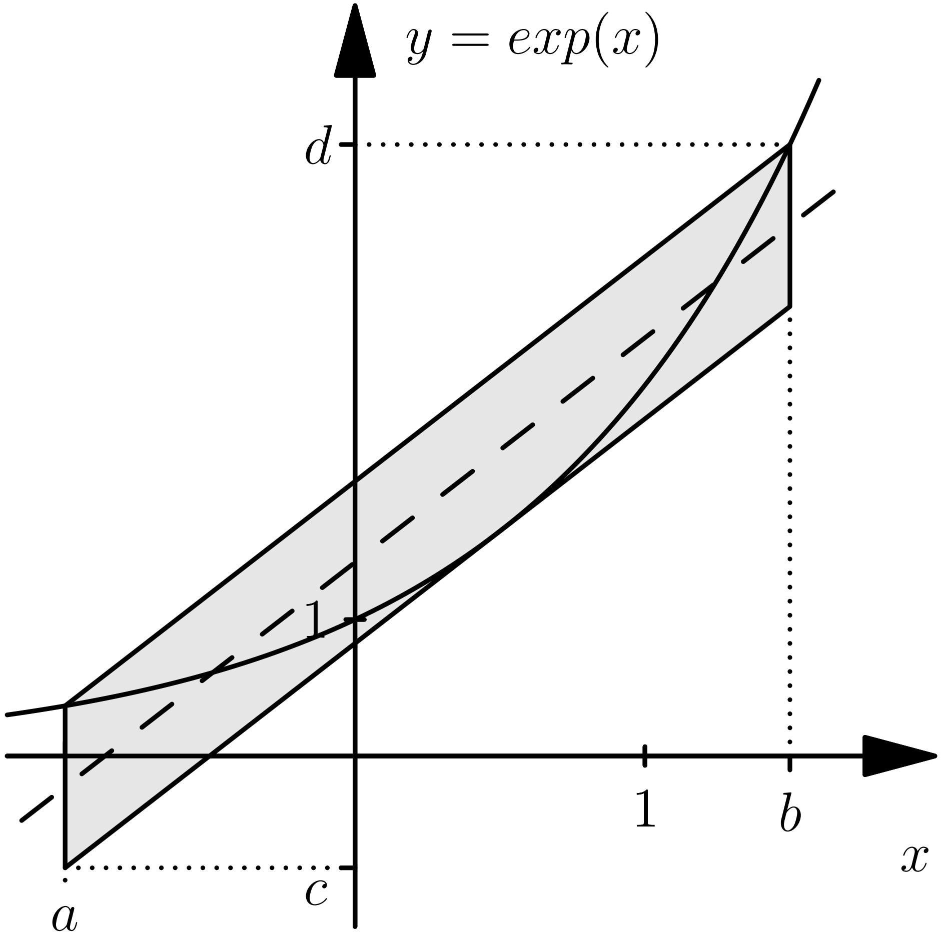
  $X = x_0 + x_1 \cdot \varepsilon_1 \qquad -1 \leq \varepsilon_1 \leq 1$

  $(x_0 + x_1 \cdot \varepsilon_1) - (x_0 + x_1 \cdot \varepsilon_1) = [\,0, 0]$

- Similarly, affine operations are ideally treated (apart from the rounding error)

Non-affine operations

A new (unused) variable is introduced to rigorously enclose the approximation error



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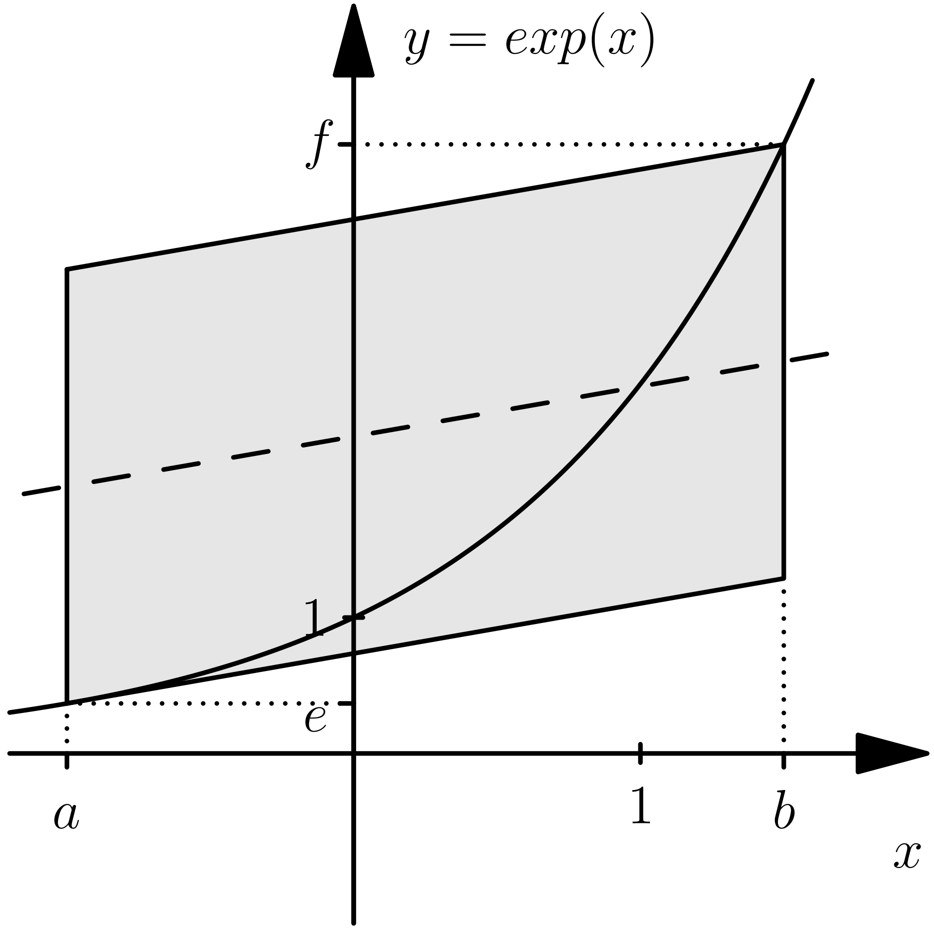
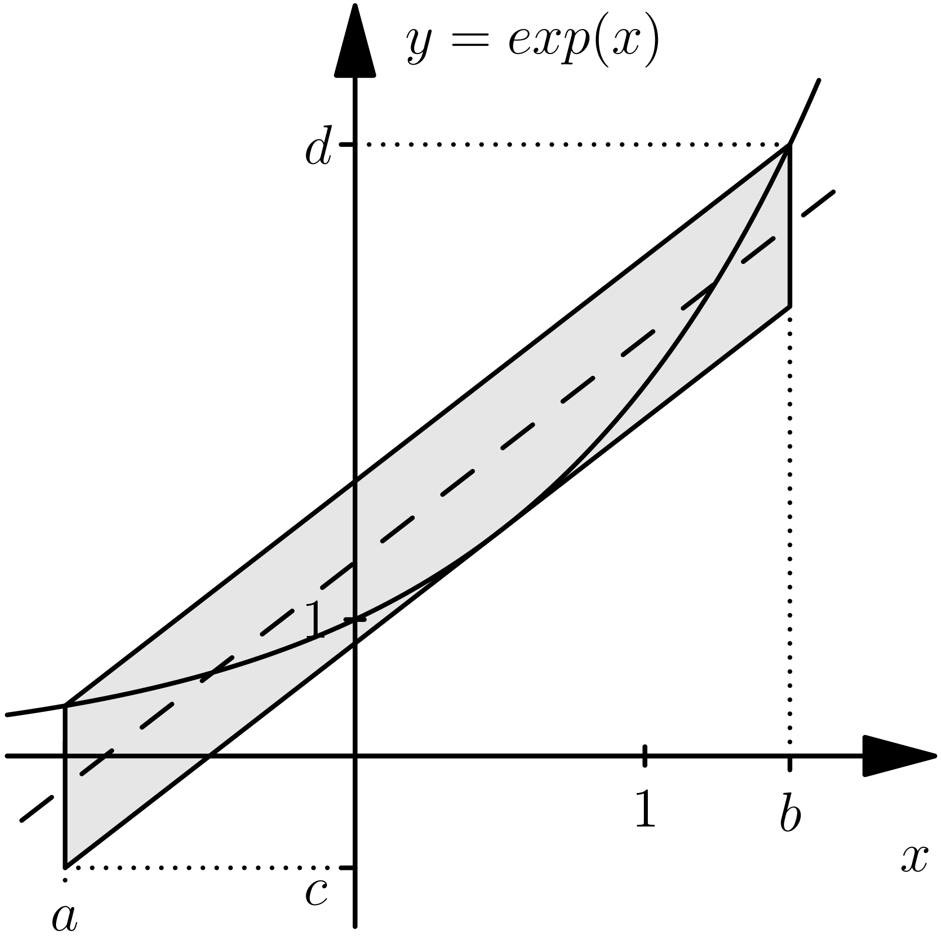


minrange

Non-affine operations (continued)

A new (unused) variable is introduced to rigorously enclose the approximation error



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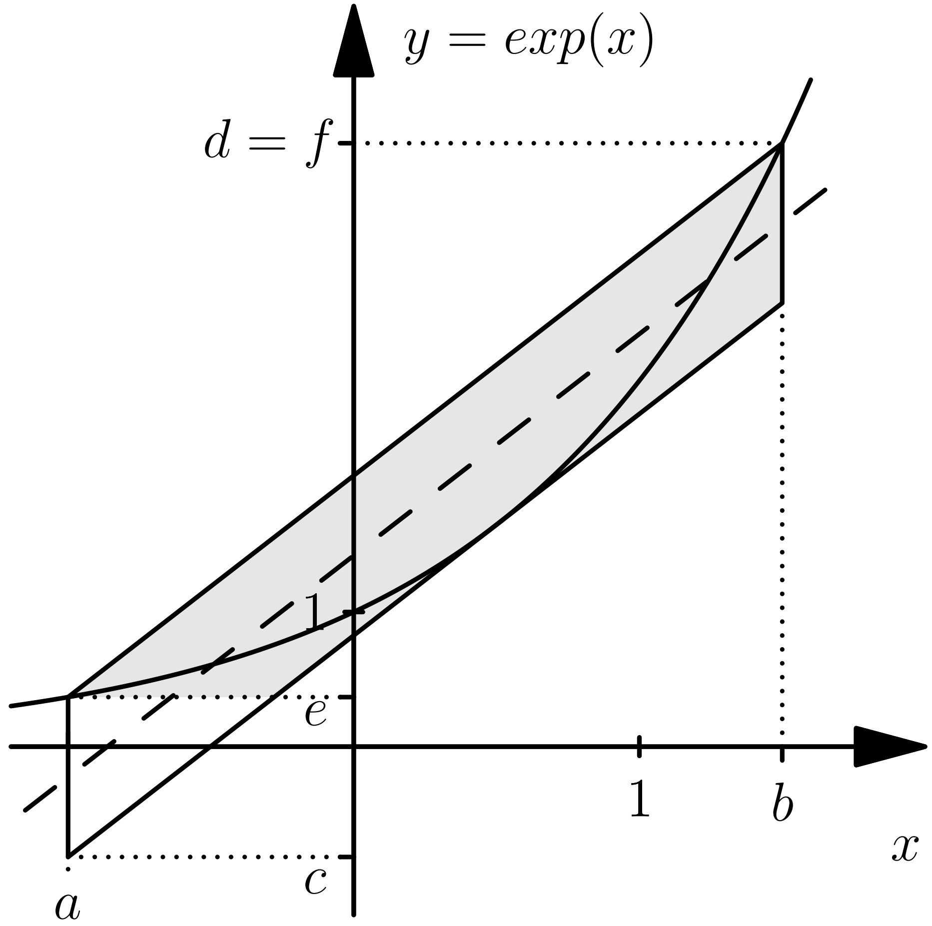


mixed AA/IA

Binary operations

- With ordinary **interval arithmetic**

  $A(B+C) \in AB+AC$ (subdistributivity)

  $X/X \neq [1, 1]$

- The modified **affine arithmetic** of Kolev'04

  $A(B+C) = AB+AC$ if B and C are independent

  $X/X = [1, 1]$

- Optimal multiplication w.r.t. range Kolev'07
- Optimal multiplication w.r.t. width Miyajima'03

Root-finding procedure

Major components

- **Linearization**

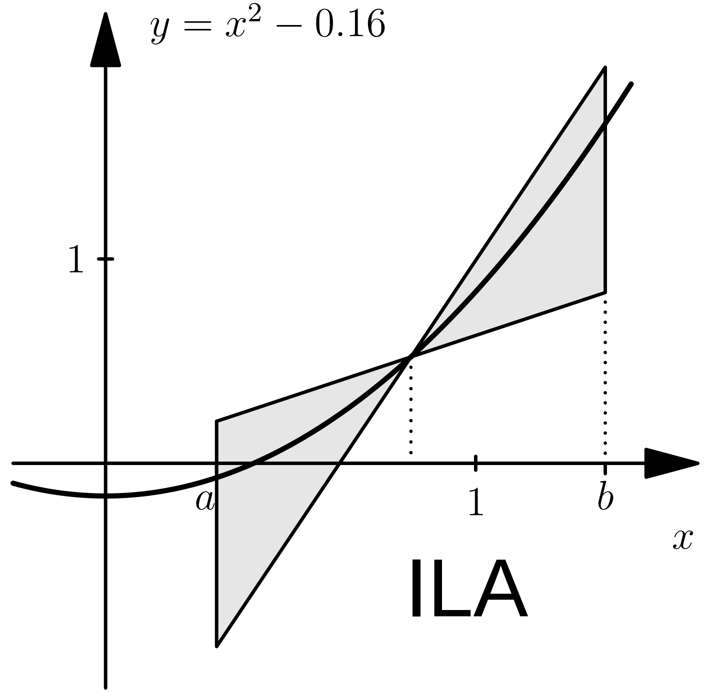
  ILA* or LIA*

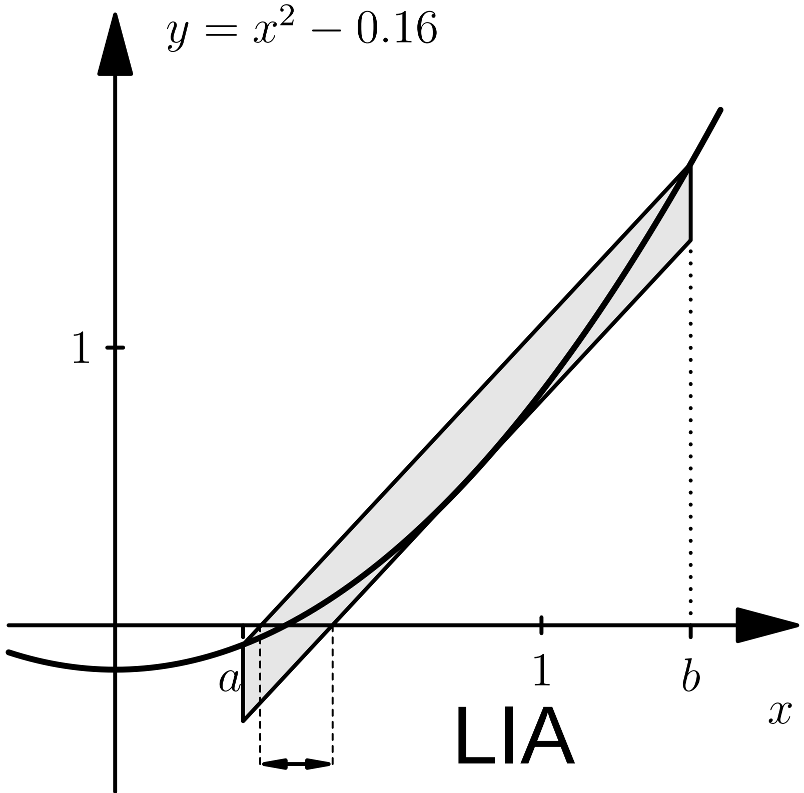
- **Pruning the box**

  based on CP, LP

- **Splitting the box**

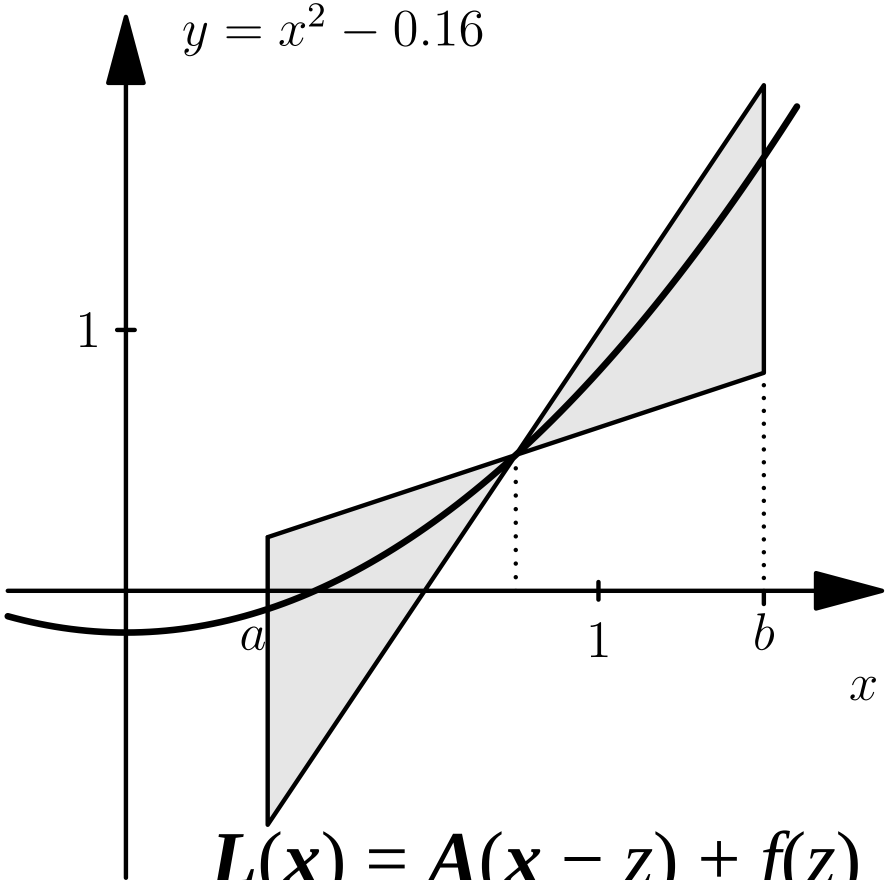
  (not discussed here)





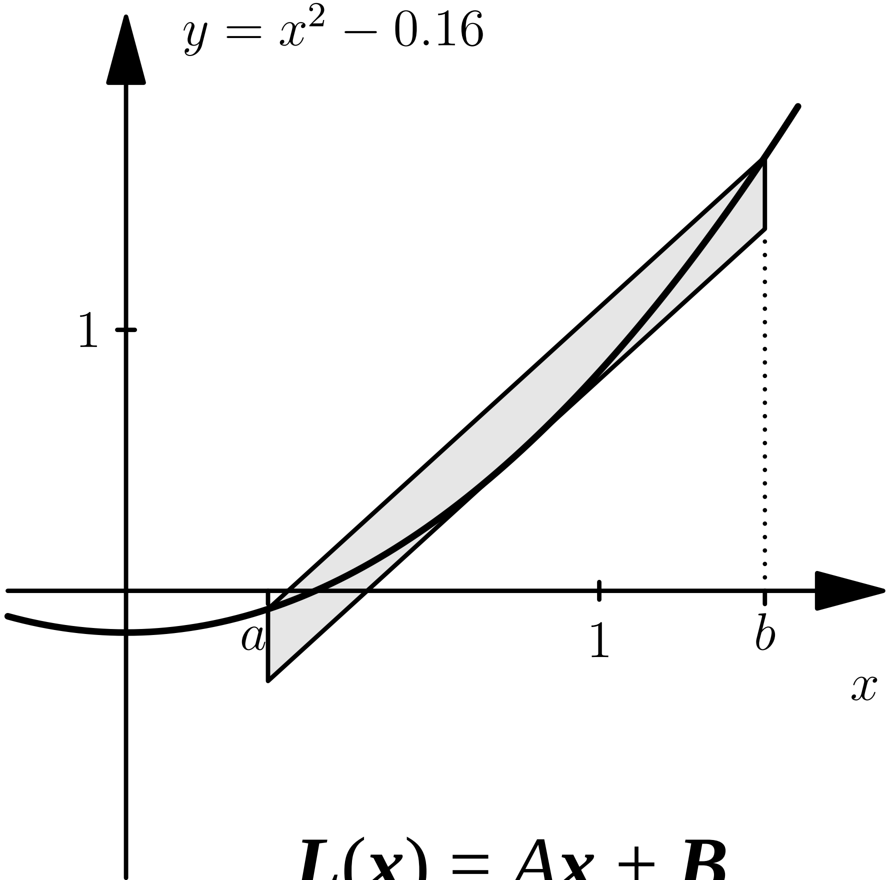
* Kolev'06

Interval Linear Approximation



$$\boldsymbol{L}(\boldsymbol{x}) = \boldsymbol{A}(\boldsymbol{x} - z) + f(z)$$

Linear Interval Approximation



$$\boldsymbol{L}(\boldsymbol{x}) = A\boldsymbol{x} + \boldsymbol{B}$$

Advantages of LIA

- Keeps track of dependencies (coefficient matrix)
- The solution set has a simpler form (convex)
- LP is directly applicable

Pruning

$$\boldsymbol{L}(x) = Ax + \boldsymbol{B} \quad x \in \boldsymbol{X}$$

- Hull solution is straightforward

$$\boldsymbol{Y} = -A^{-1}\boldsymbol{B}$$

$$\boldsymbol{X}^{new} = \boldsymbol{X} \bigcap \boldsymbol{Y}$$

- In the LP pruning, the following $2n$ LP subproblems have to be solved

$$\text{min/max} \quad x_j \quad \text{for all } j$$

$$\text{subject to}$$

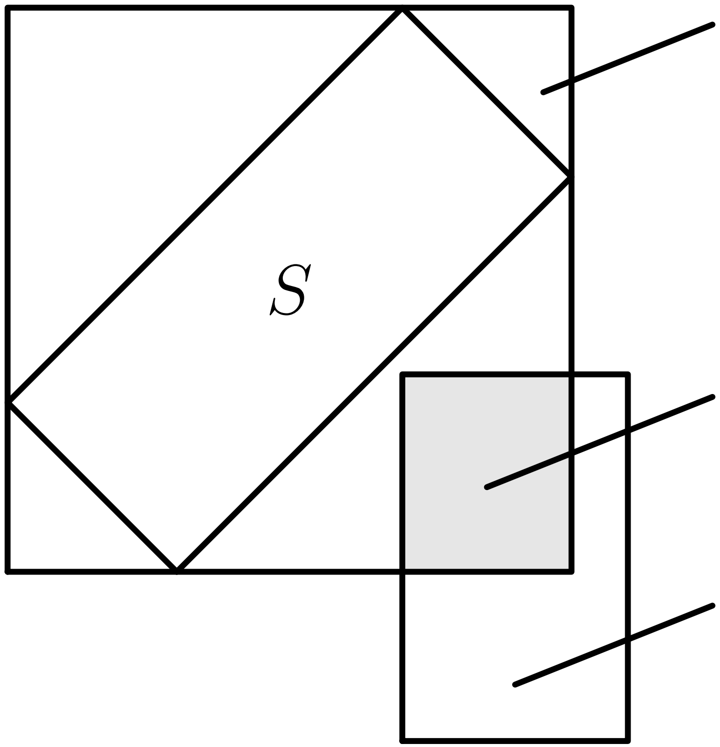
$$-b_U \le Ax \le -b_L$$

$$x_L \le x \le x_U$$

Comparing the pruning techniques I

$$L(x) = Ax + B \quad x \in X$$

No solution in ***X***



$Y = -A^{-1}B$

$X_{LP}^{new} = \emptyset$ Discarded with LP

$X^{new} = X \cap Y$ Not disc. with CP

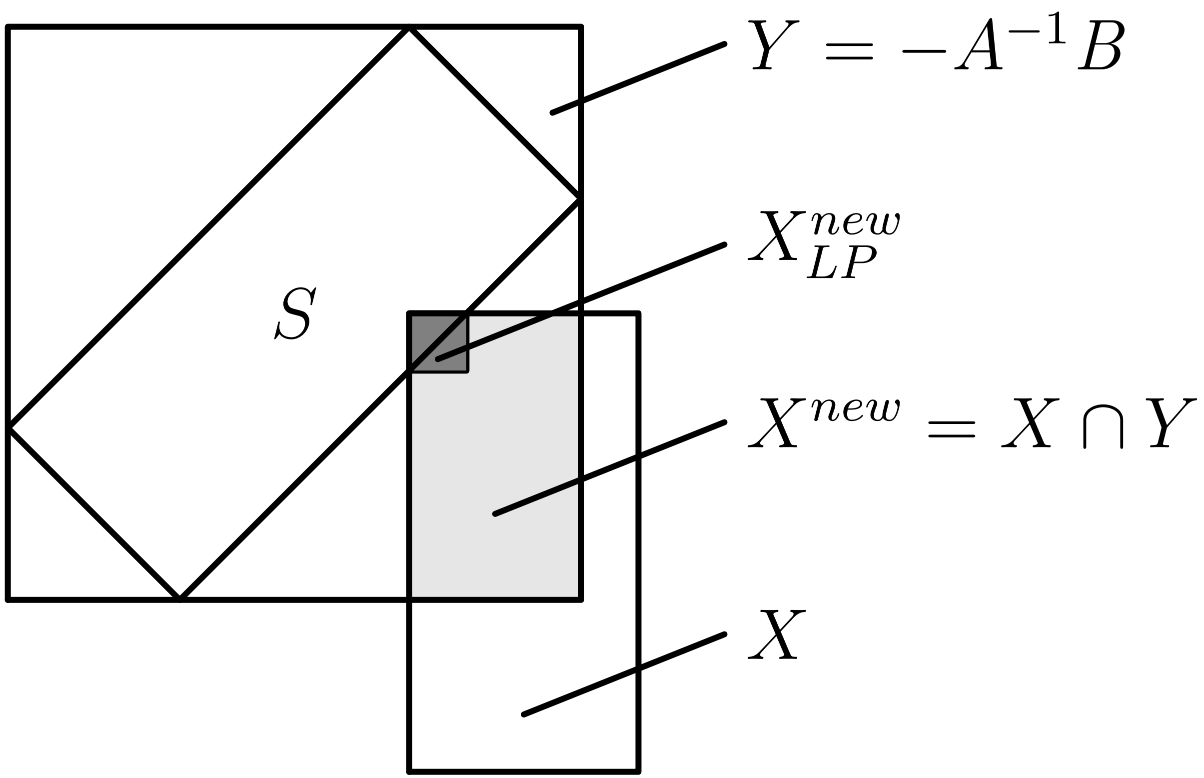
X

Kolev'06

Comparing the pruning techniques II

$$\boldsymbol{L}(x) = Ax + \boldsymbol{B} \quad x \in \boldsymbol{X}$$

There may be a solution in ***X***



Much smaller part is kept with LP pruning

Kolev’06

Revised LP pruning

$$\min/\max \quad x_j \quad \text{for all } j$$
$$\text{subject to}$$
$$-b_U \leq Ax \leq -b_L$$
$$x_L \leq x \leq x_U$$

According to the ideas of *Tobias Achterberg*

- Only the first LP subproblem has to be solved from scratch, after that just Phase II is used
- If $x_j = x_{j,\mathrm{L}}$ / $x_{j,\mathrm{U}}$ then $\min / \max x_j$ can be skipped, resp.
- Sequence of variables: find the non-basic variable that is the closest to its lower / upper bound and has not yet been considered in the pruning step
- LP object is not deallocated between two iteration (memory pool)

Numerical examples
(Separations)

Liquid-liquid equilibrium (LLE)

Two liquid phases are separated, components are distributed between phases

Solution for the necessary conditions is computed (nonlinear system of equations)

Liquid-liquid equilibrium (LLE)

$$\sum_i x_i = 1$$

$$\sum_i y_i = 1 \qquad\qquad i = 1, 2, \ldots, C$$

$$\lambda \cdot x_i + (1-\lambda) \cdot y_i = z_i$$

$$\ln \gamma_i(\mathbf{x}) + \ln x_i = \ln \gamma_i(\mathbf{y}) + \ln y_i$$

$$\sum_{i=1}^{C-1} (x_i - y_i)^2 > \varepsilon$$

$$\ln \gamma_i(\mathbf{x}) = \frac{\sum_{j=1}^{C} \tau_{ji} G_{ji} x_j}{\sum_{k=1}^{C} G_{ki} x_k} + \sum_{j=1}^{C} \frac{x_j G_{ij}}{\sum_{k=1}^{C} G_{kj} x_k} \cdot \left(\tau_{ij} - \frac{\sum_{l=1}^{C} \tau_{lj} G_{lj} x_l}{\sum_{k=1}^{C} G_{kj} x_k} \right)$$

LLE results

$C = 2$

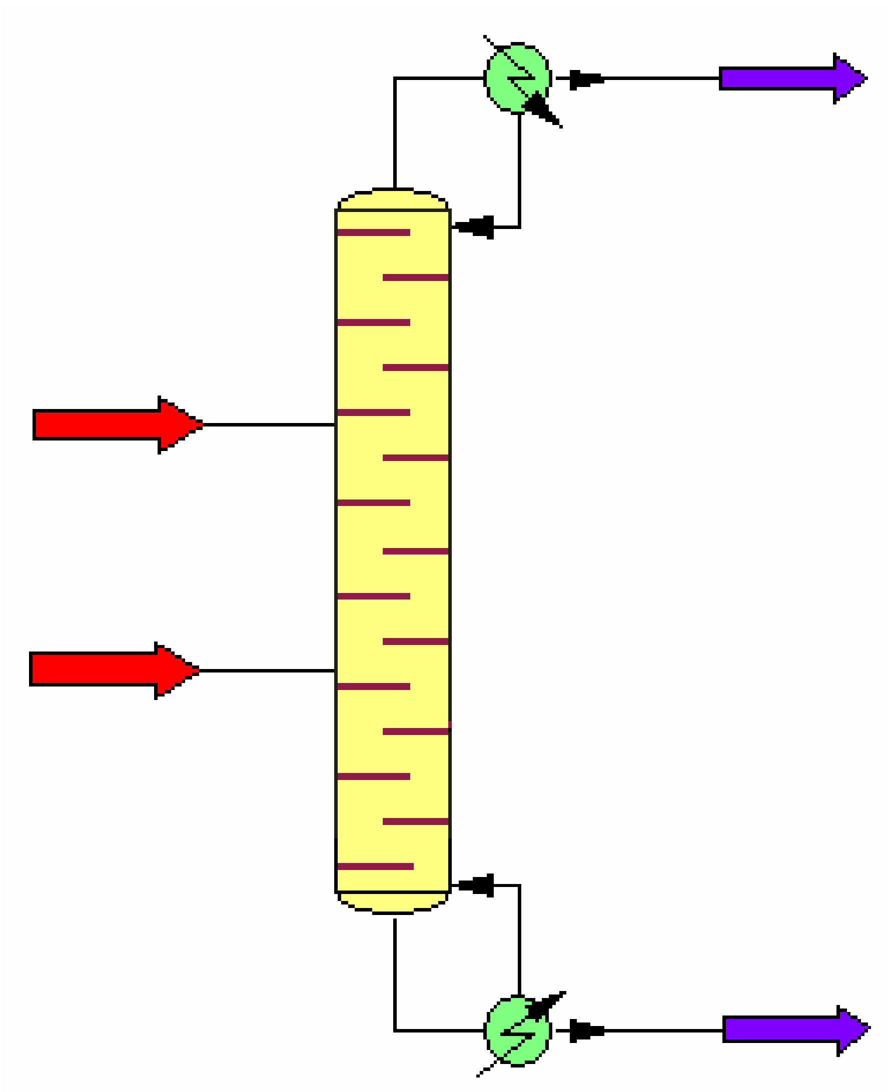
Method	total time [s]	$\frac{\text{total time}}{\text{total time}_{AA/CP}}$	iterations	$\frac{\text{iterations}}{\text{iterations}_{AA/CP}}$	cycle time [μs]	$\frac{\text{cycle time}}{\text{cycle time}_{AA/CP}}$
IN/GS	26.1	22.7	120234	85.5	217	0.27
AA/CP	1.15	1.00	1407	1.00	817	1.00

$C = 3$

Method	total time [s]	$\frac{\text{total time}}{\text{total time}_{AA/CP}}$	iterations	$\frac{\text{iterations}}{\text{iterations}_{AA/CP}}$	cycle time [ms]	$\frac{\text{cycle time}}{\text{cycle time}_{AA/CP}}$
IN/GS	>318000	$>1.36\cdot 10^4$	—	—	—	—
AA/CP	23.3	1.00	7715	1.00	3.01	1.00

Baharev'08 Not *state-of-the-art* IN/GB! (C-XSC)

Distillation columns



Distillation columns

for $j = 1, \ldots, N$ (*i.e.* for each stage)

$$\sum_i x_{i,j} = 1$$

$$\sum_i y_{i,j} = 1 \qquad\qquad i = 1,\ 2,\ \ldots,\ C$$

$$L_{j-1} x_{i,j-1} + V_{j+1} y_{i,j+1} + F_j z_{i,j} = L_j x_{i,j} + V_j y_{i,j}$$

$$V_j \sum_i \lambda_i\, y_{i,j} = V_{j+1} \sum_i \lambda_i\, y_{i,j+1}$$

$$\ln \gamma_{i,j}(\mathbf{x}_j, T_j) + \ln x_{i,j} + (A_i - B_i /(C_i + T_j) = \ln y_{i,j} + \ln P$$

$$\ln \gamma_i(\mathbf{x}, T) = -\ln\left(\sum_{a=1}^{C} x_a \Lambda_{ia}\right) + 1 - \sum_{b=1}^{C} \frac{x_b \Lambda_{bi}}{\sum_{a=1}^{C} x_a \Lambda_{ia}} \quad ; \quad \Lambda_{ab}(T) = \frac{V_b^m}{V_a^m} \exp\left(-\frac{k_{ab}}{R_G T}\right)$$

Results with a single stage

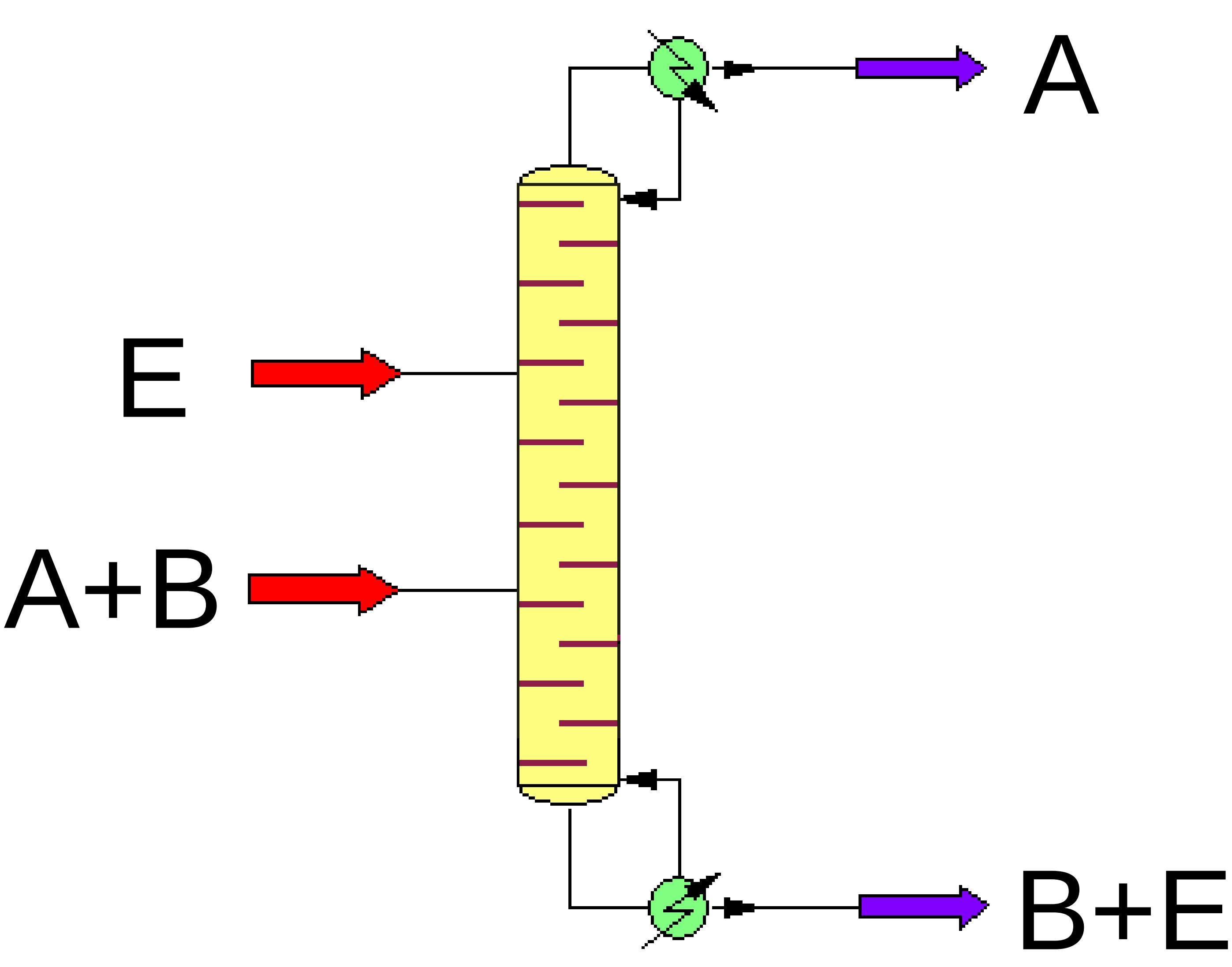
Linearization techniques ($N = 1$)

Method	time [s]	$\frac{\text{total time}_{IN/GS}}{\text{total time}_{AA/CP}}$	cycles	$\frac{\text{cycles}_{IN/GS}}{\text{cycles}_{AA/CP}}$	cycle time [ms]	$\frac{\text{cycle time}_{IN/GS}}{\text{cycle time}_{AA/CP}}$	Cluster boxes
IN/GS	280.7	63.2	271491	160.9	1.03	0.39	3
AA/CP	4.44	1.00	1687	1.00	2.63	1.00	8

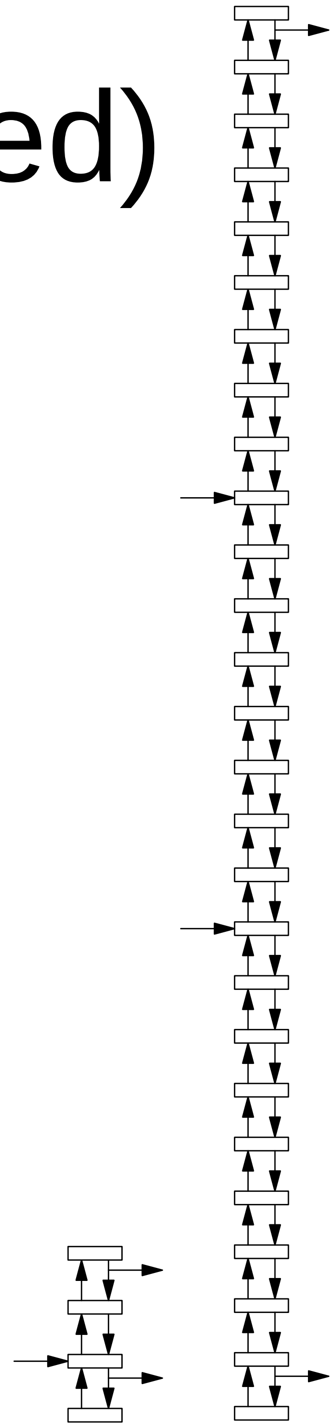
Pruning techniques

Method	time [s]	$\frac{\text{total time}_{IN/GS}}{\text{total time}_{AA/CP}}$	cycles	$\frac{\text{cycles}_{IN/GS}}{\text{cycles}_{AA/CP}}$	cycle time [ms]	$\frac{\text{cycle time}_{IN/GS}}{\text{cycle time}_{AA/CP}}$	Cluster boxes
AA/CP	4.44	4.23	1687	5.68	2.63	0.74	8
AA/LP	1.05	1.00	297	1.00	3.54	1.00	1

Extractive distillation column



Distillation column (continued)



Initial intervals are fairly wide

Hundreds of variables

N	time (s)	boxes	simplex iterations
12	22.10	19	247522
16	54.15	29	500041
22	92.13	33	709058

Revised implementation: memory pool, LP pruning enhanced

Distillation columns

for $j = 1, \ldots, N$ (*i.e.* for each stage)

$$\sum_i x_{i,j} = 1$$

$$\sum_i y_{i,j} = 1 \qquad i = 1, 2, \ldots, C$$

$$L_{j-1} x_{i,j-1} + V_{j+1} y_{i,j+1} + F_j z_{i,j} = L_j x_{i,j} + V_j y_{i,j}$$

$$V_j \sum_i \lambda_i \, y_{i,j} = V_{j+1} \sum_i \lambda_i \, y_{i,j+1}$$

$$\ln \gamma_{i,j}(\mathbf{x}_j, T_j) + \ln x_{i,j} + (A_i - B_i/(C_i + T_j) = \ln y_{i,j} + \ln P$$

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Convex envelopes in LP pruning

$$z = xy$$

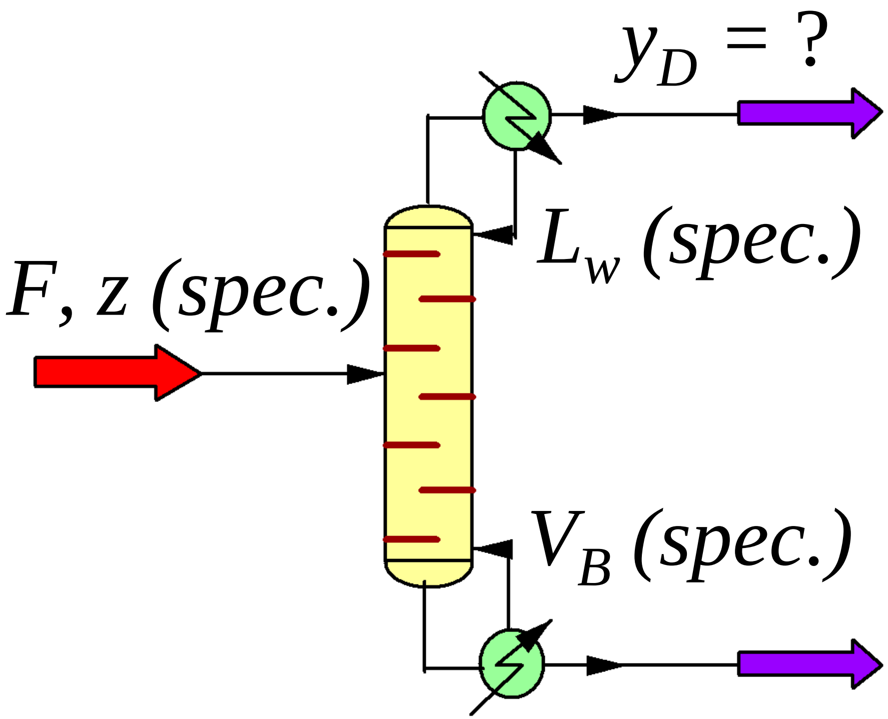
$$z \geq x_L\, y + y_L\, x - x_L\, y_L$$
$$z \geq x_U\, y + y_U\, x - x_U\, y_U$$
$$z \leq x_L\, y + y_U\, x - x_L\, y_U$$
$$z \leq x_U\, y + y_L\, x - x_U\, y_L$$

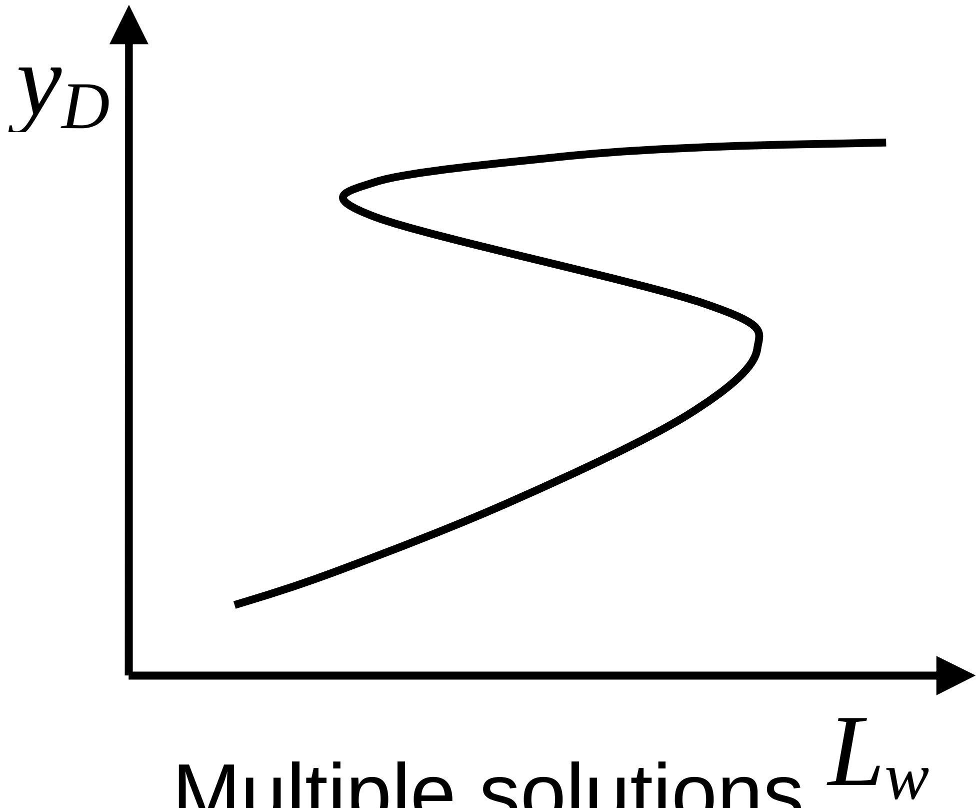
The initial intervals are varied

	with env.	without env.	with / without env.
time (s)	42.65	9.49	4.50
boxes examined	7	9	0.78
simplex iterations	176411	78803	2.24

	with env.	without env.	with / without env.
time (s)	161.1	54.15	2.97
boxes examined	17	29	0.59
simplex iterations	656571	500041	1.31

Multiple steady states





Binary mixture (C = 2)
Jacobsen'91

Multiple solutions

Instead of the complicated equations of γ:

$$y_j = \alpha x_j / ((\alpha - 1)\, x_j + 1)$$

Multiple steady states (results)

Only convex envelopes are used + LP pruning

L_w (kg/min)	V (kmol/min)	number of solutions	time (s)	box	cluster box
58.50	2.0	3	1427	48175	341
96.00	3.0	5	>3600	−	−
98.75	3.0	3	>3600	−	−

Mixed AA/IA

L_w (kg/min)	V (kmol/min)	number of solutions	time (s)	box	cluster box
58.50	2.0	3	0.22	507	0
96.00	3.0	5	0.25	267	0
98.75	3.0	3	0.20	227	0

Conclusions

Conclusions

- Numerical evidence suggests that affine arithmetic is a competing linearization compared to the Interval Newton method
- The revised LP pruning proved to be an efficient pruning technique in certain cases
- The solver written in C++ should be interfaced with a modeling language
- DAG based propagation technique should be studied

Acknowledgement

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