Practical aspects of MINLP

January, 2013

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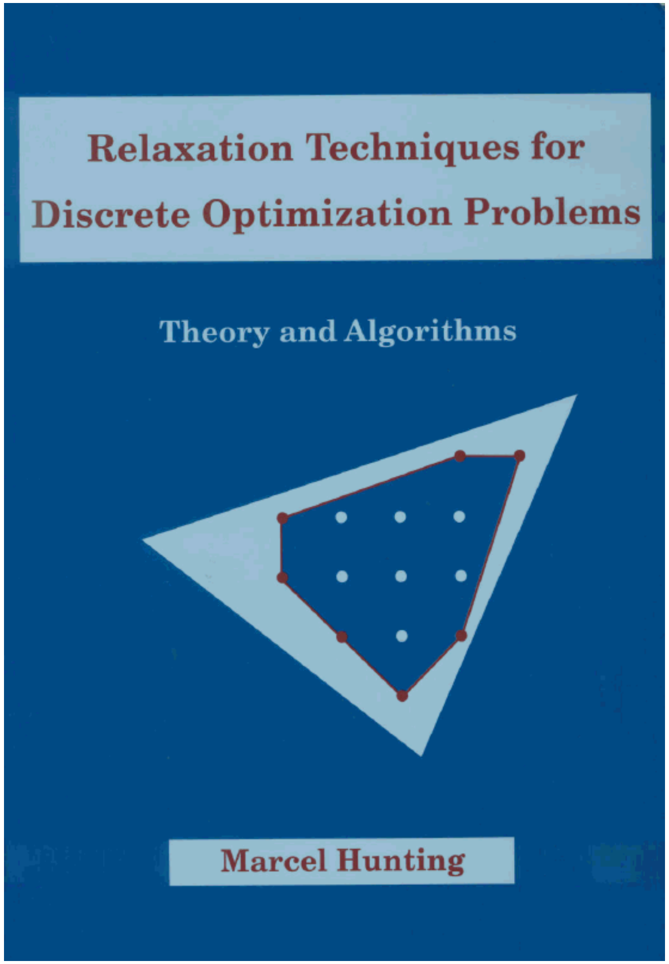
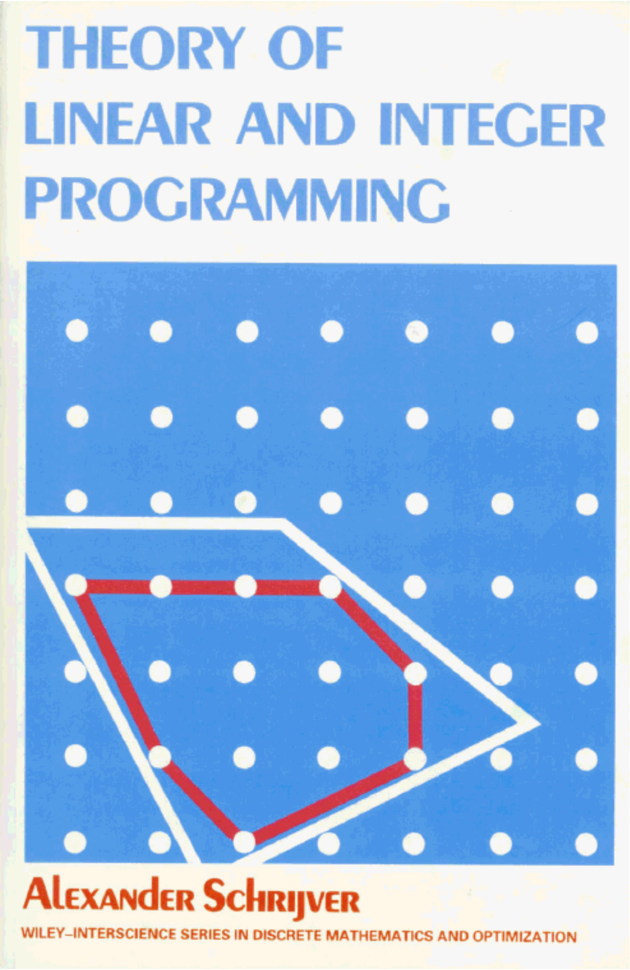
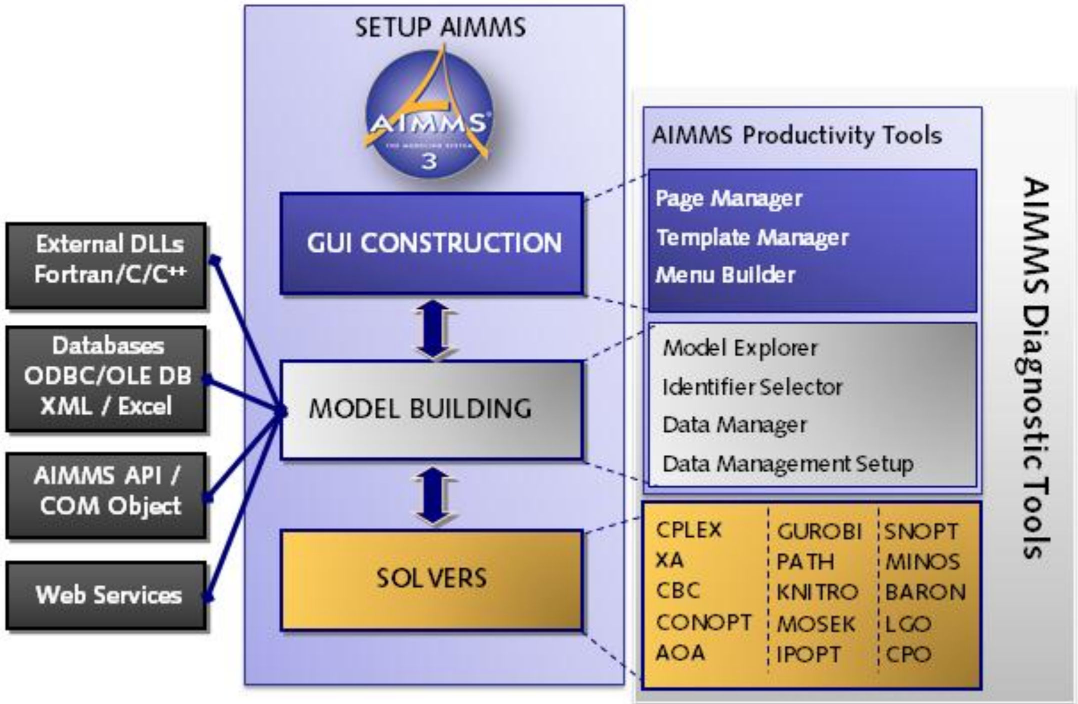
AIMMS Software Developer


Relaxation Techniques for
Discrete Optimization Problems
Theory and Algorithms
Marcel Hunting


THEORY OF
LINEAR AND INTEGER
PROGRAMMING
Alexander Schrijver
WILEY–INTERSCIENCE SERIES IN DISCRETE MATHEMATICS AND OPTIMIZATION

Paragon Decision Technology

- Founded in 1989
- Privately owned company
- About 30 employees
- Offices in
  - The Netherlands
  - USA
  - Singapore
  - China
- Developer of **AIMMS**:
  Modeling system for optimization-based applications



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Overview

- MINLP solvers
- MINLP algorithms
- Preprocessing
- Conclusions

Mixed-Integer Nonlinear Program

minimize	$f(x,y)$	
subject to	$g_j(x,y) \leq 0$	$j \in J$
	$Ax + By \leq b$	
	x continuous	
	y integer	

Important special cases:

- Convex MINLP: f and g_j are convex functions
- MIQCP: g_j are quadratic functions (and f is linear or quadratic)
- MISOCP: g_j are second-order cone constraints (and f is linear or quadratic)

Global MINLP solvers

Reference: Bussieck and Vigerske (2012)

Solver	Modeling language	Algorithm
BARON	GAMS, AIMMS	Spatial Branch & Bound
Couenne	AMPL, GAMS	Spatial Branch & Bound
GloMIQO	GAMS	Spatial Branch & Bound
LaGO	AMPL, GAMS	Spatial Branch & Bound
Lindo API	GAMS, MPL	Branch & Cut
Minotaur	AMPL	Spatial Branch & Bound
SCIP	AMPL, GAMS	Spatial Branch & Bound

- GloMIQO only for problems with quadratic (and linear) constraints
- Solving RMINLP can be harder than solving MINLP

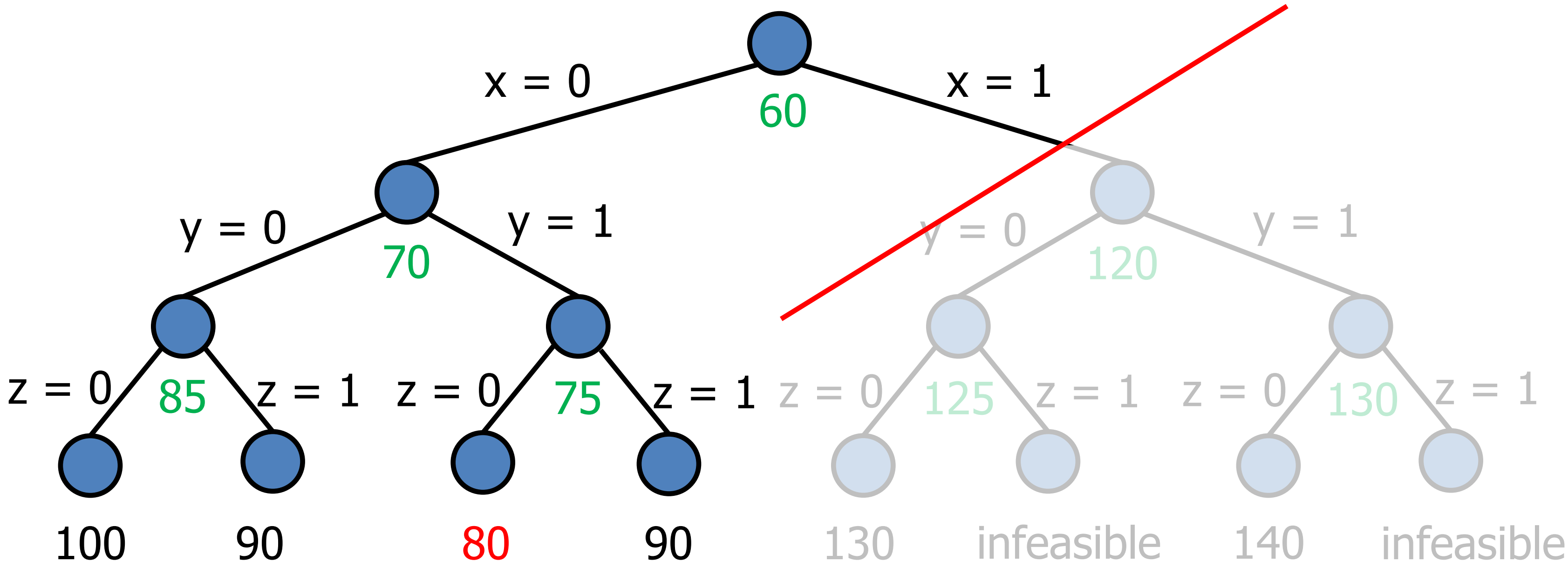
Local MINLP solvers

Solver	Modeling language	Algorithm
AlphaECP	GAMS	Extended cutting plane
AOA/COA	AIMMS	Outer approximation
BONMIN	AMPL, GAMS	Outer approximation / Branch & Bound
DICOPT	GAMS	Outer approximation
FilMINT	AMPL	Outer approximation
Knitro	AMPL, GAMS, MPL, AIMMS	Branch & Bound
MINLP_BB	AMPL	Branch & Bound
Minotaur	AMPL	Outer approximation / Branch & Bound
OQNLP	GAMS	Multistart scatter search
SBB	GAMS	Branch & Bound

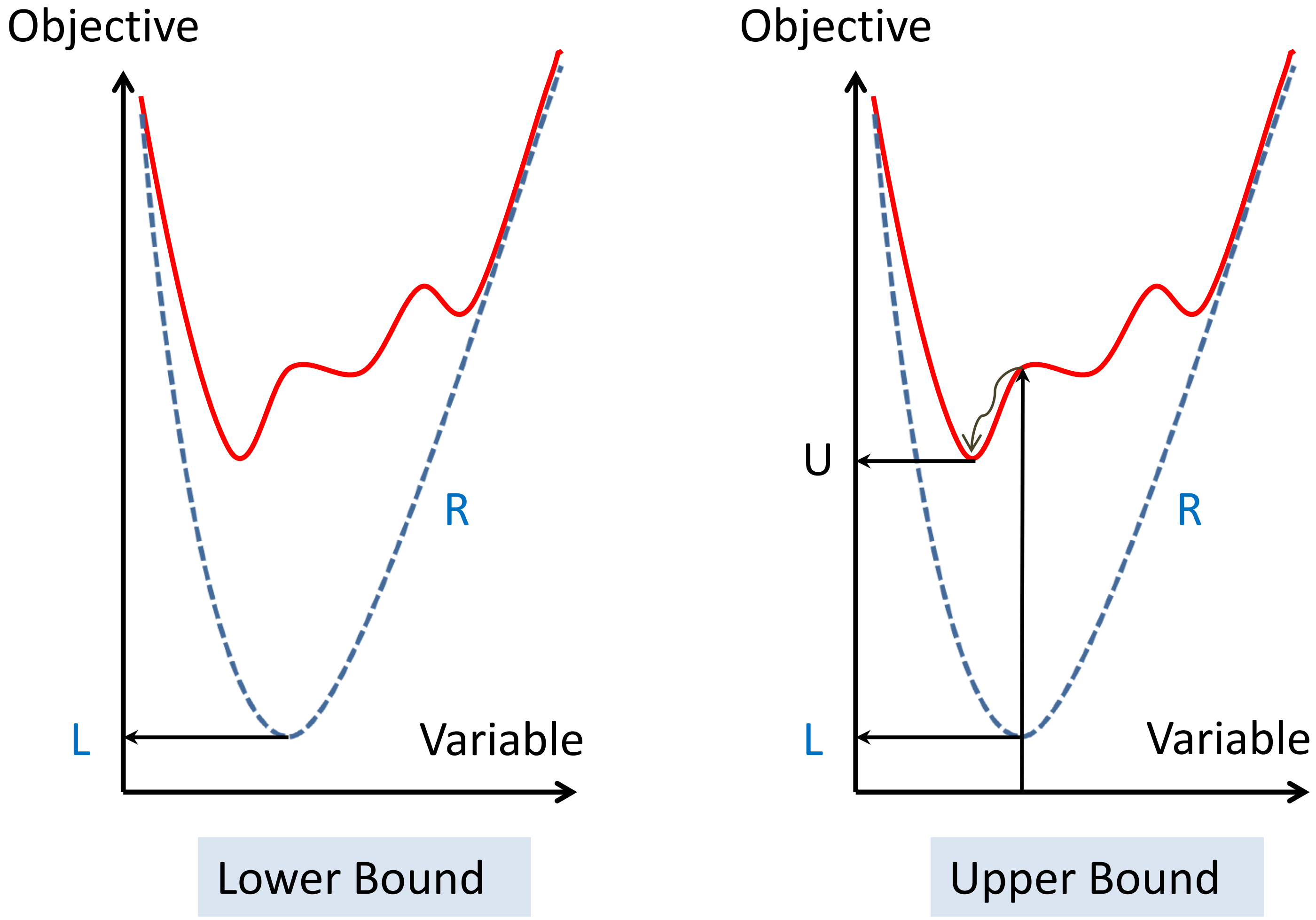
Branch-and-Bound

Integer problem (minimizing) with 3 binary variables: x, y, z

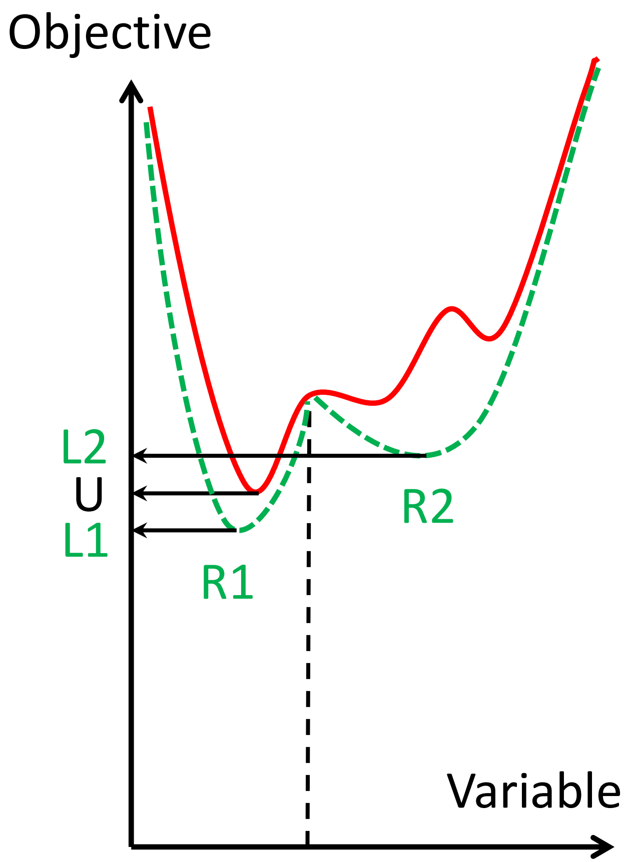
Heuristic finds solution (x,y,z) = (0,0,0) with objective value 100



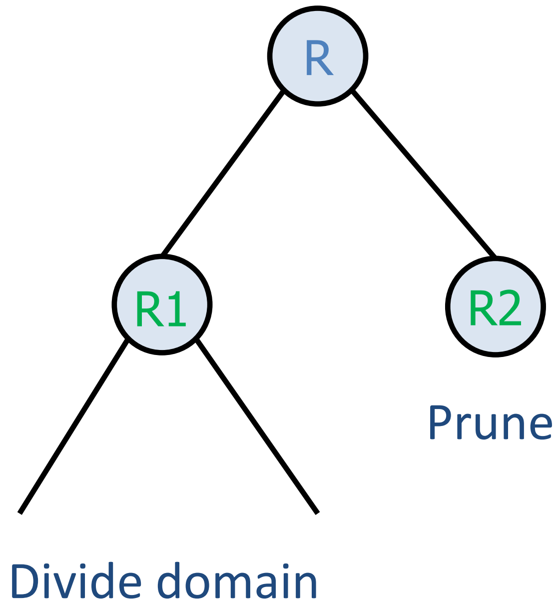
Spatial Branch-and-Bound



Spatial Branch-and-Bound

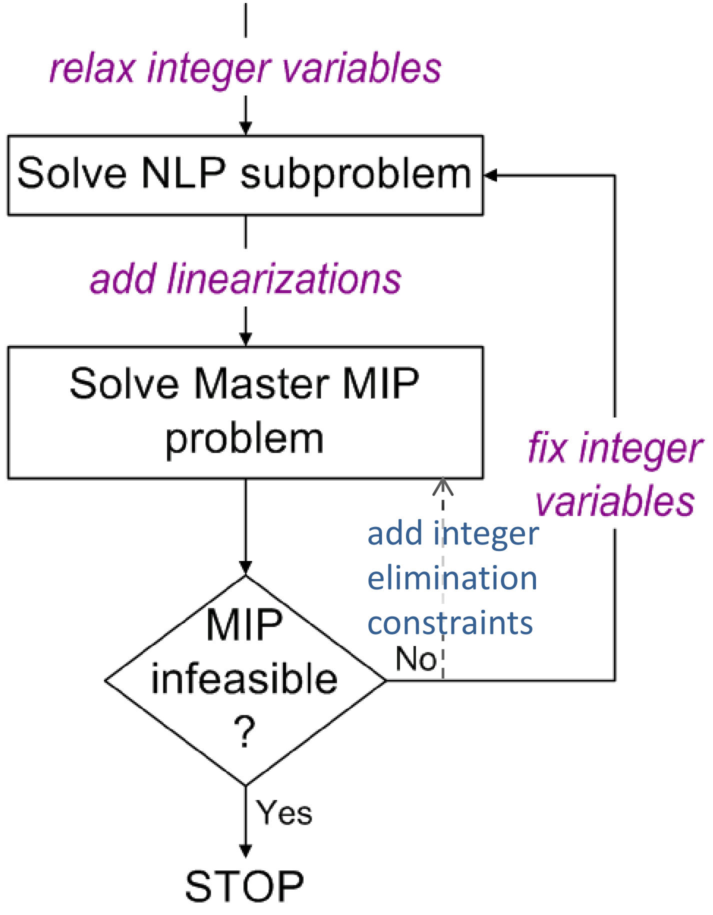


Domain Division



Search Tree

Outer Approximation



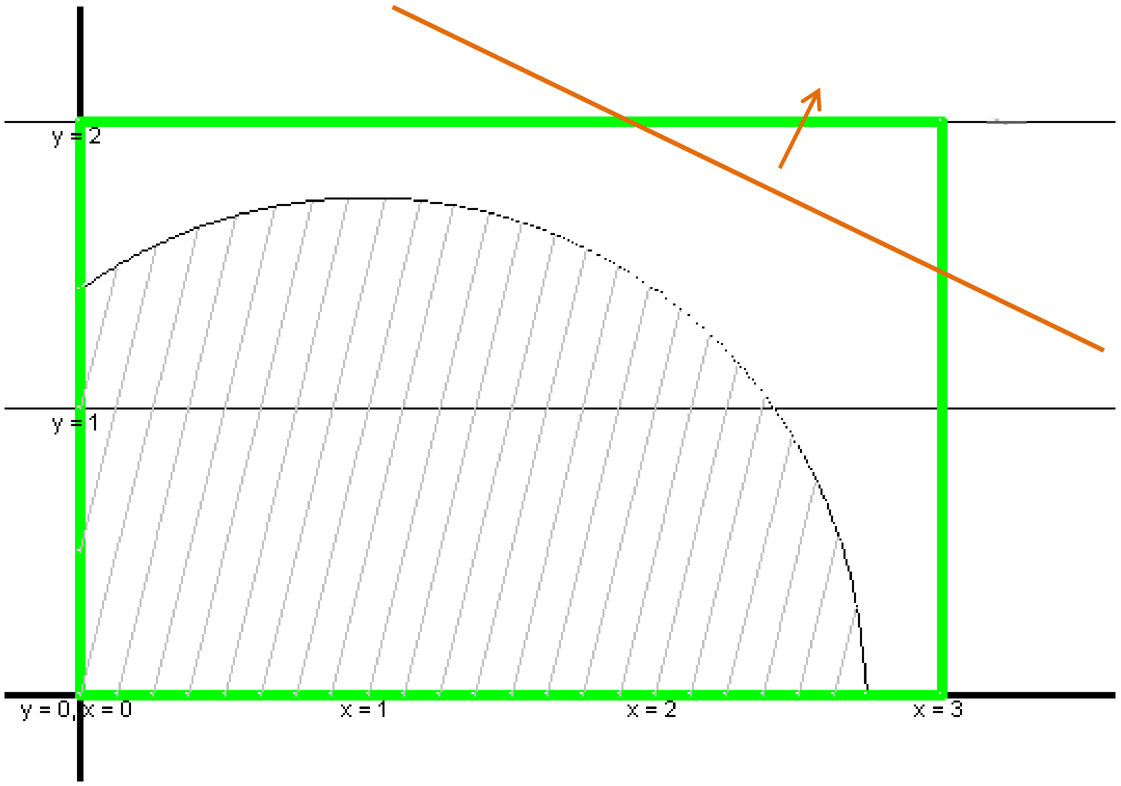
Outer Approximation: Example

max $0.5\,x + y$

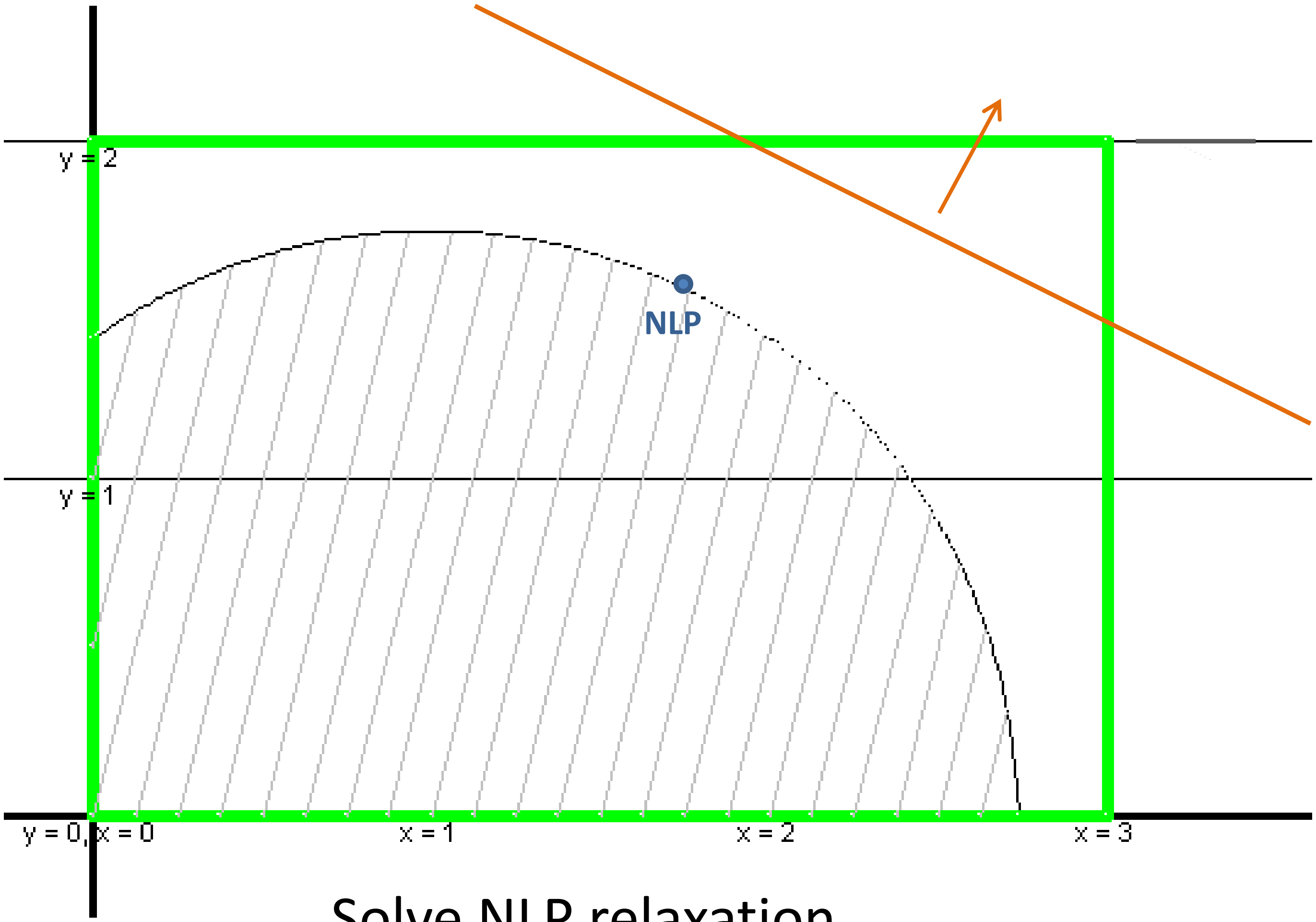
s.t. $(x-1)^2 + y^2 \leq 3$

$x \in [0,3]$

$y \in \{0..2\}$

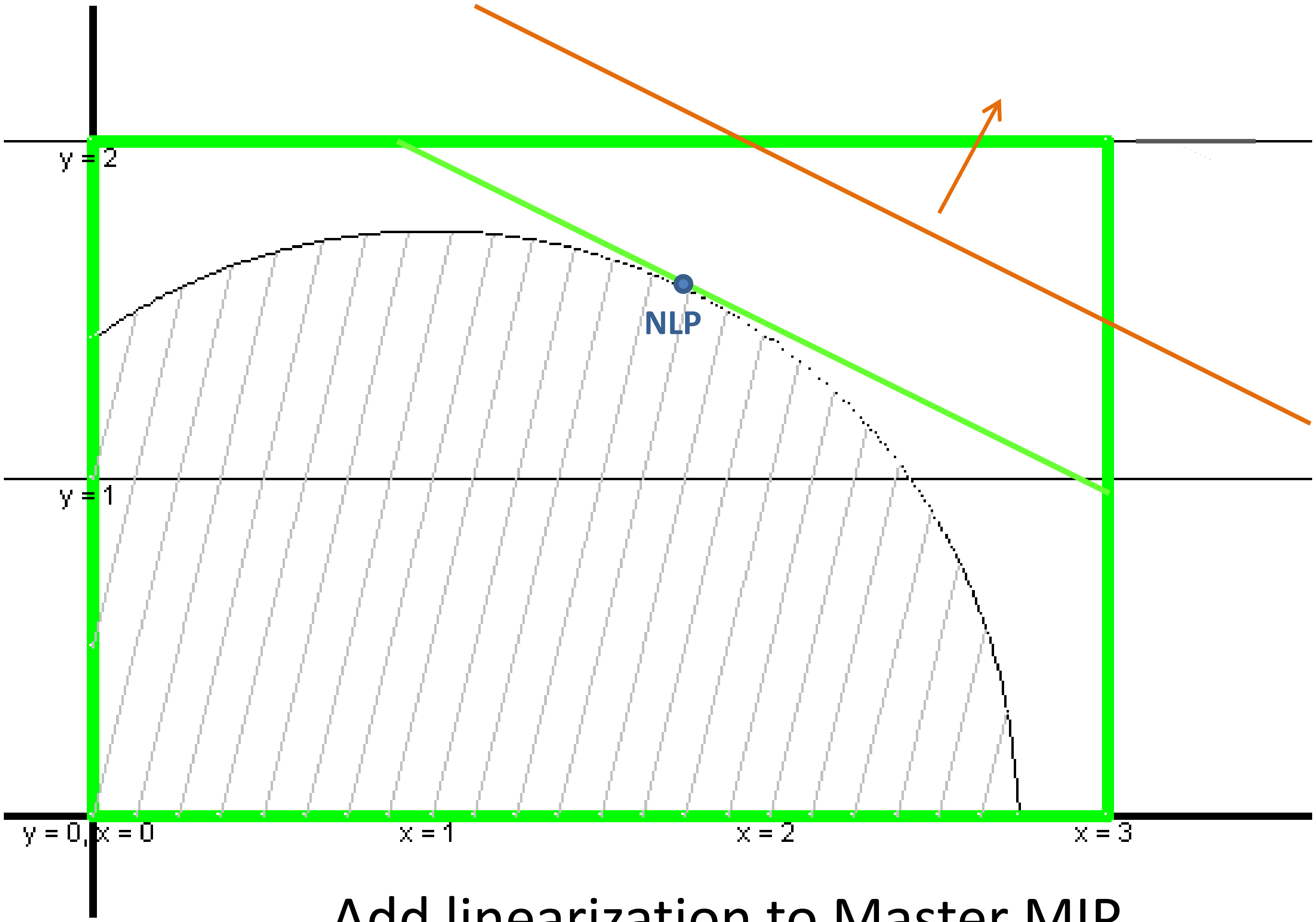


Outer Approximation: Example



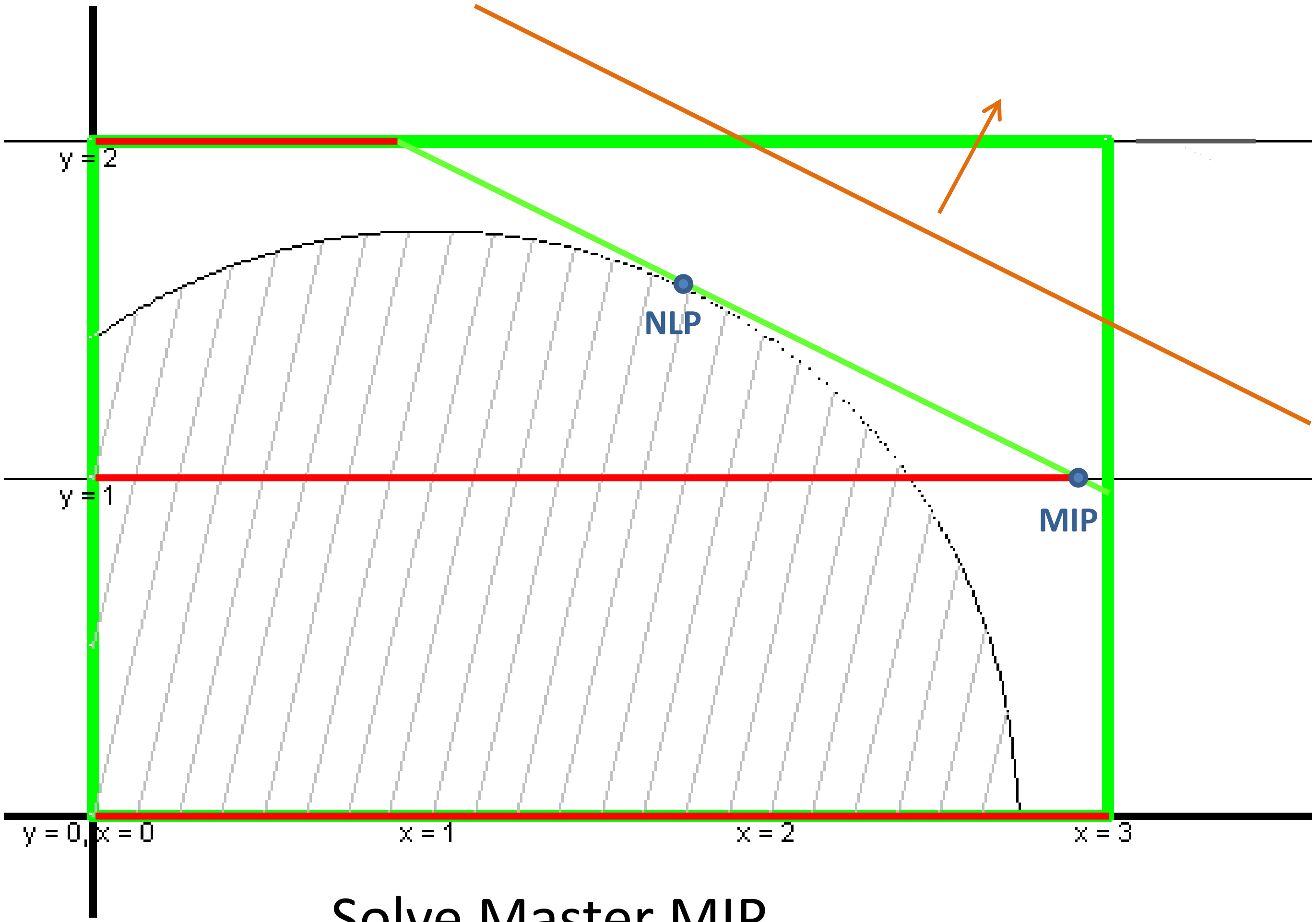
Solve NLP relaxation

Outer Approximation: Example



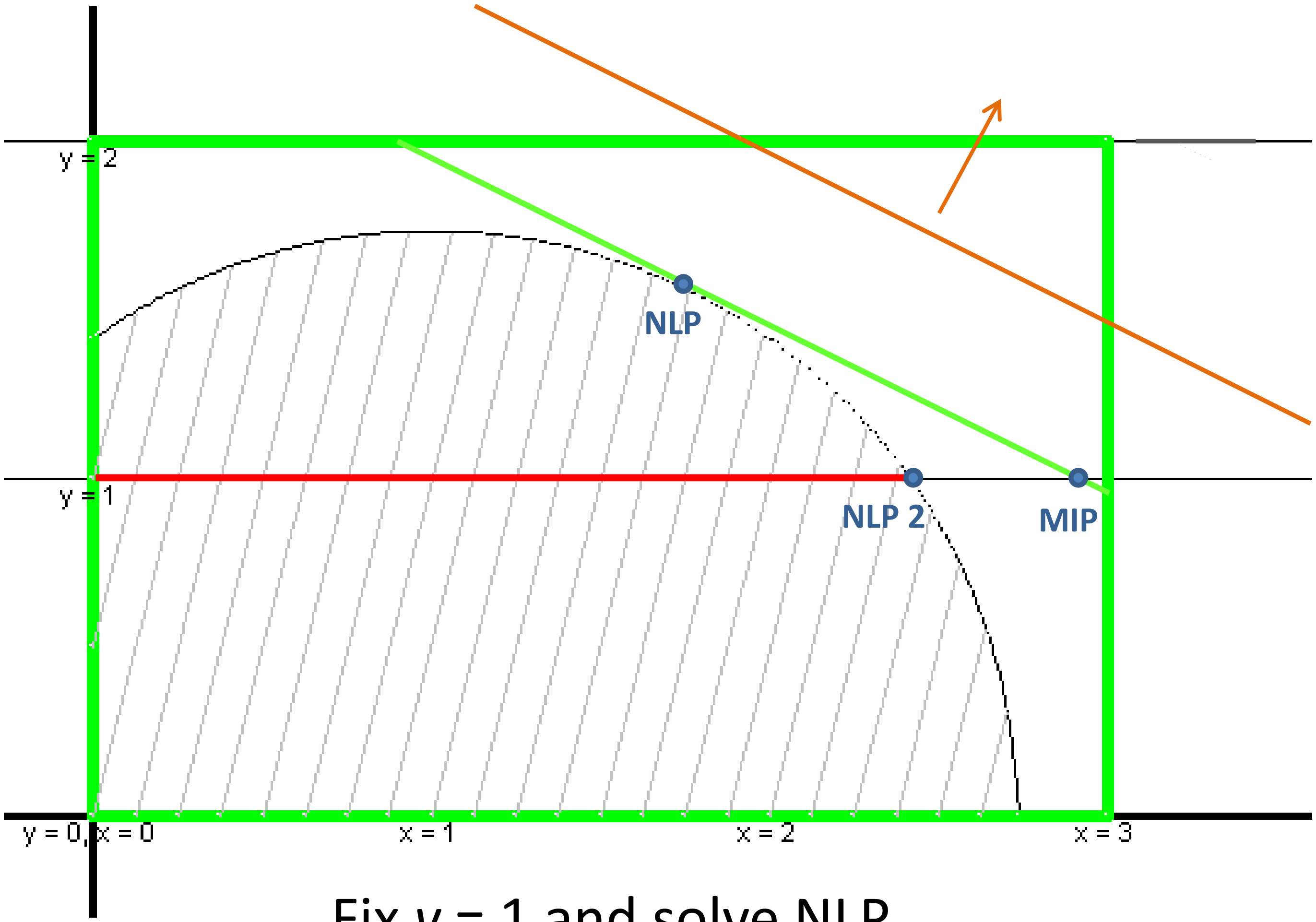
Add linearization to Master MIP

Outer Approximation: Example



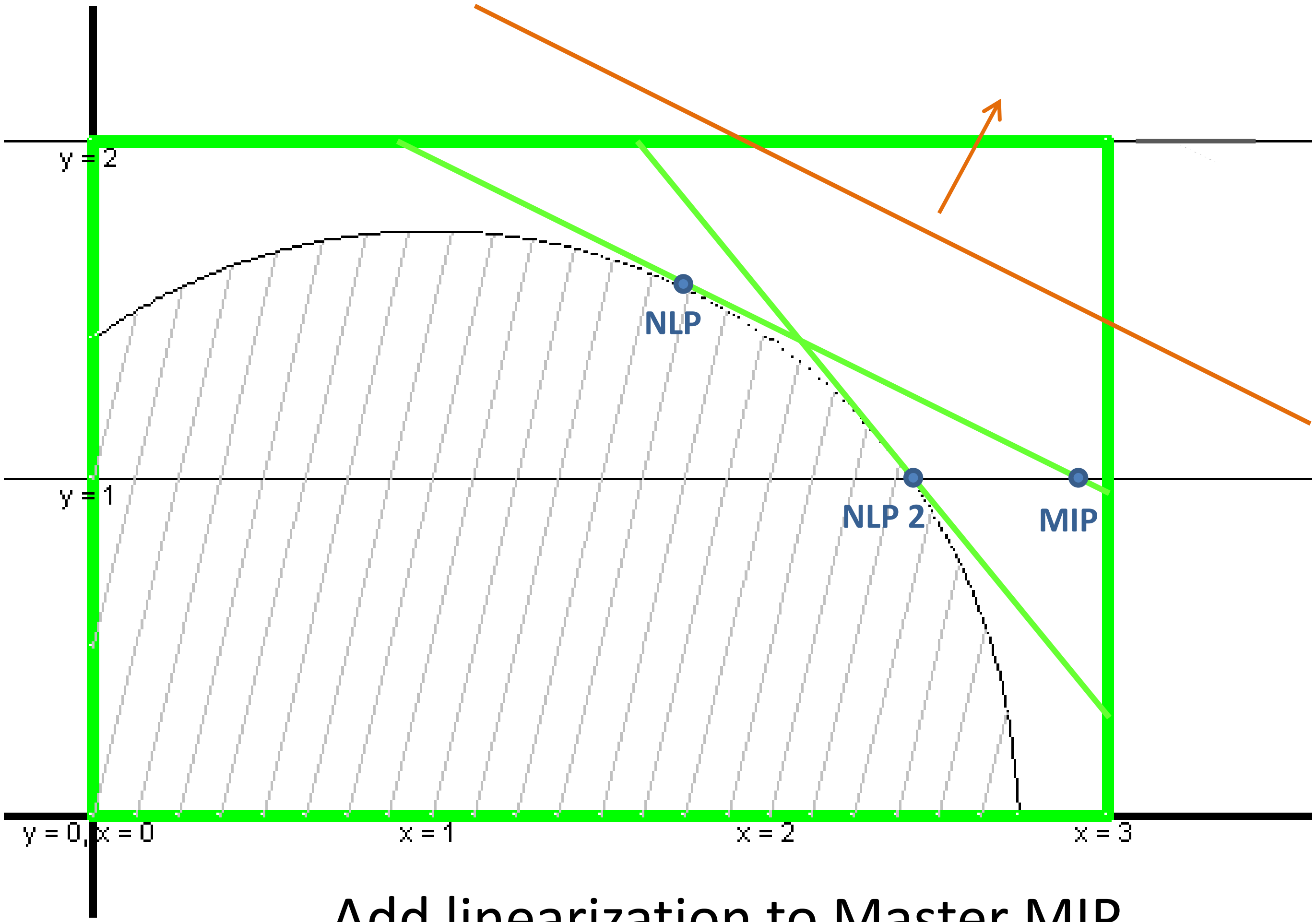
Solve Master MIP

Outer Approximation: Example



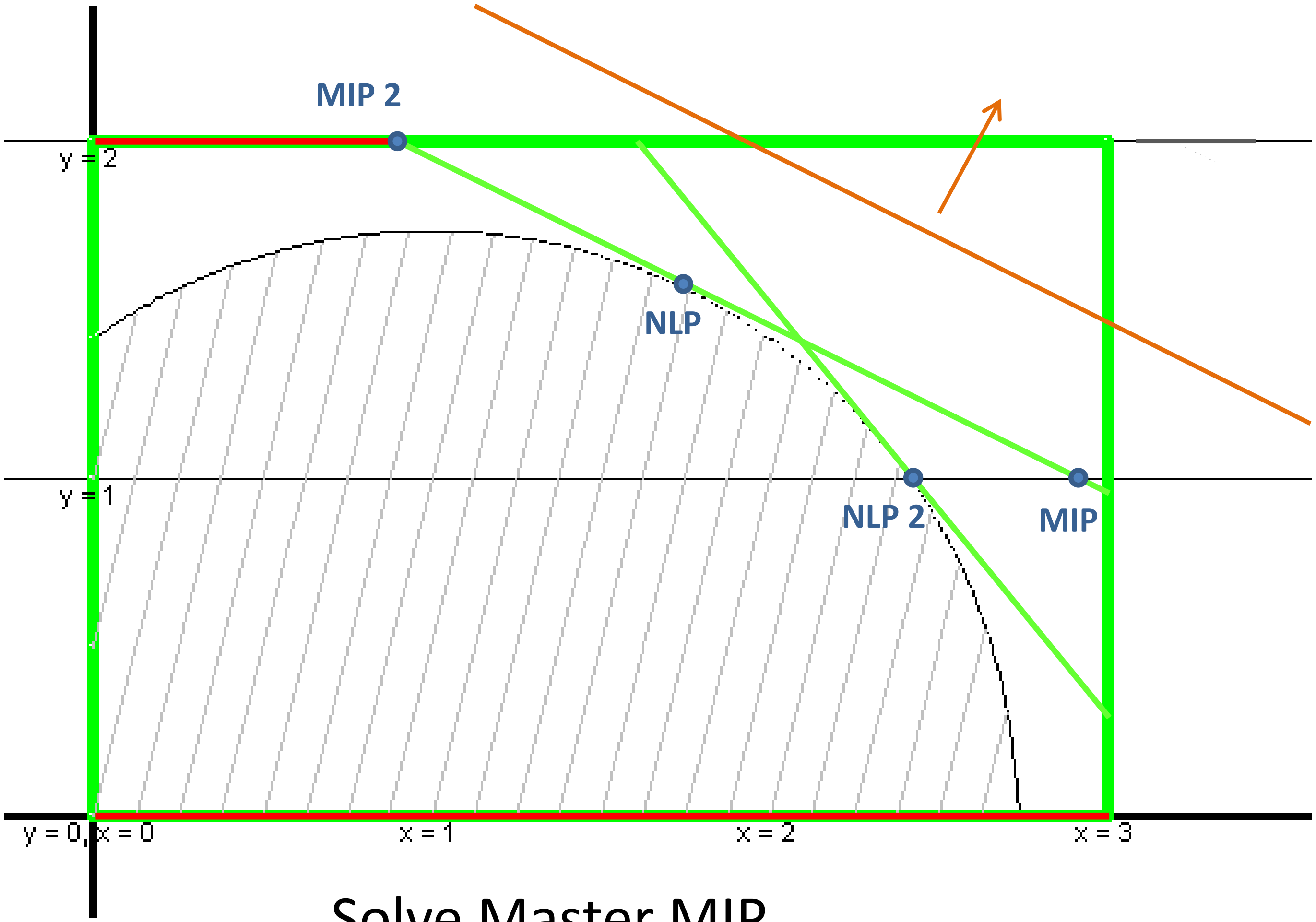
Fix y = 1 and solve NLP

Outer Approximation: Example



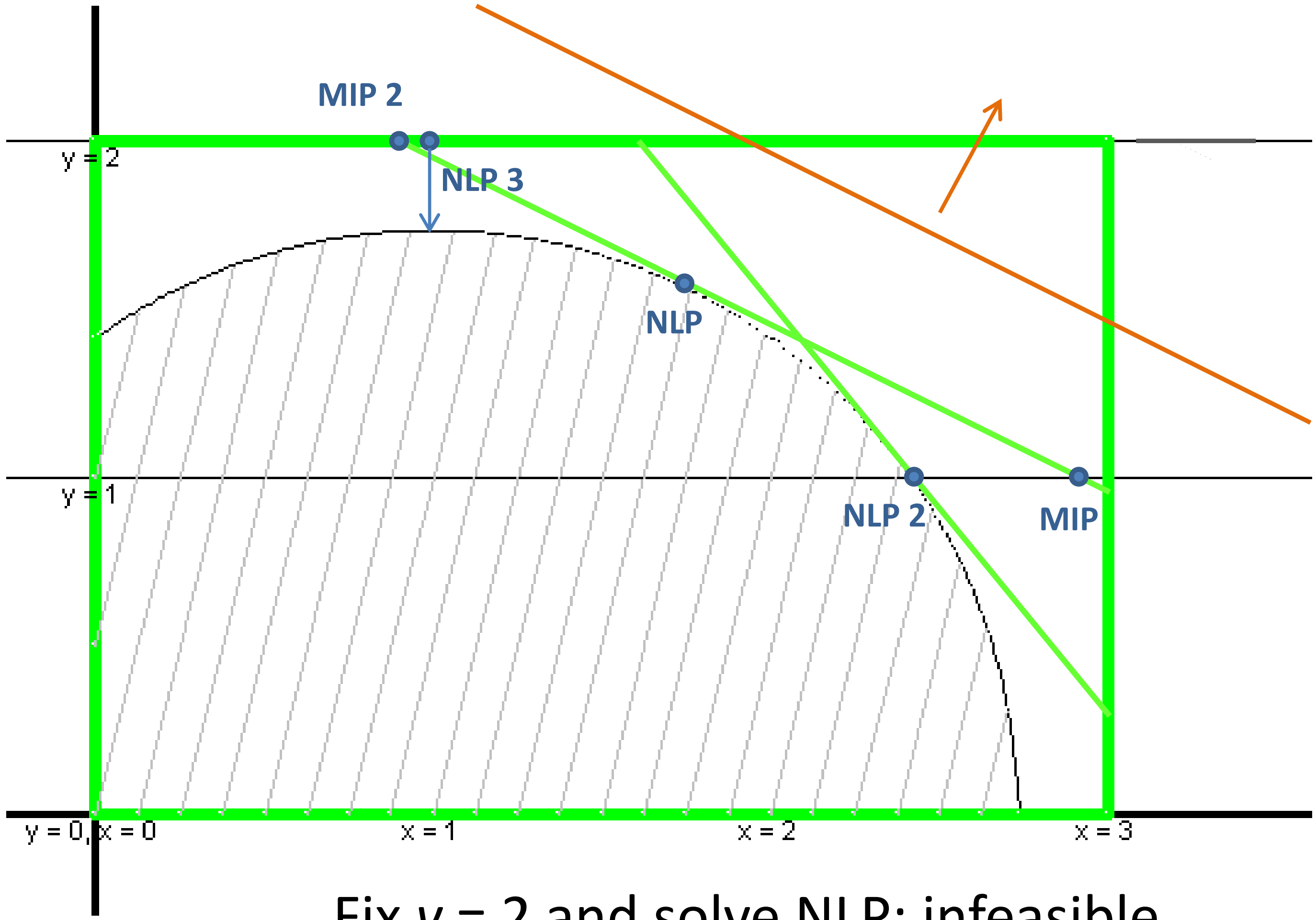
Add linearization to Master MIP

Outer Approximation: Example



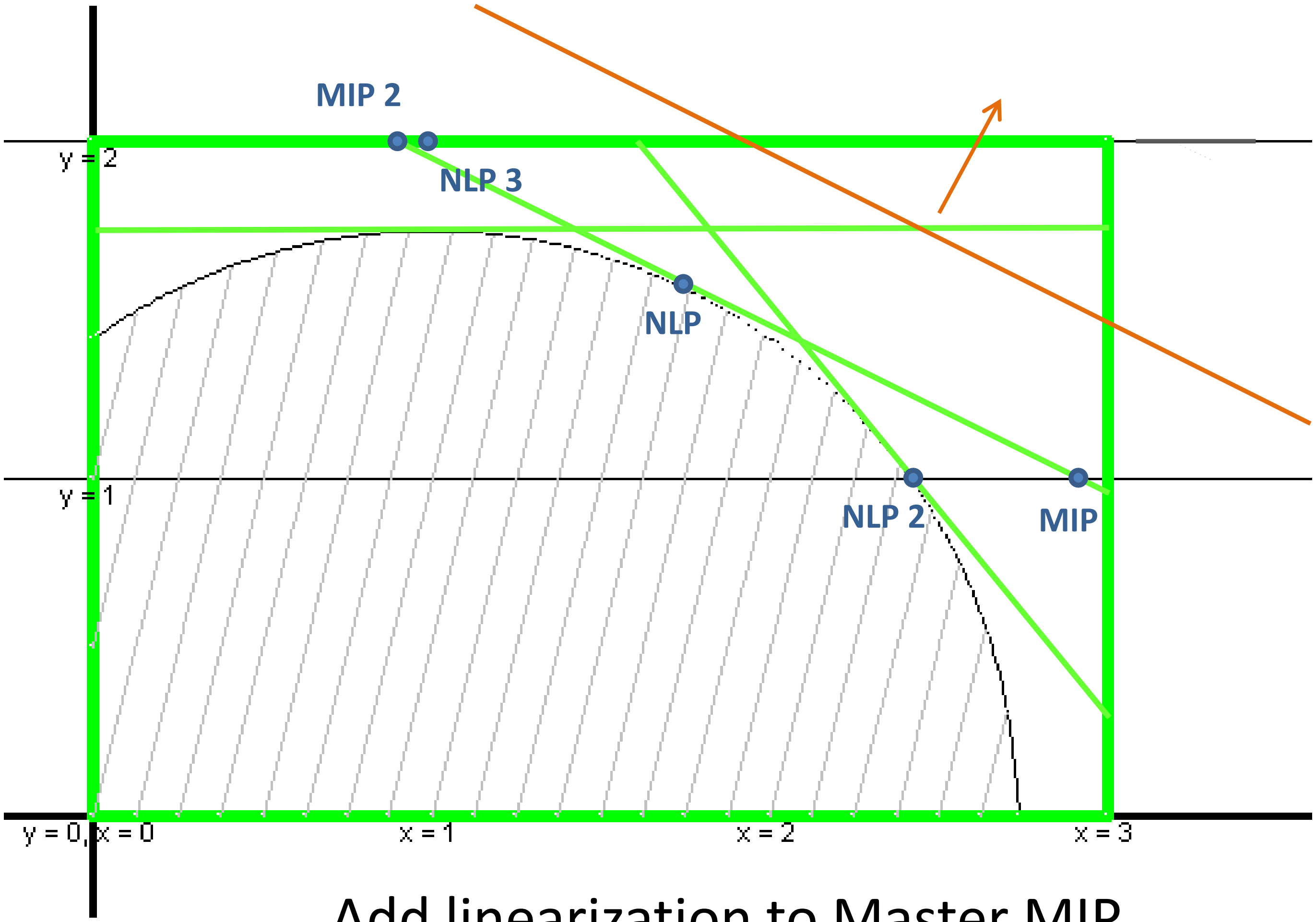
Solve Master MIP

Outer Approximation: Example



Fix *y* = 2 and solve NLP: infeasible

Outer Approximation: Example



Add linearization to Master MIP

Global MINLP: subproblem solvers

Solver	NLP	LP	MIP
BARON	MINOS, SNOPT, IPOPT, CONOPT	CPLEX, XPRESS, CLP	
Couenne	IPOPT	CPLEX, CLP	
GloMIQO	SNOPT, CONOPT		CPLEX
LaGO	IPOPT	CPLEX, CLP	
Lindo API	CONOPT		
Minotaur	IPOPT, FilterSQP	CLP	
SCIP	IPOPT	CPLEX	

Local MINLP: subproblem solvers

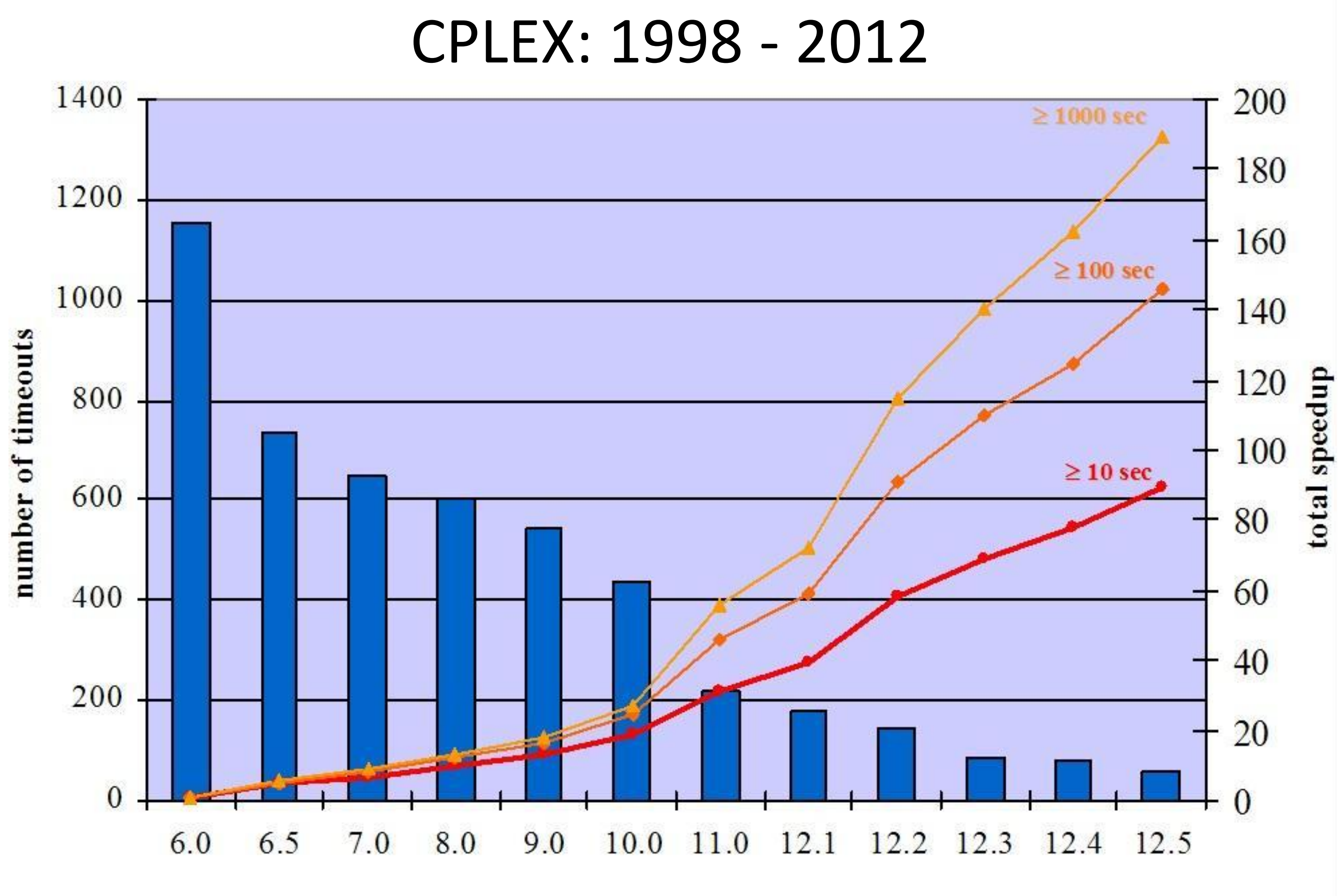
Solver	NLP	MIP
AlphaECP	CONOPT, SNOPT, Knitro, etc	CPLEX, GUROBI, etc
AOA/COA	CONOPT, SNOPT, Knitro, etc	CPLEX, GUROBI, etc
BONMIN	IPOPT	CPLEX, CBC
DICOPT	CONOPT, SNOPT, Knitro, etc	CPLEX, GUROBI, etc
FilMINT	FilterSQP	MINTO
Knitro	Knitro	
MINLP_BB	FilterSQP	
Minotaur	IPOPT, FilterSQP	CPLEX, CBC
OQNLP	CONOPT, SNOPT, Knitro, etc	
SBB	CONOPT, SNOPT, MINOS	

NLP/LP Performance Improvement

- Local NLP solvers:
  - Many “old” solvers without major updates: CONOPT, SNOPT, MINOS, FilterSQP
  - New solvers that are updated regularly but without much progress: Knitro, IPOPT

- LP solvers:
  - Dual simplex: modest progress since 2004 (1.4x)
  - Bixby: “In practice LP is viewed as a solved problem”

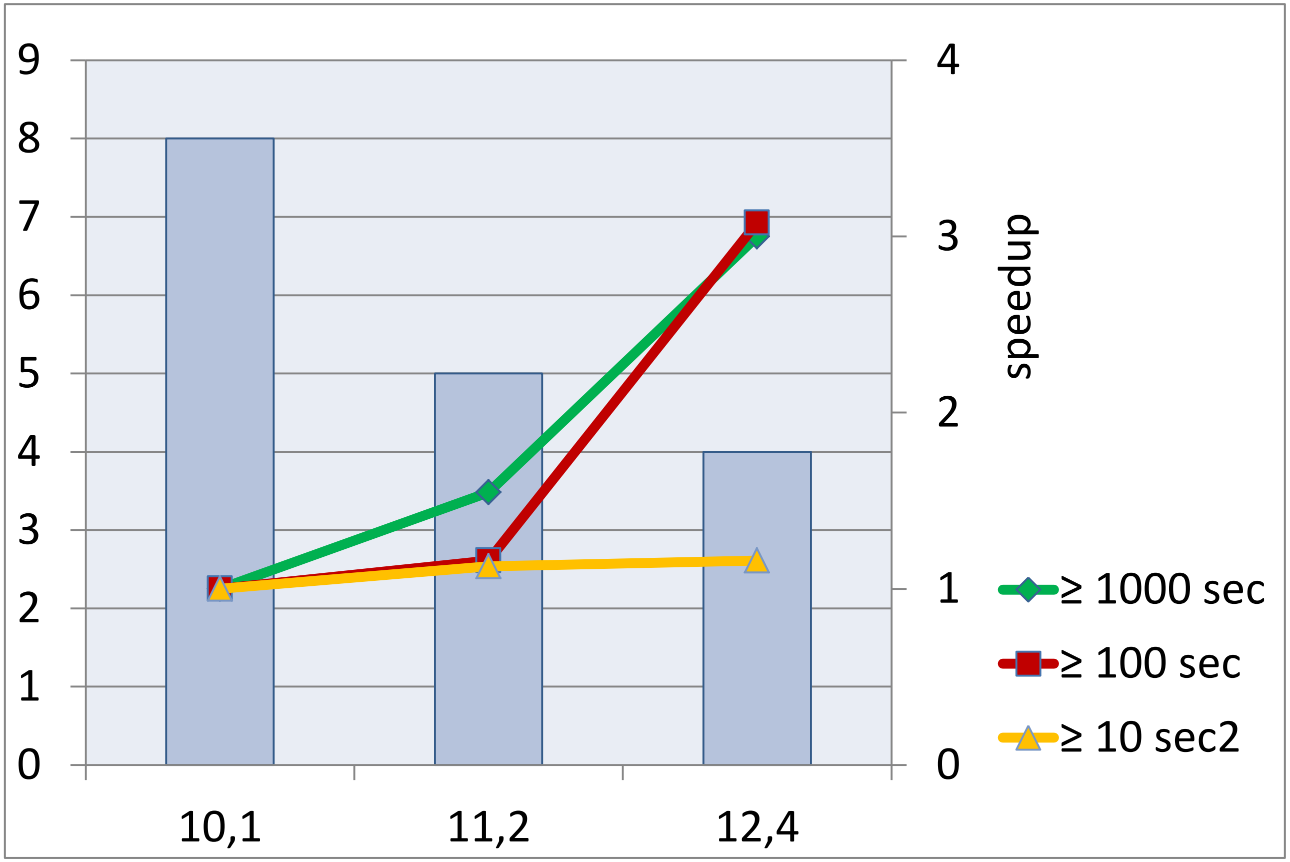
MIP Performance Improvement



Source: Jean-François Puget (IBM)

OA Performance Improvement

Thanks to MIP



Outer Approximation History

- Duran & Grossmann [1986]:
  - Binary variables
  - Convex functions
  - Optimal solution after final number of steps
- Viswanathan & Grossmann [1990]:
  - Integer variables
  - Nonconvex functions

BONMIN, AOA, DICOPT, Minotaur

- Quesada & Grossmann [1992]:
  - Use one branch-and-bound tree (convex)

BONMIN, FilMINT, Minotaur, COA

- Leyffer [2001]:
  - Quadratic Outer Approximation

Results AOA - COA

Problem	AOA	COA
BatchS151208M	17	6
BatchS201210M	41	6
CLay0205H	17	5
CLay0305H	31	8
FLay04H	33	2
FLay05H	> 3hr	172
fo7_2	54	11
fo9	1161	5183
netmod_dol2	388	63
netmod_kar1	142	5
no7_ar3_1	142	265

Problem	AOA	COA
o7	4494	629
o7_ar4_1	2923	643
RSyn0840M04H	7	8
RSyn0840M04M	33	15
SLay08H	63	5
SLay09M	48	5
SLay10H	> 3hr	505
Syn40M04H	2	2
trimloss4	356	17
Water0303	13	5
Water0303R	22	12

Results COA: 1 versus 4 Threads

Problem	1 thr	4 thr
CLay0305H	8	3
FLay05H	172	62
fo7_2	11	5
fo9	5183	937
netmod_dol2	63	22
no7_ar3_1	265	33
o7	629	323

Problem	1 thr	4 thr
o7_ar4_1	643	432
RSyn0840M04H	8	8
RSyn0840M04M	15	7
SLay09H	17	24
SLay10H	505	191
trimloss4	17	13
Water0303R	12	13

Preprocessing Techniques

- Delete redundant constraints & fixed variables

- Bounds Tightening
  - Variable *x*: range [0,inf) → range [10,55]
  - Linear / nonlinear constraints
  - Feasibility based / optimality based

- Linearize nonlinear constraints

- Improving coefficients

Feasibility Based Bound Tightening

Constraint:

$$L \leq x + f(y_1,\ldots,y_n) \leq U$$

Assume for some l_f and u_f:

$$l_f \leq f(y_1,\ldots,y_n) \leq u_f$$

Then:

$$x \geq L - u_f$$

$$x \leq U - l_f$$

FBBT: Example

x: range [10,100]

y: range [5,8]

z: range [1,2]

Constraint: $x + 4\,y - 2\,z^3 = 60$

$$x = 60 - 4\,y + 2\,z^3 \leq 60 - 20 + 16 = 56$$

$$x = 60 - 4\,y + 2\,z^3 \geq 60 - 32 + 2 = 30$$

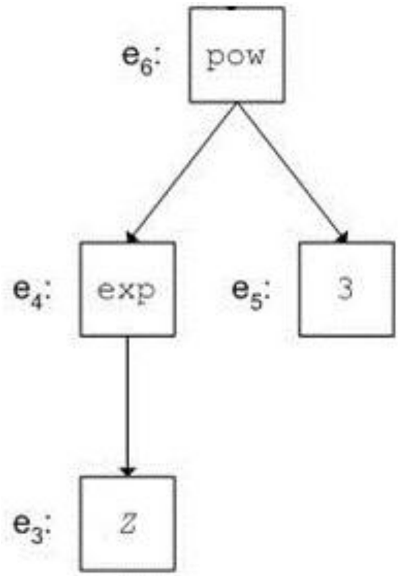
→ x: range [30,56]

FBBT: Expression Tree

$(e^z)^3 \in$ [0,8]

tighten bounds variables

$e^z \in$ [0,2]

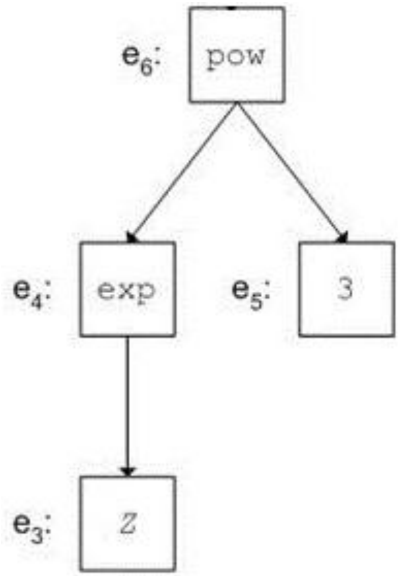


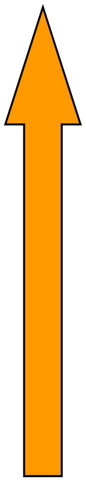
$z \in$ (−inf,ln(2)]

FBBT: Expression Tree

$(e^z)^3 \in [8,64]$

$e^z \in [2,4]$

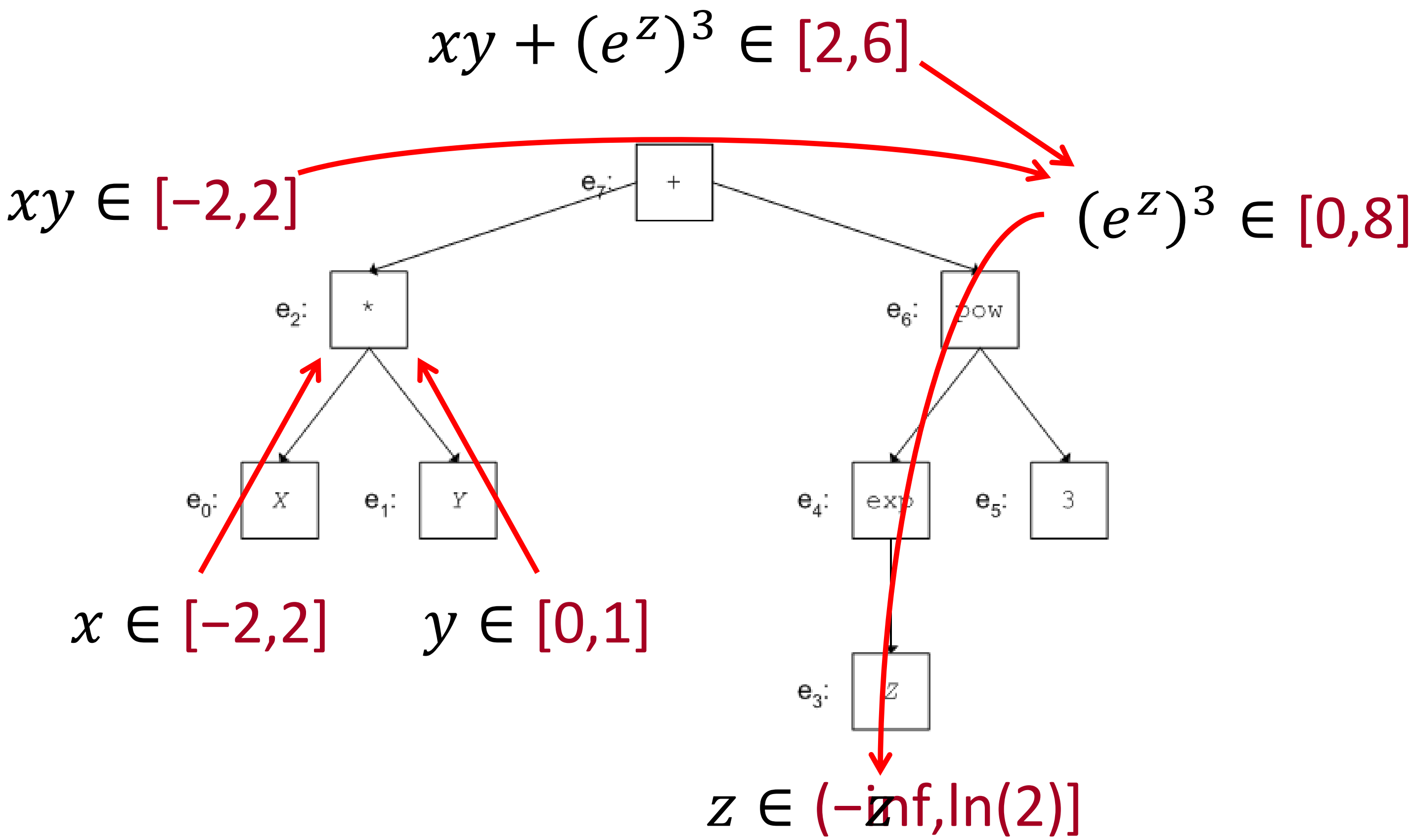




tighten bounds expression

$z \in [\ln(2), \ln(4)]$

FBBT: Binary Operator



Optimality Based Bound Tightening

$$\begin{array}{lll} \text{minimize} & f(x,y) & \\ \text{subject to} & g_j(x,y) \leq 0 & j \in J \\ & Ax + By \leq b & \\ & x \ \text{continuous} & \\ & y \ \text{integer} & \end{array}$$

Lower bound on x_i:

$$\begin{array}{ll} \text{minimize} & x_i \\ \text{subject to} & Ax + By \leq b \\ & x \ \text{continuous} \\ & y \ \text{integer} \end{array}$$

Optimality Based Bound Tightening

$$
\begin{array}{lll}
\text{minimize} & f(x,y) & \\
\text{subject to} & g_j(x,y) \leq 0 & j \in J \\
 & Ax + By \leq b & \\
 & x \;\; \text{continuous} & \\
 & y \;\; \text{integer} &
\end{array}
$$

Upper bound on x_i:

$$
\begin{array}{ll}
\text{maximize} & x_i \\
\text{subject to} & Ax + By \leq b \\
 & x \;\; \text{continuous} \\
 & y \;\; \text{integer}
\end{array}
$$

Linearize constraints

Constraint

$$(1 - x_t)\, y_t \leq y_{t-1}$$

with

$$x_t \text{ binary},\ \ y_t \in [0,100]$$

$x_t = 1 \rightarrow y_{t-1} \geq 0$

$x_t = 0 \rightarrow y_t \leq y_{t-1}$

$$y_t \leq y_{t-1} + 100\, x_t$$

Linearize constraints (cont'd)

Constraint

$$z_t + u_t \geq x_t y_t$$

with

$$x_t \text{ binary}, \;\; y_t \in [20{,}100], \;\; z_t \text{ free}, \;\; u_t \text{ free}$$

$x_t = 1 \;\rightarrow\; z_t + u_t \geq y_t$

$x_t = 0 \;\rightarrow\; z_t + u_t \geq 0$

$$z_t + u_t \geq y_t + 100\,(x_t - 1)$$
$$z_t + u_t \geq 20\,x_t$$

Linearize constraints – Trade off

Term

$x_i\, x_j$

with

x_i binary

↓

$y_{ij} \leq x_i$
$y_{ij} \leq x_j$
$x_i + x_j - y_{ij} \leq 1$
$0 \leq y_{ij} \leq 1$

Improving Coefficients

$y + 12\,x \leq 20$

x binary

$0 \leq y \leq 14$

$y + 6\,x \leq 14$

x binary

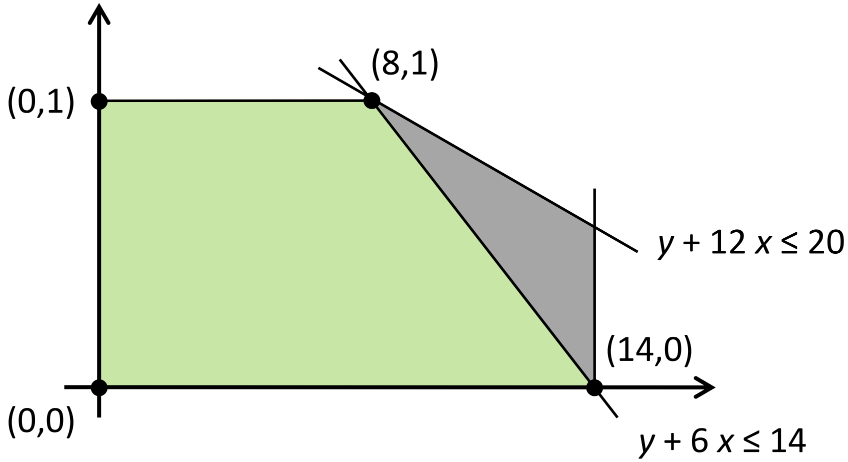
$0 \leq y \leq 14$

$x = 0 \rightarrow y \leq 20$ loose

$x = 1 \rightarrow y \leq 8$ tight

$x = 0 \rightarrow y \leq 14$ tight

$x = 1 \rightarrow y \leq 8$ tight



Improving Coefficients: Nonlinear

$$g(y_1,\dots,y_k) + Mx \le b$$
$$x \text{ binary}$$

If we have an upper bound g^u on g such that $g^u < b$ then reformulate

$$g(y_1,\dots,y_k) + (M - b + g^u)\,x \le g^u$$
$$x \text{ binary}$$

Improving Coefficients: Probing

$$g(y_1,\ldots,y_k) + Mx \le b$$

$$x \text{ binary}$$

$$y \ge 0$$

$$y_i \le m_i\, x \qquad\qquad i = 1,\ldots,k$$

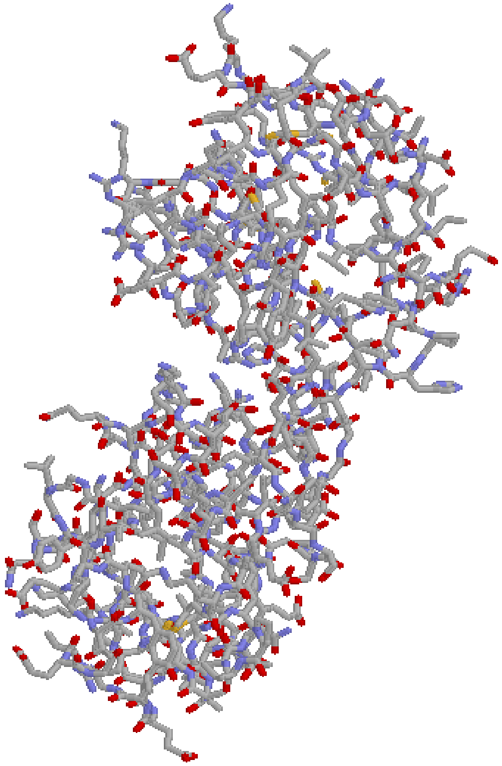
$x = 0 \rightarrow y_1 = \ldots = y_k = 0$ (implication)

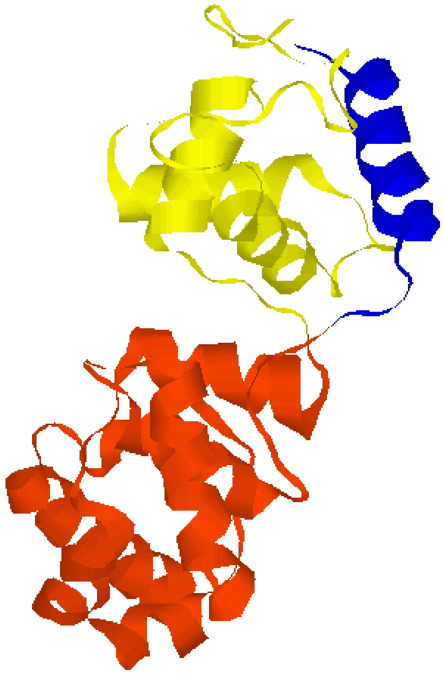
If $g(0,\ldots,0) < b \rightarrow$ tighten

Conclusions

- MINLP gets more important
- Challenging problems
- Recent developments focus on:
  - Convexification in Global Optimization
  - Preprocessing
  - Heuristics

Protein Folding





$$\frac{c(D1{:}D2)}{|D1||D2|}$$

Protein Folding