

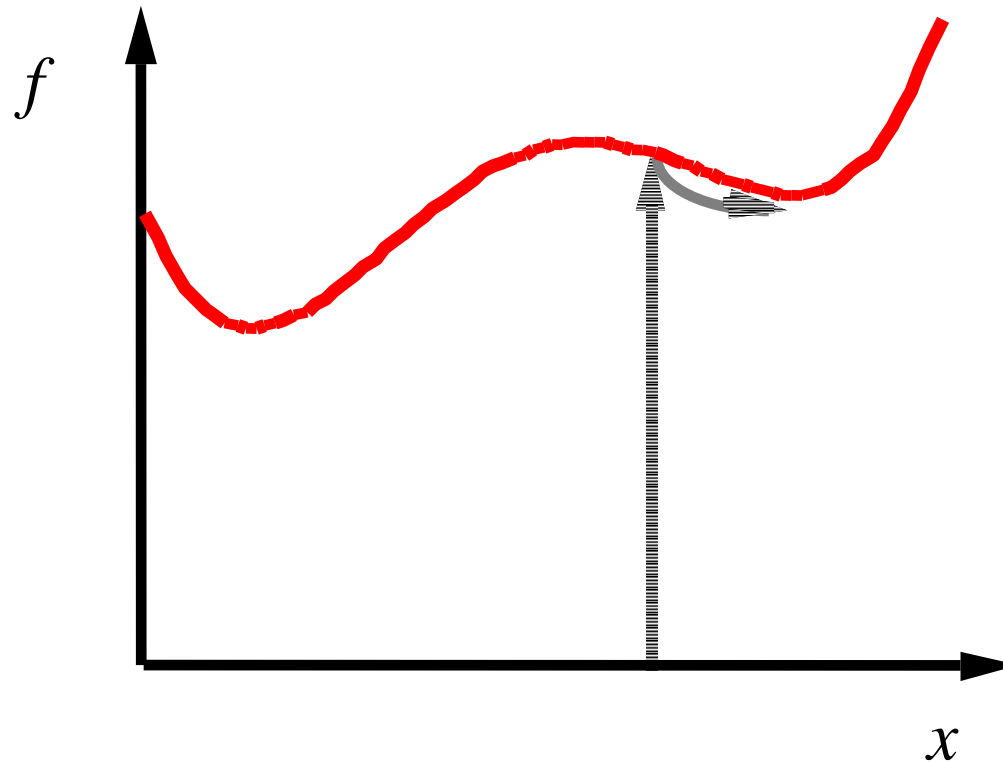
# GLOBAL OPTIMIZATION WITH BRANCH-AND-REDUCE



**Nick Sahinidis**  
Department of Chemical Engineering  
Carnegie Mellon University  
[sahinidis@cmu.edu](mailto:sahinidis@cmu.edu)

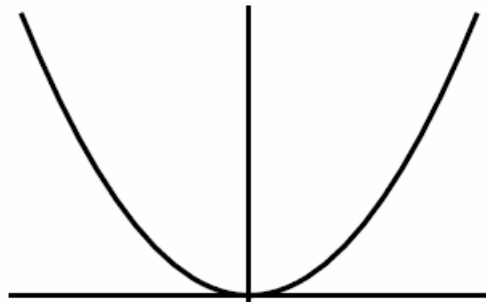
EWO seminar, 23 October 2007

# THE MULTIPLE-MINIMA DIFFICULTY IN OPTIMIZATION

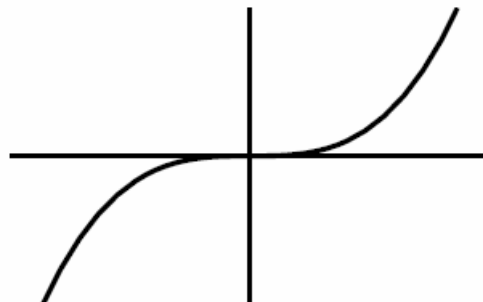


- **Classical optimality conditions are necessary but not sufficient**
- **Classical optimization provides the local minimum “closest” to the starting point used**

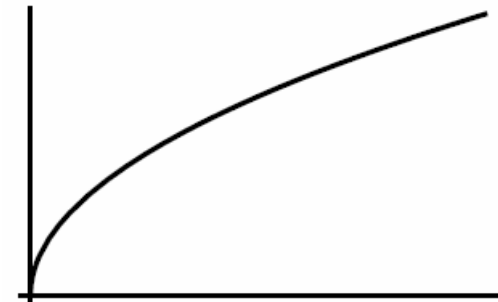
# COMMON FUNCTIONS IN MODELING



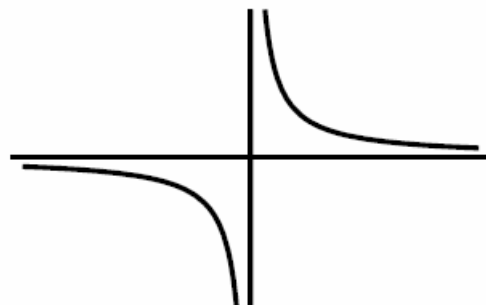
$$x^2$$



$$x^3$$



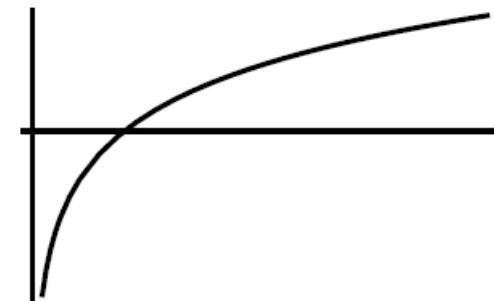
$$\sqrt{x}$$



$$\frac{1}{x}$$

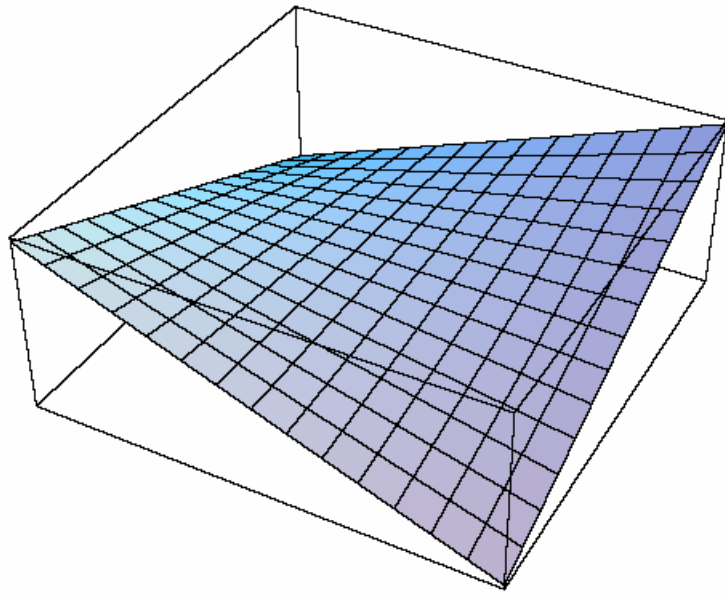


$$\exp(x)$$

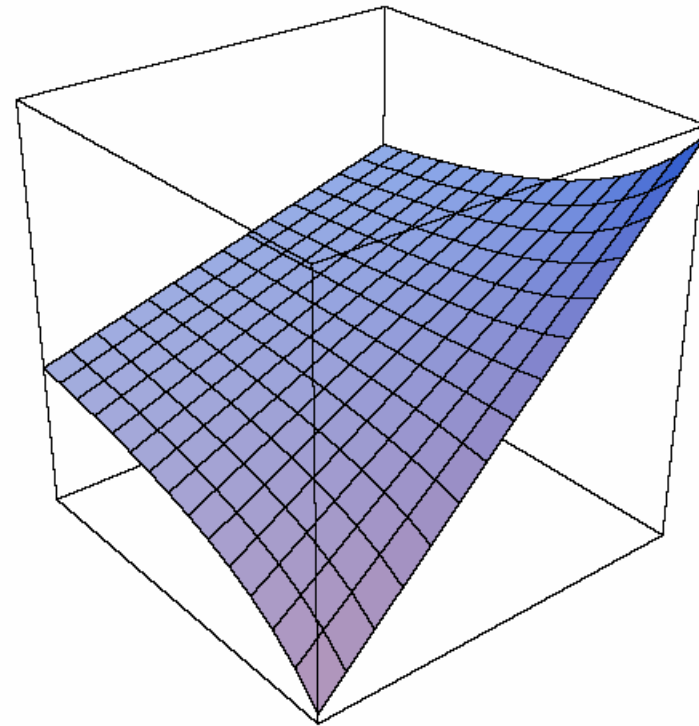


$$\log(x)$$

# COMMON FUNCTIONS IN MODELING



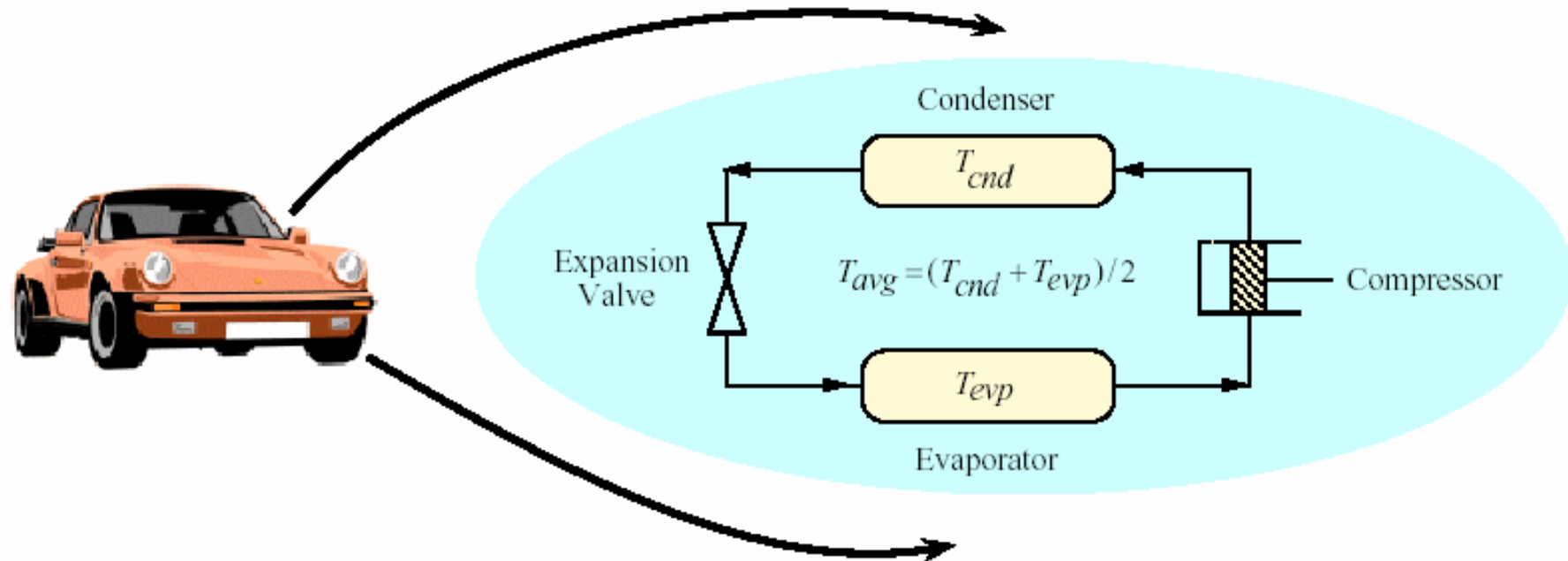
$$x_1 * x_2$$



$$\frac{x_1}{x_2}$$

# AUTOMOTIVE REFRIGERANT DESIGN

## (Joback and Stephanopoulos, 1990)



- Higher enthalpy of vaporization ( $\Delta H_{ve}$ ) reduces the amount of refrigerant
- Lower liquid heat capacity ( $C_{pla}$ ) reduces amount of vapor generated in expansion valve
- Maximize  $\Delta H_{ve} / C_{pla}$ , subject to:  $\Delta H_{ve} \geq 18.4$ ,  $C_{pla} \leq 32.2$

# FUNCTIONAL GROUPS CONSIDERED

Acyclic Groups	Cyclic Groups	Halogen Groups	Oxygen Groups	Nitrogen Groups	Sulfur Groups
$-\text{CH}_3$	$^r-\text{CH}_2-^r$	$-\text{F}$	$-\text{OH}$	$-\text{NH}_2$	$-\text{SH}$
$-\text{CH}_2-$	$^r_r > \text{CH}-^r$	$-\text{Cl}$	$-\text{O}-$	$> \text{NH}$	$-\text{S}-$
$> \text{CH}-$	$^r_r > \text{CH}-^r$	$-\text{Br}$	$^r-\text{O}-^r$	$^r_r > \text{NH}$	$^r-\text{S}-^r$
$> \text{C} <$	$^r_r > \text{C} <^r_r$	$-\text{I}$	$> \text{CO}$	$> \text{N}-$	
$= \text{CH}_2$	$^r_r > \text{C} <^r_r$		$^r_r > \text{CO}$	$= \text{N}-$	
$= \text{CH}-$	$> \text{C} <^r_r$		$-\text{CHO}$	$^r = \text{N}-^r$	
$= \text{C} <$	$^r = \text{CH}-^r$		$-\text{COOH}$	$-\text{CN}$	
$= \text{C} =$	$^r = \text{C} <^r_r$		$-\text{COO}-$	$-\text{NO}_2$	
$\equiv \text{CH}$	$^r = \text{C} <_r$		$= \text{O}$		
$\equiv \text{C}-$	$= \text{C} <^r_r$				

Number of Groups = 44

Maximum Selection Size = 15

Candidates = 39, 895, 566, 894, 524

# PROPERTY PREDICTION

$$T_b = 198.2 + \sum_{i=1}^N n_i T_{bi}$$

$$T_c = \frac{T_b}{0.584 + 0.965 \sum_{i=1}^N n_i T_{ci} - (\sum_{i=1}^N n_i T_{ci})^2}$$

$$P_c = \frac{1}{(0.113 + 0.0032 \sum_{i=1}^N n_i a_i - \sum_{i=1}^N n_i P_{ci})^2}$$

$$C_{p0a} = \sum_{i=1}^N n_i C_{p0ai} - 37.93 + \left( \sum_{i=1}^N n_i C_{p0bi} + 0.21 \right) T_{avg} \\ + \left( \sum_{i=1}^N n_i C_{p0ci} - 3.91 \times 10^{-4} \right) T_{avg}^2 \\ + \left( \sum_{i=1}^N n_i C_{p0di} + 2.06 \times 10^{-7} \right) T_{avg}^3$$

$$T_{br} = \frac{T_b}{T_c}$$

$$T_{avgr} = \frac{T_{avg}}{T_c}$$

$$T_{cndr} = \frac{T_{cnd}}{T_c}$$

$$T_{evpr} = \frac{T_{evp}}{T_c}$$

$$\alpha = -5.97214 - \ln \left( \frac{P_c}{1.013} \right) + \frac{6.09648}{T_{br}} + 1.28862 \ln(T_{br})$$

$$-0.169347 T_{br}^6$$

$$\beta = 15.2518 - \frac{15.6875}{T_{br}} - 13.4721 \ln(T_{br}) + 0.43577 T_{br}^6$$

$$\omega = \frac{\alpha}{\beta}$$

$$C_{pla} = \frac{1}{4.1868} \left\{ C_{p0a} + 8.314 \left[ 1.45 + \frac{0.45}{1 - T_{avgr}} + 0.25 \omega \right. \right. \\ \left. \left. \left( 17.11 + 25.2 \frac{(1 - T_{avgr})^{1/3}}{T_{avgr}} + \frac{1.742}{1 - T_{avgr}} \right) \right] \right\}$$

$$\Delta H_{vb} = 15.3 + \sum_{i=1}^N n_i \Delta H_{vbi}$$

$$\Delta H_{ve} = \Delta H_{vb} \left( \frac{1 - T_{evp}/T_c}{1 - T_b/T_c} \right)^{0.38}$$

$$h = \frac{T_{br} \ln(P_c/1.013)}{1 - T_{br}}$$

$$G = 0.4835 + 0.4605h$$

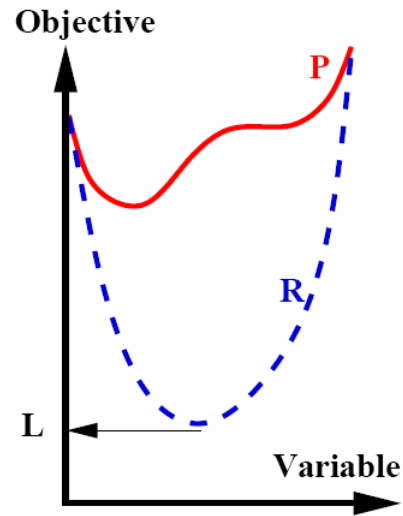
$$k = \frac{h/G - (1 + T_{br})}{(3 + T_{br})(1 - T_{br})^2}$$

$$\ln P_{vpcr} = \frac{-G}{T_{cndr}} \left[ 1 - T_{cndr}^2 + k(3 + T_{cndr})(1 - T_{cndr})^3 \right]$$

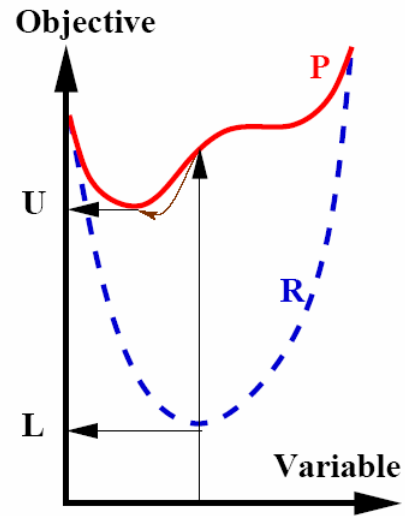
$$\ln P_{vper} = \frac{-G}{T_{evpr}} \left[ 1 - T_{evpr}^2 + k(3 + T_{evpr})(1 - T_{evpr})^3 \right]$$

$n_i$  integer

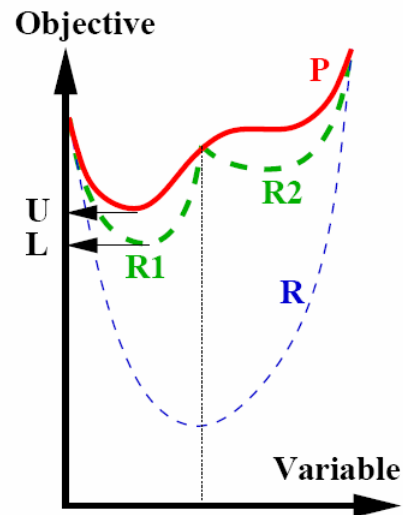
# BRANCH-AND-BOUND



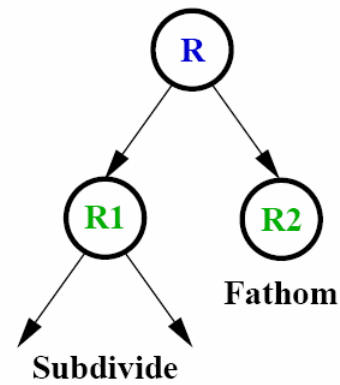
a. Lower Bounding



b. Upper Bounding



c. Domain Subdivision



d. Search Tree

# MOLECULAR DESIGN AFTER 150 CPU HOURS IN 1995

- One feasible solution identified
  - Optimality not proved
- 
- **First attempt:**
    - IBM RS/6000 43P with 128 MB RAM
  - **Second attempt:**
    - IBM SP/2 Single Processor with **2 GB RAM**

# MOLECULAR DESIGN IN 2000

	Molecular Structure	$\frac{\Delta H_{ve}}{C_{pla}}$
FNO	F – N = O	1.2880
FSH	F – SH	1.1697
CH <sub>3</sub> Cl	CH <sub>3</sub> – Cl	1.1219
CIFO	(Cl–)(–O–)(–F)	0.9822
C <sub>2</sub> HClO <sub>2</sub>	O = C < (–CH = O)(–Cl)	1.1207
C <sub>3</sub> H <sub>4</sub> O	CH <sub>3</sub> – CH = C = O	0.9619
C <sub>3</sub> H <sub>4</sub>	CH <sub>3</sub> – C ≡ CH	0.9278
C <sub>2</sub> F <sub>2</sub>	F – C ≡ C – F	0.9229
CH <sub>2</sub> ClF	F – CH <sub>2</sub> – Cl	0.9202
C <sub>2</sub> HO <sub>2</sub> F	F – O – CH = C = O	0.8705
C <sub>3</sub> H <sub>4</sub>	CH <sub>2</sub> = C = CH <sub>2</sub>	0.8656
C <sub>2</sub> H <sub>6</sub>	CH <sub>3</sub> – CH <sub>3</sub>	0.8632
C <sub>3</sub> H <sub>3</sub> FO	(F–)(CH <sub>3</sub> –) > C = C = O	0.8531
NHF <sub>2</sub>	F – NH – F	0.8468
C <sub>2</sub> HOF	CH ≡ C – O – F	0.8263

	Molecular Structure	$\frac{\Delta H_{ve}}{C_{pla}}$
C <sub>3</sub> H <sub>3</sub> F	CH ≡ C – CH <sub>2</sub> – F	0.7802
CHF <sub>2</sub> Cl	(F–)(F–) > CH – Cl	0.7770
C <sub>2</sub> H <sub>3</sub> OF	CH <sub>2</sub> = CH – O – F	0.7685
NF <sub>2</sub> Cl	(F–)(F–) > N – Cl	0.7658
C <sub>2</sub> H <sub>6</sub> NF	(CH <sub>3</sub> –)(CH <sub>3</sub> –) > N – F	0.6817
N <sub>2</sub> HF <sub>3</sub>	(F–)(F–) > N – NH – F	0.6711
C <sub>2</sub> H <sub>2</sub> OF <sub>2</sub>	CH <sub>2</sub> = C < (–O – F)(–F)	0.6705
C <sub>3</sub> H <sub>2</sub> F <sub>2</sub>	(F–)(F–) > CH – C ≡ CH	0.6686
C <sub>2</sub> HNF <sub>2</sub>	CH ≡ C – N < (–F)(–F)	0.6587
C <sub>3</sub> H <sub>4</sub> F <sub>2</sub>	(F–)(F – CH <sub>2</sub> –) > C = CH <sub>2</sub>	0.6377
C <sub>3</sub> H <sub>4</sub> F <sub>2</sub>	(F–)(F–) > CH – CH = CH <sub>2</sub>	0.6263
C <sub>2</sub> H <sub>3</sub> NF <sub>2</sub>	CH <sub>2</sub> = CH – N < (–F)(–F)	0.6176
CH <sub>3</sub> NOF <sub>2</sub>	(F–)(CH <sub>3</sub> –) > N – O – F	0.6139
C <sub>3</sub> H <sub>3</sub> F <sub>3</sub>	(r > CH– 'r) <sub>3</sub> (–F) <sub>3</sub>	0.5977

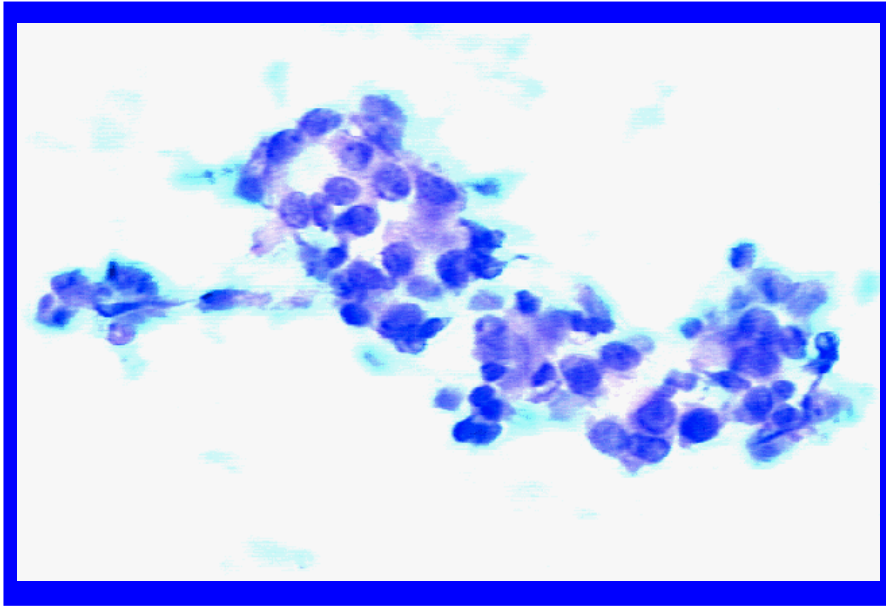
For CCl<sub>2</sub>F<sub>2</sub>,  $\Delta H_{ve}/C_{pla} \approx 0.57$

In 30 CPU minutes

# BREAST CANCER DIAGNOSIS

- **200,000 cases diagnosed in the U.S. a year**
- **40,000 deaths a year**
  
- **Most breast cancers are first diagnosed by the patient as a lump in the breast**
- **Majority of breast lumps are benign**
  
- **Available diagnosis methods:**
  - **Mammography (68% to 79% correct)**
  - **Surgical biopsy (100% correct but invasive and costly)**
  - **Fine needle aspirate (FNA)**
    - » **With visual inspection: 65% to 98% correct**
    - » **Automated diagnosis: 95% correct**
      - **Linear programming techniques**
      - **Mangasarian and Wolberg in 1990s**

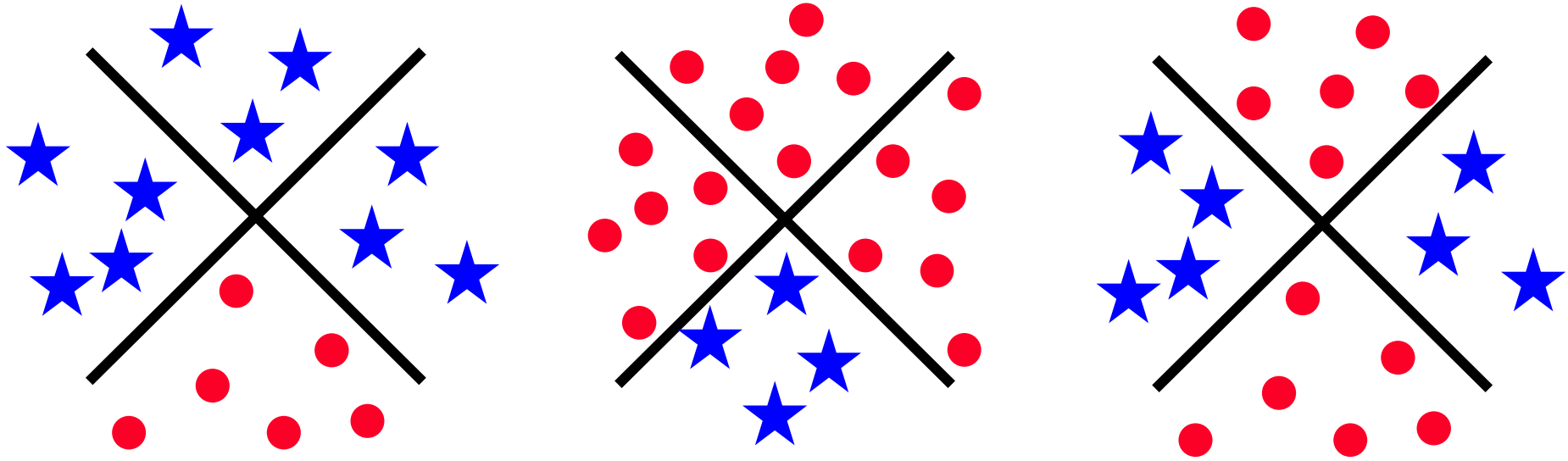
# WISCONSIN DIAGNOSTIC BREAST CANCER (WDBC) DATABASE



From Wolberg, Street, & Mangasarian, 1993

- **653 patients**
- **9 cytological characteristics:**
  - Clump thickness
  - Uniformity of cell size
  - Uniformity of cell shape
  - Marginal adhesion
  - Single epithelial cell size
  - Bare nuclei
  - Bland chromatin
  - Normal nucleoli
  - Mitoses
- **Biopsy classified these 653 patients in two classes:**
  - Benign
  - Malignant

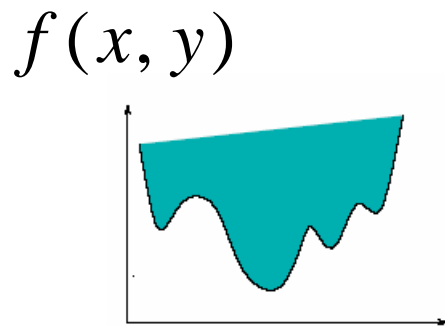
# BILINEAR (IN-)SEPARABILITY OF TWO SETS IN $R^n$



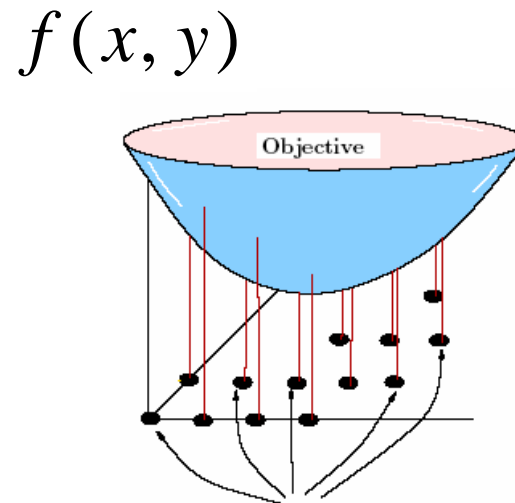
**Requires the solution of three nonconvex bilinear programs**

# CHALLENGES IN GLOBAL OPTIMIZATION

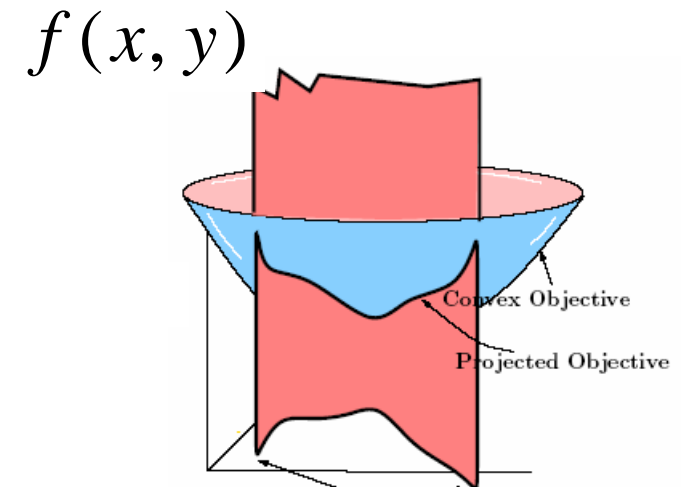
$$\begin{aligned} \min \quad & f(x, y) \\ \text{s.t.} \quad & g(x, y) \leq 0 \\ & x \in R^n, \quad y \in Z^p \end{aligned}$$



Multimodal objective



Integrality conditions



Nonconvex constraints

## NP-HARD PROBLEM

# GLOBAL OPTIMIZATION ALGORITHMS

- **Stochastic and deterministic algorithms**
- **Branch-and-Bound**
  - Bound problem over successively refined partitions
    - » Falk and Soland, 1969
    - » McCormick, 1976
- **Convexification**
  - Outer-approximate with increasingly tighter convex programs
  - Tuy, 1964
  - Serali and Adams, 1994
- **Horst and Tuy, *Global Optimization: Deterministic Approaches*, 1996**
  - Over 800 citations
- **Our approach**
  - **Branch-and-Reduce**
    - » Ryoo and Sahinidis, 1995, 1996
    - » Sheckman and Sahinidis, 1998
  - **Constraint Propagation & Duality-Based Reduction**
    - » Ryoo and Sahinidis, 1995, 1996
    - » Tawarmalani and Sahinidis, 2002
  - **Convexification**
    - » Tawarmalani and Sahinidis, 2001, 2002, 2004, 2005
- **Tawarmalani and Sahinidis, *Convexification and Global Optimization in Continuous and Mixed-Integer Nonlinear Programming*, 2002**

# BOUNDING SEPARABLE PROGRAMS

$$\begin{aligned} \min \quad & f = -x_1 - x_2 \\ \text{s.t.} \quad & x_3^2 - x_1^2 - x_2^2 \leq 8 \\ & x_3 = x_1 + x_2 \\ & 0 \leq x_1 \leq 6 \\ & 0 \leq x_2 \leq 4 \\ & 0 \leq x_3 \leq 10 \end{aligned}$$

# BOUNDING SEPARABLE PROGRAMS

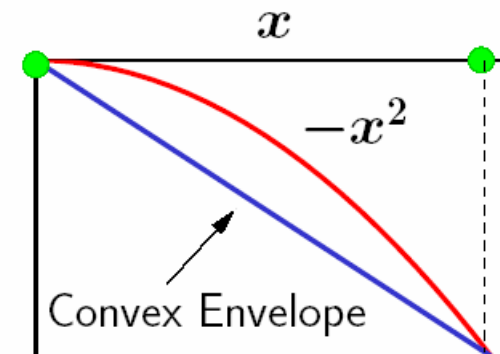
$$\begin{aligned} \min \quad & f = -x_1 - x_2 \\ \text{s.t.} \quad & x_3^2 - x_1^2 - x_2^2 \leq 8 \end{aligned}$$

$$x_3 = x_1 + x_2$$

$$0 \leq x_1 \leq 6$$

$$0 \leq x_2 \leq 4$$

$$0 \leq x_3 \leq 10$$



# BOUNDING FACTORABLE PROGRAMS

Introduce variables for intermediate quantities whose envelopes are not known

$$f(x, y, z, w) = \sqrt{\exp(xy + z \ln w) z^3}$$

$$\begin{array}{c}
 \overbrace{\hspace{10em}}^{f} \\
 \overbrace{\hspace{8em}}^{x_5} \\
 \left( \exp(\underbrace{xy}_{x_1} + \underbrace{z \ln w}_{x_2}) \underbrace{z^3}_{x_6} \right)^{0.5} \\
 \underbrace{\hspace{4em}}_{x_4} \\
 \underbrace{\hspace{10em}}_{x_7}
 \end{array}$$

$$x_1 = xy$$

$$x_2 = \ln(w)$$

$$x_3 = zx_2$$

$$x_4 = x_1 + x_3$$

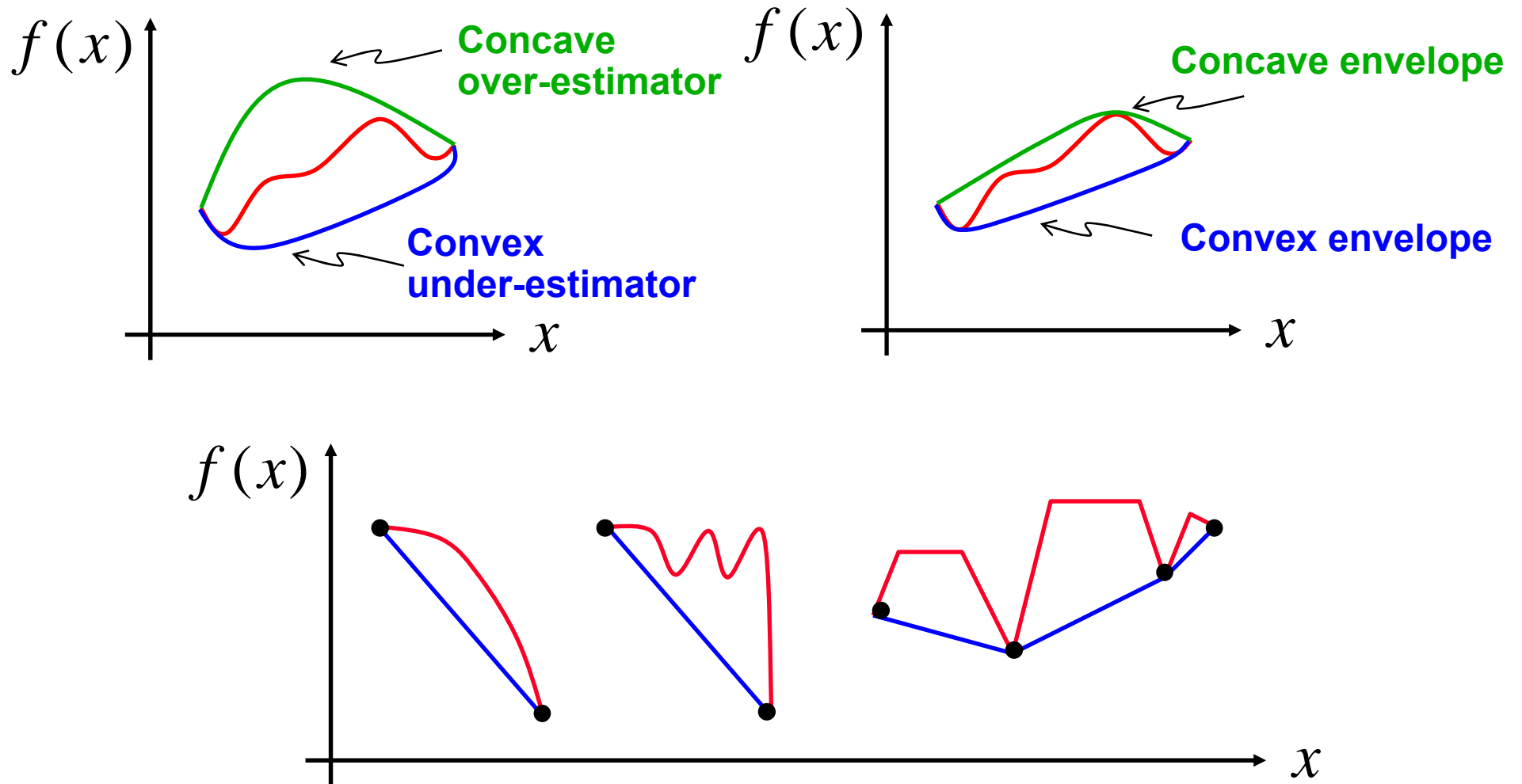
$$x_5 = \exp(x_4)$$

$$x_6 = z^3$$

$$x_7 = x_5 x_6$$

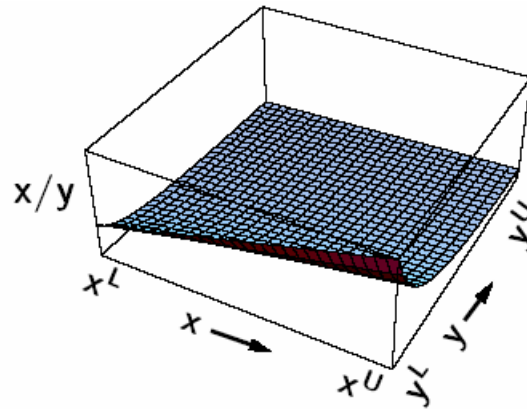
$$f = \sqrt{x_7}$$

# TIGHT RELAXATIONS



**Convex/concave envelopes often finitely generated**

# RATIO: TRADITIONAL RELAXATION



$$z \geq x/y$$

$$y^L \leq y \leq y^U$$

$$x^L \leq x \leq x^U$$

$$z \geq x/y$$

$$x^L \leq x \leq x^U$$

$$y^L \leq y \leq y^U$$

cross-multiplying

$$zy \geq x$$

$$y^L \leq y \leq y^U$$

$$x^L/y^U \leq z \leq x^U/y^L$$

$$x^L \leq x \leq x^U$$

Relaxing

$$z \geq (xy^U - yx^L + x^L y^U)/y^{U^2}$$

$$z \geq (xy^L - yx^U + x^U y^L)/y^{L^2}$$

$$y^L \leq y \leq y^U$$

$$x^L \leq x \leq x^U$$

Simplifying

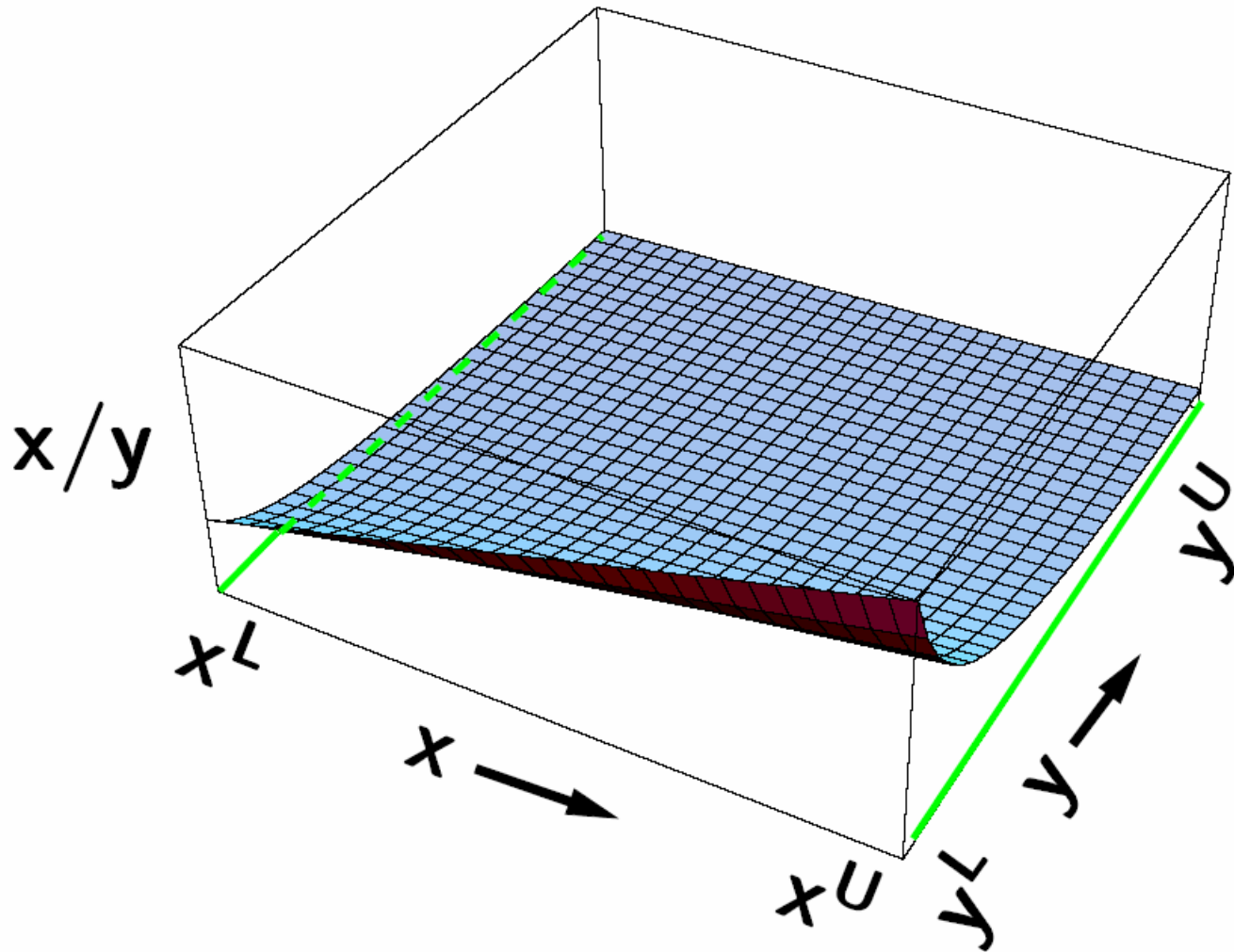
$$zy - (z - x^L/y^U)(y - y^U) \geq x$$

$$zy - (z - x^U/y^L)(y - y^L) \geq x$$

$$y^L \leq y \leq y^U$$

$$x^L \leq x \leq x^U$$

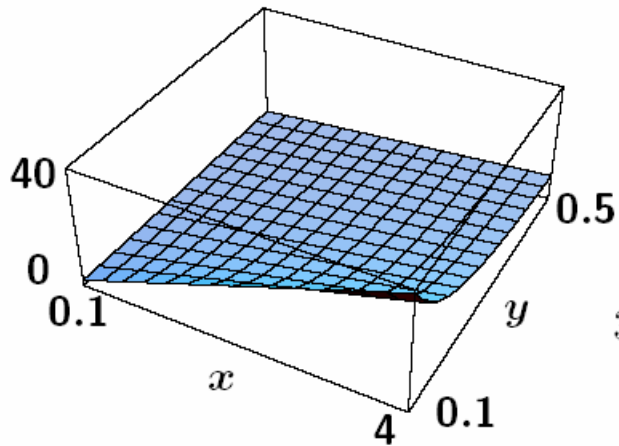
# RATIO: THE GENERATING SET



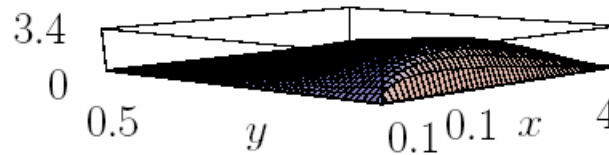
$$G^{\text{epi}}(x/y) = \{(x, y) \mid x \in \{x^L, x^U\}\}$$

# DIFFERENCE BETWEEN ENVELOPE AND TRADITIONAL RELAXATION

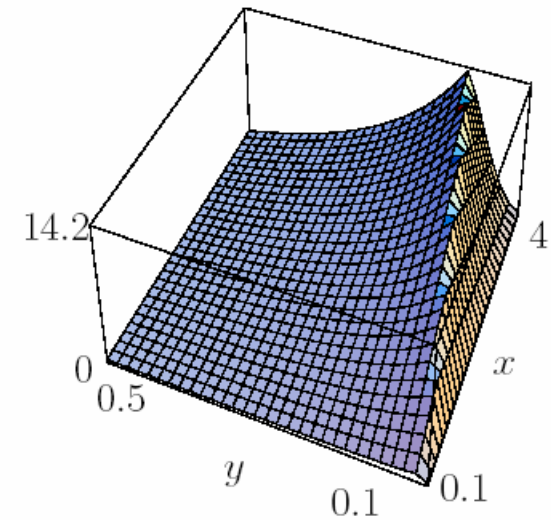
## Comparison of Tightness:



Ratio:  $x/y$



$x/y$  – Envelope



$x/y$  – Traditional

# ENVELOPES OF MULTILINEAR FUNCTIONS

- **Multilinear function over a box**

$$M(x_1, \dots, x_n) = \sum_t a_t \prod_{i=1}^{p_t} x_i, \quad -\infty < L_i \leq x_i \leq U_i < +\infty, \quad i = 1, \dots, n$$

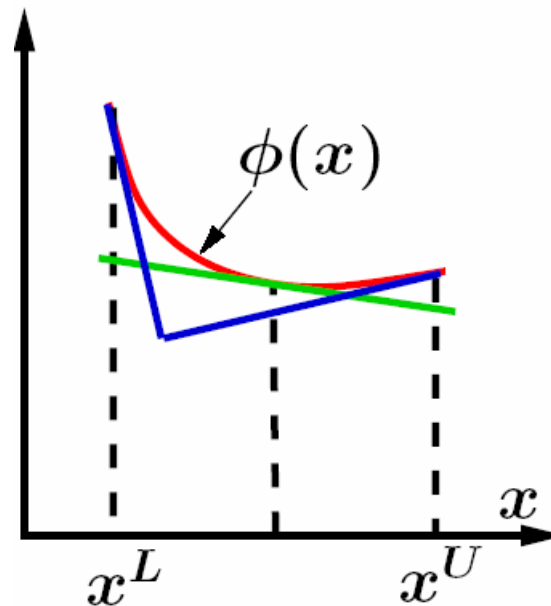
- **Generating set**

$$\text{vert} \left( \prod_{i=1}^n [L_i, U_i] \right)$$

- **Polyhedral convex encloser follows trivially from polyhedral representation theorems**

# POLYHEDRAL OUTER-APPROXIMATION

- Local NLP solvers essential for local search
- Linear programs can be solved very efficiently
- Outer-approximate convex relaxation by polyhedron



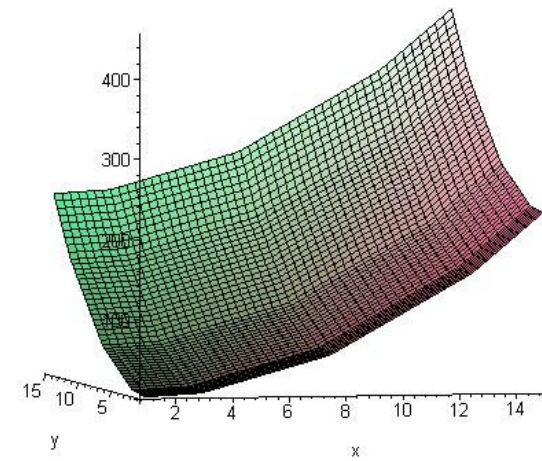
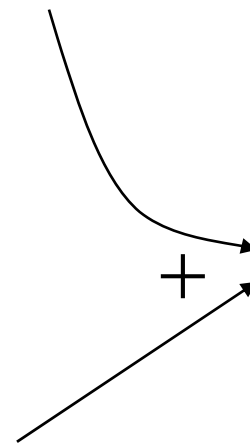
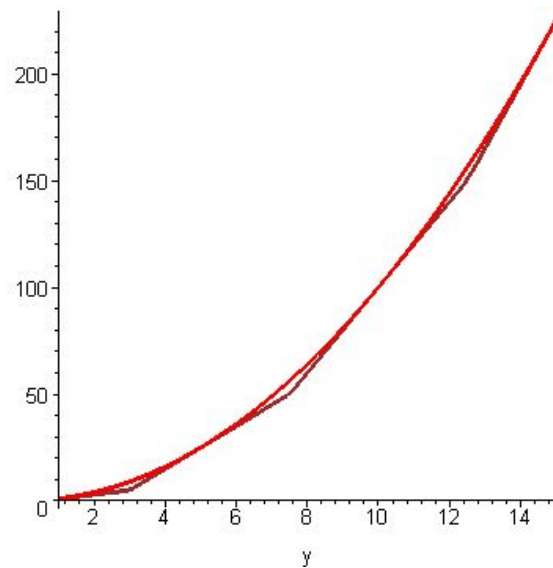
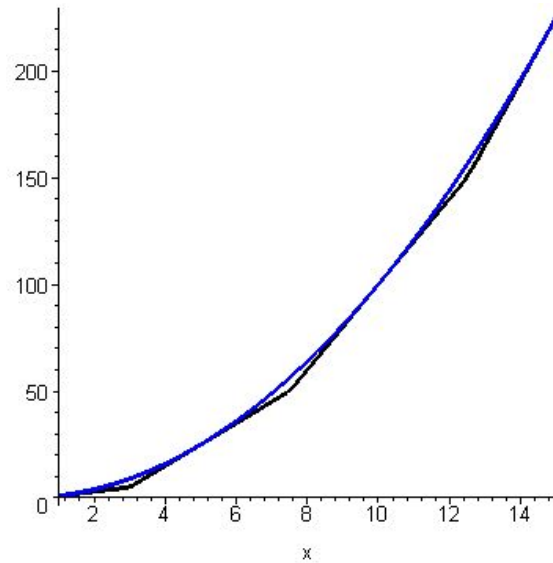
Tawarmalani and Sahinidis (*Math. Progr.*, 2004, 2005)

- Quadratically convergent sandwich algorithm
- Cutting planes for functional compositions

# RECURSIVE FUNCTIONAL COMPOSITIONS

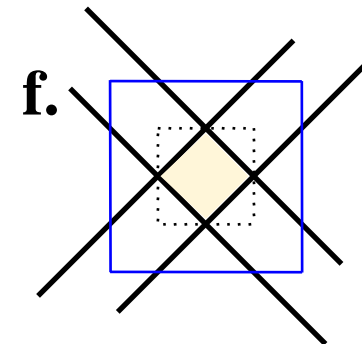
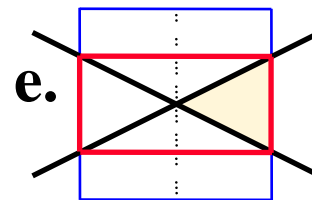
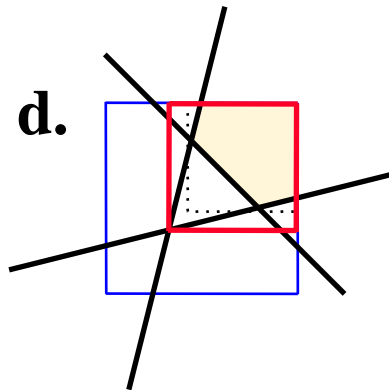
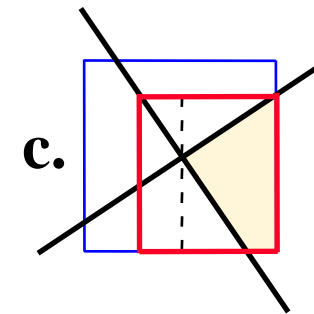
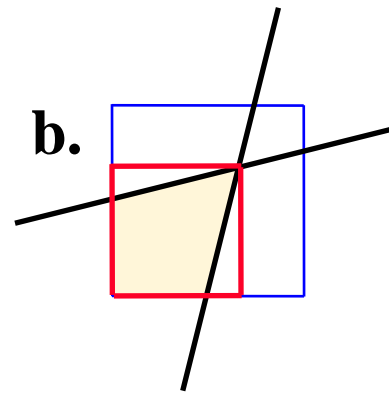
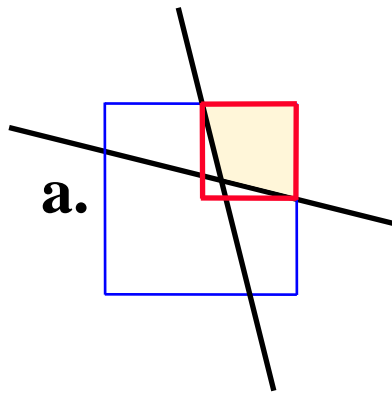
- Consider  $h=g(f)$ , where
  - $g$  and  $f$  are multivariate convex functions
  - $g$  is non-decreasing in the range of each nonlinear component of  $f$
- $h$  is convex
- Two outer approximations of the composite function  $h$ :
  - S1: a single-step procedure that constructs supporting hyperplanes of  $h$  at a predetermined number of points
  - S2: a two-step procedure that constructs supporting hyperplanes for  $g$  and  $f$  at corresponding points
- Two-step is sharper than one-step
  - If  $f$  is affine, S2=S1
  - In general, the inclusion is strict

# OUTER APPROXIMATION OF $x^2+y^2$

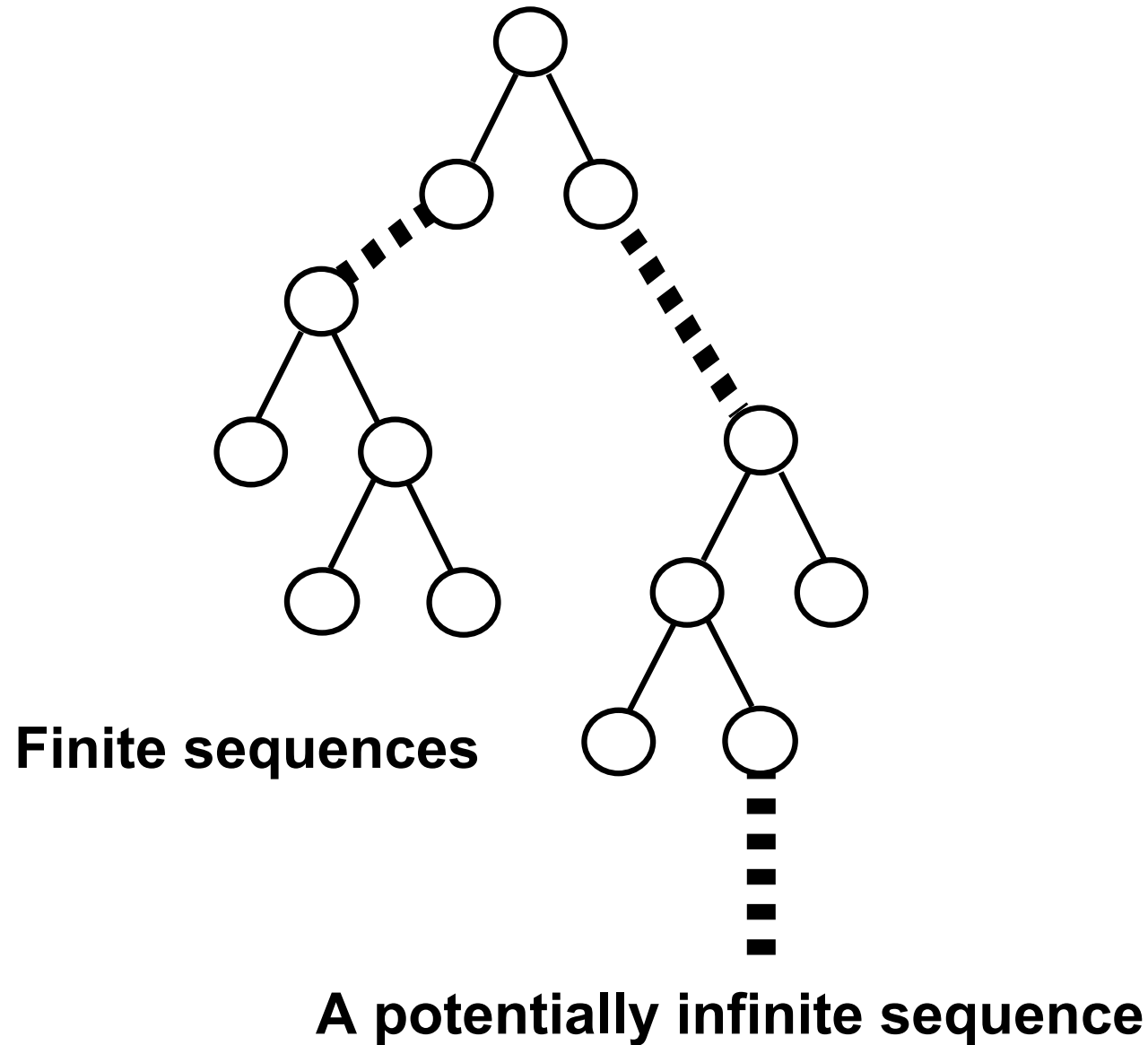




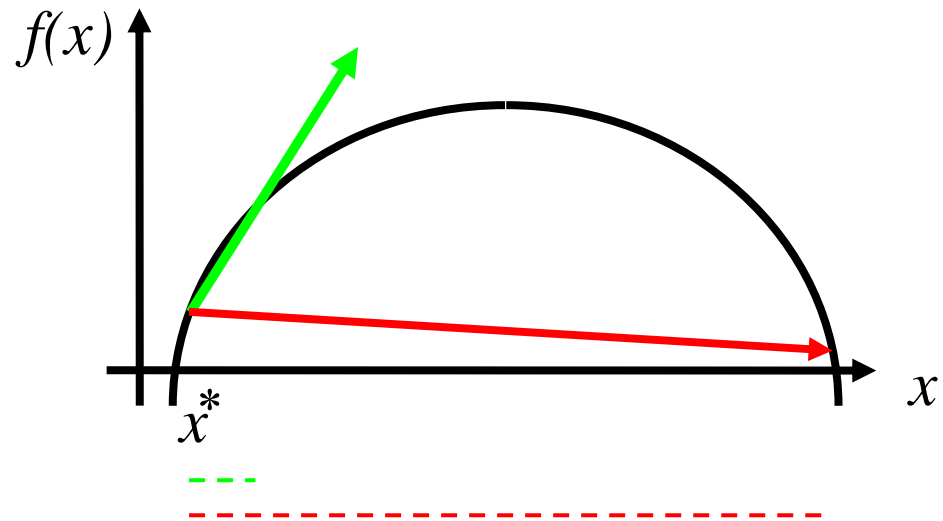
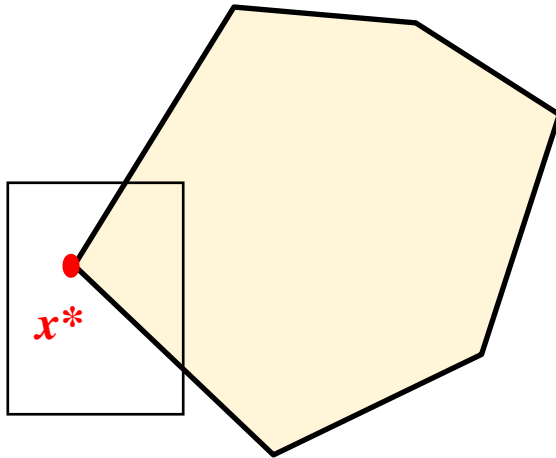
# REDUCTION VIA CONSTRAINT PROPAGATION



# FINITE VERSUS CONVERGENT BRANCH-AND-BOUND ALGORITHMS

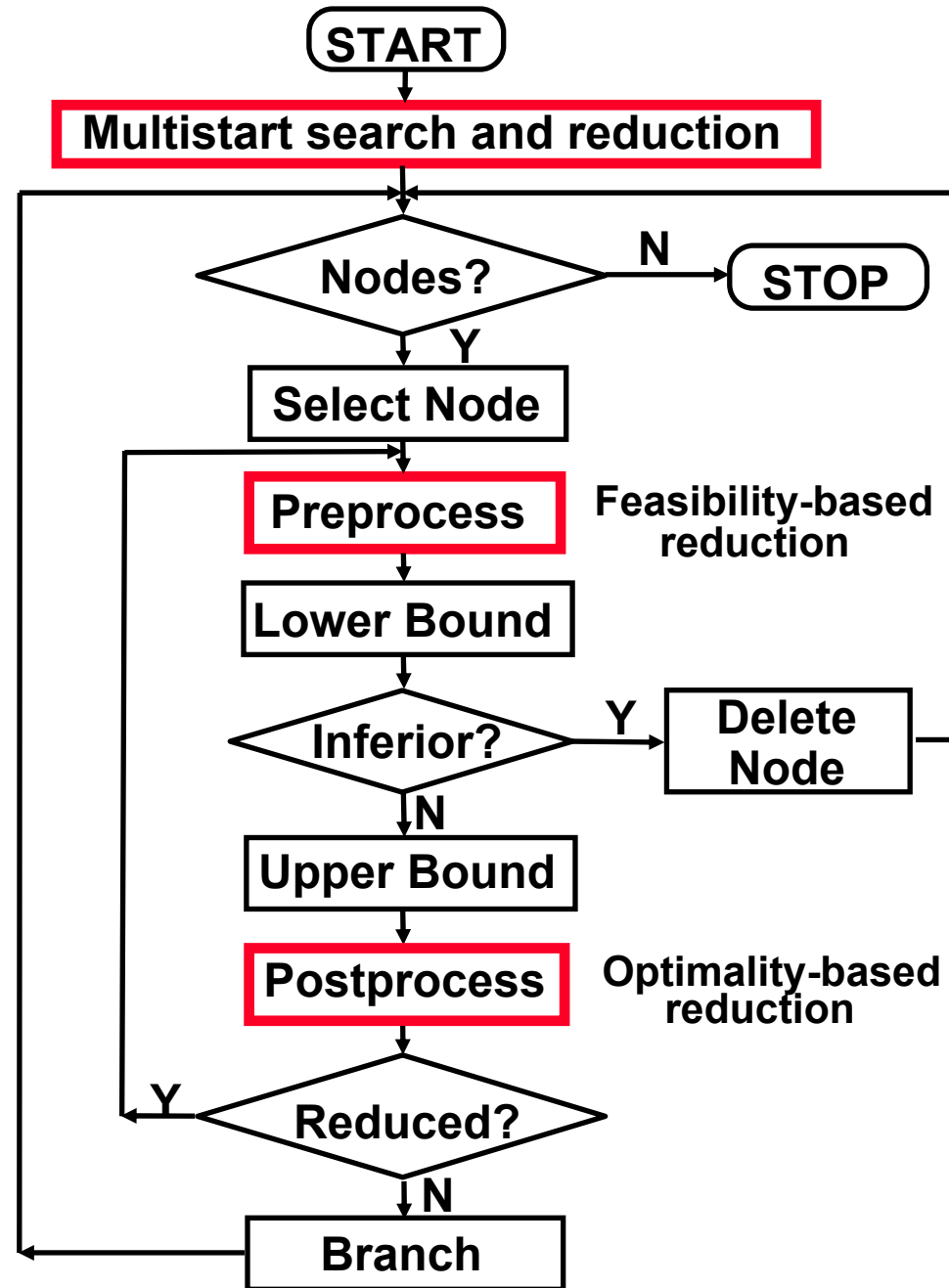


# FINITE BRANCHING RULE



- **Variable selection:**
  - Typically, select variable with largest underestimating gap
  - Occasionally, select variable corresponding to largest edge
- **Point selection:**
  - Typically, at the midpoint (exhaustiveness)
  - When possible, at the best currently known solution
- **Finite isolation of global optimum**
- **Finite termination in many cases**
  - Concave minimization over polytopes
  - 2-Stage stochastic integer programming

# BRANCH-AND-REDUCE



# Branch-And-Reduce Optimization Navigator

## Components

- Modeling language
- Preprocessor
- Data organizer
- I/O handler
- Range reduction
- Solver links
- Interval arithmetic
- Sparse matrix routines
- Automatic differentiator
- IEEE exception handler
- Debugging facilities

## Capabilities

- Core module
  - Application-independent
  - Expandable
- Fully automated MINLP solver
- Application modules
  - Multiplicative programs
  - Indefinite QPs
  - Fixed-charge programs
  - Mixed-integer SDPs
  - ...
- Solve relaxations using
  - CPLEX, MINOS, SNOPT, OSL, SDPA, ...

- Available under GAMS and AIMMS
- Available on NEOS server

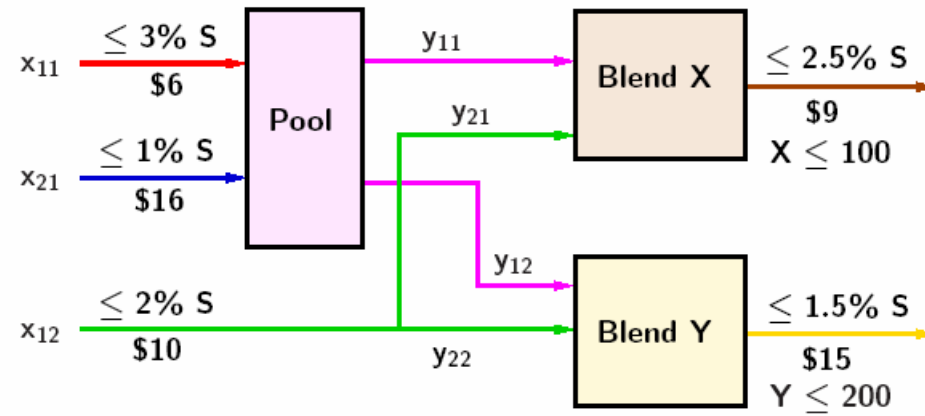
# 26 PROBLEMS FROM globallib AND minlplib

	Minimum	Maximum	Average
Constraints	2	513	76
Variables	4	1030	115
Discrete variables	0	432	63

## EFFECT OF CUTTING PLANES

	Without cuts	With cuts	% reduction
Nodes	23,031,434	253,754	99
Nodes in memory	622,339	13,772	98
CPU hrs	76	6	93

# POOLING PROBLEM: p-FORMULATION



$$\min \quad \overbrace{6x_{11} + 16x_{21} + 10x_{12}}^{\text{cost}} - \overbrace{9(y_{11} + y_{21})}^{\text{X-revenue}} - \overbrace{15(y_{12} + y_{22})}^{\text{Y-revenue}}$$

$$\text{s.t.} \quad q = \frac{3x_{11} + x_{21}}{y_{11} + y_{12}} \quad \text{Sulfur Mass Balance}$$

$$\begin{aligned} x_{11} + x_{21} &= y_{11} + y_{12} \\ x_{12} &= y_{21} + y_{22} \end{aligned} \quad \text{Mass balance}$$

$$\frac{qy_{11} + 2y_{21}}{y_{11} + y_{21}} \leq 2.5 \quad \text{Quality Requirements}$$

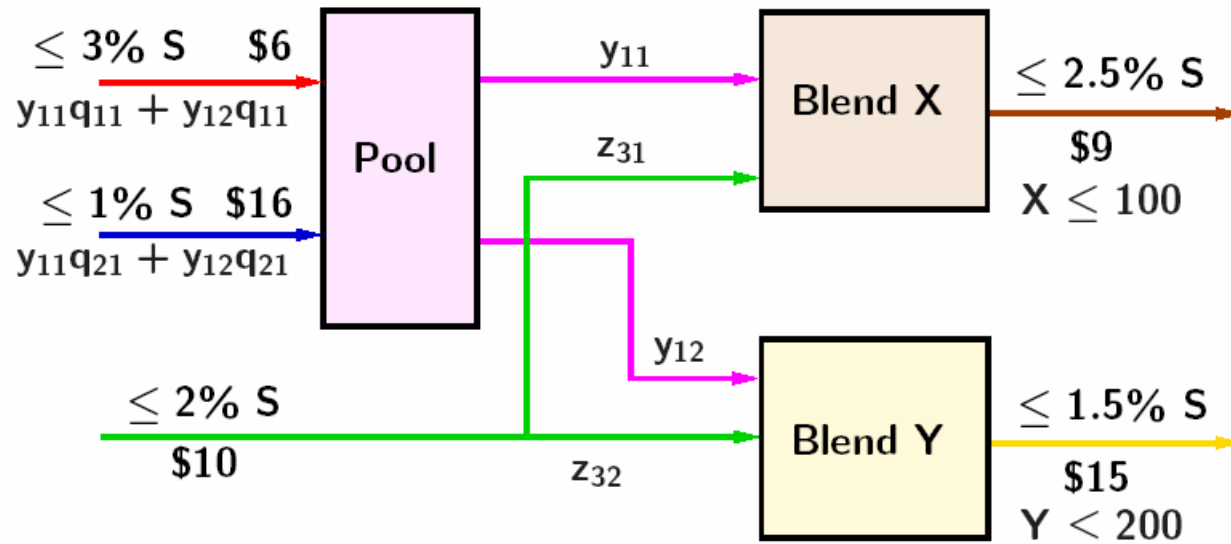
$$\frac{qy_{12} + 2y_{22}}{y_{12} + y_{22}} \leq 1.5$$

$$y_{11} + y_{21} \leq 100 \quad \text{Demands}$$

$$y_{12} + y_{22} \leq 200$$

Haverly 1978

# POOLING PROBLEM: q-FORMULATION



$$\min \quad \overbrace{6(y_{11}q_{11} + y_{12}q_{11}) + 16(y_{11}q_{21} + y_{12}q_{21}) + 10(z_{31} + z_{32})}^{\text{cost}} - \underbrace{9(y_{11} + y_{21})}_{X\text{-revenue}} - \underbrace{15(x_{12} + x_{22})}_{Y\text{-revenue}}$$

$$\text{s.t.} \quad q_{11} + q_{21} = 1$$

Mass Balance

$$-0.5z_{31} + 3y_{11}q_{11} + y_{11}q_{21} \leq 2.5y_{11}$$

$$0.5z_{32} + 3y_{12}q_{11} + y_{12}q_{21} \leq 1.5y_{12}$$

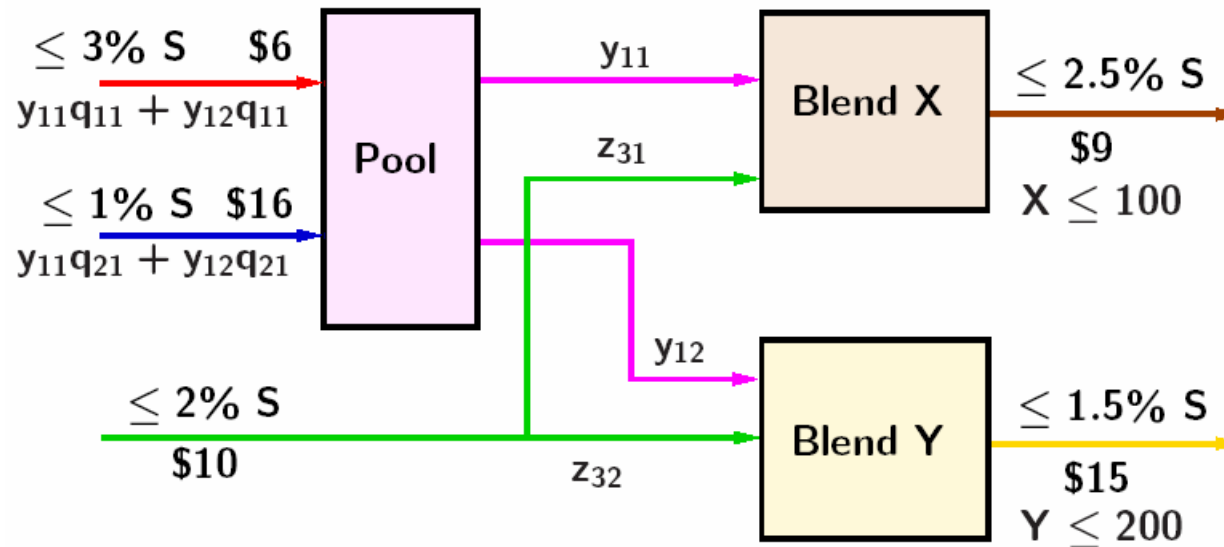
Quality Requirements

$$y_{11} + z_{31} \leq 100$$

$$y_{12} + z_{32} \leq 200$$

Demands

# POOLING PROBLEM: pq-FORMULATION



$$\begin{aligned}
 \min \quad & \overbrace{6(y_{11}q_{11} + y_{12}q_{11}) + 16(y_{11}q_{21} + y_{12}q_{21}) + 10(z_{31} + z_{32})}^{\text{cost}} \\
 & \underbrace{-9(y_{11} + y_{21})}_{\text{X-revenue}} - \underbrace{15(x_{12} + x_{22})}_{\text{Y-revenue}} \\
 \text{s.t.} \quad & q_{11} + q_{21} = 1 && \text{Mass Balance} \\
 & -0.5z_{31} + 3y_{11}q_{11} + y_{11}q_{21} \leq 2.5y_{11} \\
 & 0.5z_{32} + 3y_{12}q_{11} + y_{12}q_{21} \leq 1.5y_{12} && \text{Quality Requirements} \\
 & y_{11} + z_{31} \leq 100 \\
 & y_{12} + z_{32} \leq 200 && \text{Demands} \\
 & y_{11}q_{11} + y_{11}q_{21} = y_{11} \\
 & y_{12}q_{11} + y_{12}q_{21} = y_{12} && \text{Convexification Constraints}
 \end{aligned}$$

# PRODUCT DISAGGREGATION

Consider the function:

$$\phi(x; y_1, \dots, y_n) = a_0 + \sum_{k=1}^n a_k y_k + xb_0 + x \sum_{k=1}^n b_k y_k$$

Let

$$H = [x^L, x^U] \times \prod_{k=1}^n [y_k^L, y_k^U]$$

Then

$$\text{convex}_H \phi = a_0 + \sum_{k=1}^n a_k y_k + xb_0 + \sum_{k=1}^n \text{convex}_{[y_k^L, y_k^U] \times [x^L, x^U]} (b_k y_k x)$$

**Disaggregated formulations are tighter**

# LOCAL SEARCH WITH CONOPT

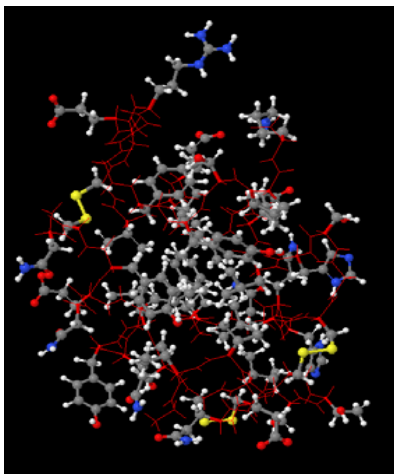
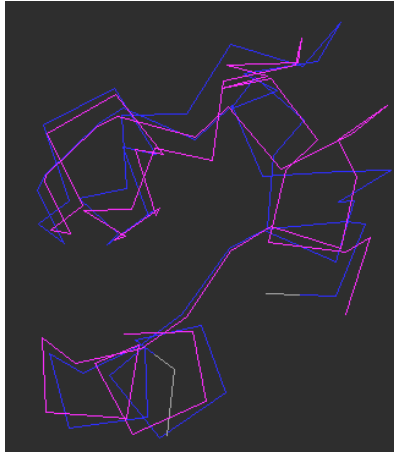
Problem	q-formulation objective	pq-formulation objective
adhya1	<b>-68.74</b>	<b>-56.67</b>
adhya2	0	0
adhya3	<b>-65</b>	<b>-57.74</b>
adhya4	<b>-470.83</b>	<b>-470.83</b>
bental4	0	0
bental5	<b>-2900</b>	<b>-2700</b>
foulds2	<b>-1000</b>	<b>-600</b>
foulds3	<b>-6.5</b>	<b>-6.5</b>
foulds4	<b>-6</b>	<b>-6.5</b>
foulds5	<b>-7</b>	<b>-6.5</b>
haverly1	<b>-400</b>	0
haverly2	<b>-400</b>	0
haverly3	<b>-750</b>	0
rt97	<b>Infeasible</b>	<b>-4330.78</b>

# GLOBAL SEARCH WITH BARON

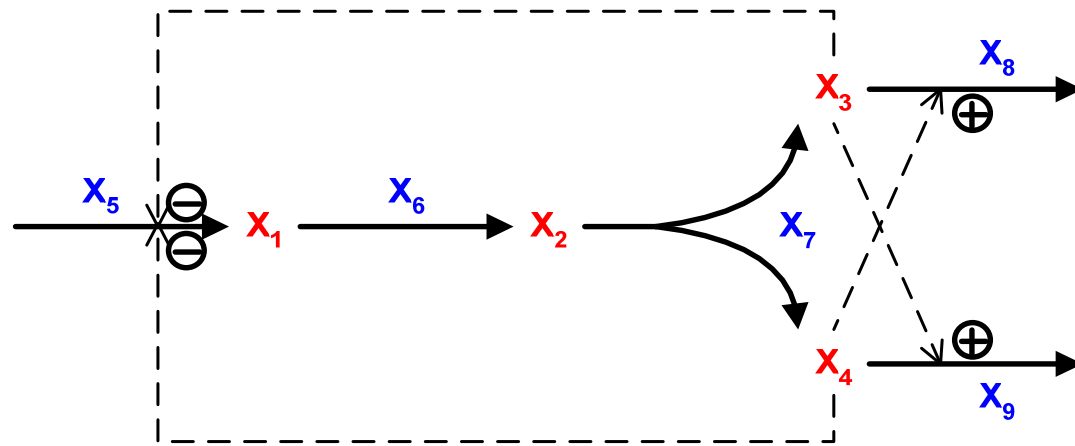
Problem	p-formulation		pq-formulation	
	Nodes	CPU sec	Nodes	CPU sec
adhya1	573	17	24	0.5
adhya2	501	20	17	0.5
adhya3	>9248	>1200	31	1.5
adhya4	>6129	>1200	1	1
bental4	101	0.5	1	0.5
bental5	>6445	>1200	-1	0
foulds2	1061	16	-1	0
foulds3	>348	>1200	-1	5
foulds4	>326	>1200	-1	1
foulds5	>389	>1200	-1	1
haverly1	25	0	1	0
haverly2	17	0	1	0
haverly3	3	0	1	0
rt97	5629	174	6	0.5

# ONGOING DEVELOPMENT OF BARON

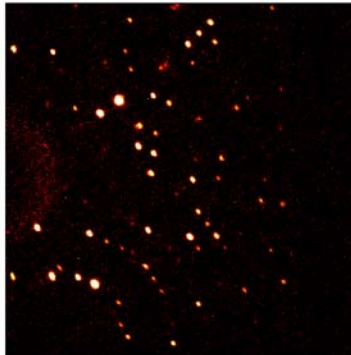
## Structural Bioinformatics



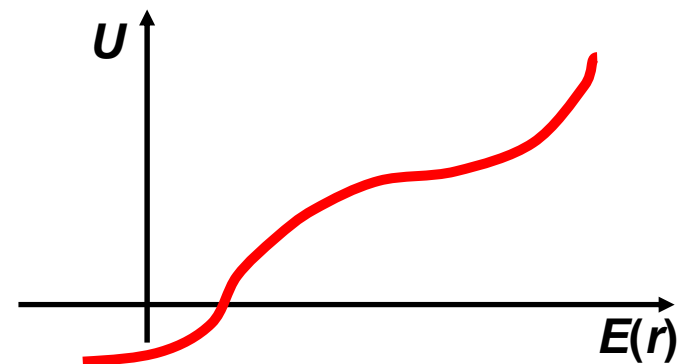
## Systems biology



## X-ray imaging



## Portfolio optimization



# BARON IN APPLICATIONS

- Development of new **Runge-Kutta methods** for partial differential equations
  - Ruuth and Spiteri, *SIAM J. Numerical Analysis*, 2004
- **Energy policy** making
  - Manne and Barreto, *Energy Economics*, 2004
- Design of **metabolic pathways**
  - Grossmann, Domach and others, *Computers & Chemical Engineering*, 2005
- Model estimation for automatic **control**
  - Bemporand and Ljung, *Automatica*, 2004
- Agricultural **economics**
  - Cabrini et al., *Manufacturing and Service Operations Management*, 2005

# GLOBAL/MINLP SOFTWARE

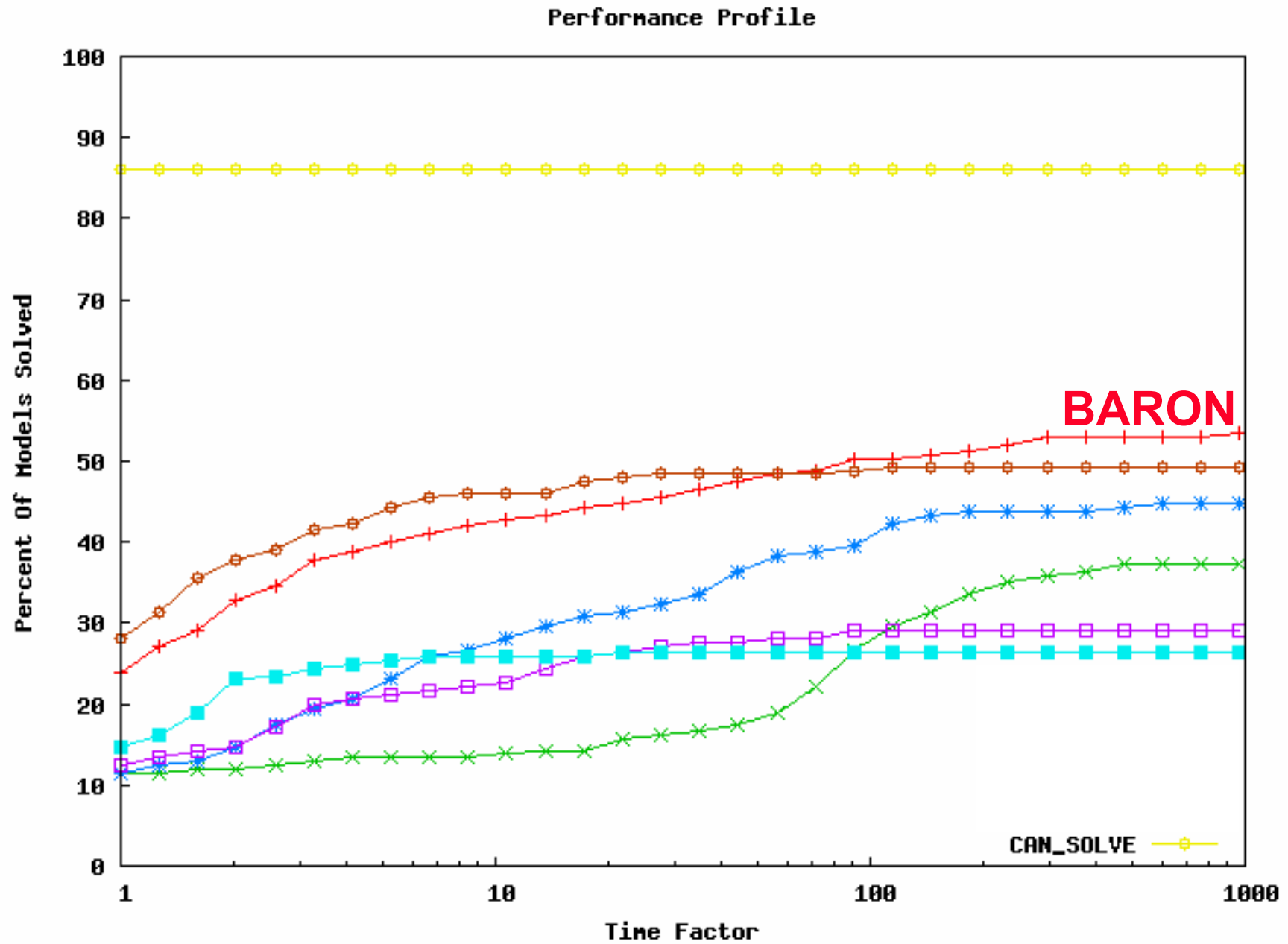
- **AlphaECP**—Exploits pseudoconvexity
- **BARON**—Branch-And-Reduce
- **BONMIN**—Integer programming technology (CMU/IBM)
- **DICOPT**—Decomposition
- **GlobSol**—Interval arithmetic
- **Interval Solver (Frontline)**—Interval solver; Excel
- **LaGO**—Lagrangian relaxations (COIN/OR)
- **LGO**—Stochastic search; black-box optimization
- **LINGO**—Trigonometric functions; IF-THEN-ELSE; ...
- **MSNLP, OQNLP**—Stochastic search
- **SBB**—Simple branch-and-bound

**NLP/MINLP**

**NLP**

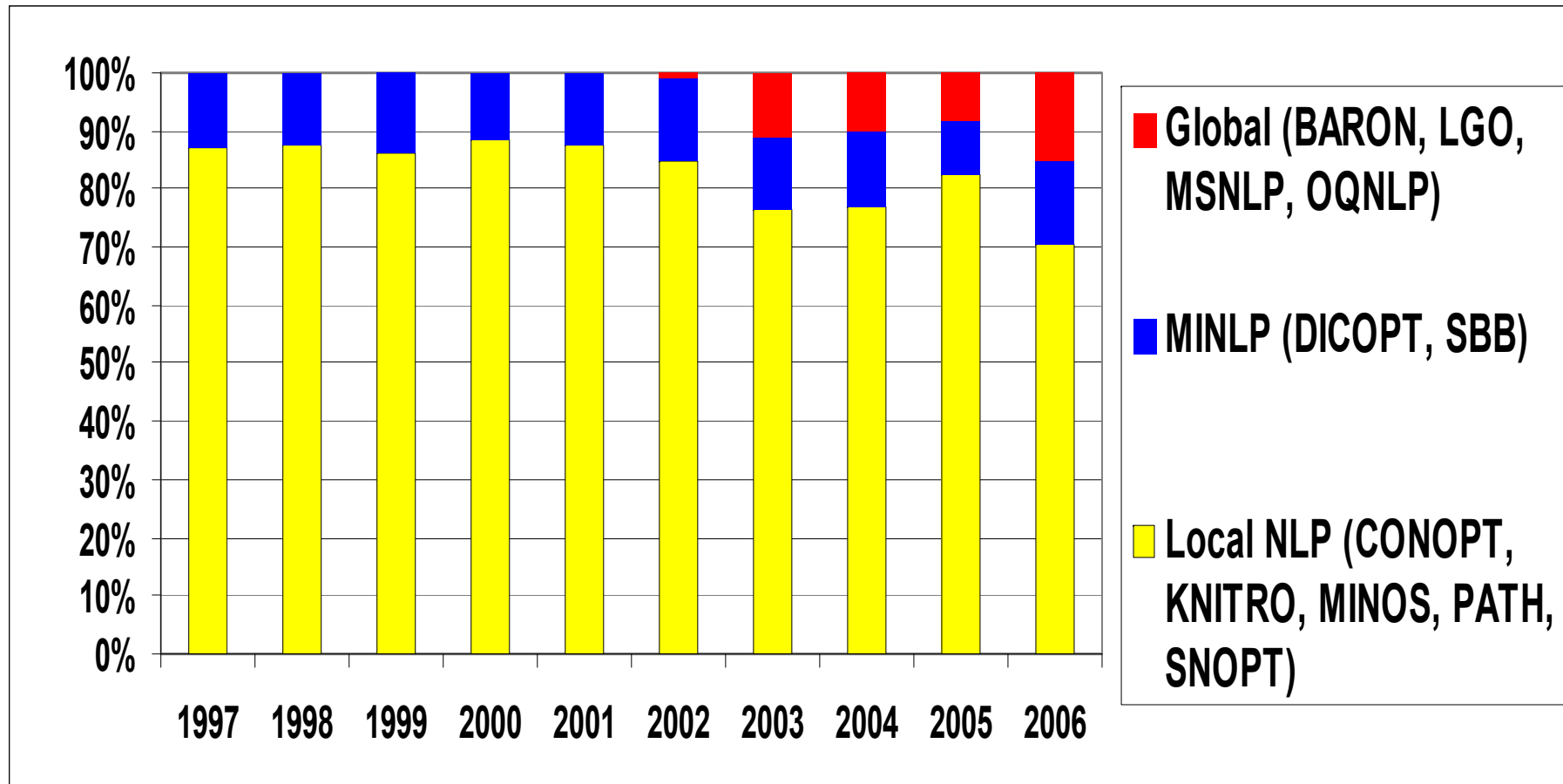
**MINLP**

# COMPARISONS ON MINLPLIB



# GAMS SALES

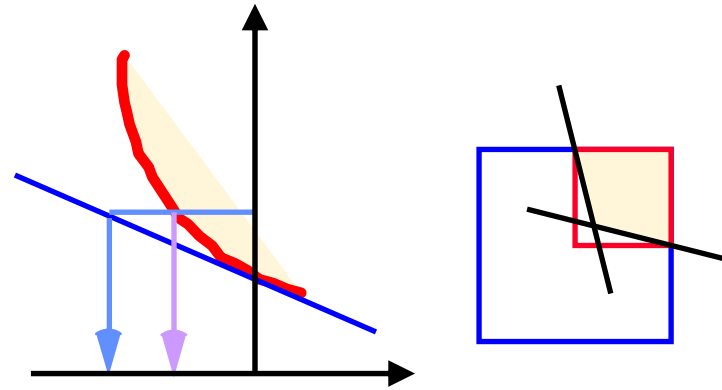
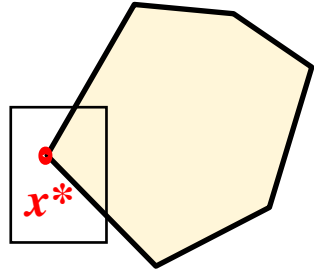
## Commercial and academic users



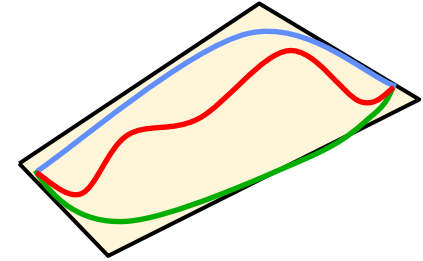
Data courtesy of Alex Meeraus

# Range Reduction

**Finiteness**



**Convexification**



## BRANCH-AND-REDUCE

