

# **GLOBAL OPTIMIZATION WITH BRANCH-AND-REDUCE**

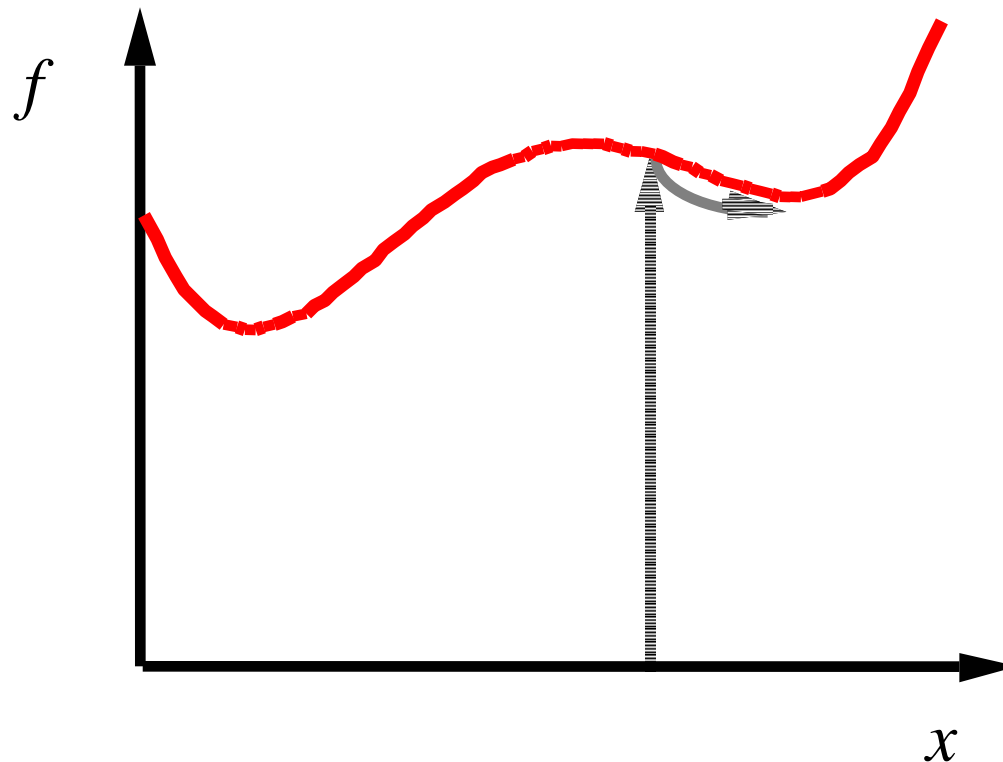
**5<sup>th</sup> Annual MOPTA Conference  
July 27, 2005, Windsor, ON, Canada**

**Nick Sahinidis**



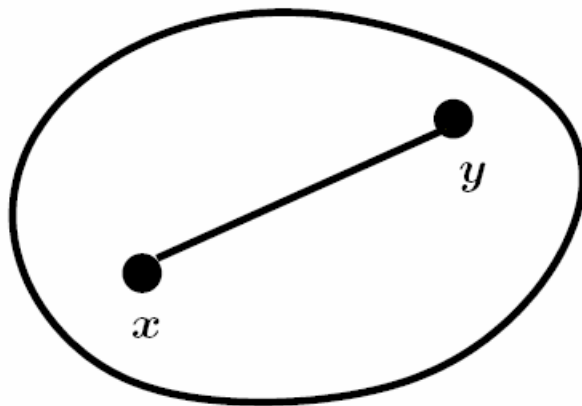
**University of Illinois at Urbana-Champaign  
Chemical and Biomolecular Engineering**

# THE MULTIPLE-MINIMA DIFFICULTY

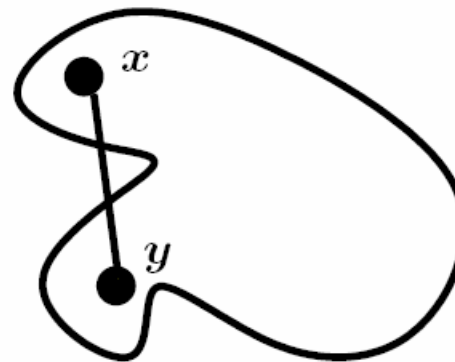


- **Classical optimality conditions are necessary but not sufficient**
- **Classical optimization provides the local minimum “closest” to the starting point used**

# CONVEX AND NONCONVEX SETS

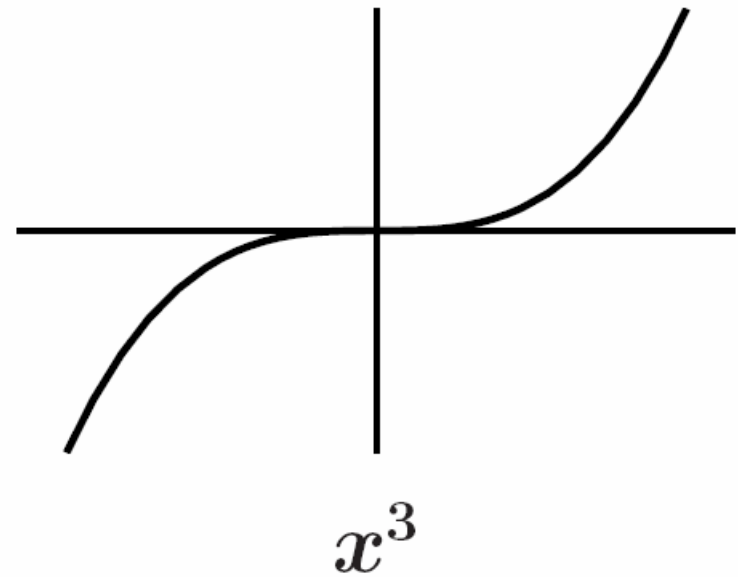
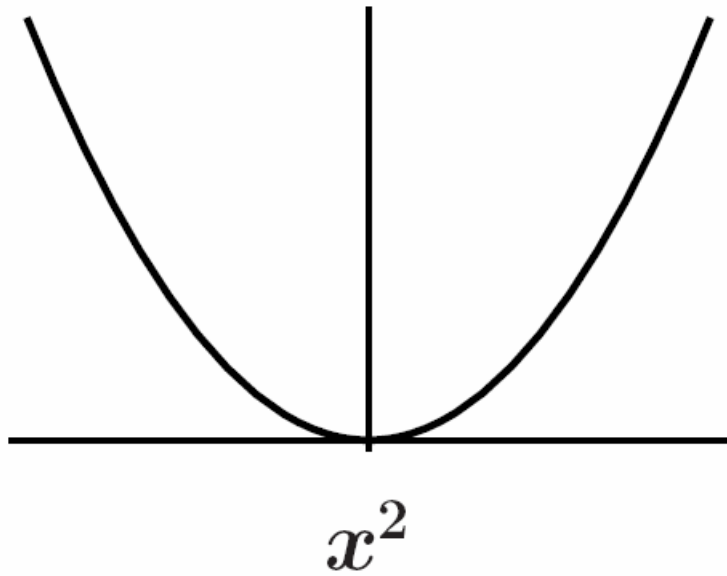


Convex Set

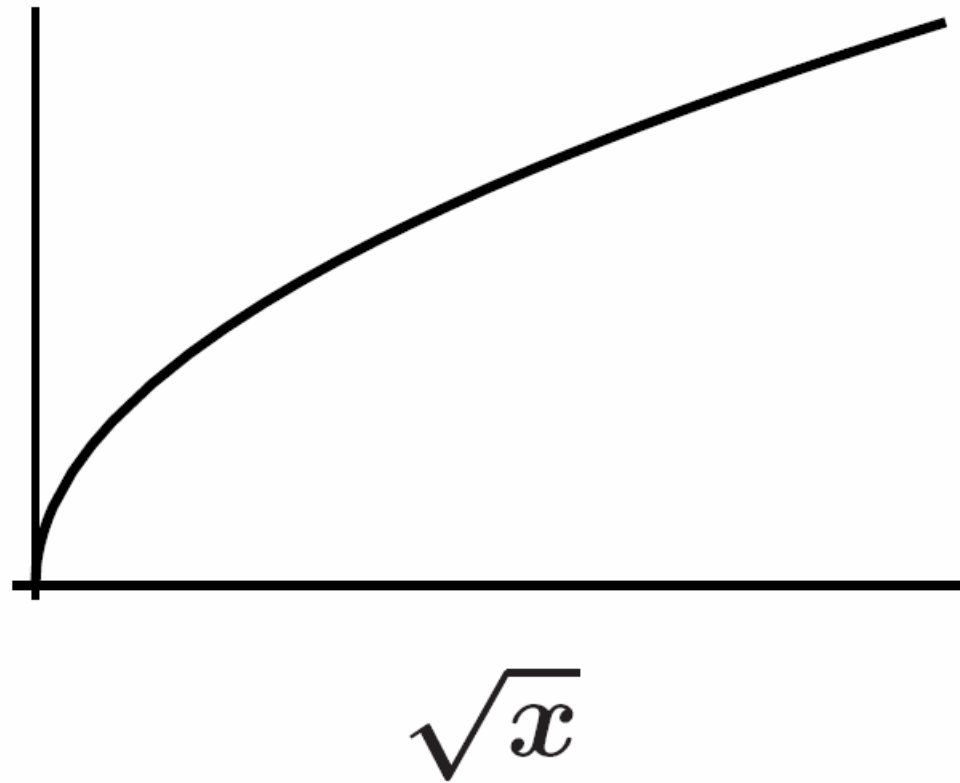


Nonconvex Set

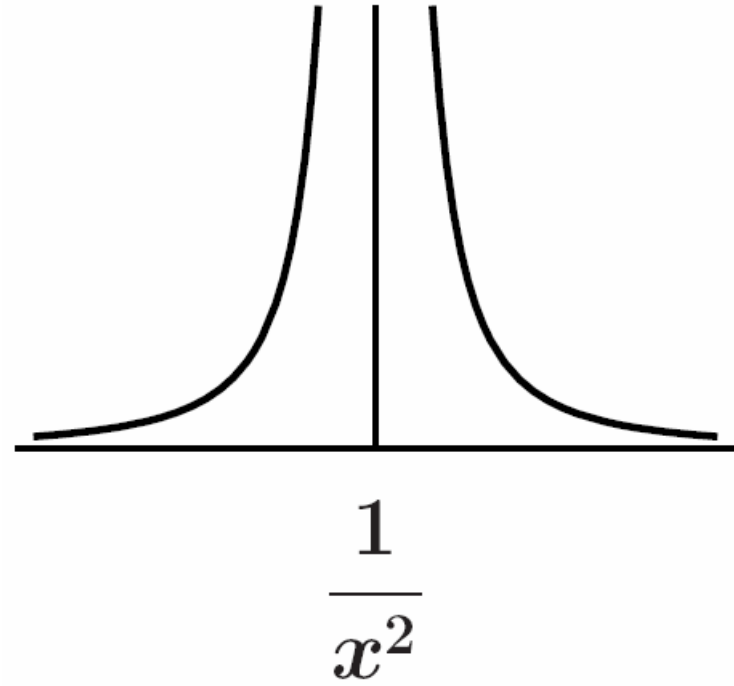
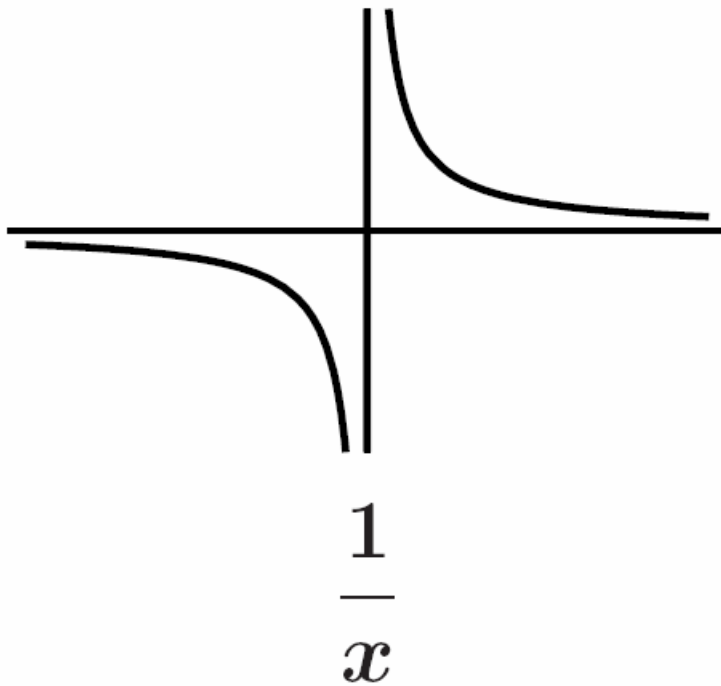
# COMMON FUNCTIONS IN MODELING



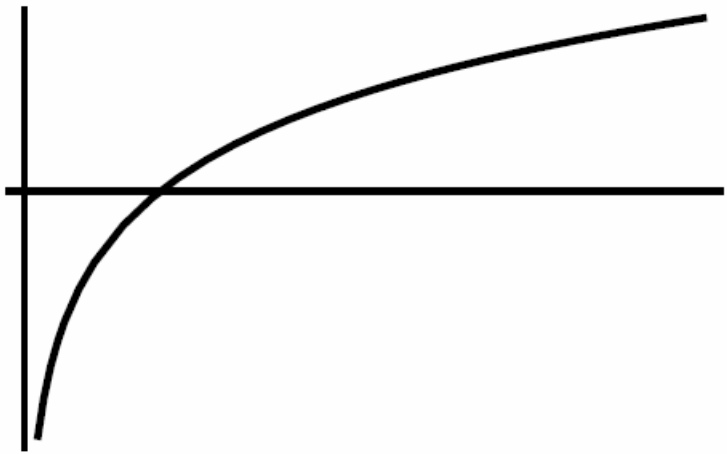
# COMMON FUNCTIONS IN MODELING



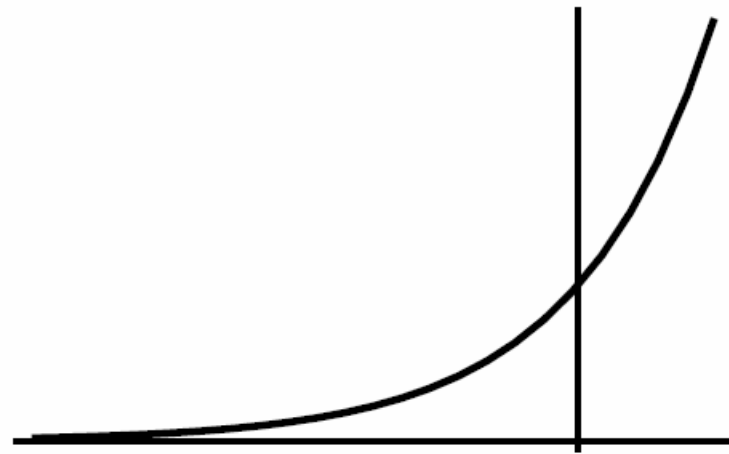
# COMMON FUNCTIONS IN MODELING



# COMMON FUNCTIONS IN MODELING

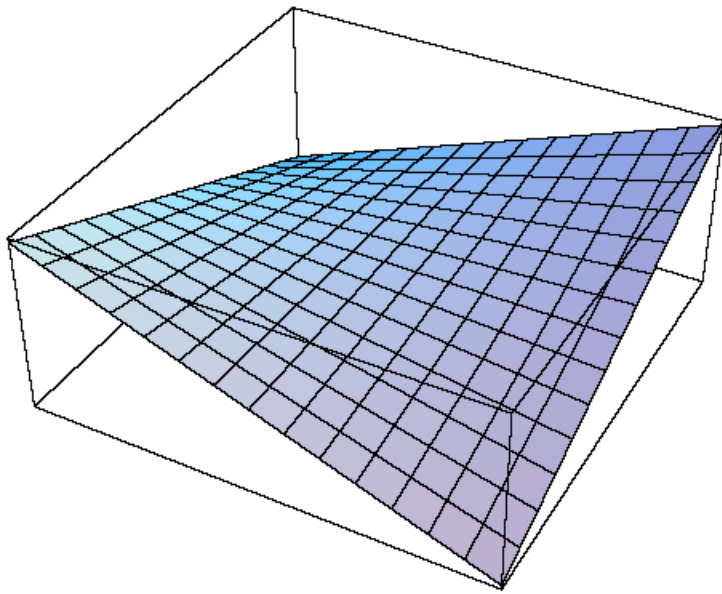


$\log(x)$

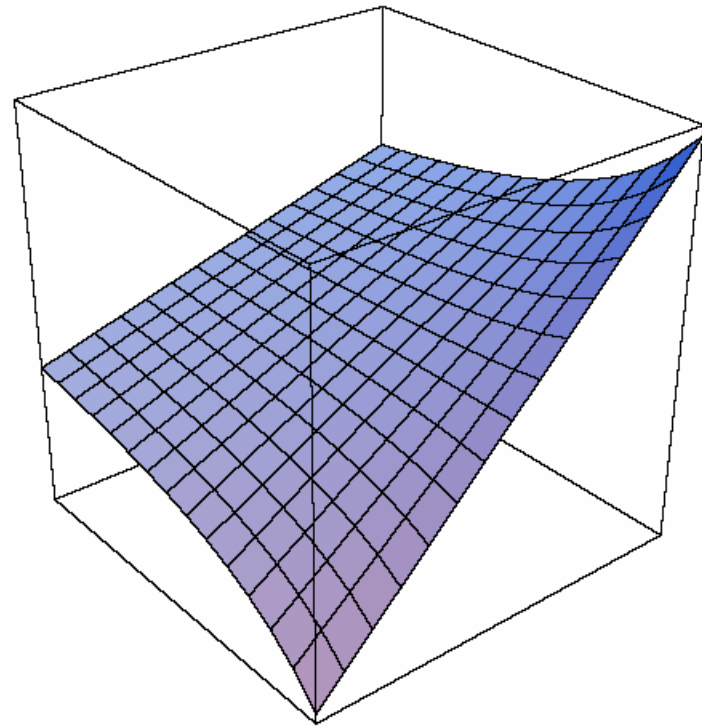


$\exp(x)$

# COMMON FUNCTIONS IN MODELING

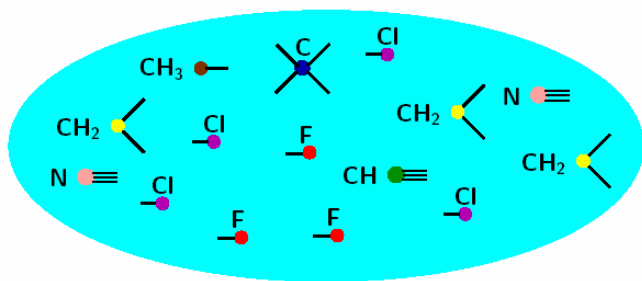


$$x_1 * x_2$$

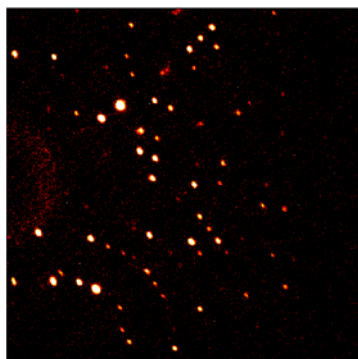


$$\frac{x_1}{x_2}$$

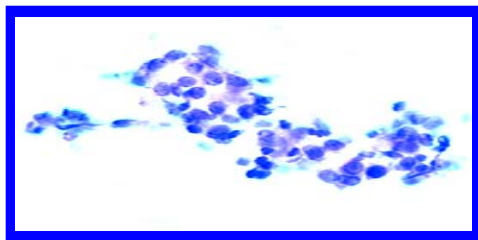
# INFORMATICS PROBLEMS IN CHEMISTRY, BIOLOGY, AND MEDICINE



- Design of automotive refrigerants



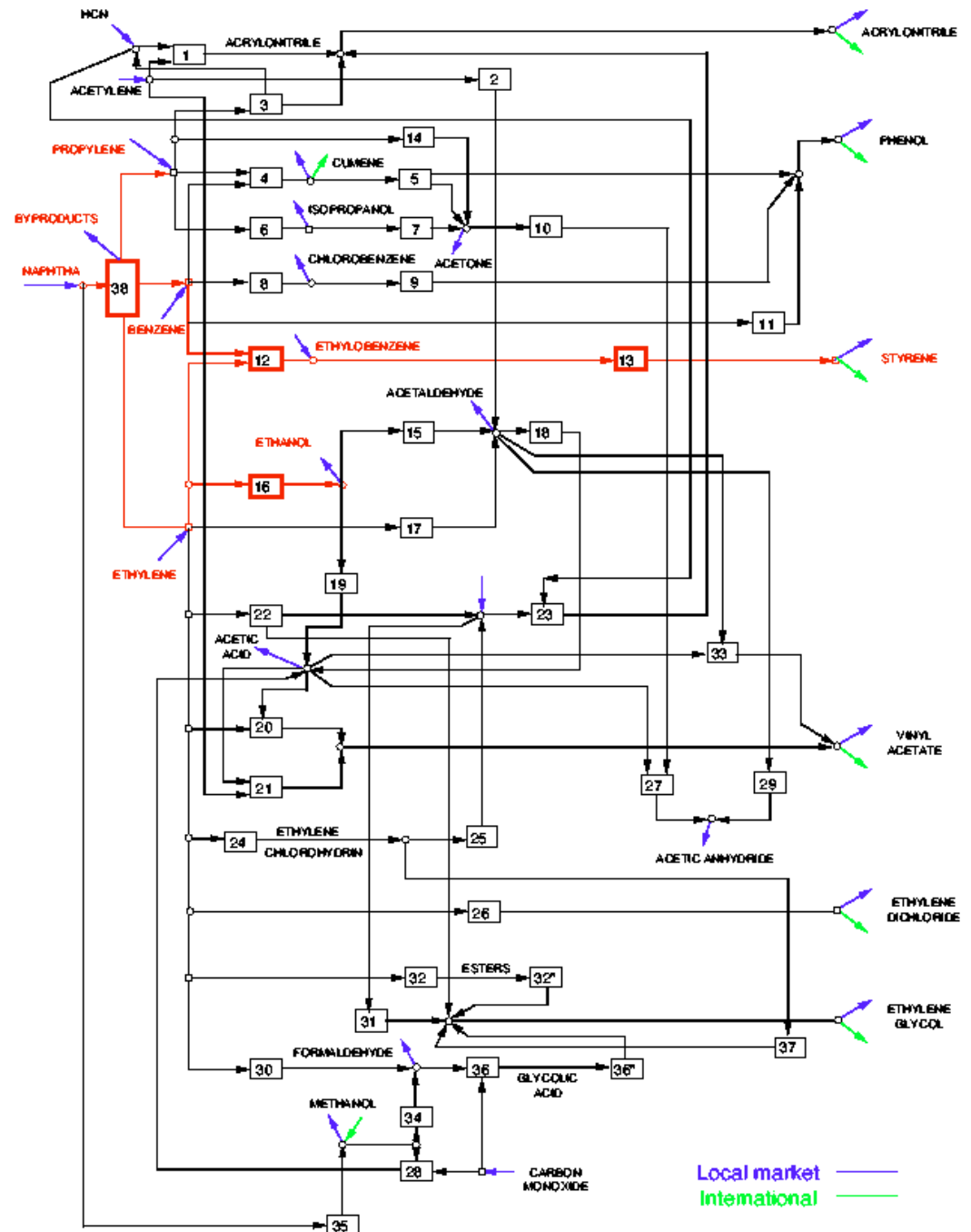
- Molecular structure determination via X-ray crystallography



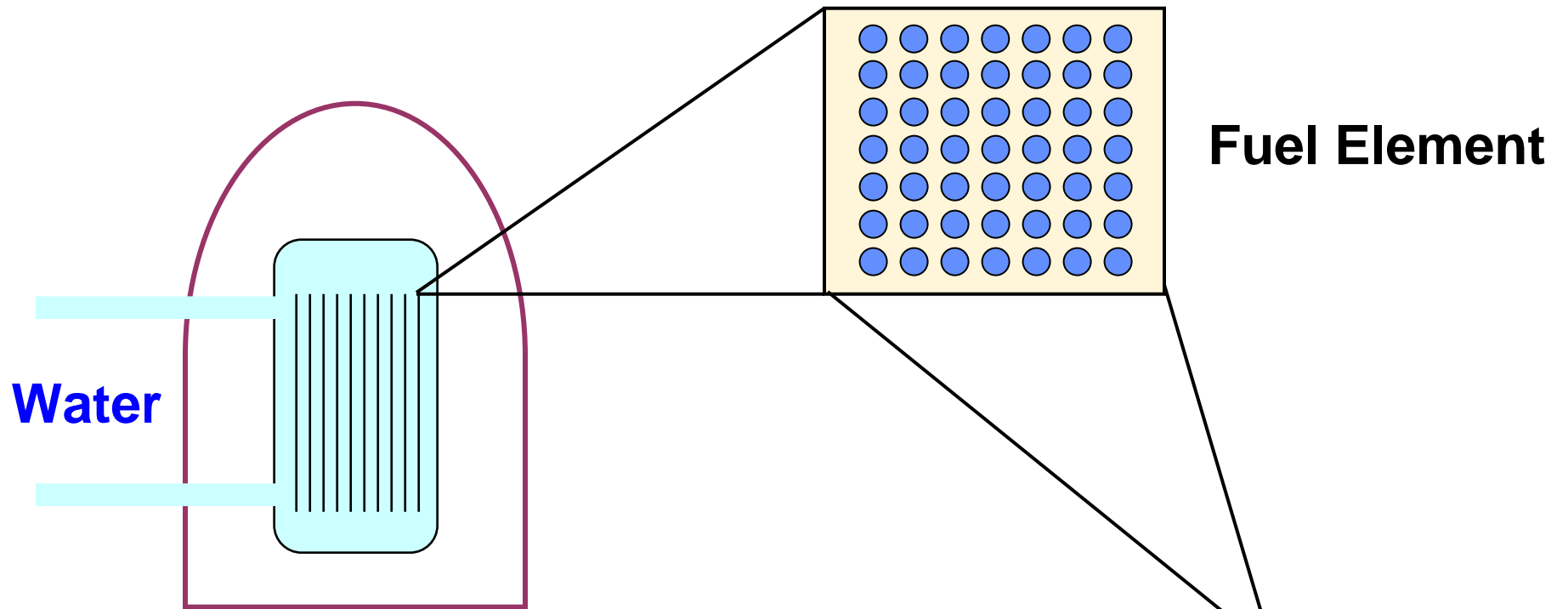
- Breast cancer diagnosis

# SUPPLY CHAIN DESIGN & OPERATIONS

- Technology selection
- Facility location
- Capacity expansion
- Blending and pooling
- Uncertainty
- Portfolio optimization
- Very large-scale decision making problems

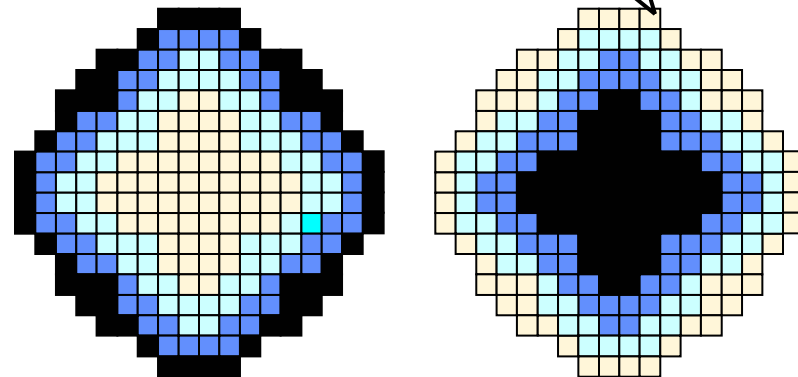


# NUCLEAR REACTOR FUEL MANAGEMENT



## Fuel Element Age

- Fresh
- One year old
- Two year old
- Three year old

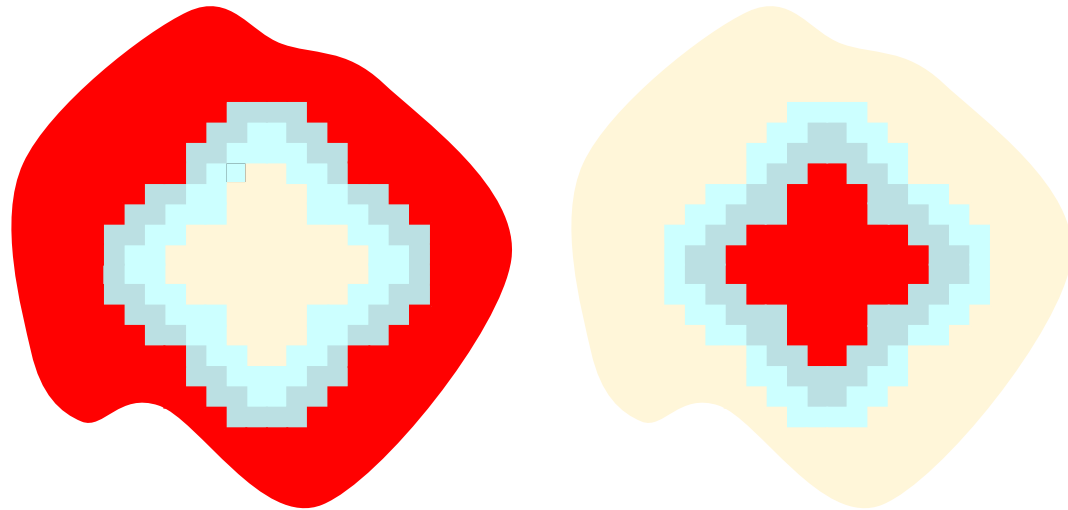


Reactor Loading Patterns

# DRUG RELEASE CONTROL

Drug Concentration

- None
- Low
- Medium
- High



- Which parts of the tumor to cut?
  - Integer decision variables
- What is the optimal concentration profile?
  - Continuous decision variables

# APPLICATIONS OF GLOBAL OPTIMIZATION

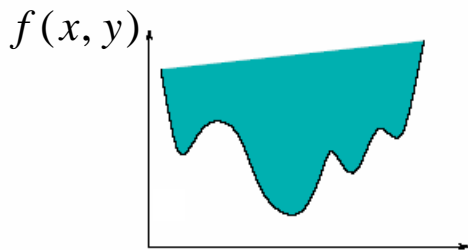
- **Engineering design & manufacturing:**
  - Product & process design
  - Production planning-scheduling-logistics
- **Computational chemical sciences:**
  - Chemical & phase equilibria
  - Molecular design
- **Informatics problems in biology and medicine**
  - Molecular structure prediction
  - Diagnosis



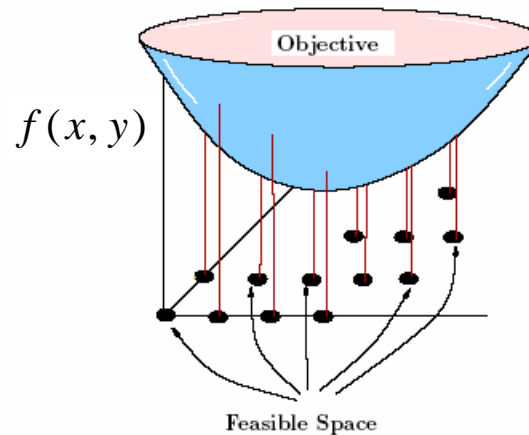
**Global optimization is an empowering  
technology in science and engineering**

# MIXED-INTEGER NONLINEAR PROGRAMMING

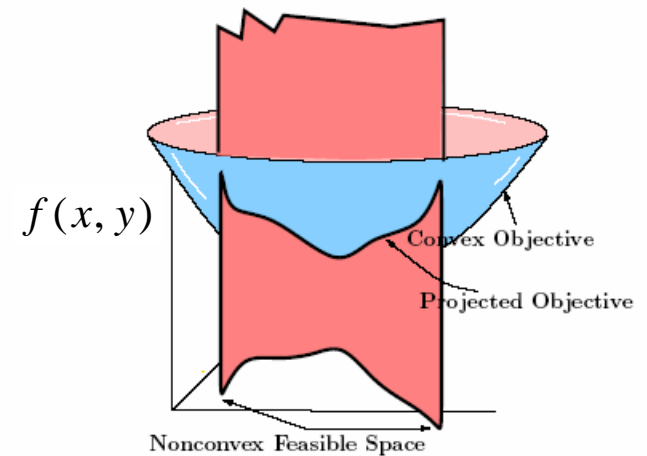
$$\begin{aligned} \min \quad & f(x, y) \\ \text{s.t.} \quad & g(x, y) \leq 0 \\ & x \in R^n, y \in Z^p \end{aligned}$$



**Multimodal objective**

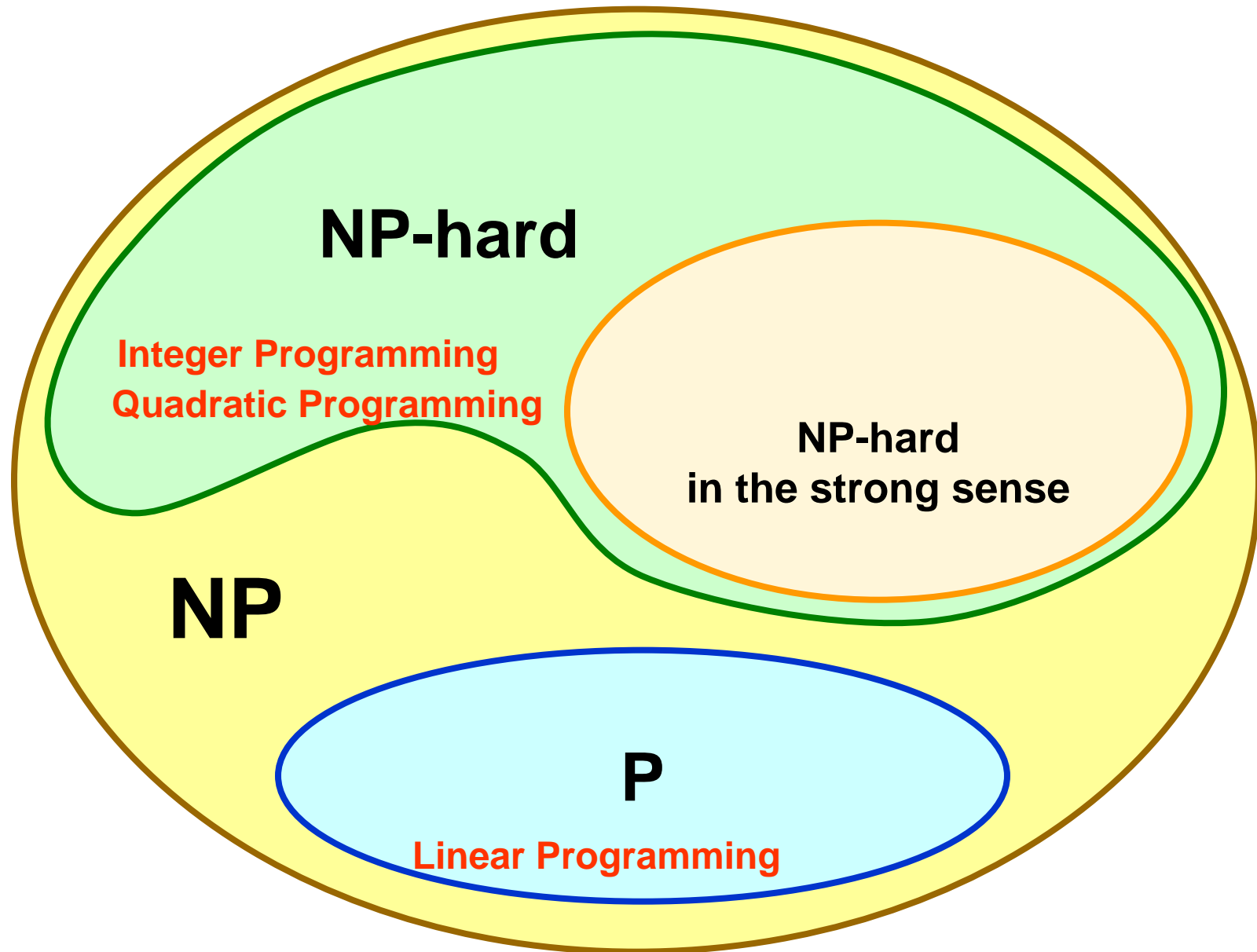


**Integrality conditions**

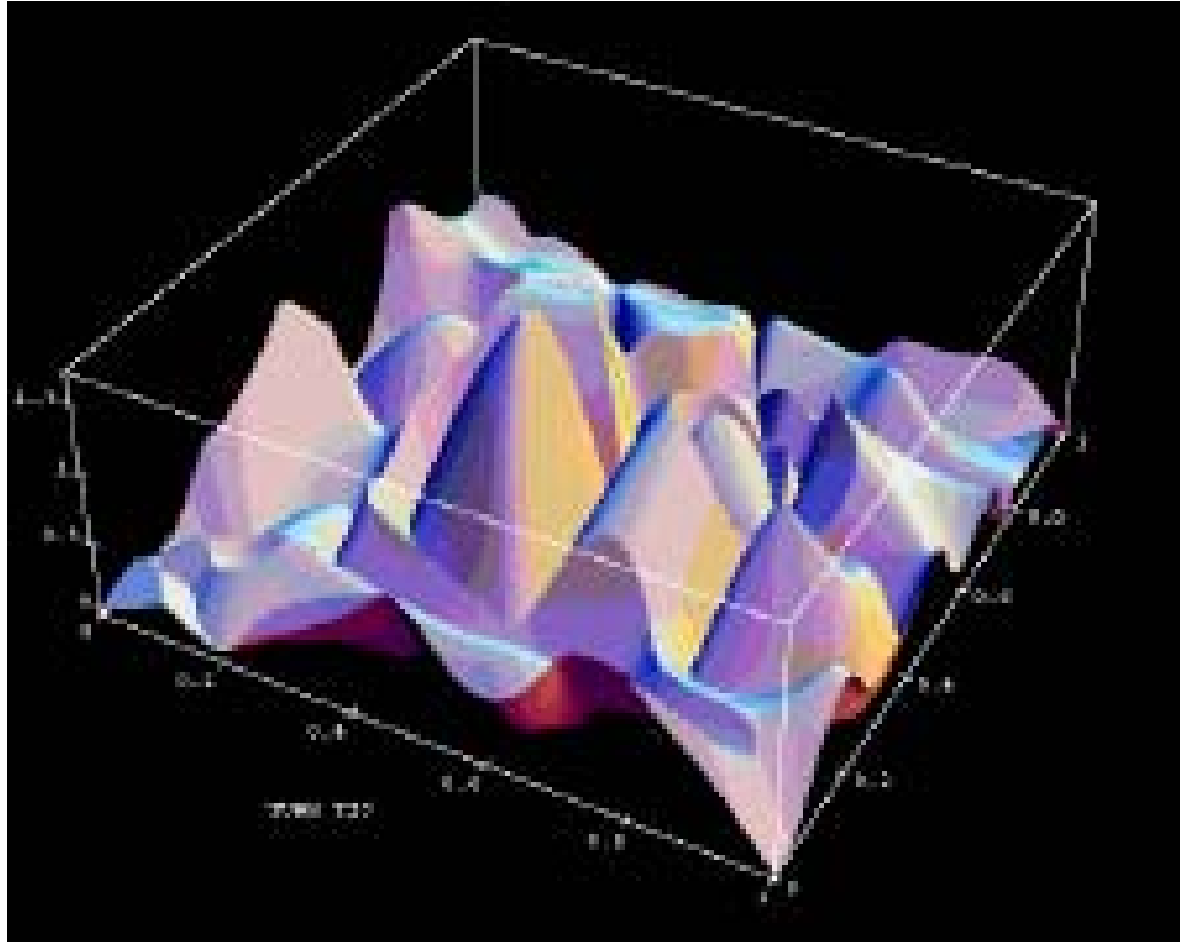


**Nonconvex constraints**

# GLOBAL OPTIMIZATION PROBLEMS ARE NP-HARD

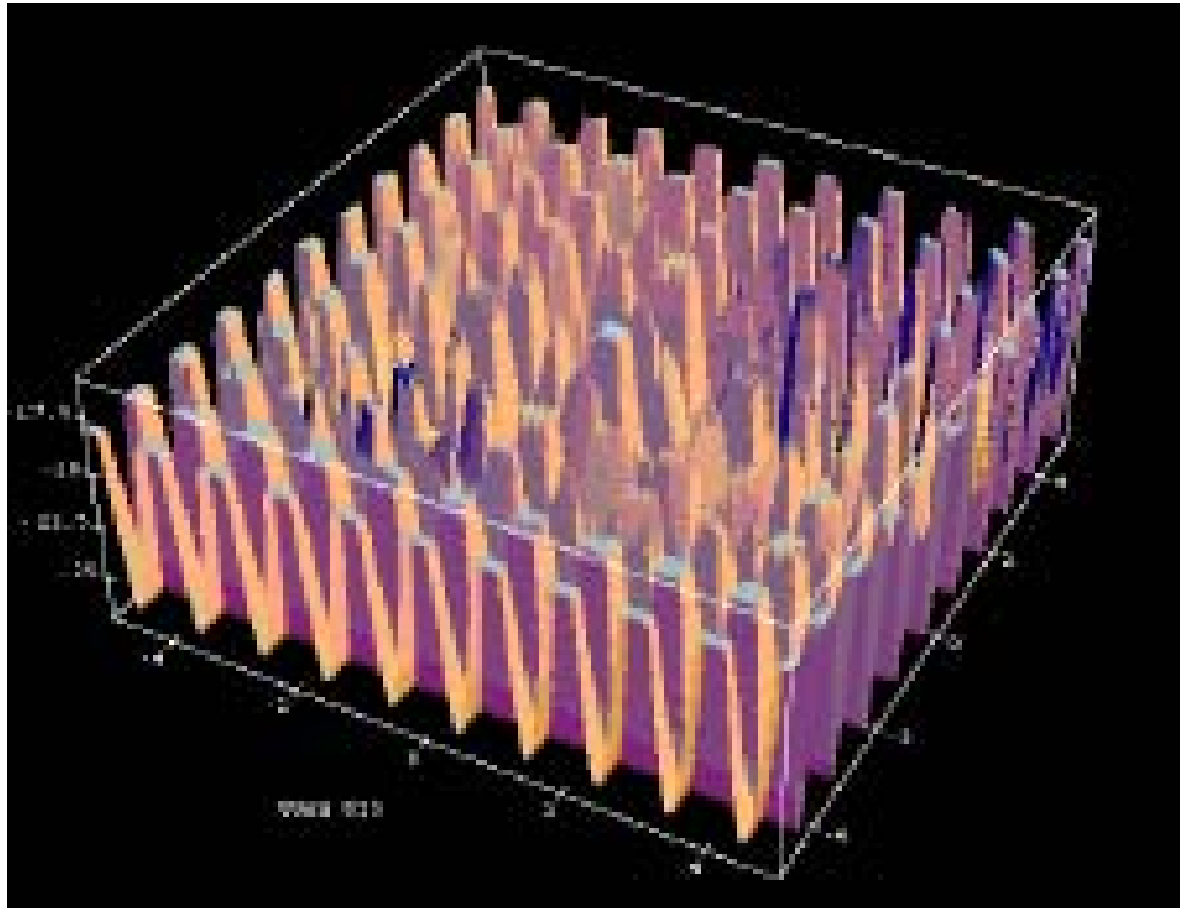


# NONCONVEX FUNCTIONS— MOUNTAINS



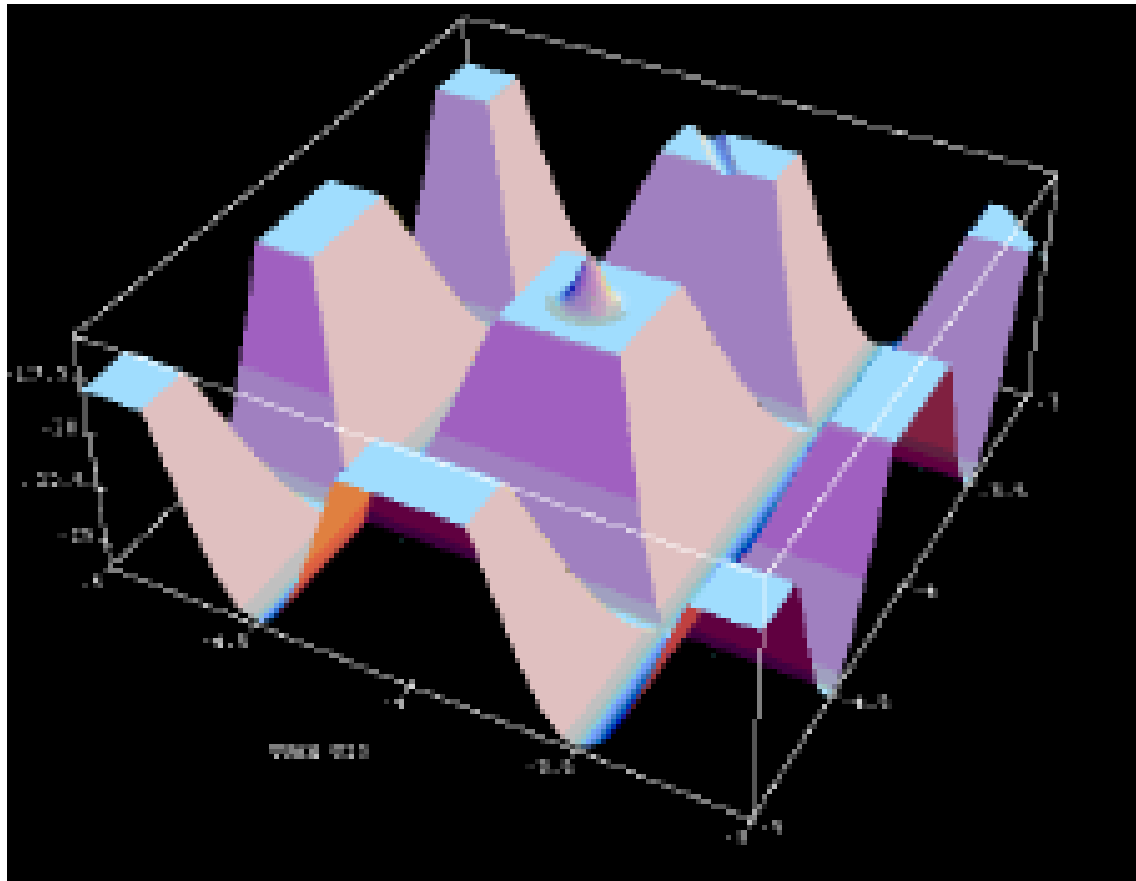
Taken from <http://www.ti3.tu-harburg.de/english/globopt.html>

# NONCONVEX FUNCTIONS— PLATEAUS



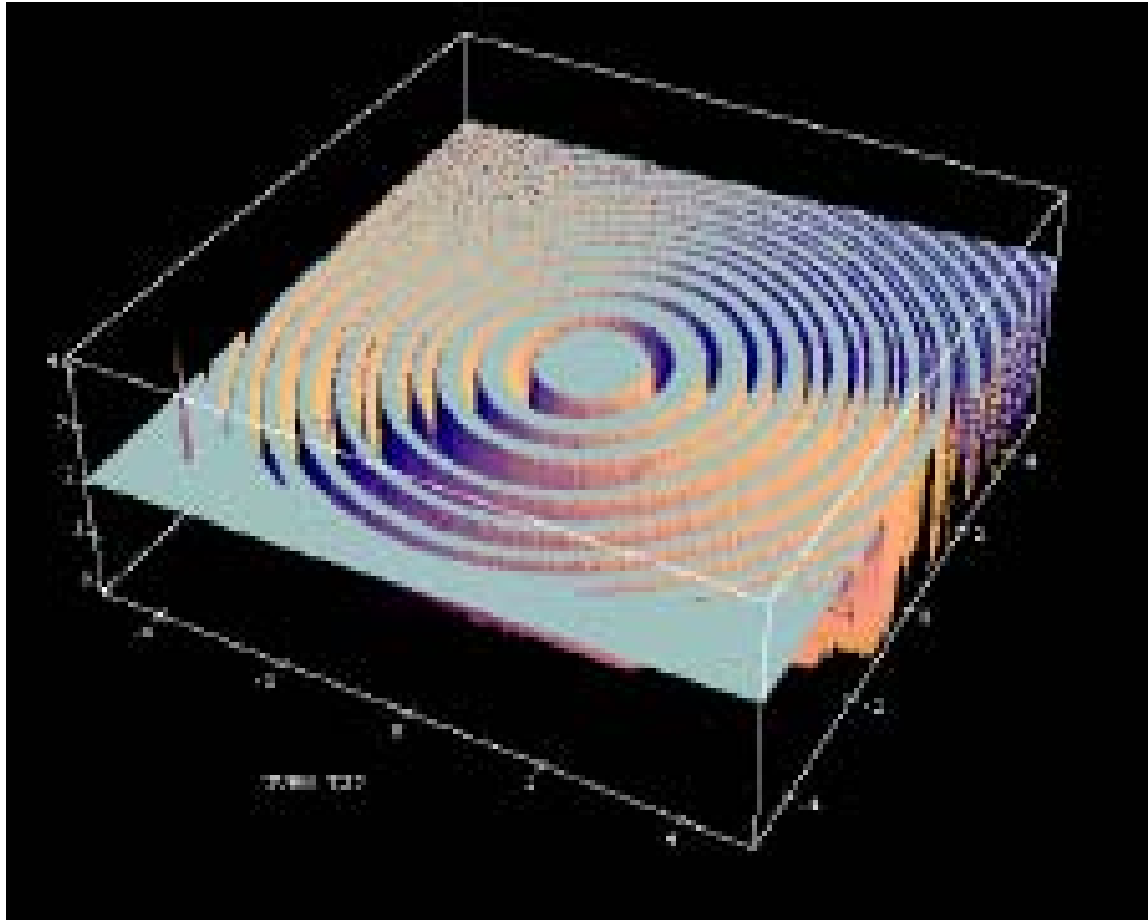
Taken from <http://www.ti3.tu-harburg.de/english/globopt.html>

# NONCONVEX FUNCTIONS— DETAILS OF PLATEAUS



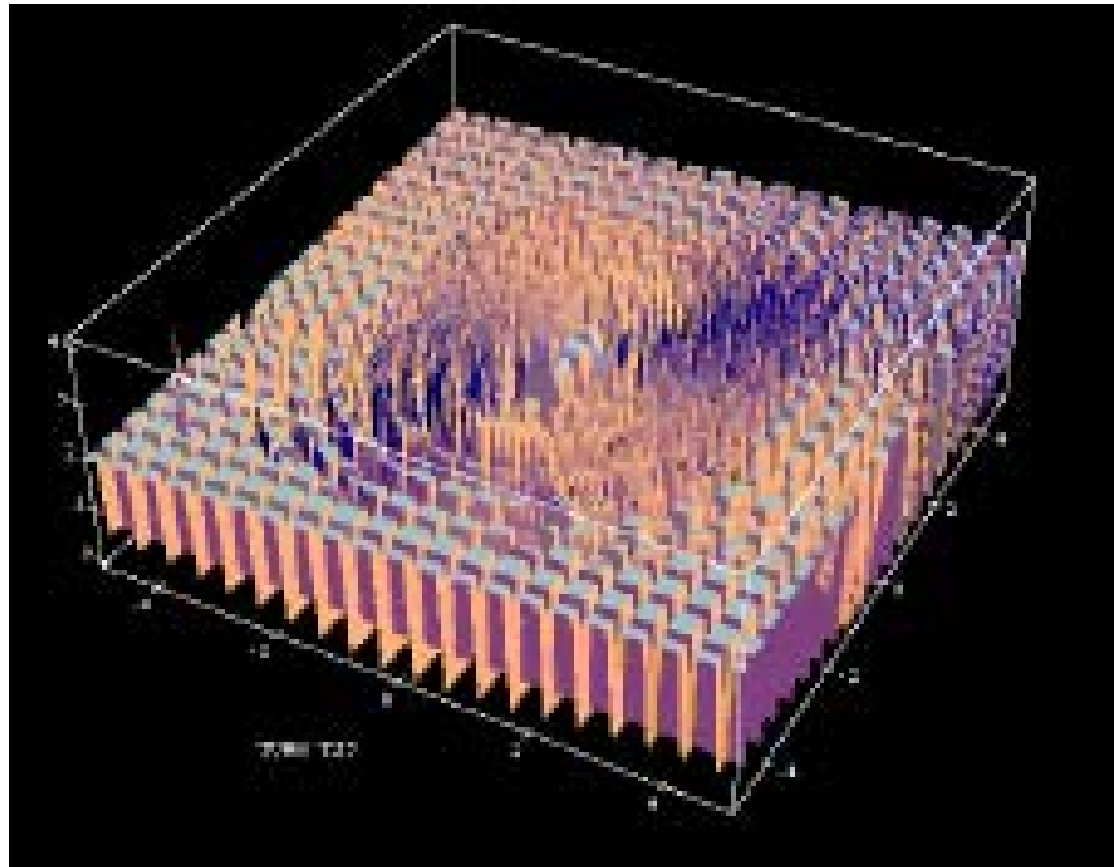
Taken from <http://www.ti3.tu-harburg.de/english/globopt.html>

# NONCONVEX FUNCTIONS— DARTBOARD WITH ARROW



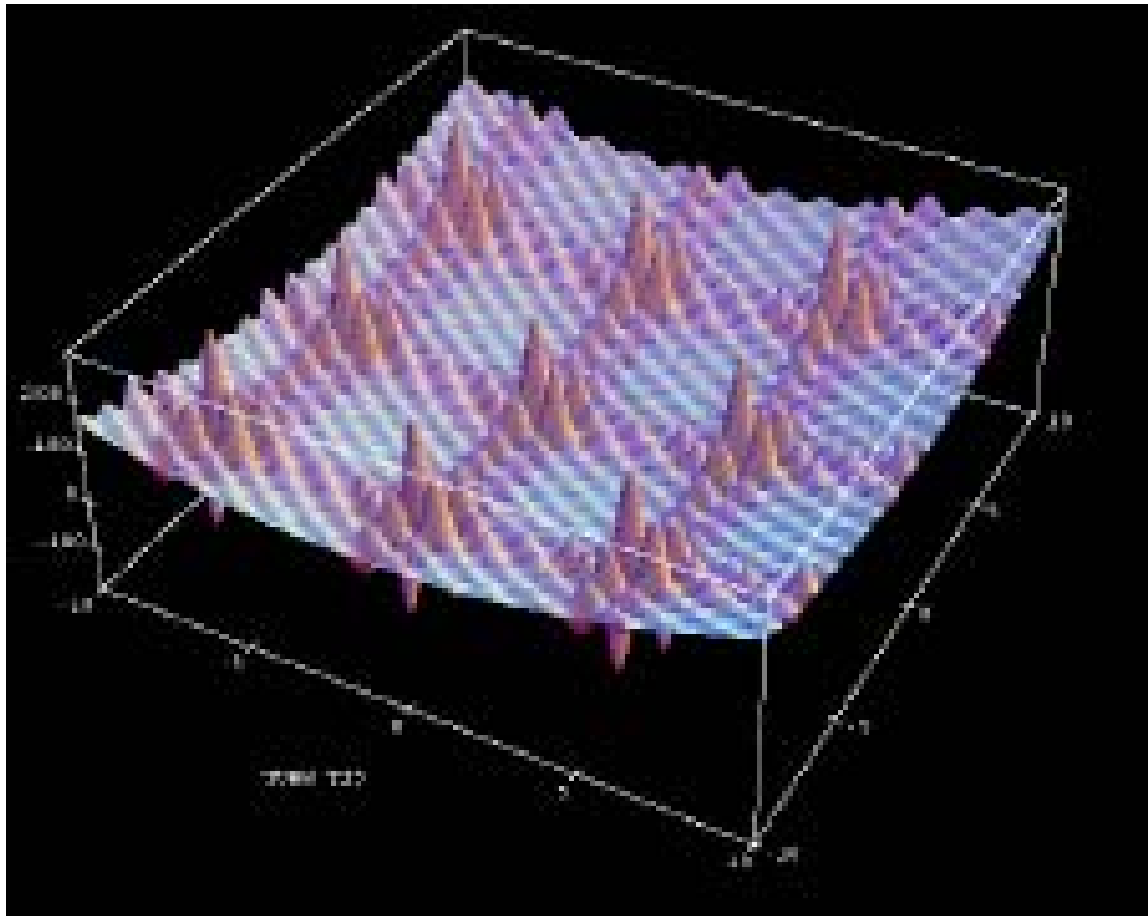
Taken from <http://www.ti3.tu-harburg.de/english/globopt.html>

# NONCONVEX FUNCTIONS— BRYCE CANYON



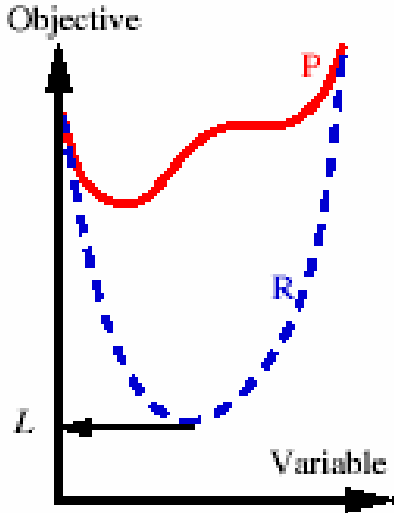
Taken from <http://www.ti3.tu-harburg.de/english/globopt.html>

# NONCONVEX FUNCTIONS— LEVY'S BENT EGG CARDBOARD

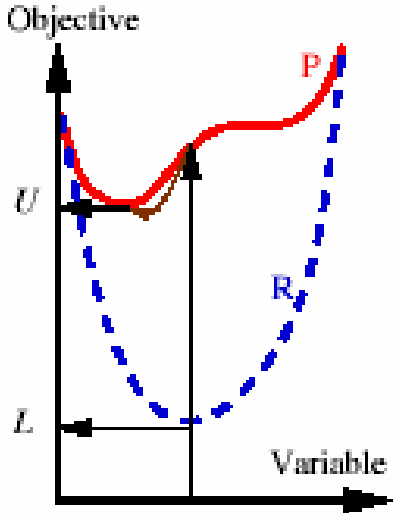


Taken from <http://www.ti3.tu-harburg.de/english/globopt.html>

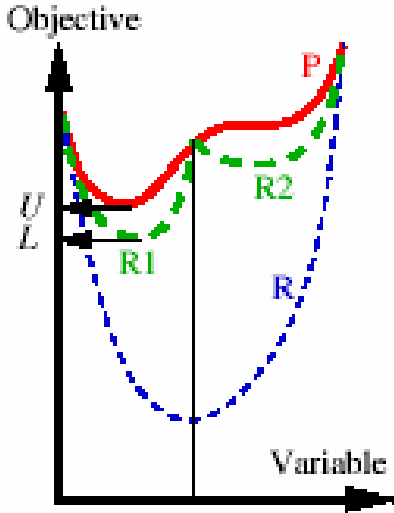
# BRANCH-AND-BOUND



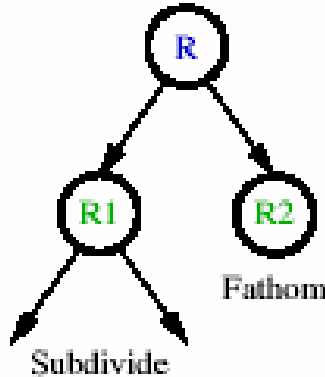
a. Lower Bounding



b. Upper Bounding



c. Domain Subdivision

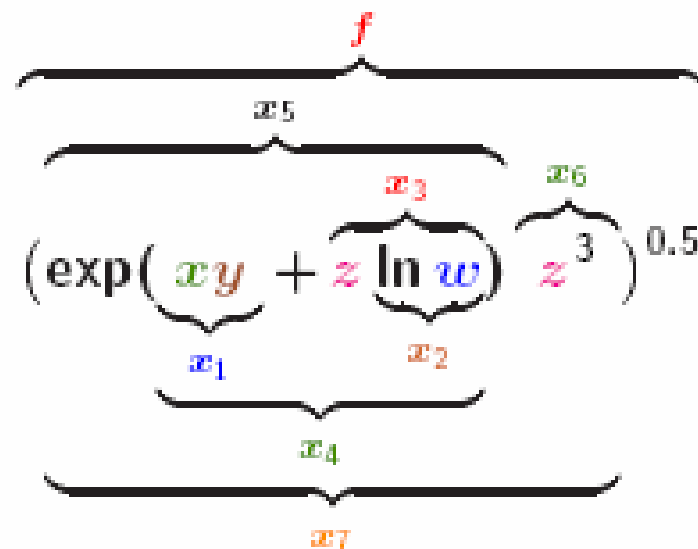


d. Search Tree

# PROCEDURE FOR BOUNDING FACTORABLE PROGRAMS

Introduce variables for intermediate quantities whose envelopes are not known

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



$$x_1 = xy$$

$$x_2 = \ln(w)$$

$$x_3 = z$$

$$x_4 = x_1 + x_3$$

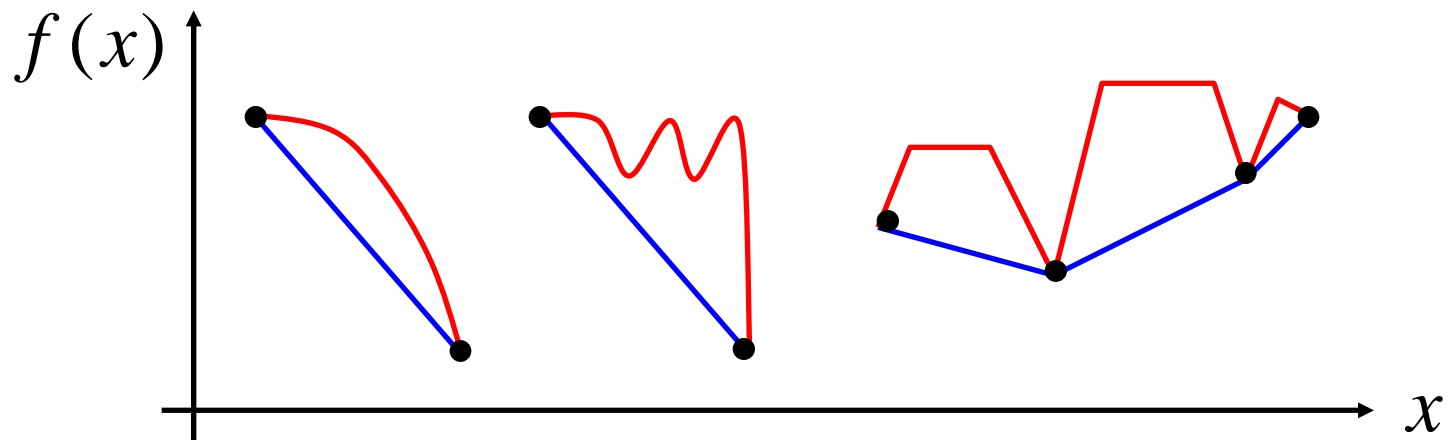
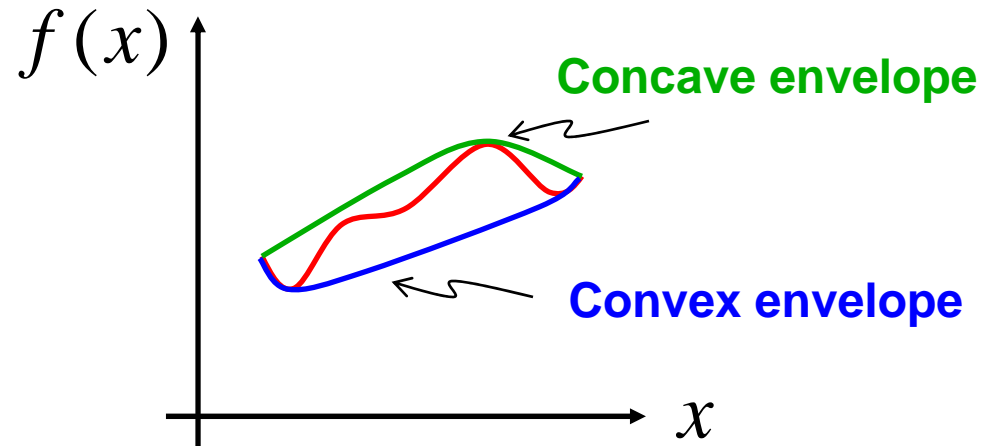
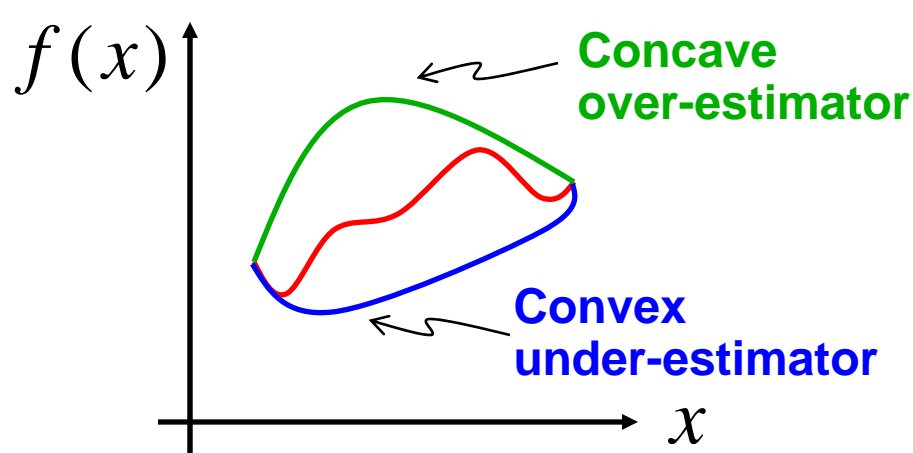
$$x_5 = \exp(x_4)$$

$$x_6 = z^3$$

$$x_7 = x_5 x_6$$

$$f = \sqrt{x_7}$$

# CONVEX/CONCAVE ENVELOPES OFTEN FINITELY GENERATED



# TWO-STEP CONVEX ENVELOPE CONSTRUCTION VIA CONVEX EXTENSIONS

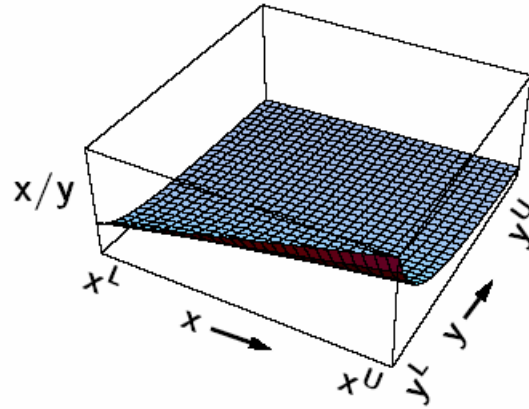
## 1. **Identify generating set** (Tawarmalani and Sahinidis, 2002):

- **Key result:** A point in set  $X$  is *not* in the generating set if it is not in the generating set over a neighborhood of  $X$  that contains it

## 2. **Use disjunctive programming techniques to construct epigraph over the generating set**

- Rockafellar (1970)
- Balas (1974)

# RATIO: FACTORABLE 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

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

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

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

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

Simplifying

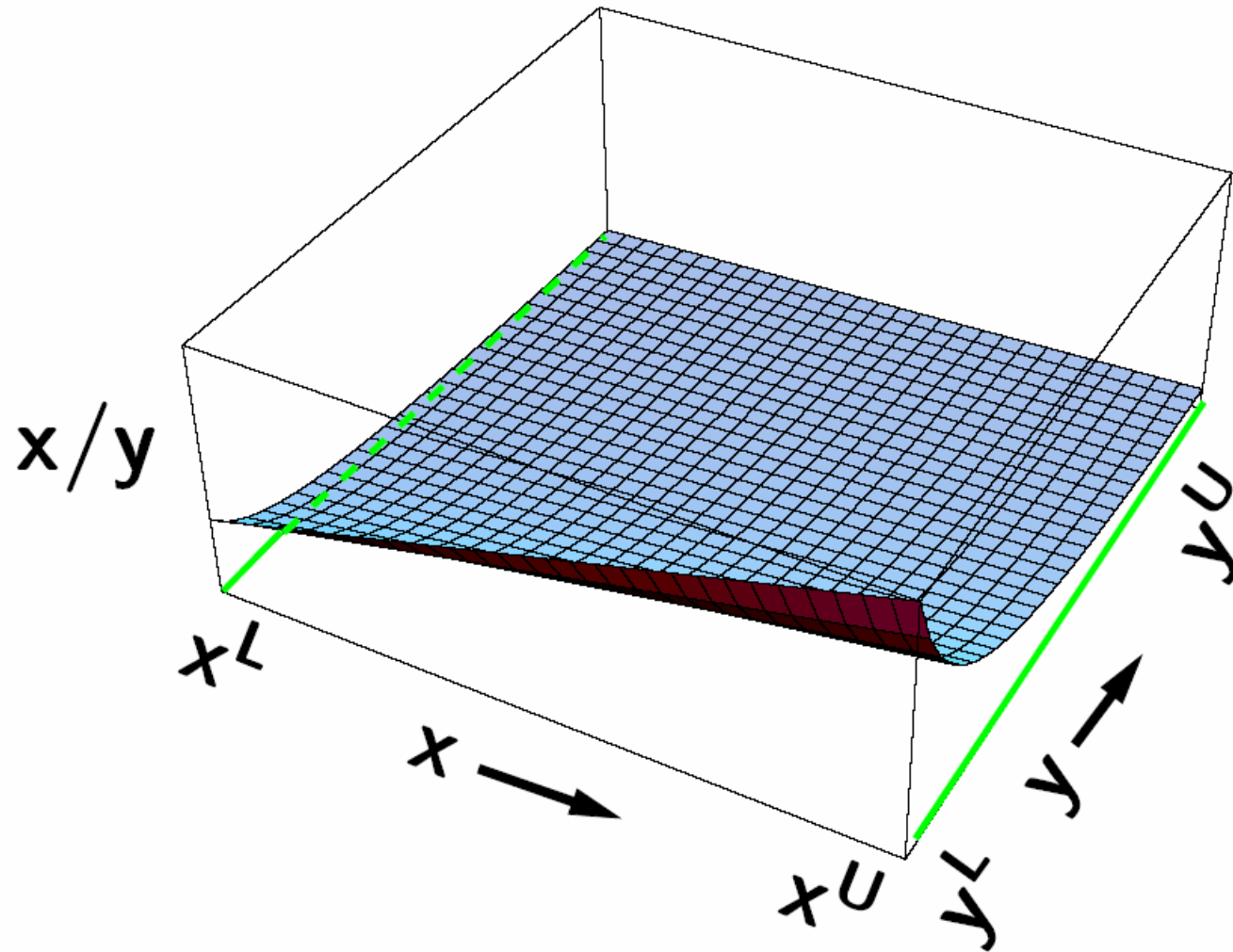
$$z \geq (xy^U - yx^L + x^L y^U)/y^{U^2}$$

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

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

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

# RATIO: THE GENERATING SET



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

# 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**

# PRODUCT DISAGGREGATION

Consider the function:

$$\phi(x; y_1, \dots, y_n) = a_0 + \sum_{k=1}^n a_k y_k + x b_0 + x \sum_{k=1}^n b_k y_k$$

Let

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

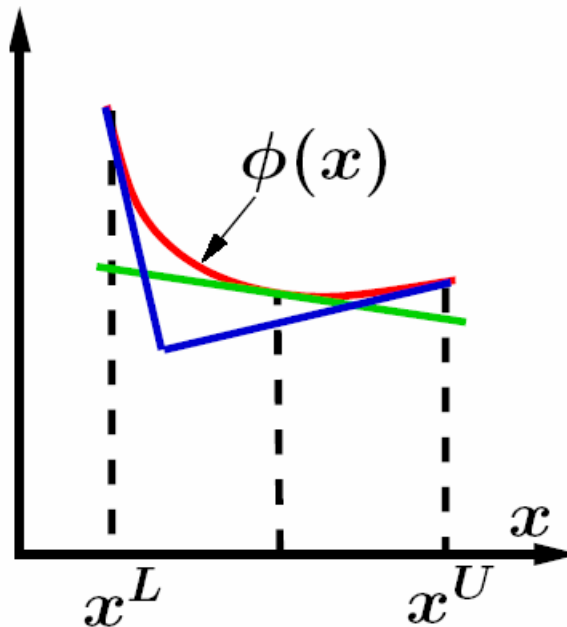
Then

$$\text{convex}_H \phi = a_0 + \sum_{k=1}^n a_k y_k + x b_0 + \sum_{k=1}^n \text{convex}_{[y_k^L, y_k^U] \times [x^L, x^U]} (b_k y_k x)$$

**Disaggregated formulations are tighter**

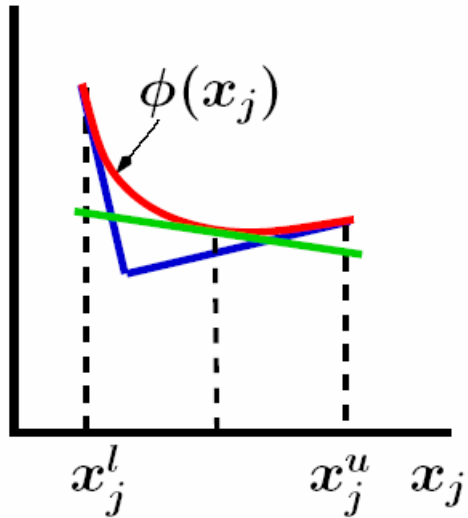
# POLYHEDRAL OUTER APPROXIMATION

- Convex NLP solvers are not as robust as LP solvers
- Linear programs can be solved efficiently
- Outer-approximate convex relaxation by polyhedron

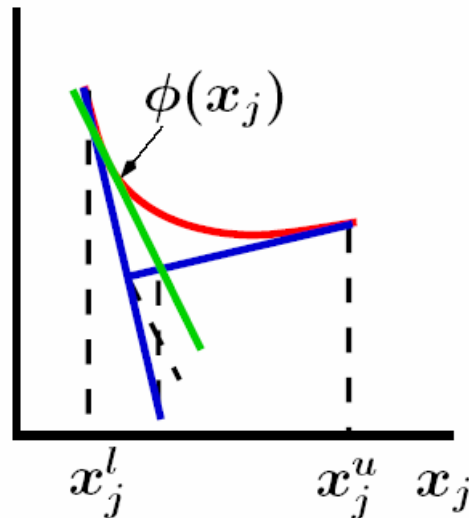


Enjoys quadratic convergence

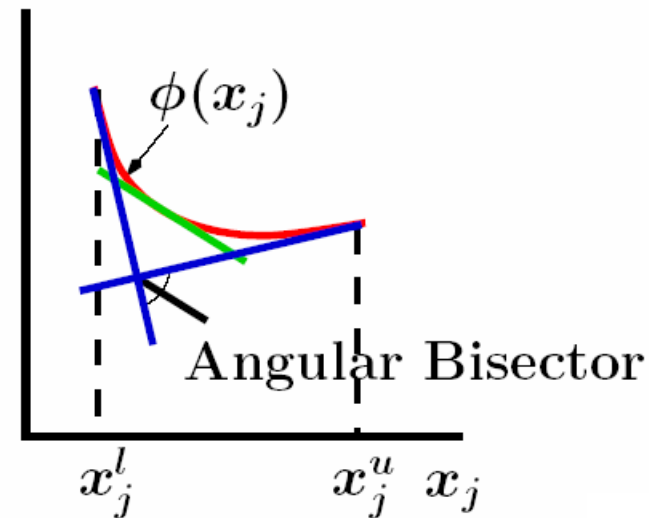
# TANGENT LOCATION RULES



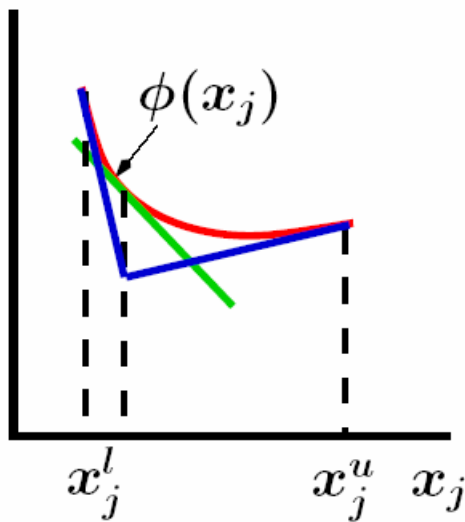
Interval bisection



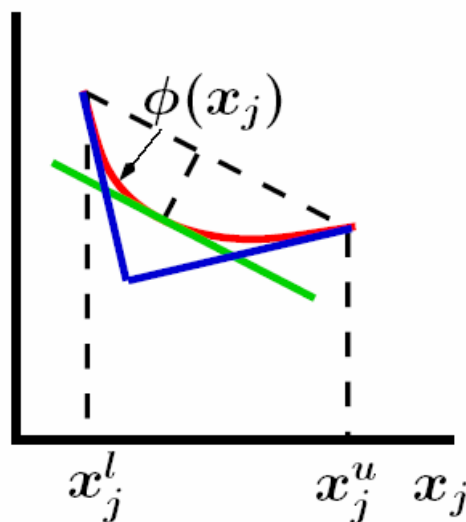
Slope Bisection



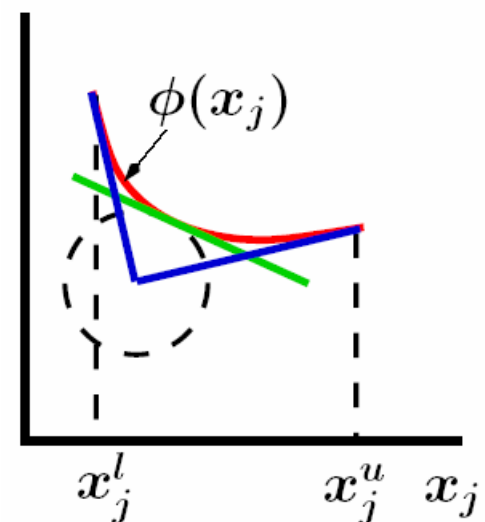
Angle bisection



Maximum error rule

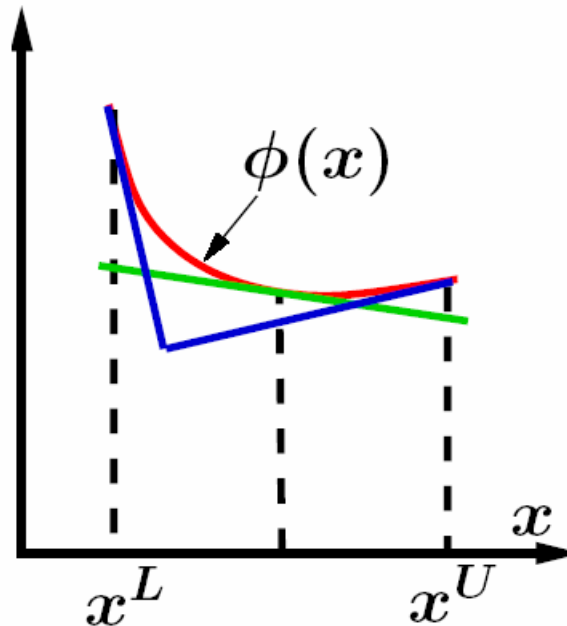


Chord rule



Maximum projective error

# EXPLOITING CONVEXITY

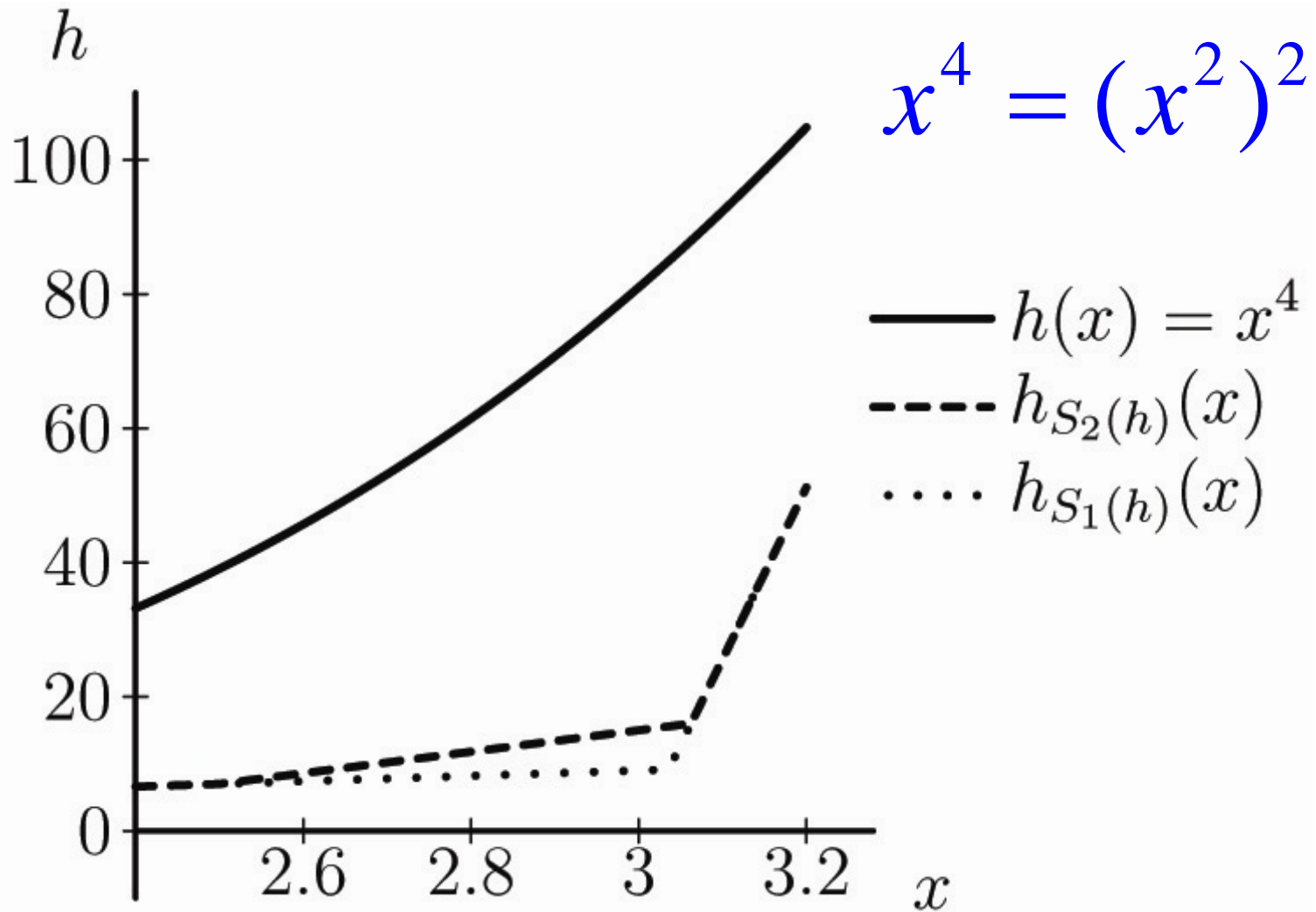


- **Polyhedral relaxations of univariate functions facilitate reliable lower bounding via fast LP routines**
- **Outstanding issues:**
  - Lower bound itself weakens
  - Effect of functional decomposition
  - Polyhedral relaxations of convex multivariate functions
    - Gruber (1993), Böröczky and Reitzner (2004)

# RECURSIVE FUNCTIONAL COMPOSITIONS

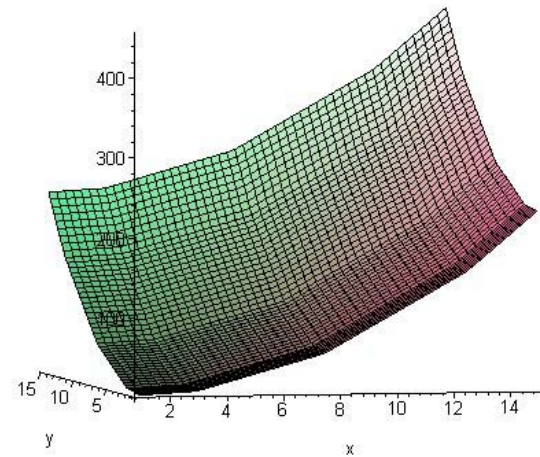
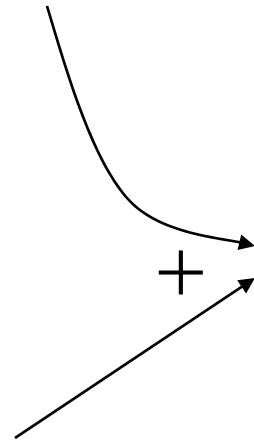
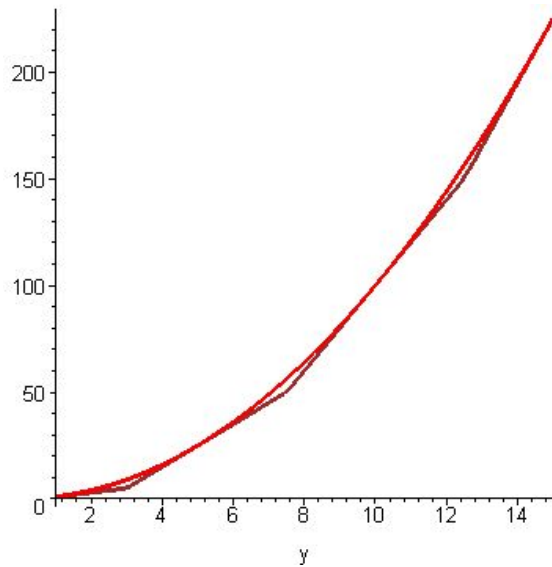
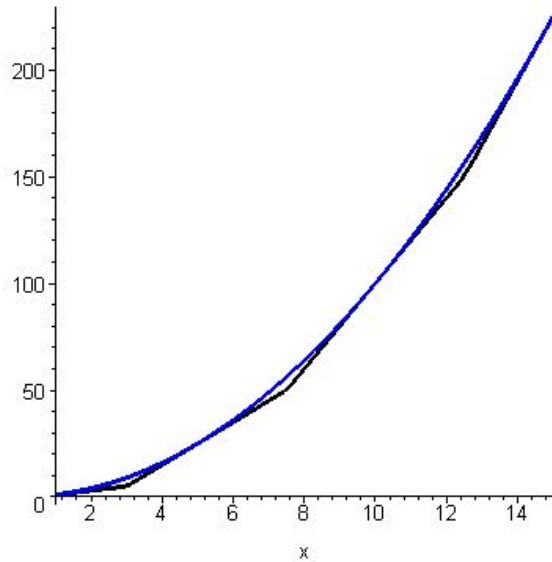
- Consider  $h=g(f)$ , where
  - $g$  and  $f$  are multivariate convex functions
  - $g$  is non-decreasing in the range of each nonlinear component of  $f$
- $h$  is convex
- Two outer approximations of the composite function  $h$ :
  - S1: a single-step procedure that constructs supporting hyperplanes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

# STRICT INCLUSION



Outer - approximating  $x^4$  at  $x = 1$  and  $x = 4$

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



# TWO-STEP IS BETTER

- **Theorem:** An exponential number of supporting hyperplanes in S1 may be required to cover S2

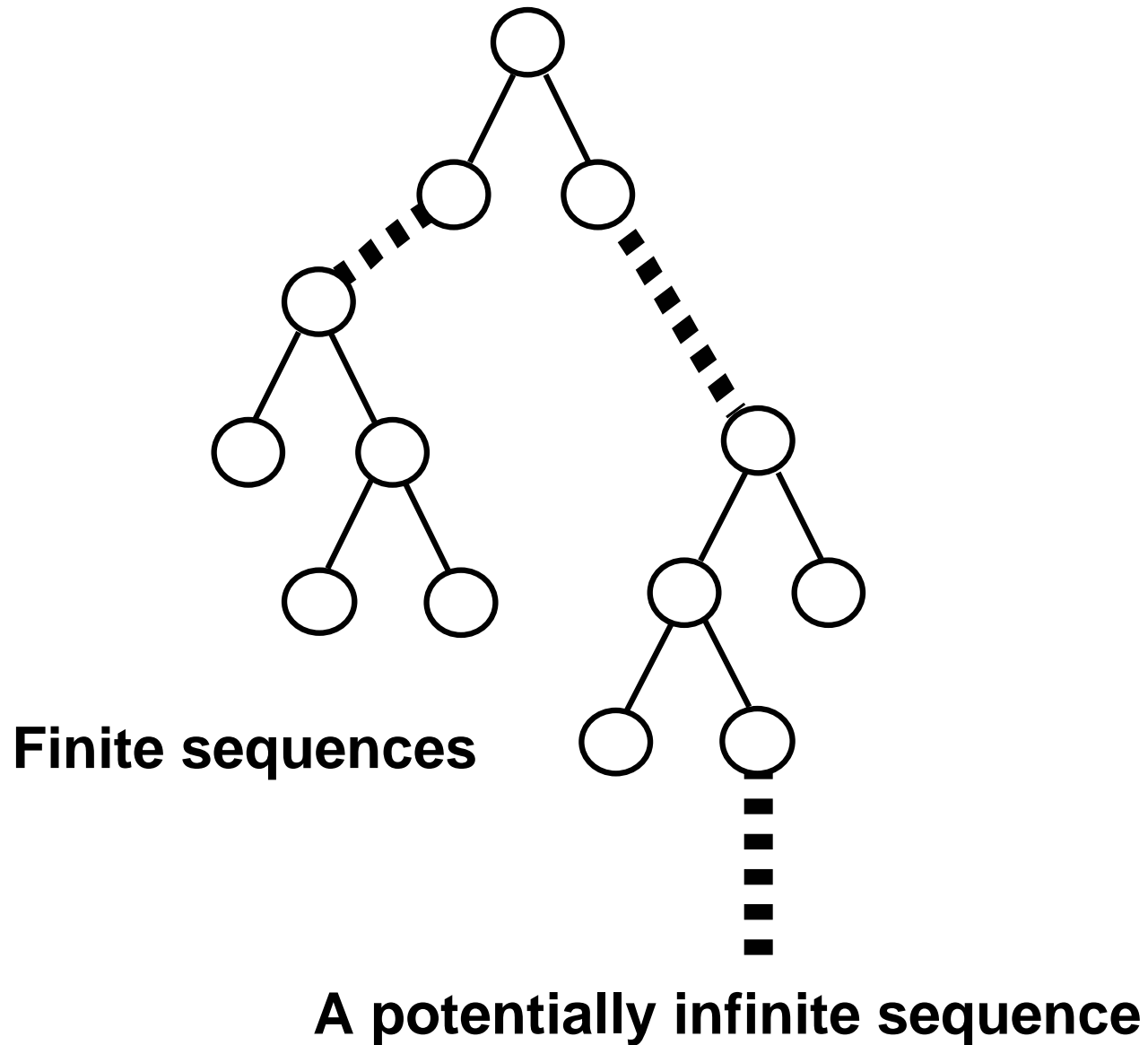
$h = f_1(x_1) + \dots + f_m(x_m)$  where each  $f_i$  is strictly convex

- Separable functions are quite common in nonconvex optimization
- S2 has the potential of providing much tighter polyhedral outer approximations than S1 with a comparable number of supporting hyperplanes

# AUTOMATIC DETECTION AND EXPLOITATION OF CONVEXITY

- **Composition rule:  $h = g(f)$ , where**
  - $g$  and  $f$  are multivariate convex functions
  - $g$  is non-decreasing in the range of each nonlinear component of  $f$
- **Subsumes many known rules for detecting convexity/concavity**
  - $g$  univariate convex,  $f$  linear
  - $g = \max\{f_1(x), \dots, f_m(x)\}$ , each  $f_i$  convex
  - $g = \exp(f(x))$
  - ...
- **Automatic exploitation of convexity is not essential for constructing polyhedral outer approximations in these cases**
  - However,  $\text{logexp}(x) = \log(e^{x_1} + \dots + e^{x_n})$
  - **CONVEX\_EQUATIONS** modeling language construct

# FINITE VERSUS CONVERGENT BRANCH-AND-BOUND ALGORITHMS

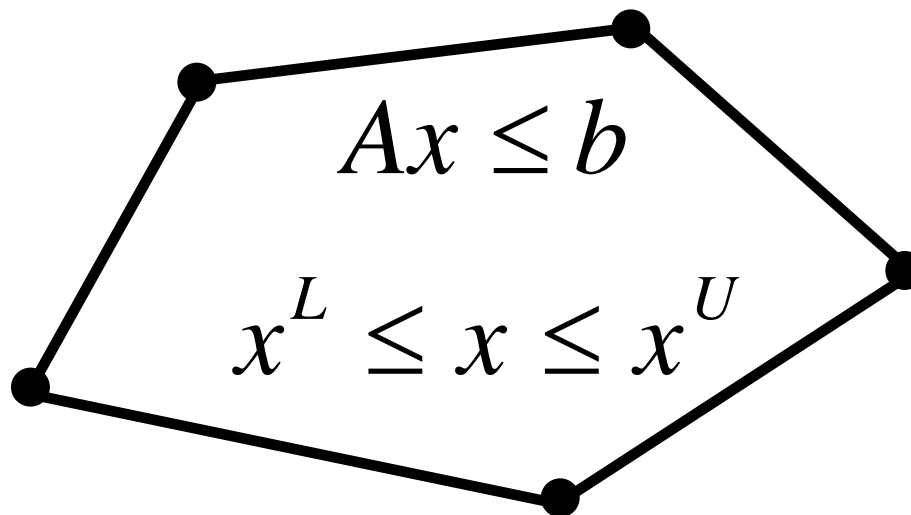


# SEPARABLE CONCAVE MINIMIZATION

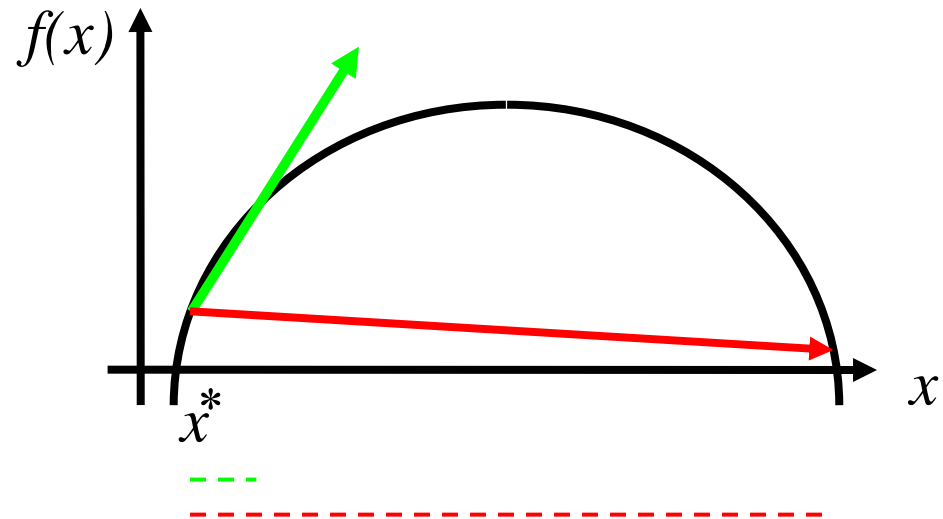
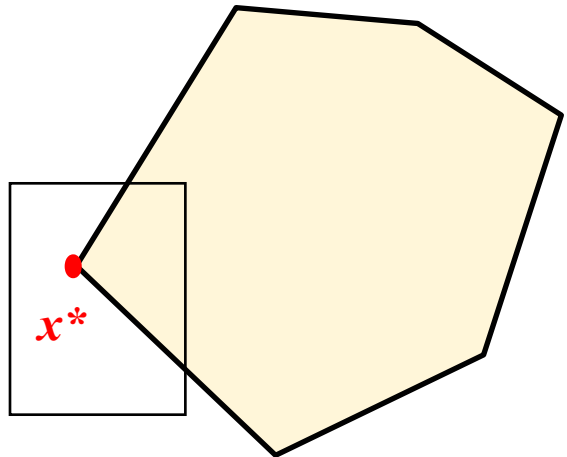
Consider  $f_k(x_k)$  concave,  $\forall k$ .

$$\min f(x) = \sum_k f_k(x_k)$$

s.t.



# FINITE BRANCHING RULE



- **Branching variable selection:**
  - Typically, select variable with largest underestimating gap
  - Occasionally, select variable corresponding to largest edge
- **Branching point selection:**
  - Typically, at the midpoint (exhaustiveness)
  - When possible, at the best currently known solution
    - Makes underestimators exact at the candidate solutions
- **Finite isolation of global optimum**
- **Ascend directions of LP also ascend directions of concave program**

# STOCHASTIC INTEGER PROGRAMMING

$$\min f(x_1, x_2) = -1.5x_1 - 4x_2 + \sum_{s=1}^4 \frac{1}{4} Q^s(x_1, x_2)$$

$$s.t. \quad 0 \leq x_1, x_2 \leq 5$$

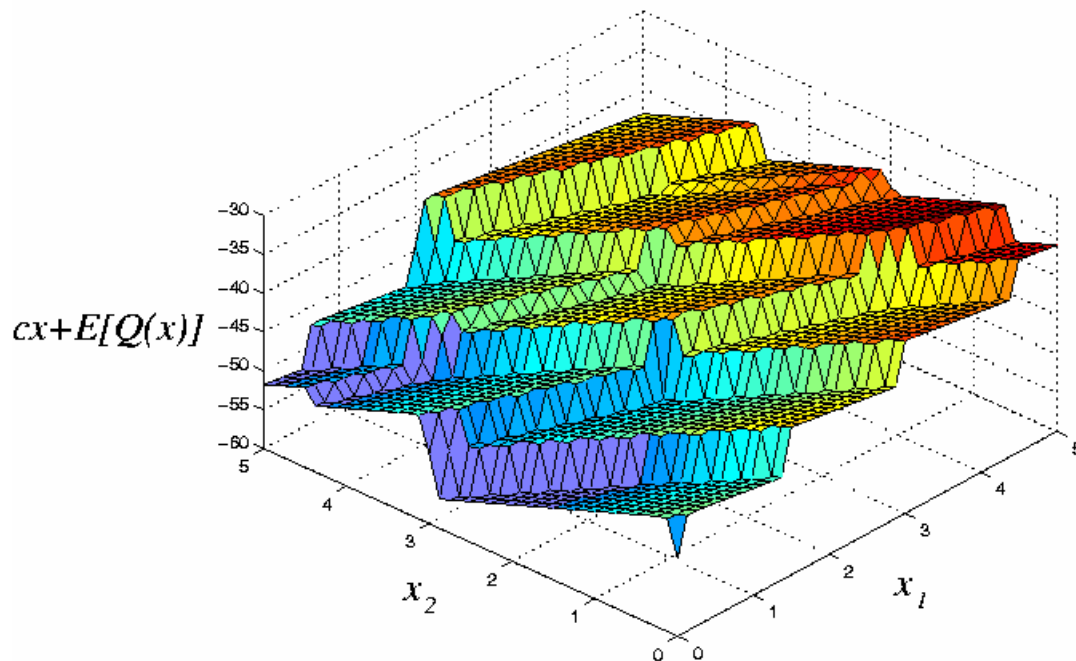
$$Q^s(x_1, x_2) := \min -16y_1 - 19y_2 - 23y_3 - 28y_4$$

$$s.t. \quad 2y_1 + 3y_2 + 4y_3 + 5y_4 \leq \omega_1^s - \frac{1}{2}x_1 - \frac{2}{3}x_2$$

$$6y_1 + y_2 + 3y_3 + 2y_4 \leq \omega_2^s - \frac{2}{3}x_1 - \frac{1}{3}x_2$$

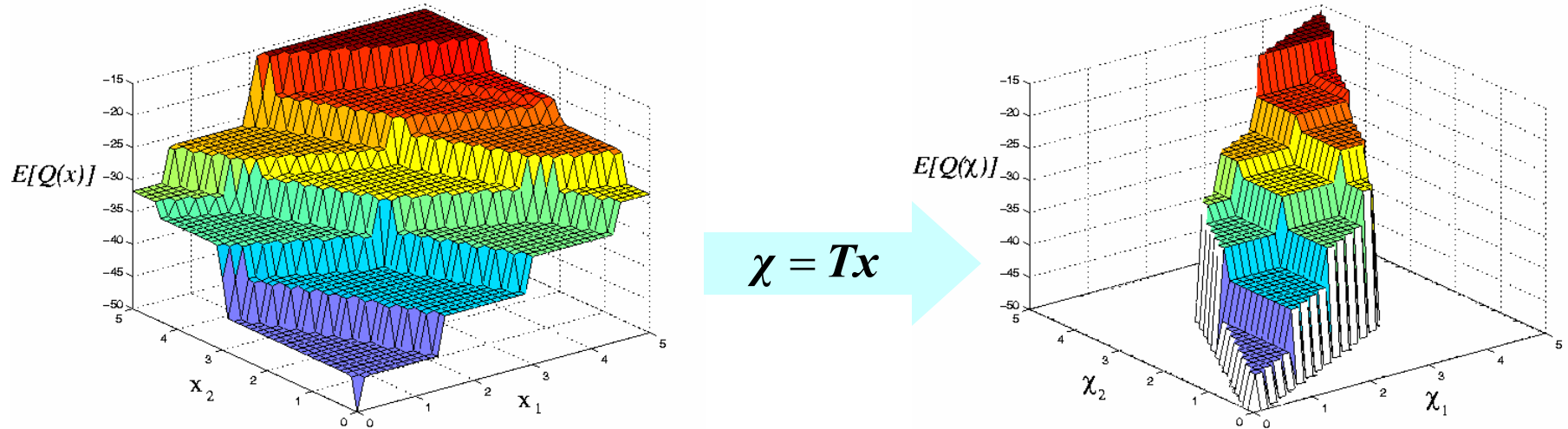
$$y_i \in \{0,1\} \quad \text{for } i=1,\dots,4$$

where  $(\omega_1, \omega_2) \in \{5,15\} \times \{5,15\}$



- Discontinuous
- Highly non-convex
- Many local minima

# VARIABLE TRANSFORMATION

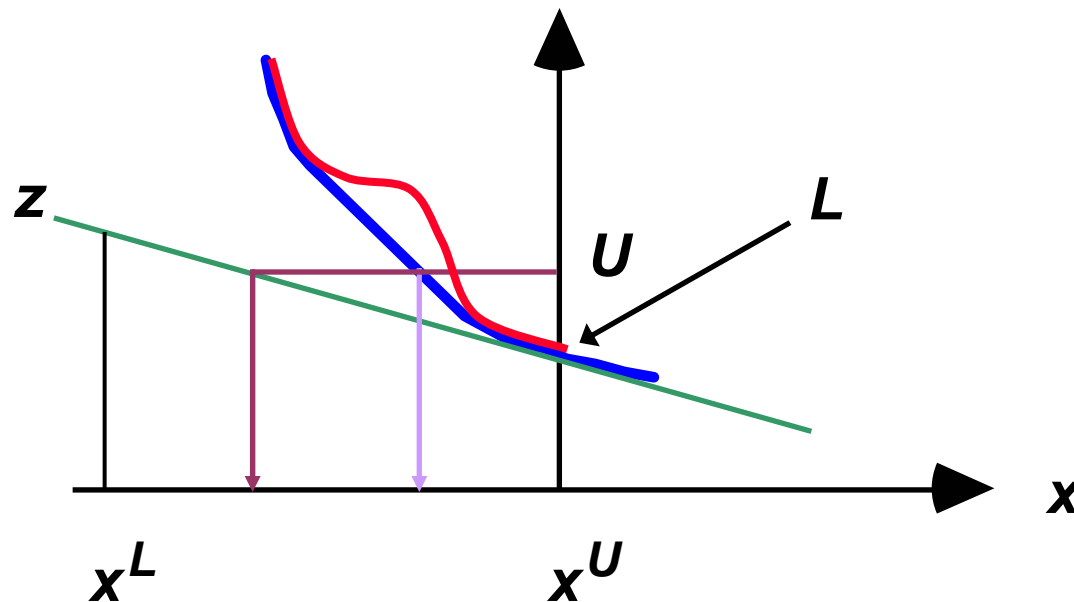


## Ahmed, Tawarmalani and Sahinidis (2004)

- Solve the problem in the space of the “tender variables”
- Variable transformation aligns discontinuities orthogonal to variable axes
- Discontinuities identified based on Blair and Jeroslow (1977) results
- Finite termination

# MARGINALS-BASED RANGE REDUCTION

## Relaxed Value Function

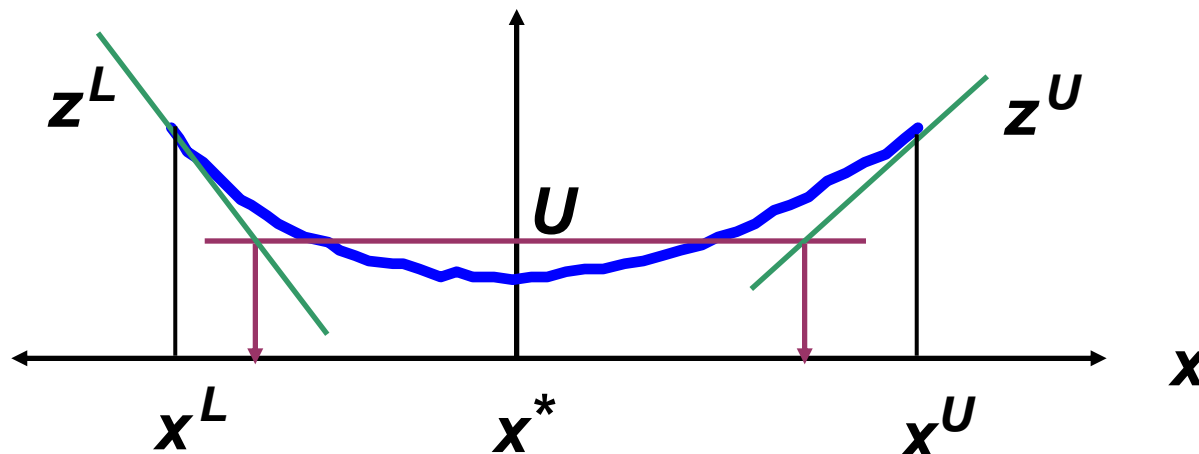


**If a variable goes to its upper bound at the relaxed problem solution, this variable's lower bound can be improved**

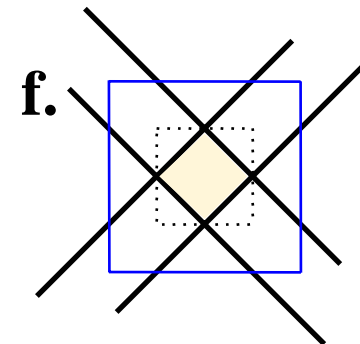
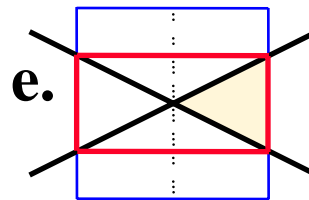
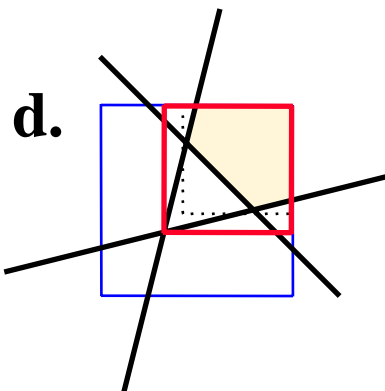
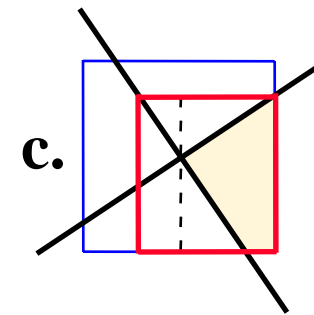
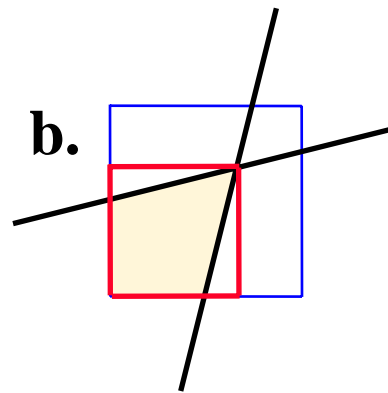
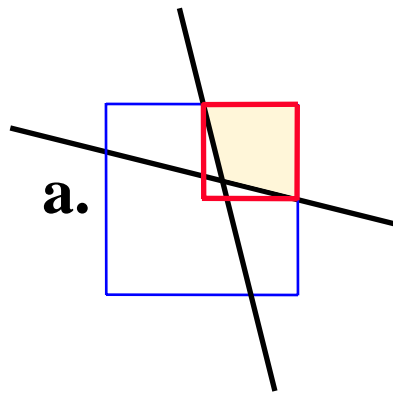
# PROBING

- Q. What if a variable does not go to a bound?
- A. Use probing: temporarily fix variable at a bound or minimize/maximize this variable over the problem constraints

## Relaxed Value Function



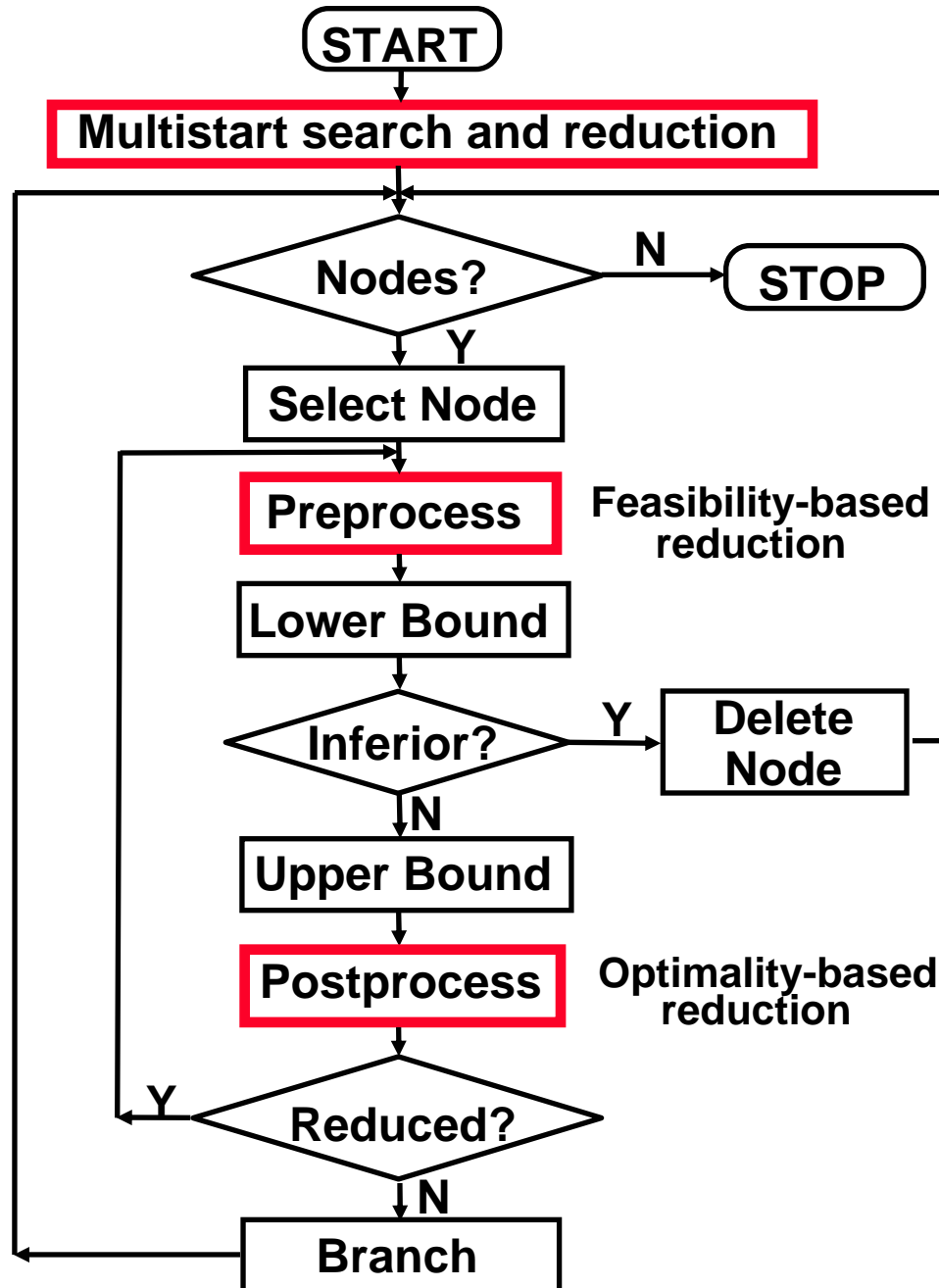
# POOR MAN'S LPs AND NLPs



# **DOMAIN REDUCTION THEORY in T&S book (2002)**

- **Draw inferences about several reduction problems from solutions of problems solved in the course of branch-and-bound**
- **Implied results:**
  - **Monotone complementarity bounds for convex programs**
    - **Mangasarian and McLinden, 1985**
  - **Linearity-based tightening in integer programming**
    - **Andersen and Andersen, 1995**
  - **Marginals-based reduction**
    - **Ryoo and Sahinidis, 1995**
  - **Branch and Contract**
    - **Zamora and Grossmann, 1999**
- **New reduction strategies**
  - **Learning heuristic improves branching decisions**

# BRANCH-AND-REDUCE



# TINY TEST PROBLEMS

<b>Ex.</b>	<b>Cons.</b>	<b>Vars.</b>	<b>Source/In</b>	<b>Description</b>
1	1	2	Sahinidis & Grossmann	bilinear constraint
2	3	3	Liebman et al. (GINO)	design of a water pumping system
3	7	10	Liebman et al. (GINO)	alkylation process optimization
4	1	3	Liebman et al. (GINO)	design of insulated tank
5	3	5	Liebman et al. (GINO)	heat exchanger network design
6	3	3	Liebman et al. (GINO)	chemical equilibrium
7	7	10	Liebman et al. (GINO)	pooling problem
8	2	2	Swaney	bilinear and quadratic constraints
9	1	2	Swaney	bilinear constraints and objective
10	1	2	Soland	nonlinear equality constraint
11	2	3	Westerberg & Shah	bilinearities, economies of scale
12	3	4	Stephanopoulos & Westerberg	design of two-stage process systems
13	3	2	Kocis & Grossmann	MINLP, process synthesis
14	10	7	Yuan et al.	MINLP, process synthesis
15	6	5	Kocis & Grossmann	MINLP, process synthesis
16	9	12	Floudas & Ciric	heat exchanger network synthesis
17	2	2	GINO	design of a reinforced concrete beam
18	4	2	Visweswaran & Floudas	quadratically constrained LP
19	2	2	Manousiouthakis & Surlas	quadratically constrained QP
20	6	5	Manousiouthakis & Surlas	reactor network design
21	6	5	Stephanopoulos & Westerberg	design of three-stage process system
22	5	2	Kalantari & Rosen	linearly constrained concave QP
23	2	2	Al-Khayyal & Falk	biconvex program
24	4	2	Thakur	linearly constrained concave QP
25	4	2	Falk & Soland	nonlinear fixed charge problem

# STANDARD BRANCH-AND-BOUND

Ex.	$N_{tot}$	$N_{opt}$	$N_{mem}$	T
1	3	1	2	0.8
2	1007	1	200	210
3	2122*	1	113*	1245*
4	17	1	5	6.7
5	1000*	1	1000*	417*
6	1	1	1	0.3
7	205	1	37	43
8	43	1	8	1
9	2192*	1	1000*	330*
10	1	1	1	0.4
11	81	1	24	19
12	3	1	2	0.6
13	7	2	3	1.3
14	7	3	3	3.4
15	15	8	5	3.4
16	2323*	1	348*	1211*
17	1000*	1	1001*	166*
18	1	1	1	0.5
19	85	1	14	11.4
20	3162*	1	1001*	778*
21	7	1	4	1.2
22	9	1	4	1.2
23	75	6	13	11.7
24	7	3	2	1.5
25	17	9	9	2.9

$N_{tot}$  Total number of nodes  
 $N_{opt}$  Node where optimum found  
 $N_{mem}$  Max. no. nodes in memory  
T CPU sec (SPARC 2)

- Standard branch-and-bound converges very slowly
- It is not necessarily finite
- Tighter relaxations needed

\*: Did not converge within limits of  
 $T \leq 1200$  (=20 min), and  $N_{mem} \leq 1000$  nodes.

# REDUCTION BENEFITS

Ex.	BRANCH-AND-BOUND				BRANCH-AND-REDUCE							
	N <sub>tot</sub>	N <sub>opt</sub>	N <sub>mem</sub>	T	No probing				With Probing			
					N <sub>tot</sub>	N <sub>opt</sub>	N <sub>mem</sub>	T	N <sub>tot</sub>	N <sub>opt</sub>	N <sub>mem</sub>	T
1	3	1	2	0.8	1	1	1	0.5	1	1	1	0.7
2	1007	1	200	210	1	1	1	0.2	1	1	1	0.3
3	2122*	1	113*	1245*	31	1	7	20	9	1	5	48
4	17	1	5	6.7	3	1	2	0.4	1	1	1	0.3
5	1000*	1	1000*	417*	5	1	3	1.5	5	1	3	2.4
6	1	1	1	0.3	1	1	1	0.3	1	1	1	0.3
7	205	1	37	43	25	1	8	5.4	7	1	2	5.8
8	43	1	8	10	1	1	1	0.8	1	1	1	0.8
9	2192*	1	1000*	330*	19	1	8	5.4	13	1	4	7
10	1	1	1	0.4	1	1	1	0.4	1	1	1	0.4
11	81	1	24	19	3	1	2	0.6	1	1	1	0.7
12	3	1	2	0.6	1	1	1	0.2	1	1	1	0.2
13	7	2	3	1.3	3	1	2	0.7	1	1	1	0.7
14	7	3	3	3.4	7	3	3	2.7	3	3	2	3
15	15	8	5	3.4	1	1	1	0.3	1	1	1	0.3
16	2323*	1	348*	1211*	1	1	1	2.2	1	1	1	2.4
17	1000*	1	1001*	166*	1	1	1	3.7	1	1	1	4
18	1	1	1	0.5	1	1	1	0.5	1	1	1	0.6
19	85	1	14	11.4	9	1	4	1.8	1	1	1	1.4
20	3162*	1	1001*	778*	47	1	12	16.7	23	1	5	15.4
21	7	1	4	1.2	1	1	1	0.5	1	1	1	0.5
22	9	1	4	1.2	3	1	2	0.4	3	1	2	0.5
23	75	6	13	11.7	47	1	9	6.5	7	1	4	5
24	7	3	2	1.5	3	1	2	0.5	3	1	2	0.6
25	17	9	9	2.9	5	1	3	0.8	5	1	3	1

# 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, XA, MINOS, SNOPT, OSL, SDPA, ...

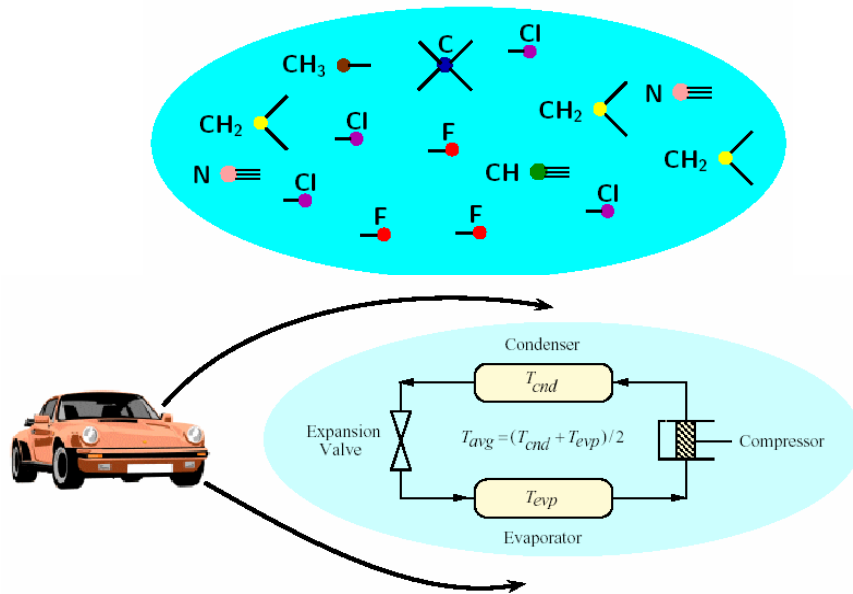
- First on the Internet in March 1995
- On-line solver between October 1999 and May 2003
  - Solved eight problems a day
- Available under GAMS and AIMMS

# BARON IN APPLICATIONS

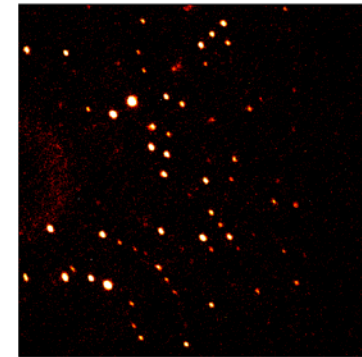
- Development of new **Runge-Kutta methods** for partial differential equations
  - Ruuth and Spiteri, *SIAM J. Numerical Analysis*, 2004
- **Energy policy** making
  - Manne and Barreto, *Energy Economics*, 2004
- Design of **metabolic pathways**
  - Grossmann, Domach and others, *Computers & Chemical Engineering*, 2005
- Automatic **control**
  - Bemporand and Ljung, *Automatica*, 2004
- Product and process **design**
  - Koksalan and Plante, *Manufacturing and Service Operations Management*, 2003
- **Design** of containerships
  - Sherali and Ganesan, *Journal of Global Optimization*, 2003

# CHEM-, BIO- and MEDICAL INFORMATICS

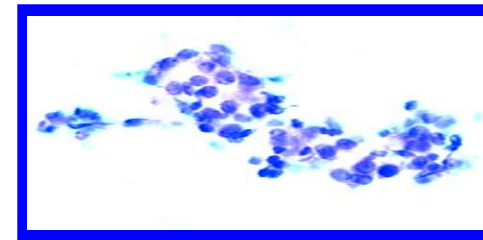
## Molecular design



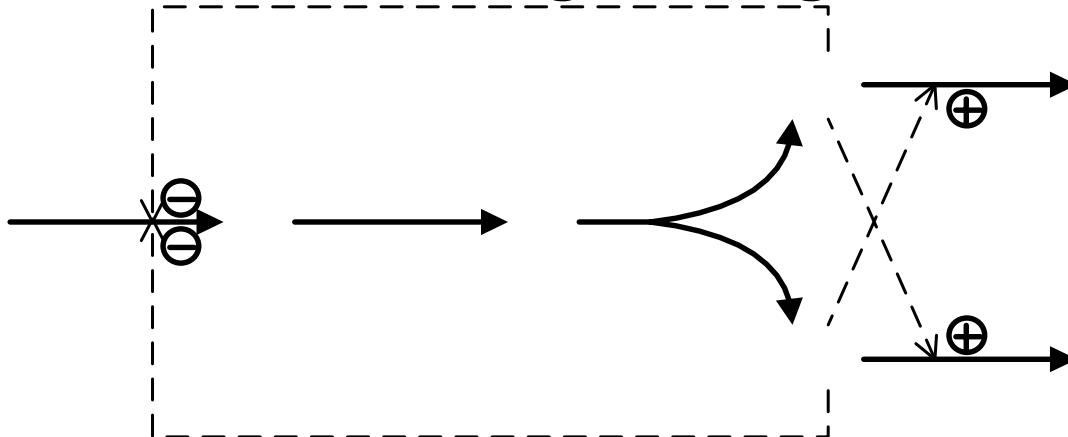
## X-ray imaging



## Breast cancer diagnosis



## Metabolic engineering



## Bioinformatics

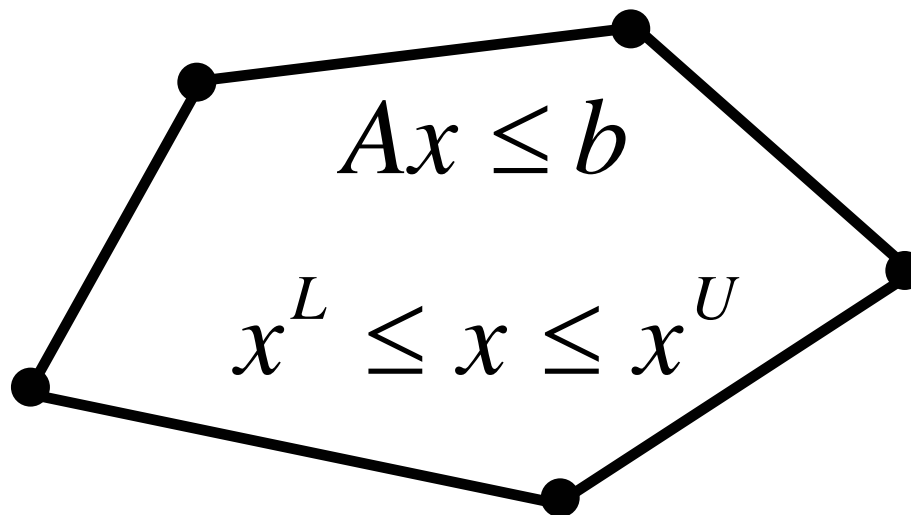
```
TTTGTGTCGTTTCACAAAATGGAAGTCCACA  
CACGGCGTCACACTTTGCTATGCCATAGCATT  
TACACAAAGTTAATAACGTGTCATGTCATG  
TGTATGCAAAAGGACGTCACATTACCGTCAGTAC  
GATCACGTTTTAGACCATTTTTTCGTCGTGAAC  
TGTGTCGTGTCGATGTGTGTCGGAGTAGA  
TTTTCGCATCTTTGTTATGCTATGTTATTTTCAT
```

# SEPARABLE CONCAVE MINIMIZATION

Consider  $f_k(x_k)$  concave,  $\forall k$ .

$$\min f(x) = \sum_k f_k(x_k)$$

s.t.



# PHILLIPS AND ROSEN PROBLEMS

			GOP (1993) E=1% (relative) HP 730		P&R (1990) E=0.1% (relative) CRAY 2 (parallel)			BARON (1996) $\epsilon=.000001$ (absolute) IBM RS/6000 Power PC		
m	n	k	avg	std dev	min	avg	max	min	avg	max
20	25	0	0.5	0.01	1	2	4	0.3	0.4	0.5
20	25	50	2	2	1	1	1	1	1	1
20	25	100	17	20	1	2	3	1	2	3
20	25	200	33	28	2	7	17	2	4	6
20	25	400	82	58	7	14	32	4	10	16
20	50	0	0.6	0.01	3	6	13	1	1	1
20	50	50	17	31	1	2	3	2	2.5	3
20	50	100	47	49	2	5	14	2	4	7
20	50	200	109	80	4	9	28	4	8	19
20	50	400			20	32	45	11	20	48
40	25	0	0.5	0.02				0.3	0.4	0.4
40	25	50	1	0.6				1	1	1
40	25	100	3	4				1	2	3
40	25	200	25	26				2	4	5
40	25	400						6	15	22
50	100	0						6	7	14
50	100	50						8	12	18
50	100	100						9	17	27
50	100	200						14	65	160
50	100	400						131	345	663

- (m, n/k) = number of constraints, concave/linear variables.
- HP 730 is 3-4 times faster than IBM RS/6000 Power PC.
- CRAY 2 is 10+ times faster than IBM RS/6000 Power PC.

# CUTTING PLANE GENERATION

- **Use supporting hyperplanes (outer approximation) of convex functions from:**
  - Univariate convex functions of original problem
  - Univariate convex functions obtained from functional decomposition of multivariate functions
  - Convex envelopes of nonconvex functions
  - Multivariate functions identified by `CONVEX_EQUATIONS` modeling language construct by the user
- **Supporting hyperplanes generated only if they are violated by LP solution**
- **Process:**
  - Start with a rough outer approximation
  - Solve LP
  - Add some cuts
  - Repeat process at current node

# ILLUSTRATIVE EXAMPLE 1: CUTS FROM CONVEX ENVELOPES

$$\begin{array}{ll} \min & x^2 - 100x + y^2 - 30y + 1000\frac{x}{y} \\ \text{s.t.} & 0 \leq x \leq 1000 \\ & 1 \leq y \leq 1000 \end{array}$$

**Solution -1118  
at (34.3, 31.8)**

Iteration    Lower bound    Relaxation optimal solution

1            -7500.9             $x_1 = (65.3, 66.5)$

2            -3832.2             $x_2 = (33.1, 34.1)$

3            -2839.5             $x_3 = (49.2, 19.0)$

4            -2325.7             $x_4 = (41.1, 25.6)$

5            -2057.5             $x_5 = (37.1, 22.3)$

6            -2041.1             $x_6 = (39.1, 23.9)$

**Cutting planes  
reduce root-node  
gap by 86%**

**With cuts: 7 nodes  
Without: 47 nodes**

# ILLUSTRATIVE EXAMPLE 2: CONVEX\_EQUATIONS CONSTRUCT

$$\begin{aligned} \min \quad & 100 \log(e^{x_1} + e^{x_2} + e^{x_3}) + x_1^2 - 40x_1 \\ & + x_2x_3 - 10 \log(x_1) + x_2^2 - 20x_2 - 50x_3 \\ \text{s.t.} \quad & 1 \leq x_1 \leq 10 \\ & 1 \leq x_2 \leq 10 \\ & 1 \leq x_3 \leq 10 \end{aligned}$$

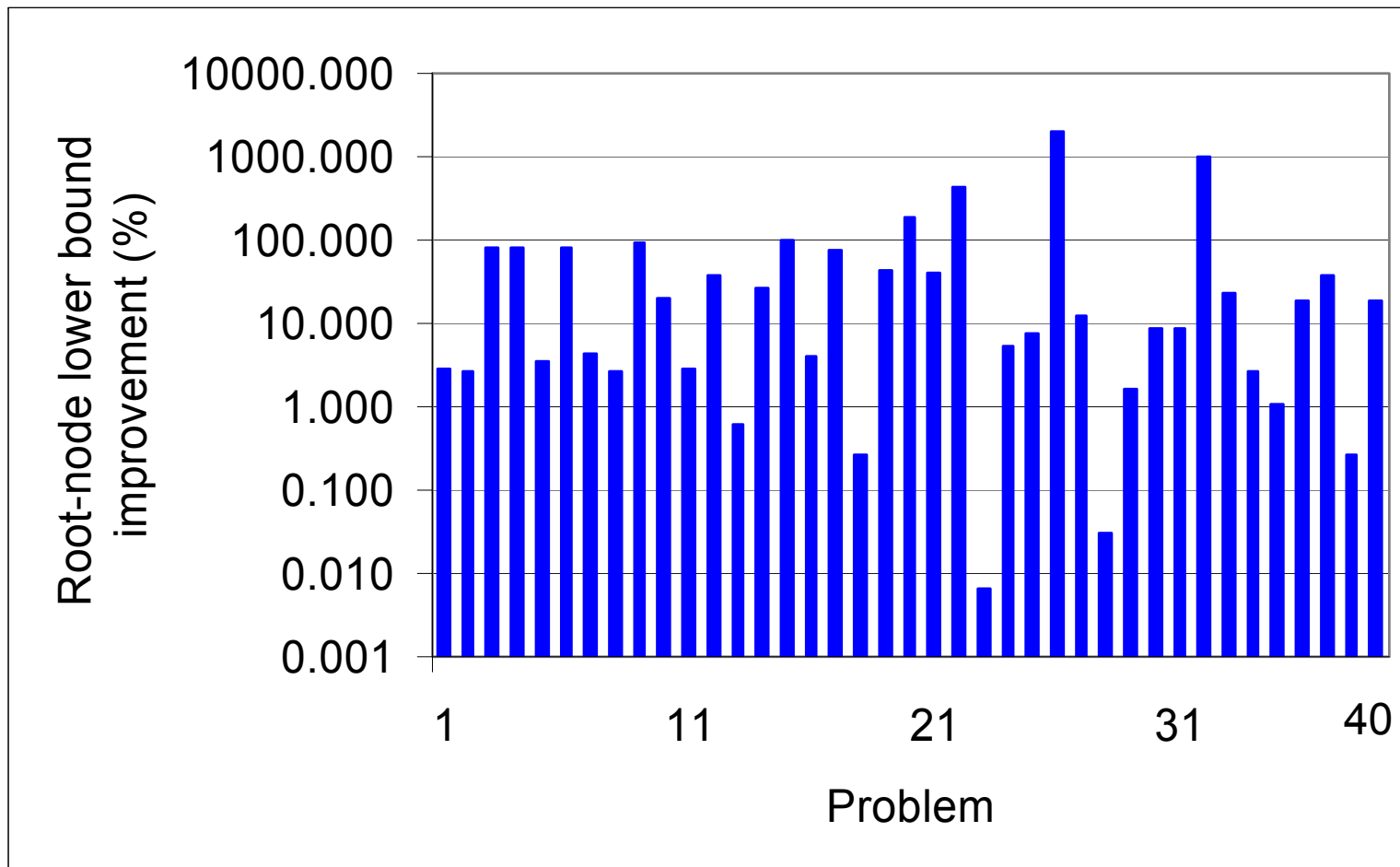
**Solution 83.28**

Iteration	Lower bound 1	Lower bound 2
1	-586.9	62.5
2	-514.9	78.9
3	-445.8	79.6
4	-436.2	80.2
5	-432.9	80.6

**Cutting planes  
reduce root-node  
gap by 99.5%**

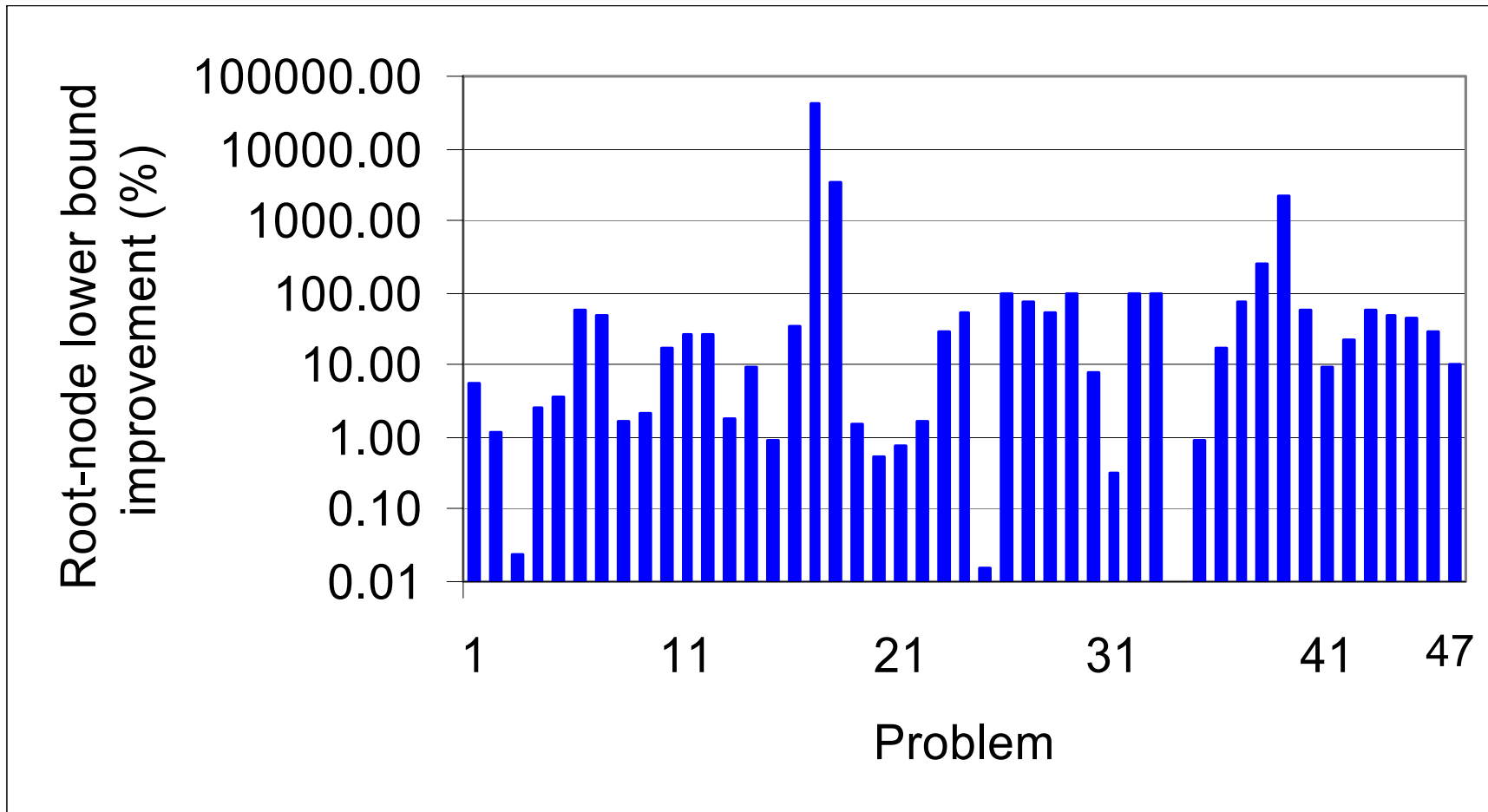
**With cuts: 35 nodes  
Without: 1793 nodes**

# ROOT-NODE LOWER BOUND IMPROVEMENTS FOR `globallib`



**Up to 2000% improvement**

# ROOT-NODE LOWER BOUND IMPROVEMENTS FOR `minlp1ib`



**Up to 41357% improvement**

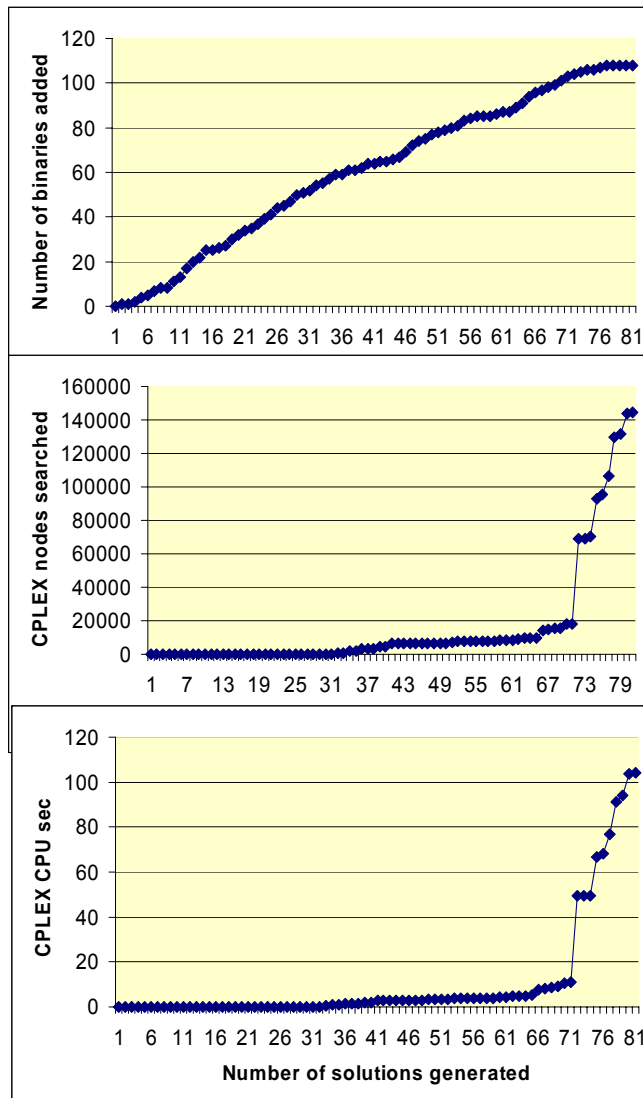
# 26 PROBLEMS FROM globallib AND minlp1ib

	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 sec	275,163	20,430	93

# FINDING THE $K$ -BEST OR ALL FEASIBLE SOLUTIONS



Typically found through repetitive applications of branch-and-bound and generation of “integer cuts”

$$\min \sum_{i=1}^4 10^{4-i} x_i$$

$$\text{s.t. } 2 \leq x_i \leq 4, \quad i = 1, \dots, 4$$

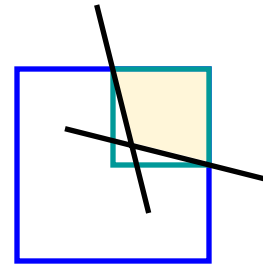
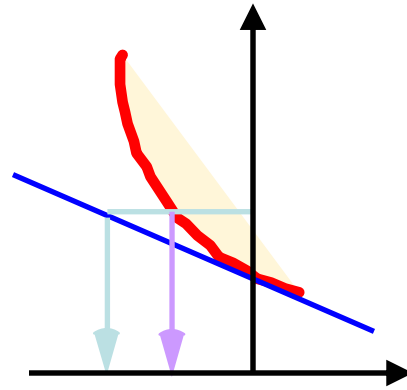
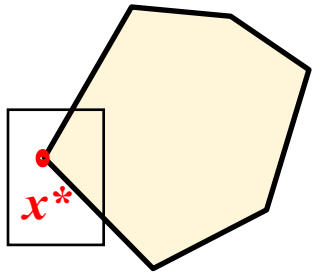
$$x \text{ integer}$$

**BARON finds all solutions:**

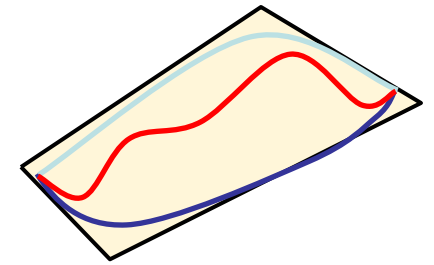
- No integer cuts
- Fathom nodes that are infeasible or points
- Single search tree
- 511 nodes; 0.56 seconds
- Applicable to discrete and continuous spaces

# Range Reduction

**Finiteness**



**Convexification**



## **BRANCH-AND-REDUCE**

**Engineering design**

**Supply chain operations**

**Chem-,  
Bio-,  
Medical  
Informatics**

# ACKNOWLEDGEMENTS

- **N. Adhya (i2)**
- **S. Ahmed**
  - Georgia Institute of Technology
- **Y. Chang**
- **J. Elble**
- **K. Furman (ExxonMobil)**
- **V. Ghildyal (Sabre)**
- **M. L. Liu**
  - National Chengchi University
- **G. Nanda (Sabre)**
- **H. Ryoo**
  - Korea University
- **J. Sheckman**
- **A. Smith**
- **M. Tawarmalani**
  - Purdue University
- **A. Vaia (BPAmoco)**
- **R. Vander Wiel (3M)**
- **Y. Voudouris (Merck)**
- **M. Yu**

- **American Chemical Society**
- **DuPont**
- **ExxonMobil**
- **Lucent Technologies**
- **Mitsubishi Chemicals**
- **National Institutes of Health**
  - General Medical Sciences
- **National Science Foundation**
  - Bioengineering and Environmental Sciences
  - Chemical and Thermal Systems
  - Design and Manufacturing
  - Electrical and Communication Systems
  - Operations Research
- **TAPPI**
- **University of Illinois at U-C**
  - Chemical Engineering
  - Computational Science and Engineering
  - Mechanical and Industrial Engineering
  - Research Board