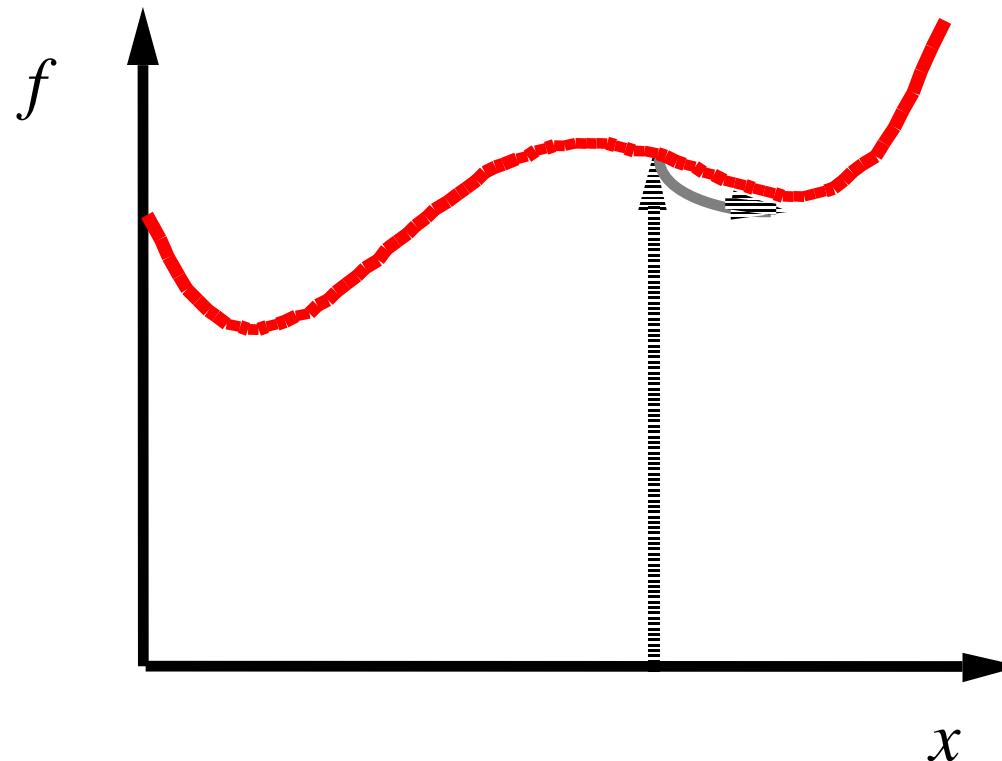


GLOBAL OPTIMIZATION OF NONCONVEX NLPs AND MINLPs with BARON



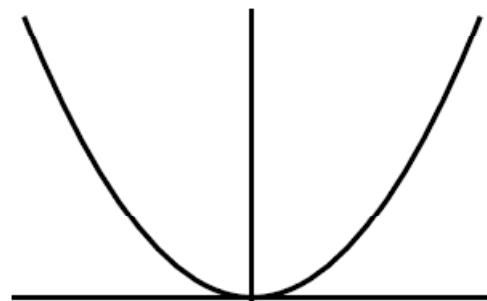
Nick Sahinidis
Department of Chemical Engineering
Carnegie Mellon University
sahinidis@cmu.edu

THE MULTIPLE-MINIMA DIFFICULTY IN OPTIMIZATION

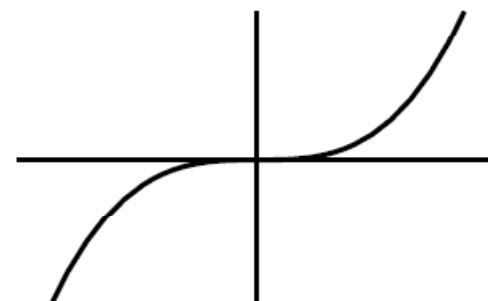


- Classical optimality conditions are necessary but not sufficient
- Classical optimization provides the local minimum “closest” to the starting point used

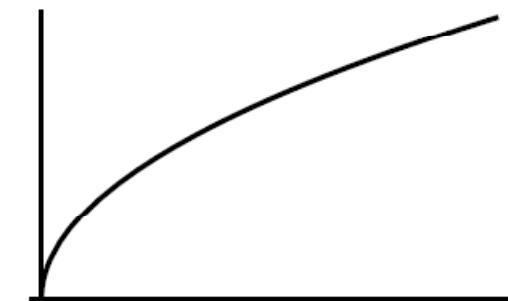
COMMON FUNCTIONS IN MODELING



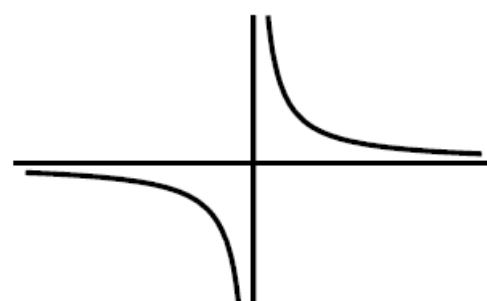
$$x^2$$



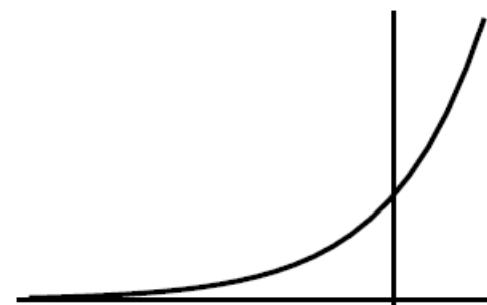
$$x^3$$



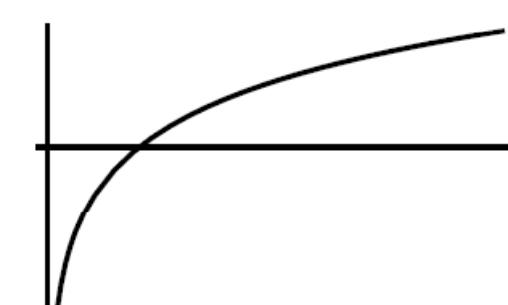
$$\sqrt{x}$$



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

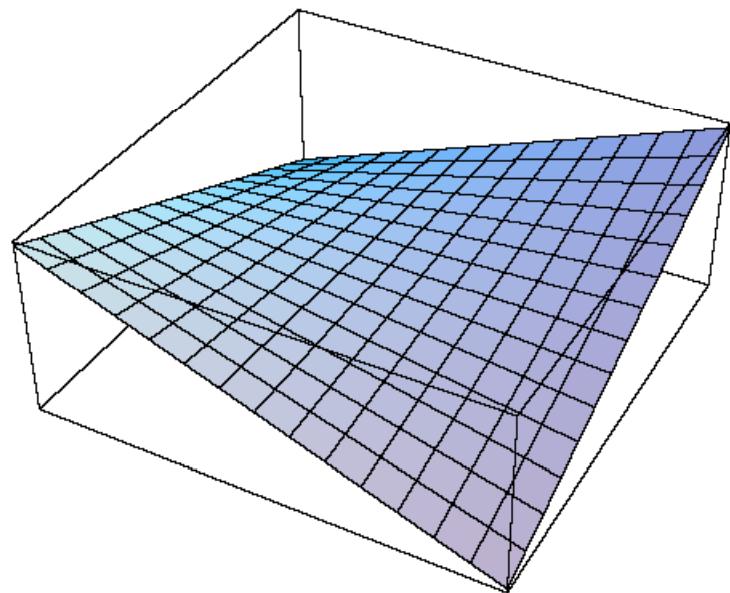


$$\exp(x)$$

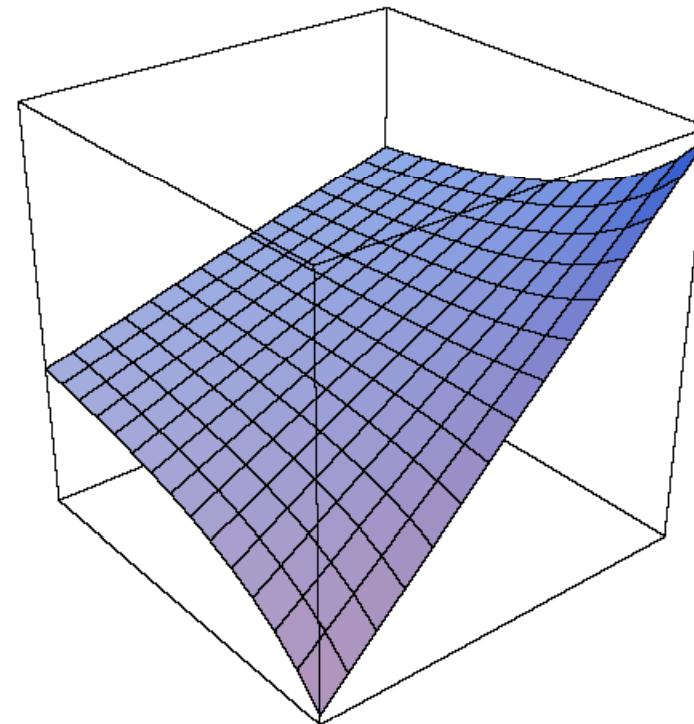


$$\log(x)$$

COMMON FUNCTIONS IN MODELING



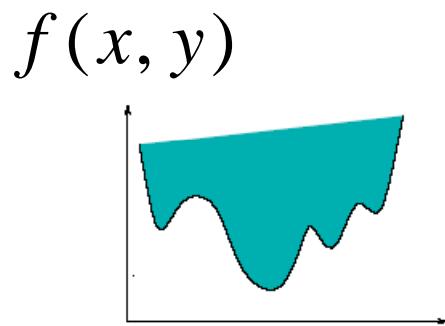
$$x_1 * x_2$$



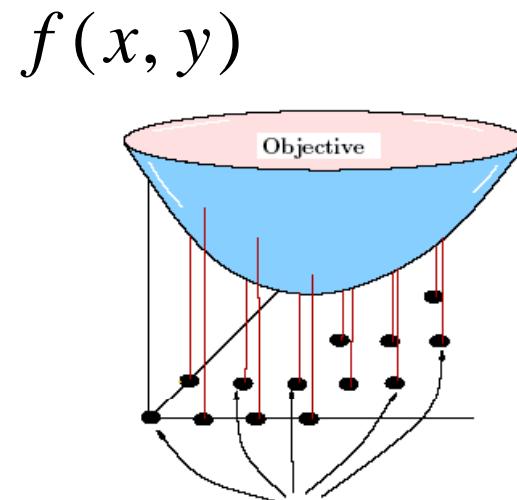
$$\frac{x_1}{x_2}$$

CHALLENGES IN GLOBAL OPTIMIZATION

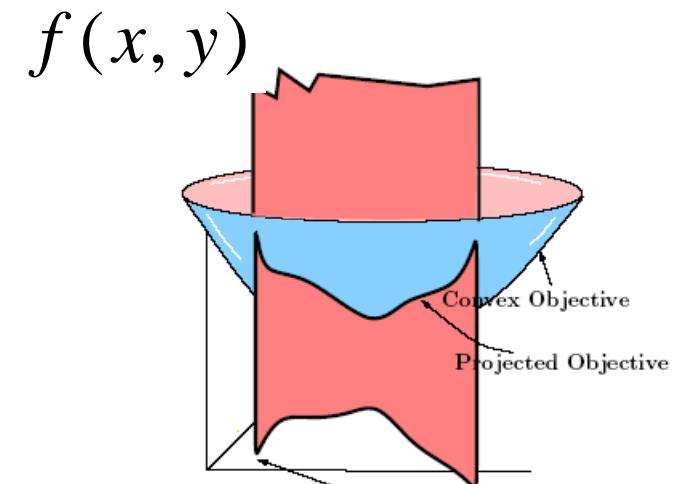
$$\begin{aligned} & \min \quad f(x, y) \\ \text{s.t.} \quad & g(x, y) \leq 0 \\ & x \in R^n, \quad y \in Z^p \end{aligned}$$



Multimodal objective



Integrality conditions

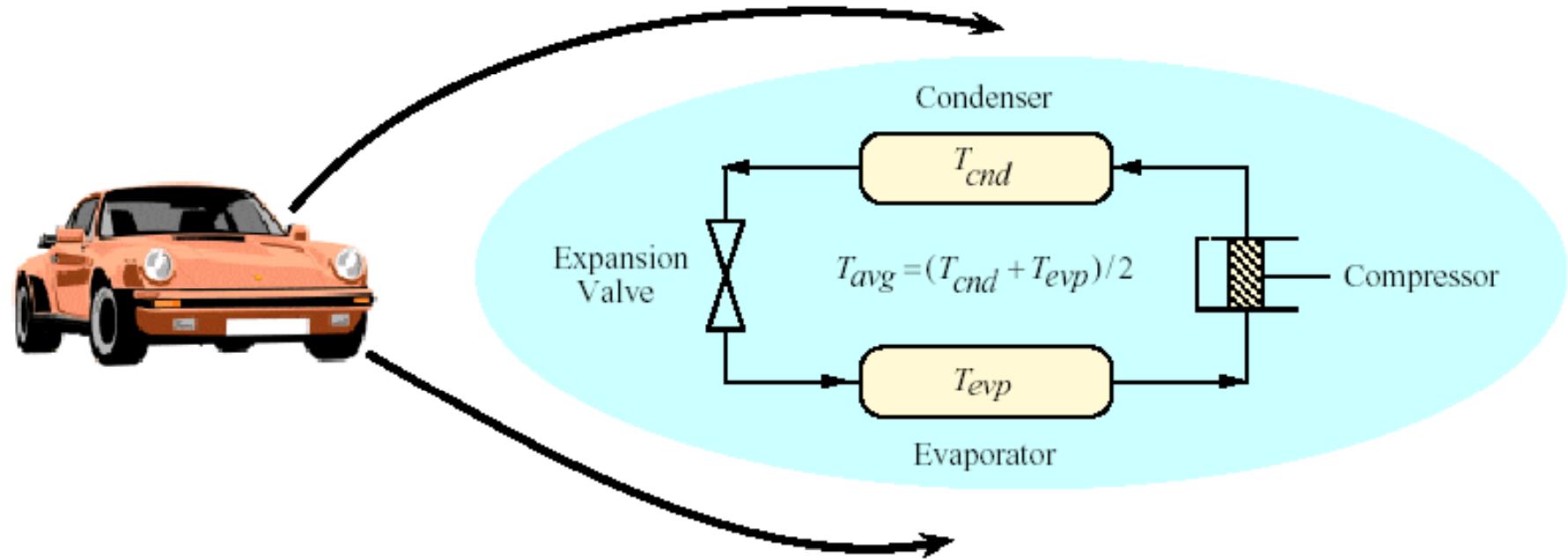


Nonconvex constraints

NP-HARD PROBLEM

AUTOMOTIVE REFRIGERANT DESIGN

(Joback and Stephanopoulos, 1990)



- Higher enthalpy of vaporization (ΔH_{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
$-\text{CH}_3$	$\text{r} - \text{CH}_2 - \text{r}$	$-\text{F}$	$-\text{OH}$	$-\text{NH}_2$	$-\text{SH}$
$-\text{CH}_2-$	$\text{r} > \text{CH} - \text{r}$	$-\text{Cl}$	$-\text{O}-$	$> \text{NH}$	$-\text{S}-$
$> \text{CH}-$	$\text{r} > \text{CH} - \text{r}$	$-\text{Br}$	$\text{r} - \text{O} - \text{r}$	$\text{r} > \text{NH}$	$\text{r} - \text{S} - \text{r}$
$> \text{C} <$	$\text{r} > \text{C} < \text{r}$	$-\text{I}$	$> \text{CO}$	$> \text{N}-$	
$= \text{CH}_2$	$\text{r} > \text{C} < \text{r}$		$\text{r} > \text{CO}$	$= \text{N}-$	
$= \text{CH}-$	$> \text{C} < \text{r}$		$-\text{CHO}$	$\text{r} = \text{N} - \text{r}$	
$= \text{C} <$	$\text{r} = \text{CH} - \text{r}$		$-\text{COOH}$	$-\text{CN}$	
$= \text{C} =$	$\text{r} = \text{C} < \text{r}$		$-\text{COO}-$	$-\text{NO}_2$	
$\equiv \text{CH}$	$\text{r} = \text{C} < \text{r}$		$= \text{O}$		
$\equiv \text{C}-$	$= \text{C} < \text{r}$				

Number of Groups = 44

Maximum Selection Size = 15

Candidates = 39,895,566,894,524

PROPERTY PREDICTION

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

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

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

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

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

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

$$T_{cntr} = \frac{T_{cntr}}{T_c}$$

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

$$\begin{aligned} \alpha &= -5.97214 - \ln \left(\frac{P_c}{1.013} \right) + \frac{6.09648}{T_{br}} + 1.28862 \ln(T_{br}) \\ &\quad - 0.169347 T_{br}^6 \end{aligned}$$

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

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

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

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

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

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

$$G = 0.4835 + 0.4605h$$

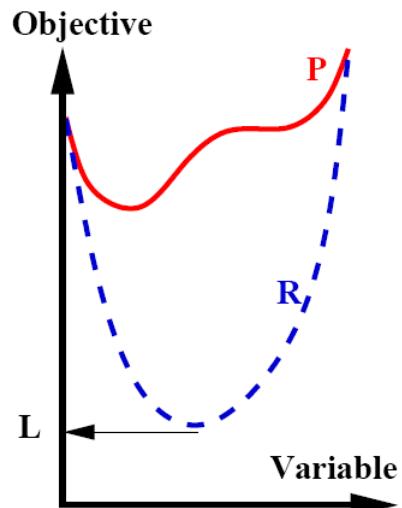
$$k = \frac{h/G - (1 + T_{br})}{(3 + T_{br})(1 - T_{br})^2}$$

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

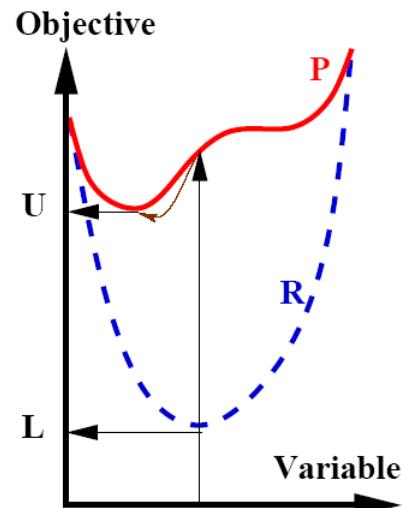
$$\ln P_{vper} = \frac{-G}{T_{evpr}} [1 - T_{evpr}^2 + k(3 + T_{evpr})(1 - T_{evpr})^3]$$

n_i integer

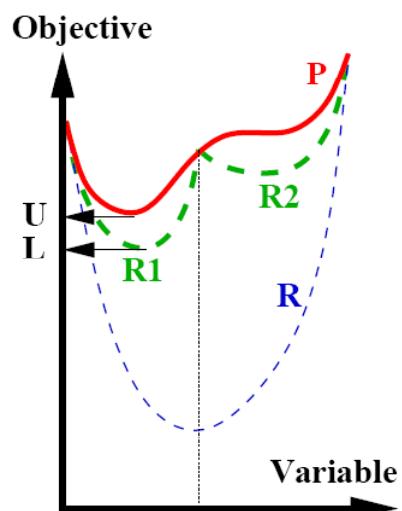
BRANCH-AND-BOUND



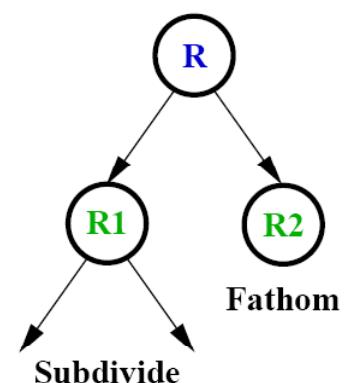
a. Lower Bounding



b. Upper Bounding



c. Domain Subdivision



d. Search Tree

MOLECULAR DESIGN AFTER 150 CPU HOURS IN 1995

- One feasible solution identified
- Optimality not proved

... on the same computer five years later

MOLECULAR DESIGN IN 2000

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

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

For CCl₂F₂, $\Delta H_{ve}/C_{pla} \approx 0.57$

In 30 CPU minutes

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
 - Sherali and Adams, 1994
- Horst and Tuy, *Global Optimization: Deterministic Approaches*, 1996
 - Over 1500 citations
- Our approach
 - Branch-and-Reduce
 - » Ryoo and Sahinidis, 1995, 1996
 - » Shectman 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

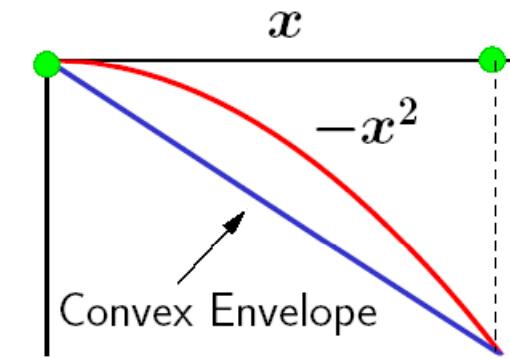
$$\begin{array}{ll}\min & f = -x_1 - x_2 \\ \text{s.t.} & x_3^2 - x_1^2 - x_2^2 \leq 8\end{array}$$

$$x_3 = x_1 + x_2$$

$$0 \leq x_1 \leq 6$$

$$0 \leq x_2 \leq 4$$

$$0 \leq x_3 \leq 10$$



BOUNDING FACTORABLE PROGRAMS

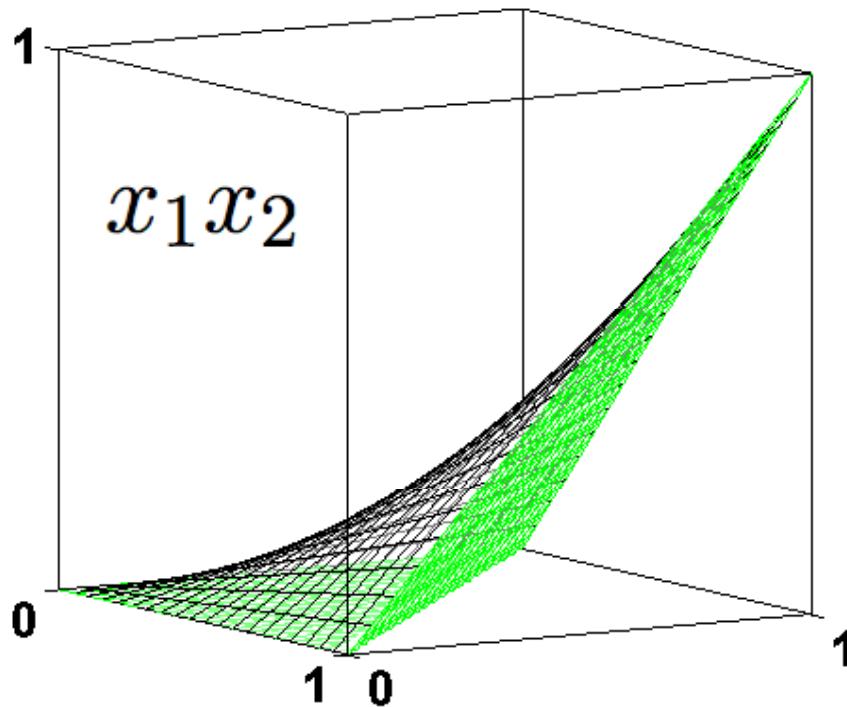
Introduce variables for intermediate quantities whose envelopes are not known

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

$$f = \exp\left(\underbrace{xy}_{x_1} + \underbrace{z \ln w}_{x_2}\right)^{\underbrace{z^3}_{x_6}} \cdot \underbrace{\exp\left(\underbrace{x_5}_{x_4}\right)^{x_7}}_{x_3}^{0.5}$$

CONVEX ENVELOPE OF BILINEAR FUNCTIONS

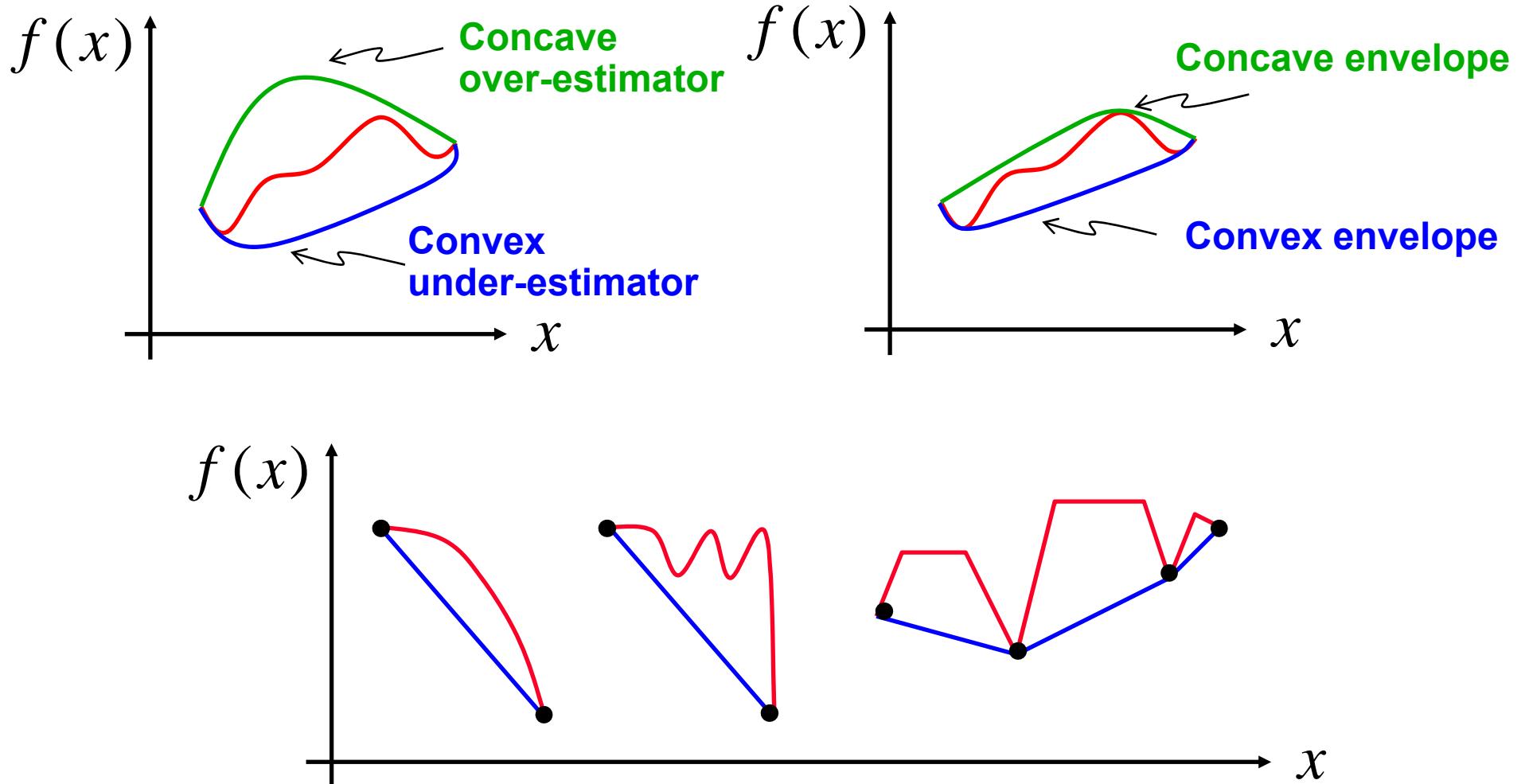
(Al-Khayyal and Falk, 1983; McCormick 1976)



$$x_1 x_2 \geq L_1 x_2 + L_2 x_1 + L_1 L_2$$

$$x_1 x_2 \geq U_1 x_2 + U_2 x_1 + U_1 U_2$$

TIGHT RELAXATIONS

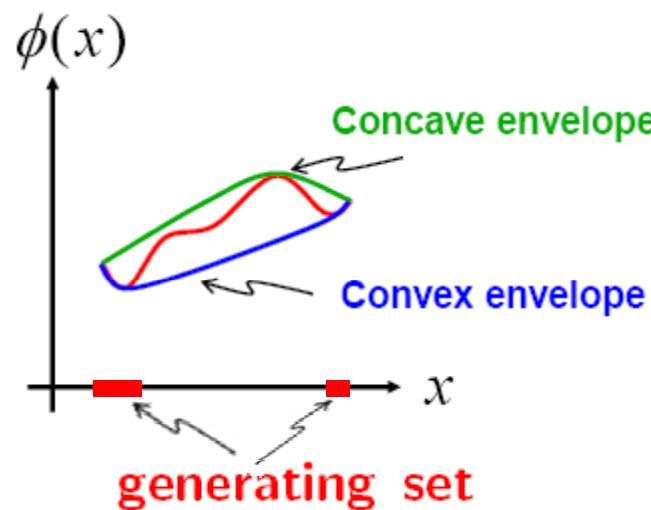


Envelopes often generated by
finitely many convex sets of points

CONVEX ENVELOPES AND THEIR GENERATORS

- The **convex envelope** of ϕ over the convex set C is the greatest convex function majorized by ϕ over C .

$$\text{conv}_C \phi(x) = \inf\{t : (x, t) \in \text{conv}_C(\text{epi}\phi(x))\}$$



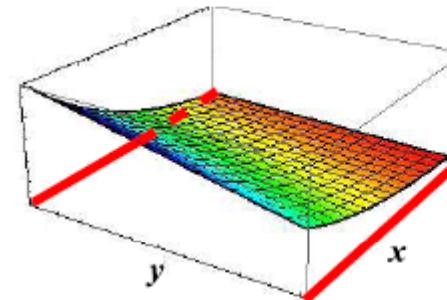
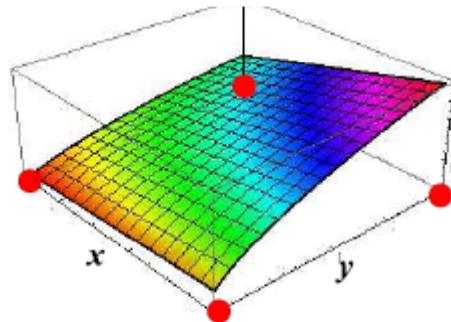
- Assume ϕ is lsc and C is compact. The **generating set** of ϕ on C , denoted by $\mathcal{G}_C \phi$ is the projection of the **set of extreme points** of the convex hull of $\text{epi}\phi$ on C .

IDENTIFYING THE GENERATING SET

- Tawarmalani and Sahinidis 2001: $x_0 \notin \mathcal{G}_C\phi(x)$ iff there exists $X \subset C$ and $x_0 \in X$ such that $x_0 \notin \mathcal{G}_X\phi(x)$

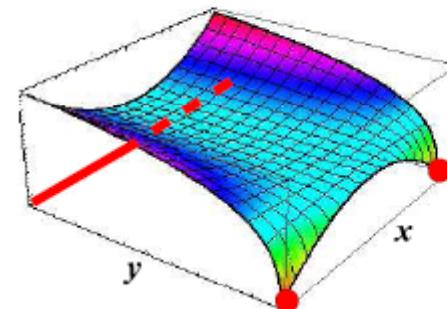
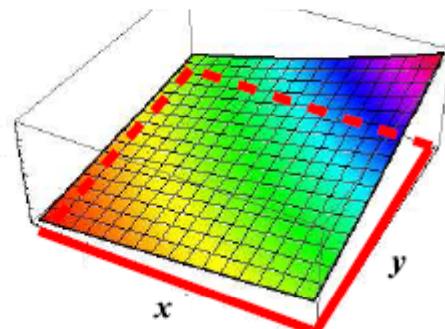
$$\phi = x\sqrt{y}, \quad x, y \geq 0$$

$$\phi = y \exp(-x), \quad y \geq 0, \quad x \in \mathbb{R}$$



$$\phi = \exp(xy), \quad x, y \in \mathbb{R}$$

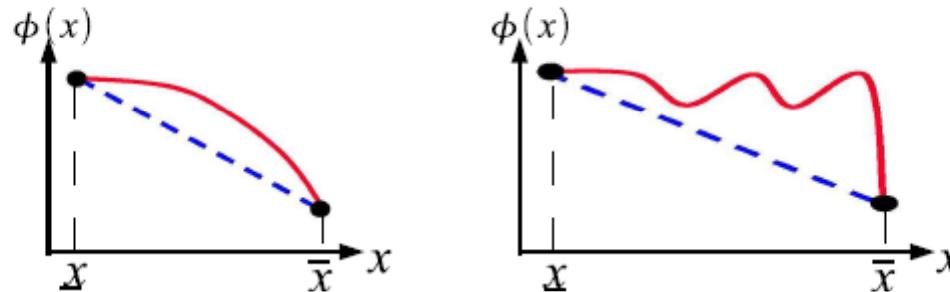
$$\phi = x^2 \log y, \quad x \in \mathbb{R} \quad \log \underline{y} < 0 < \log \bar{y}$$



$\mathcal{G}_C\phi$ is often representable as a union of finitely many convex sets

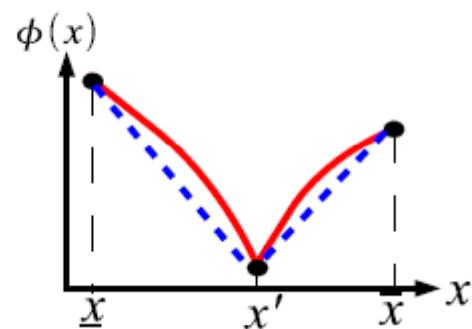
CONSTRUCTING THE CONVEX ENVELOPE

- $\phi(x), x \in C = [\underline{x}, \bar{x}] \subset \mathbb{R}, \mathcal{G}_C\phi = \{\underline{x}, \bar{x}\}$



$$\text{conv}_C\phi(x) = \lambda\phi(\underline{x}) + (1 - \lambda)\phi(\bar{x}), \quad \lambda = (x - \underline{x})/(\bar{x} - \underline{x})$$

- $\phi(x), x \in C = [\underline{x}, \bar{x}] \subset \mathbb{R}, \mathcal{G}_C\phi = \{\underline{x}, x', \bar{x}\}$



$$\begin{aligned} & \min_{\lambda_i} \quad \lambda_1\phi(\underline{x}) + \lambda_2\phi(x') + \lambda_3\phi(\bar{x}) \\ \text{s.t.} \quad & \lambda_1\underline{x} + \lambda_2x' + \lambda_3\bar{x} = x \\ & \lambda_1 + \lambda_2 + \lambda_3 = 1 \\ & \lambda_i \geq 0, \quad i = 1, 2, 3. \end{aligned}$$

$$\Rightarrow \text{conv}_C\phi(x) =$$

$$\begin{cases} \lambda_1\phi(\underline{x}) + (1 - \lambda_1)\phi(x'), \quad \lambda_1 = (x - \underline{x})/(\bar{x} - \underline{x}), & \text{if } \underline{x} \leq x \leq x' \\ (1 - \lambda_3)\phi(x') + \lambda_3\phi(\bar{x}), \quad \lambda_3 = (x - x')/(\bar{x} - x'), & \text{if } x' \leq x \leq \bar{x} \end{cases}$$

CONSTRUCTING THE CONVEX ENVELOPE–Continued

- The generating set consists of ***p* points**, $\mathcal{G}_C\phi = \{x^1, \dots, x^p\}$:

$$(LP) \quad \text{conv}_C\phi(x) = \min_{\lambda_i} \left\{ \sum_{i=1}^p \lambda_i \phi(x^i) : \sum_{i=1}^p \lambda_i x^i = x, \sum_{i=1}^p \lambda_i = 1, \lambda_i \geq 0, i = 1, \dots, p \right\}$$

- The generating set is representable as a union of **finite** number of closed **convex sets**: $\mathcal{G}_C(\phi) = \cup_{i \in I} S_i$, $I = \{1, \dots, p\}$

$$(NCX) \quad \text{conv}_C\phi(x) = \min_{z^i, \lambda_i} \left\{ \sum_{i \in I} \lambda_i \phi(z^i) : \sum_{i \in I} \lambda_i z^i = x, \sum_{i \in I} \lambda_i = 1, z^i \in S_i, \lambda_i \geq 0, \forall i \in I \right\}$$

- if S_i is a singleton for all $i \in I$, then NCX simplifies to an LP
- otherwise, NCX is highly **nonconvex** due to products: $\lambda_i \phi(z^i)$, $\lambda_i z^i$

CONVEXIFY VIA PERSPECTIVE TRANSFORMATION

- Let $S_i = \{u \in C : g_i(u) \leq 0\}$, $i \in I$, where $g_i : \mathbb{R}^n \rightarrow \mathbb{R}^{m_i}$ and g_{ij} , $j = 1, \dots, m_i$ are closed convex functions. Let $x^i = \lambda_i z^i$.

$$\begin{aligned} (\text{CX}) \quad & \min_{x^i, \lambda_i} \sum_{i \in I} \lambda_i \phi(x^i / \lambda_i) \\ \text{s.t.} \quad & \sum_{i \in I} x^i = x \\ & \sum_{i \in I} \lambda_i = 1, \lambda_i \geq 0, \forall i \in I \\ & \lambda_i g_{ij}(x^i / \lambda_i) \leq 0, j = 1, \dots, m_i, \forall i \in I. \end{aligned}$$

- Let ϕ and g_{ij} , forall i, j be twice continuously differentiable functions,
 - CX is not differentiable at points where $\lambda_i = 0$ for some $i \in I$,
 - size of CX; i.e., $|I|$ often increases exponentially with n
- Solve CX **analytically** and derive **explicit characterization** for the convex envelope of **important functional classes** (Khajavirad and Sahinidis, submitted 2010).

EXAMPLES AND COMPARISONS WITH FACTORABLE RELAXATIONS

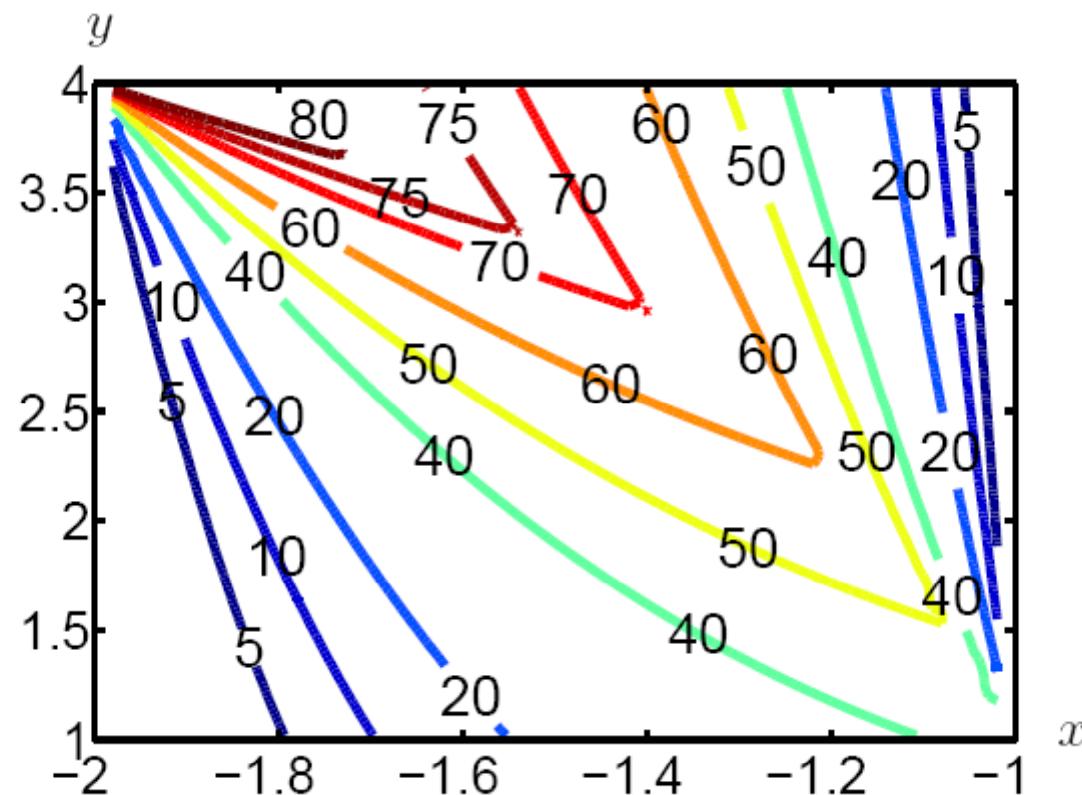
Gap closed by $\text{conv}_C \phi$ at $x \in C$:

$$\gamma = (\text{conv}\phi(x) - \tilde{\phi}(x)) / (\phi(x) - \tilde{\phi}(x)) \times 100\%,$$

where $\tilde{\phi}$ is a convex underestimator of ϕ obtained by a conventional factorable relaxation scheme.

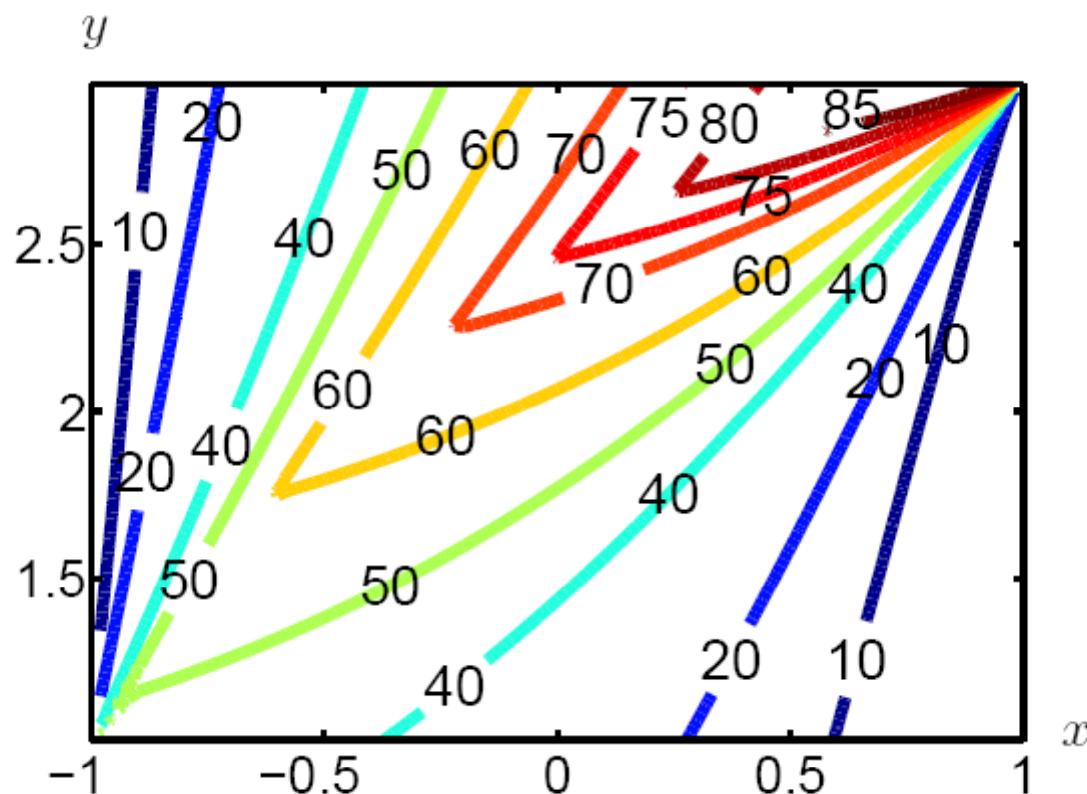
EXAMPLE 1

- $\phi = \sqrt{y}/x^2$ where $x \in [-2, -1]$, $y \in [1, 4]$
- $t_1 = \text{conv}(\sqrt{y})$, $t_2 = 1/x^2$ and $\tilde{\phi} = \text{conv}(t_1 t_2)$



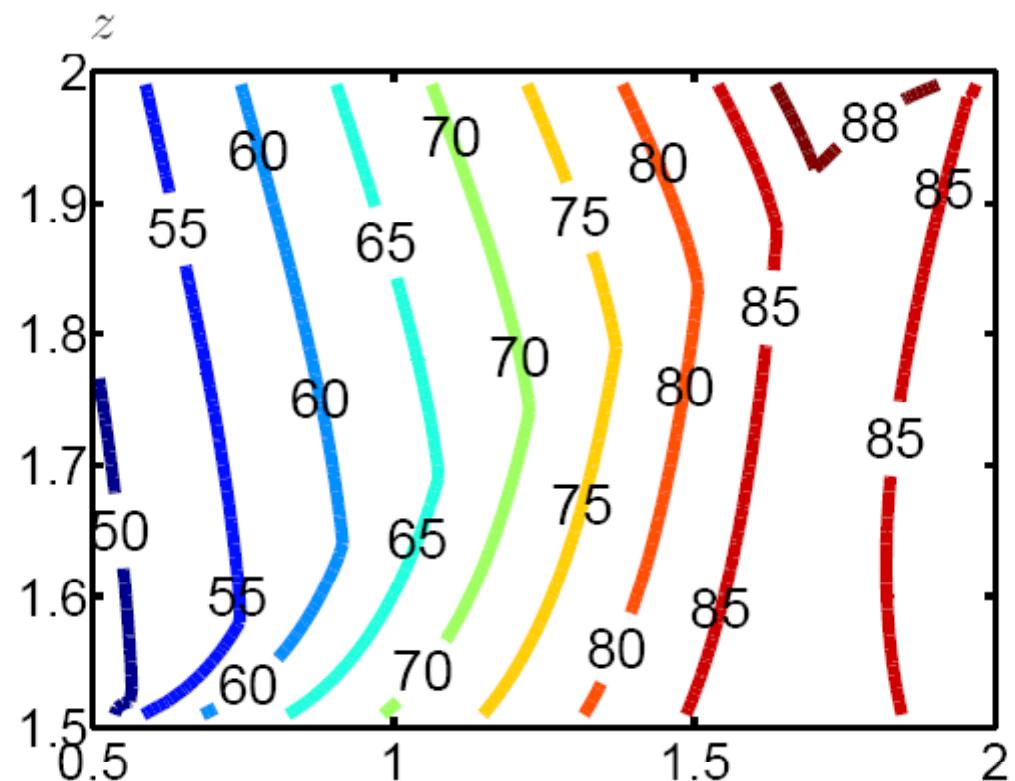
EXAMPLE 2

- $\phi = y \exp(-x)$ where $x \in [-1, 1]$, $y \in [1, 3]$
- $t = \exp(-x)$ and let $\tilde{\phi} = \text{conv}(yt)$



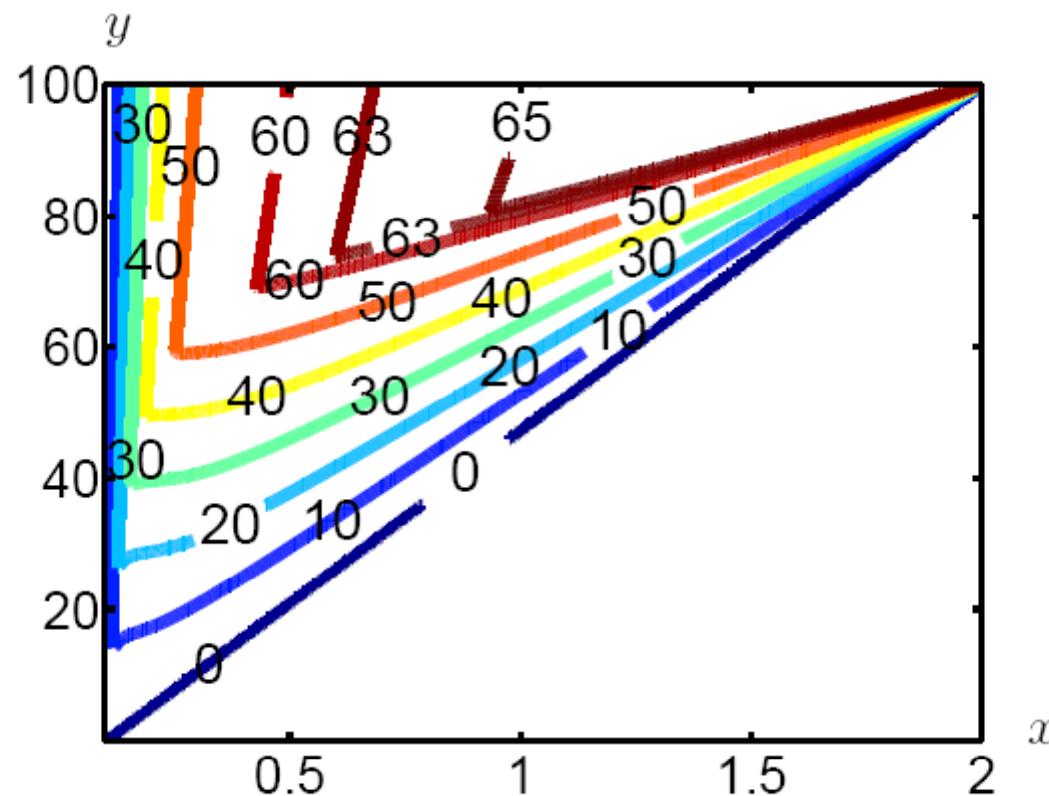
EXAMPLE 3

- $\phi = x/(yz)$ where $0.5 \leq x \leq 2$, $0.1 \leq y \leq 1$, $1.5 \leq z \leq 2$
- $t = 1/(yz)$ and let $\tilde{\phi} = \text{conv}(xt)$



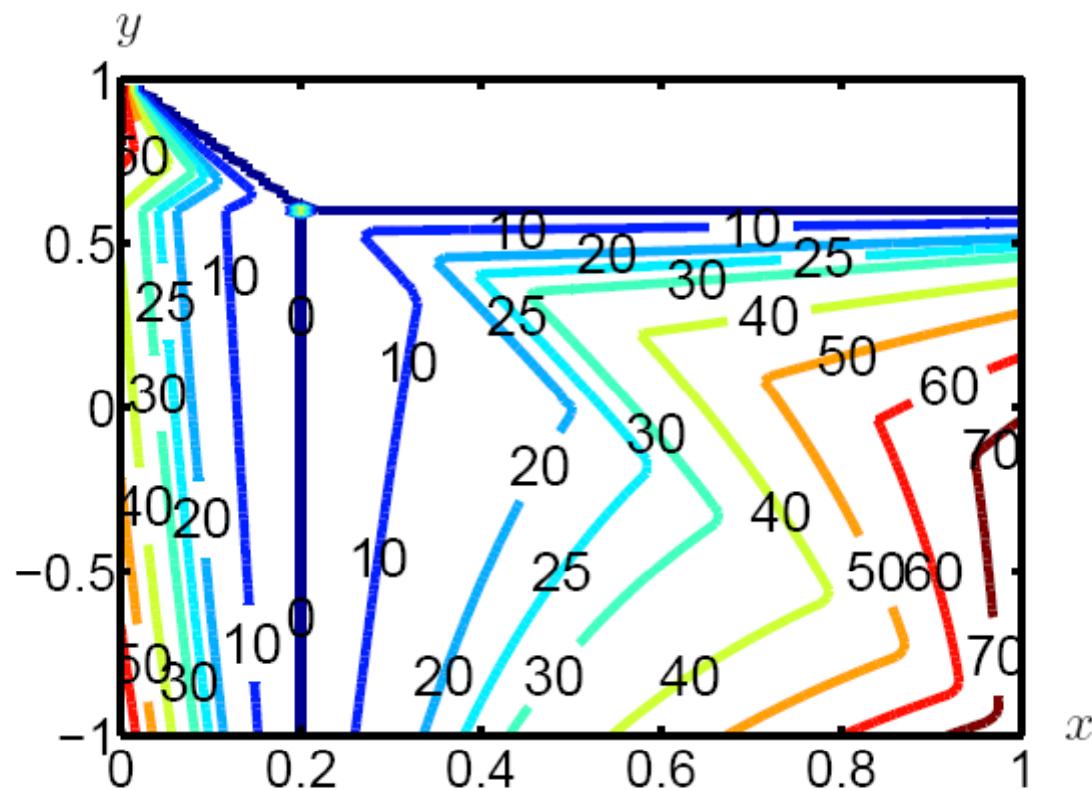
EXAMPLE 4

- $\phi = (\log_{10} y)/x^2$ where $0.1 \leq x \leq 2$, $0.1 \leq y \leq 100$
- $t_1 = \text{conv}(\log_{10} y)$, $t_2 = 1/x^2$ and $\tilde{\phi} = \text{conv}(t_1 t_2)$



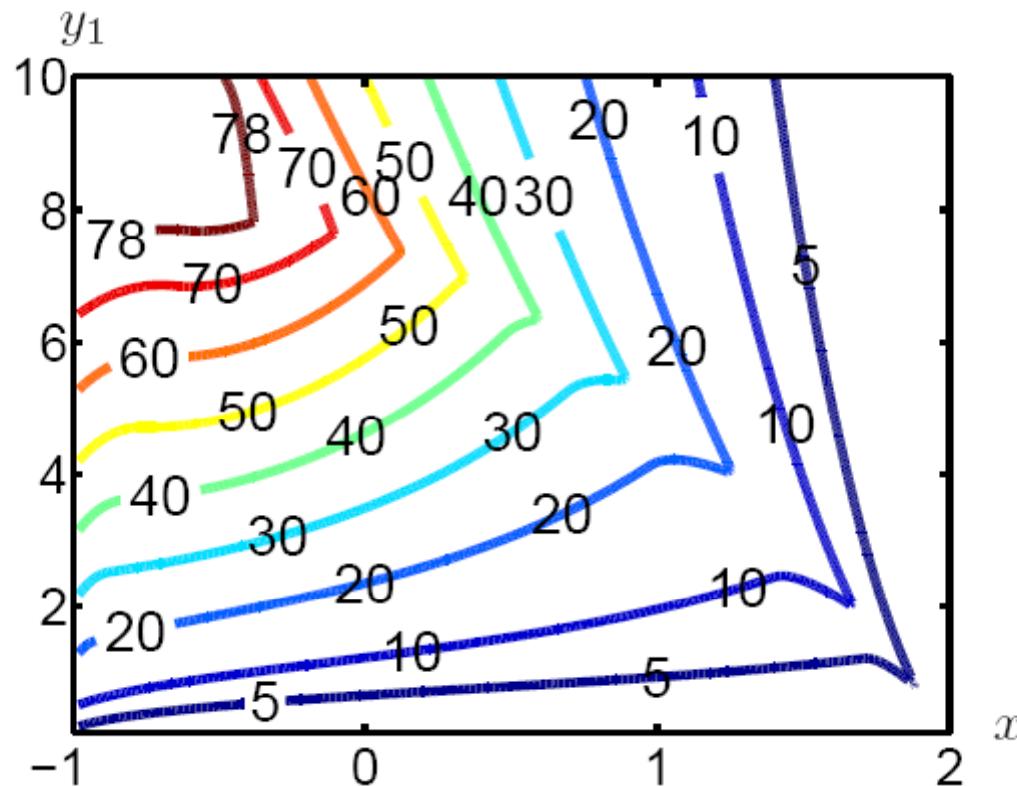
EXAMPLE 5

- $\phi = y \exp(x - z)$ where $-1 \leq y \leq 1, 0 \leq x, z \leq 1$
- $t = x - z$, and $\tilde{\phi} = \text{conv}(y \exp(t))$



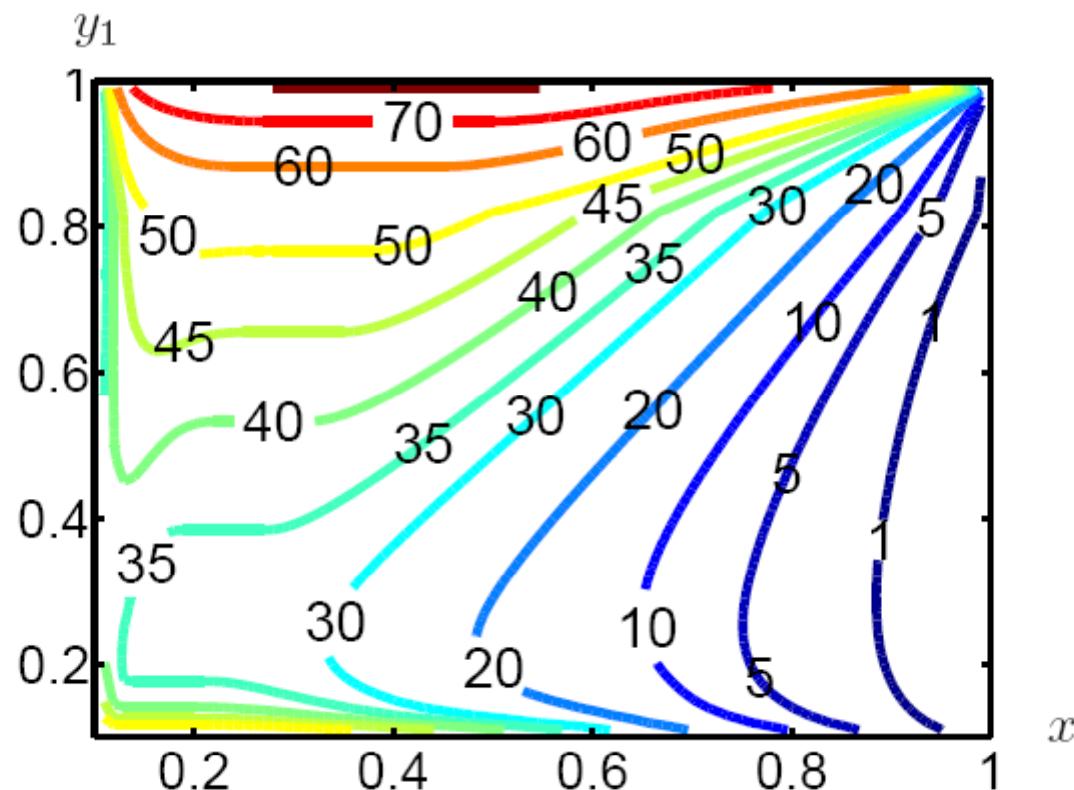
EXAMPLE 6

- $\phi = x^2 \log_{10} y$ where $-1 \leq x \leq 2$, $0.1 \leq y_1 \leq 10$
- $t_1 = x^2$, $t_2 = \text{conv}(\log_{10} y)$ and $\tilde{\phi} = \text{conv}(t_1 t_2)$.



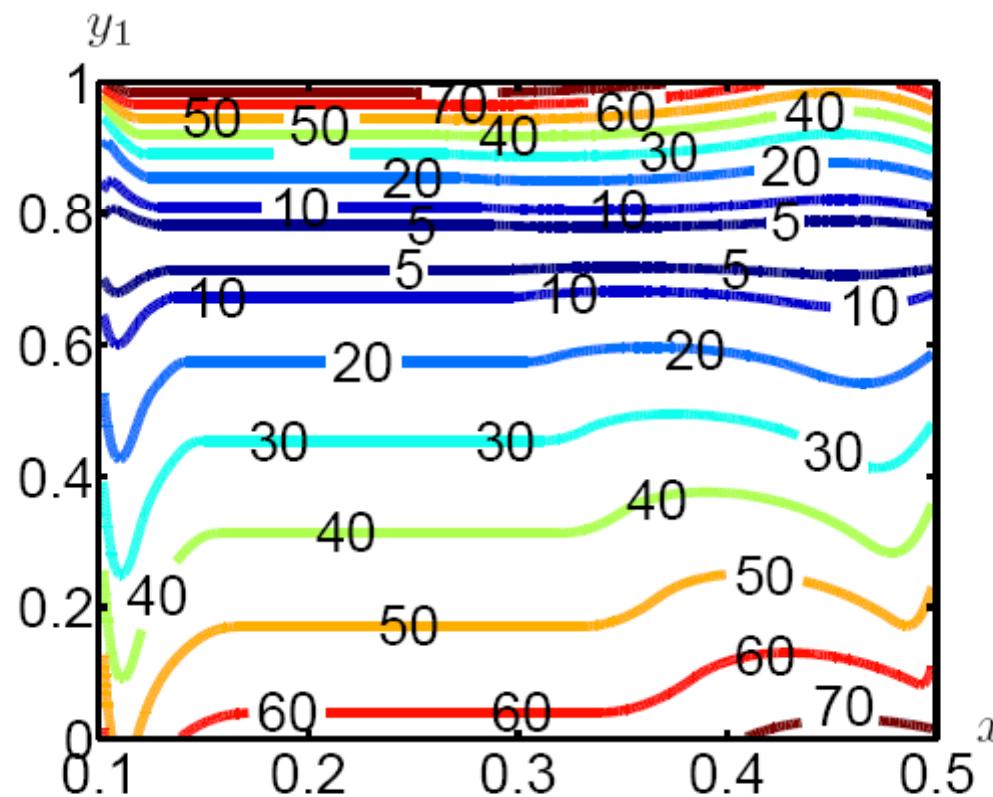
EXAMPLE 7

- $\phi = y_1 y_2 / x$ where $x \in [0.1, 1]$, $y_1 \in [0.1, 1]$, $y_2 \in [0.5, 1.5]$
- $t = \text{conv}(y_1 y_2)$ and let $\tilde{\phi} = \text{conv}(t/x)$



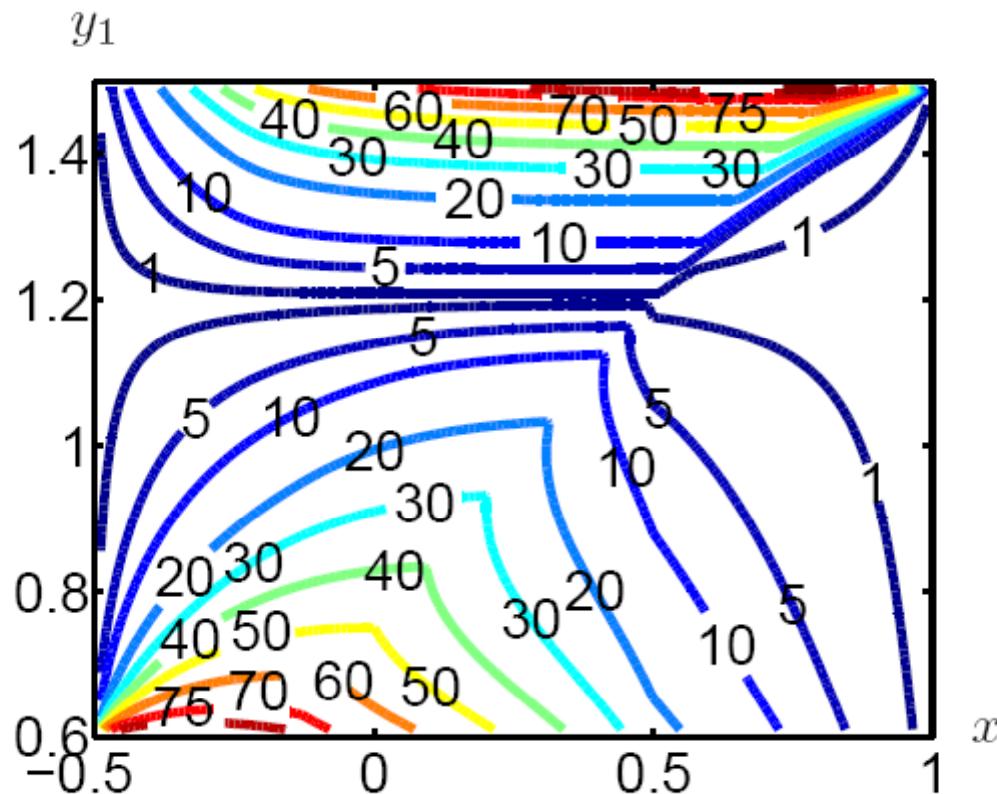
EXAMPLE 8

- $\phi = x^2\sqrt{y_1 + y_2}$ where $0.1 \leq x \leq 0.5$, $0 \leq y_1 \leq 1$, $0.5 \leq y_2 \leq 1.5$
- $t = y_1 + y_2$ and let $\tilde{\phi} = \text{conv}(x^2\sqrt{t})$



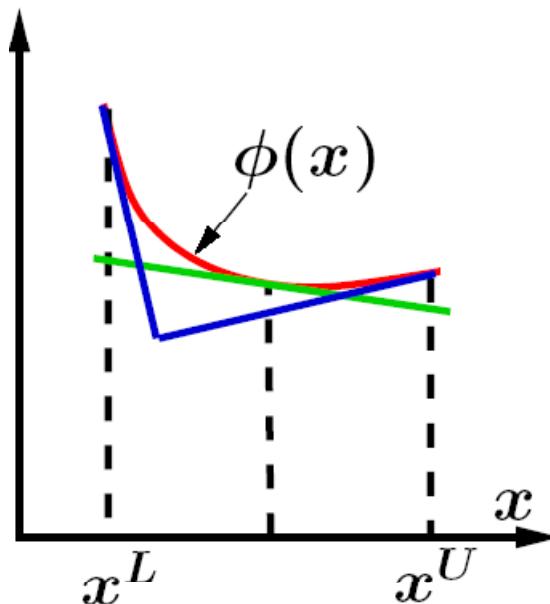
EXAMPLE 9

- $\phi = (2y_1 - y_2) \exp(-x)$ where $-0.5 \leq x \leq 1$, $0.6 \leq y_1 \leq 1.5$, $0.1 \leq y_2 \leq 1.0$
- $t = 2y_1 - y_2$ and let $\tilde{\phi} = \text{conv}(t \exp(-x))$



POLYHEDRAL OUTER-APPROXIMATION

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



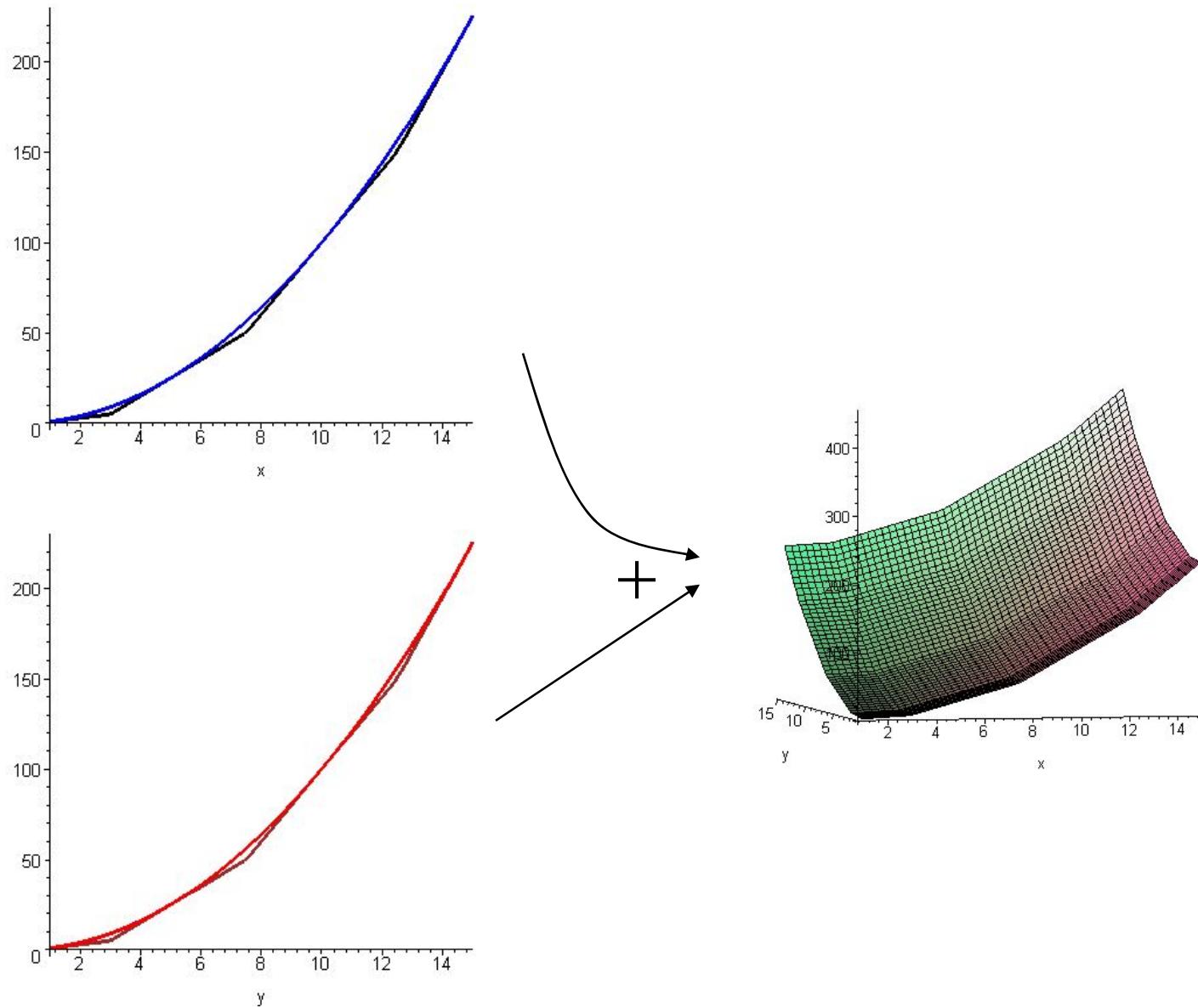
Tawarmalani and Sahinidis (*Math. Progr.*, 2004, 2005)

- Quadratically convergent sandwich algorithm
- Cutting planes for functional compositions

RECURSIVE FUNCTIONAL COMPOSITIONS

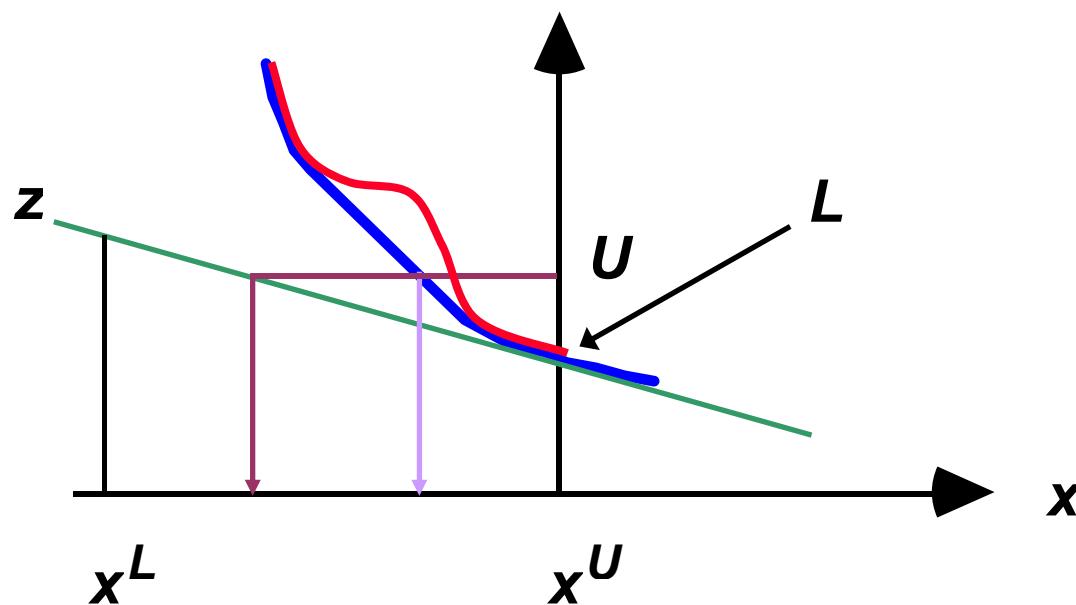
- Consider $h=g(f)$, where
 - g and f are multivariate convex functions
 - g is non-decreasing in the range of each nonlinear component of f
- **h is convex**
- **Two outer approximations of the composite function h :**
 - S1: a single-step procedure that constructs supporting hyperplanes of h at a predetermined 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



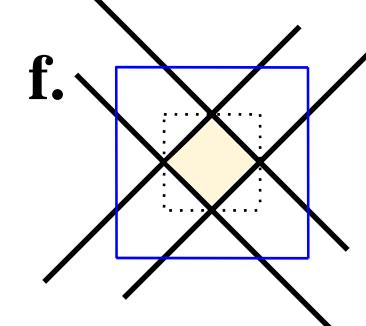
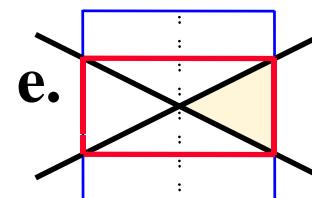
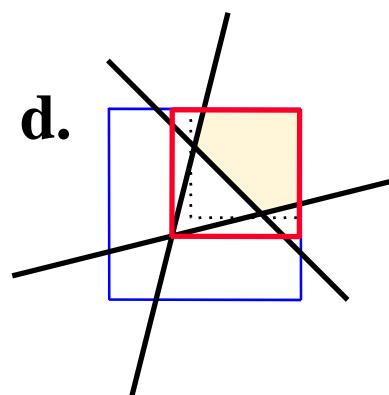
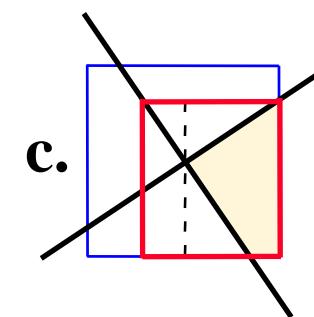
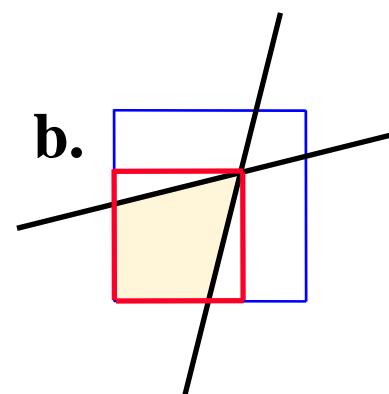
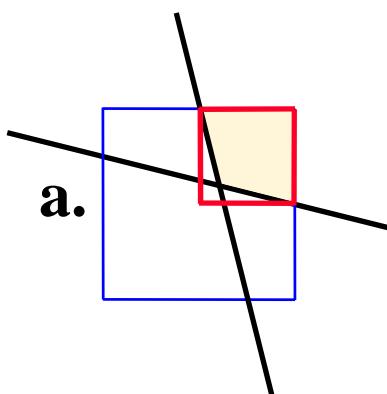
MARGINALS-BASED RANGE REDUCTION

Relaxed Value Function

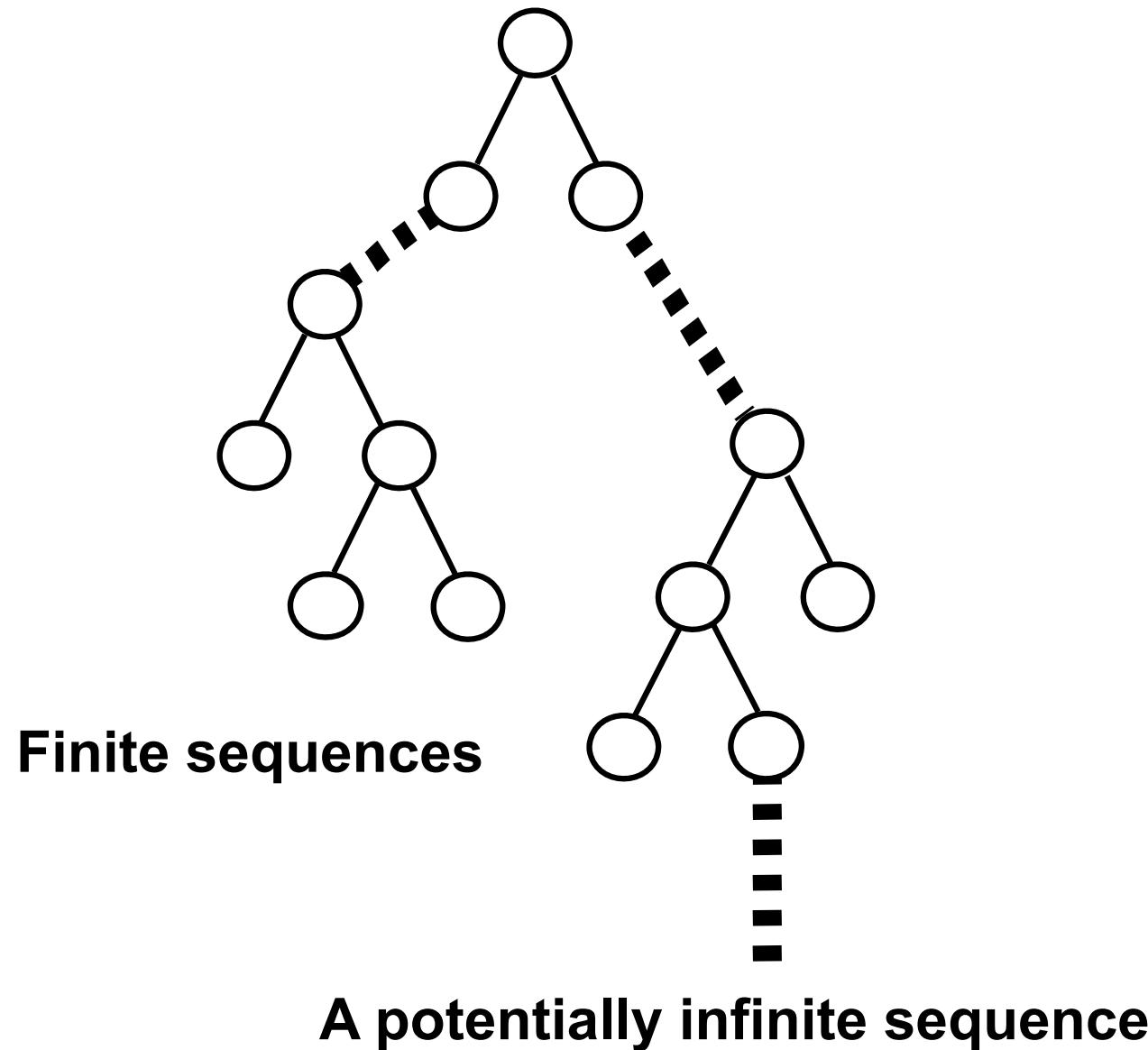


If a variable goes to its upper bound at the relaxed problem solution, this variable's lower bound can be improved

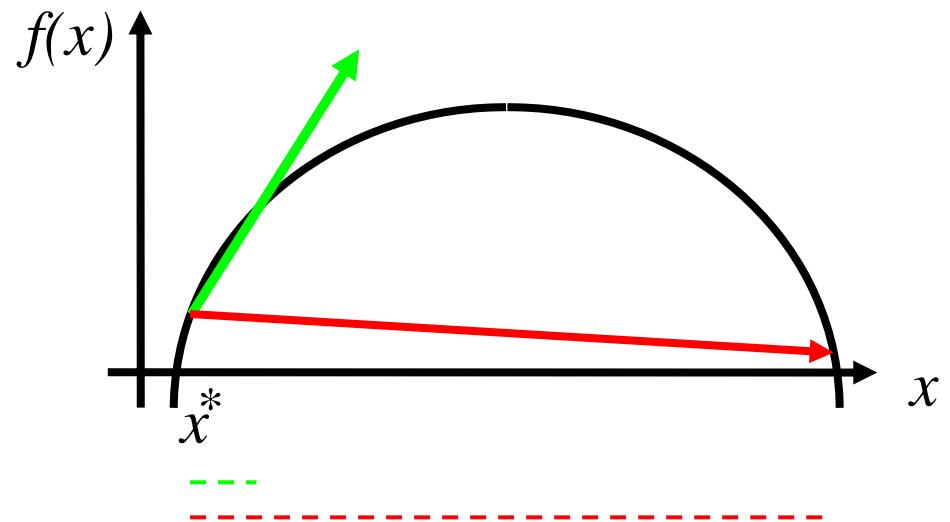
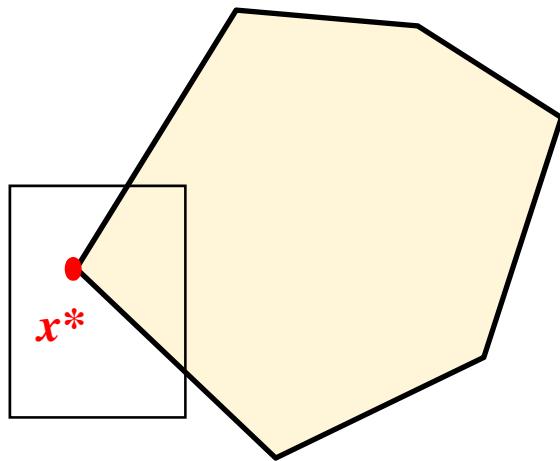
REDUCTION VIA CONSTRAINT PROPAGATION



FINITE VERSUS CONVERGENT BRANCH-AND-BOUND ALGORITHMS

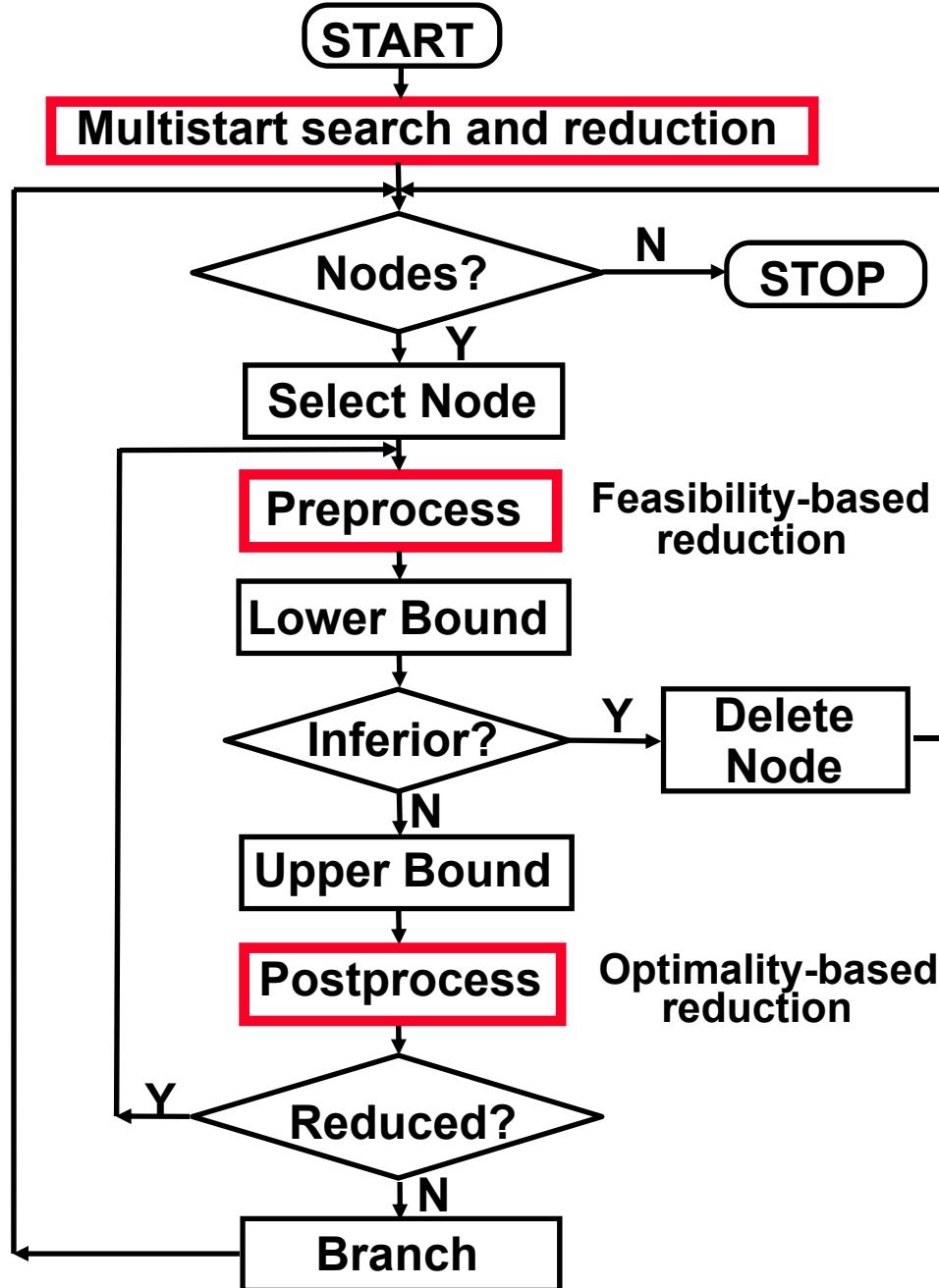


FINITE BRANCHING RULE



- **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	Capabilities
<ul style="list-style-type: none">• Modeling language• Preprocessor• Data organizer• I/O handler• Range reduction• Solver links• Interval arithmetic• Sparse matrix routines• Automatic differentiator• IEEE exception handler• Debugging facilities	<ul style="list-style-type: none">• Core module<ul style="list-style-type: none">– Application-independent– Expandable• Fully automated MINLP solver• Application modules<ul style="list-style-type: none">– Multiplicative programs– Indefinite QPs– Fixed-charge programs– Mixed-integer SDPs– ...• Solve relaxations using<ul style="list-style-type: none">– CPLEX, MINOS, SNOPT, OSL, SDPA, ...

BARON HISTORY

1991-93	Duality-based range reduction Constraint propagation
1994-95	Branch-and-bound system Finite algorithm for separable concave minimization
1996-97	Parser for factorable programs; nonlinear relaxations Links to MINOS and OSL
1997-98	Polyhedral relaxations Compressed data storage, tree traversal, ...
2002	Under GAMS
2004	Branch-and-cut
2005-07	Local search; memory management, ...
2009	Multi-term envelopes
2010-11	Multi-variate envelopes

TINY TEST PROBLEMS

Ex.	Cons.	Vars.	Source/In	Description
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 & Ceric	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 & Sourlas	quadratically constrained QP
20	6	5	Manousiouthakis & Sourlas	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) — circa 1995

- 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 _{tot}	N _{opt}	N _{mem}	T	N _{tot}	N _{opt}	N _{mem}	T	N _{tot}	N _{opt}	N _{mem}	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

26 TEST PROBLEMS FROM globallib AND minplib

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

EFFECT OF CUTTING PLANES

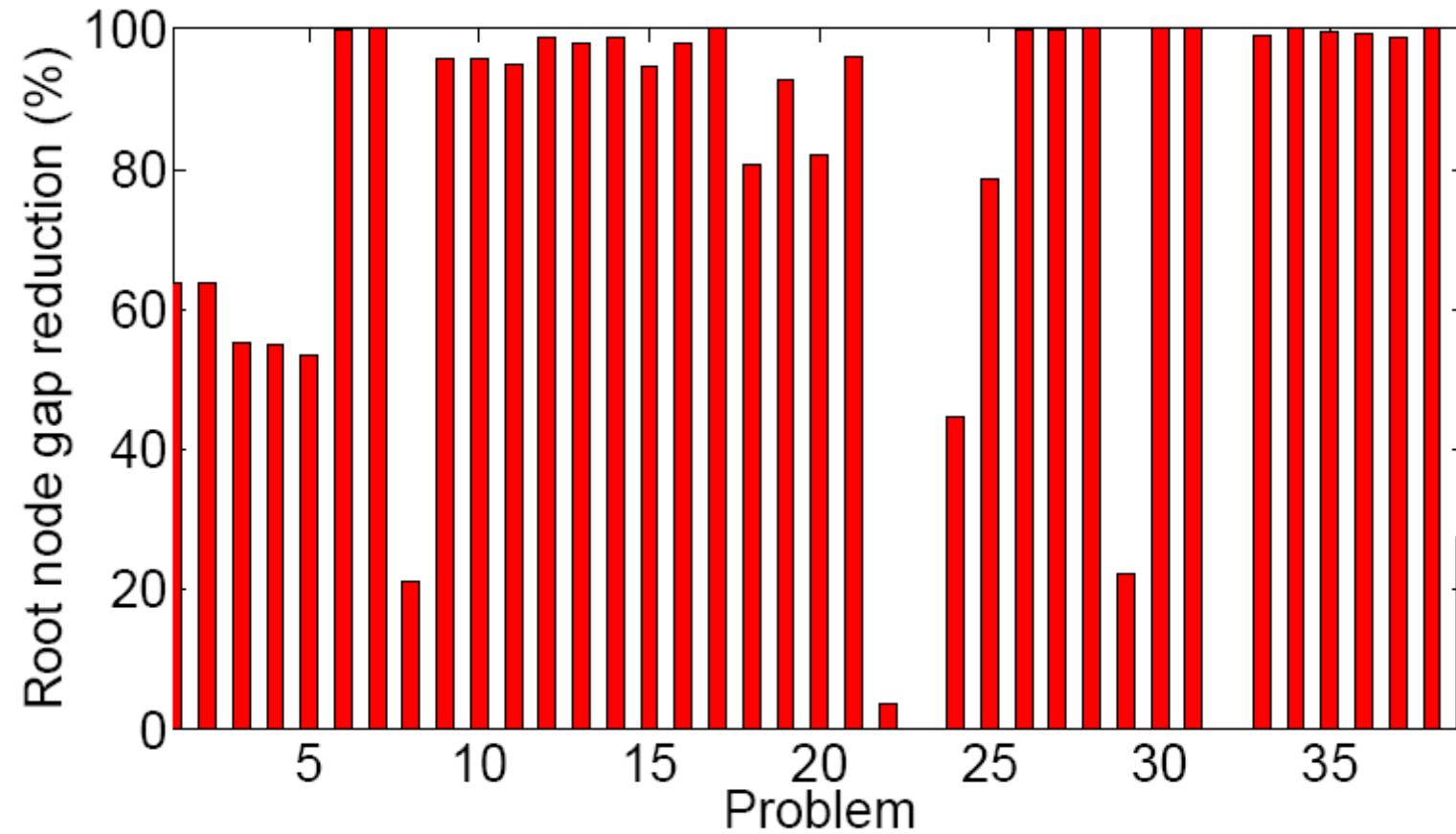
	Without cuts	With cuts	% reduction
Nodes	23,031,434	253,754	99
Nodes in memory	622,339	13,772	98
CPU hrs— circa 2004	76	6	93

EFFECT OF CONVEXITY IDENTIFICATION AND MULTIVARIATE RELAXATIONS

Problem	m	n	n _{int}	Without			With		
				N _{tot}	N _{mem}	T	N _{tot}	N _{mem}	T
chem	5	12		316963	63530	500	31	5	0
chenery	39	44		1337	104	11	1	1	0
ex6_1_1	7	9		45719	3562	48	1237	91	3
ex6_1_3	10	13		204870	10522	302	1736	175	7
ex6_1_4	5	7		385	34	0	45	11	0
ex6_2_14	3	5		1897	114	5	109	15	1
ex6_2_12	3	5		36971	2383	59	18591	1972	37
ex6_2_11	2	4		23303	1730	51	7231	384	22
ex6_2_8	2	4		8875	863	9	3365	219	5
ex6_2_6	2	4		16757	909	18	9223	871	11
ex7_2_4	5	9		313	17	1	285	22	1
ex8_4_4	13	18		193	15	1	127	12	1
ex8_5_1	5	7		1329	111	11	612	50	7
csched1	23	77	63	17505	805	41	103	37	1
csched1a	23	29	15	2605	1792	4	73	11	0
springs	11	33		11203	5441	500	2017	116	79
hs112	4	11		229315	132618	500	143	11	1
farmat2-eps	1	3		37567	1066	12	3	2	0
hs104	7	9		591	39	2	220	16	1
gold	1	3		2063	307	1	453	47	0

These relaxations will become available with BARON 10.0 in March 2011

ROOT NODE GAP REDUCTIONS

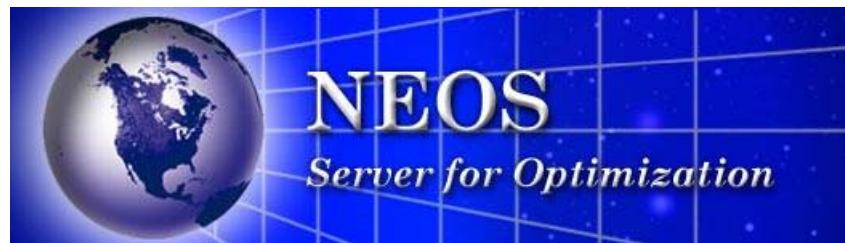


Average gap reduction = 75%



BARON SOFTWARE

- **First to offer deterministic guarantee for the global optimization of NLPs and MINLPs**
 - Inspired developments in LINDOGlobal, Couenne, ...
- **Availability**
 - Commercial under GAMS and AIMMS
 - Free through the NEOS server for optimization

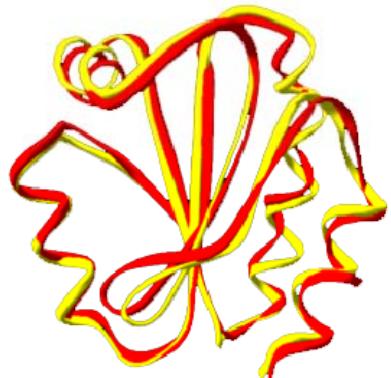


BARON IN APPLICATIONS

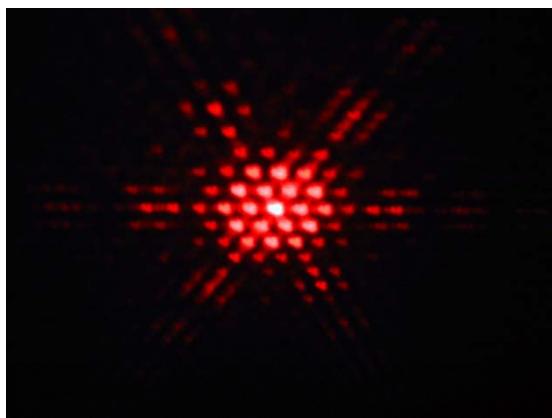
- Development of new **Runge-Kutta methods** for partial differential equations
 - Ruuth and Spiteri, *SIAM J. Numerical Analysis*, 2004
- **Energy policy making**
 - Manne and Barreto, *Energy Economics*, 2004
- Design of **metabolic pathways**
 - Grossmann, Domach and others, *Computers & Chemical Engineering*, 2005
- Model estimation for automatic **control**
 - Bemporand and Ljung, *Automatica*, 2004
- **Agricultural economics**
 - Cabrini *et al.*, *Manufacturing and Service Operations Management*, 2005
- **Portfolio optimization**
 - Rios and Sahinidis, *Annals of Operations Research*, 2010

CURRENT DEVELOPMENTS

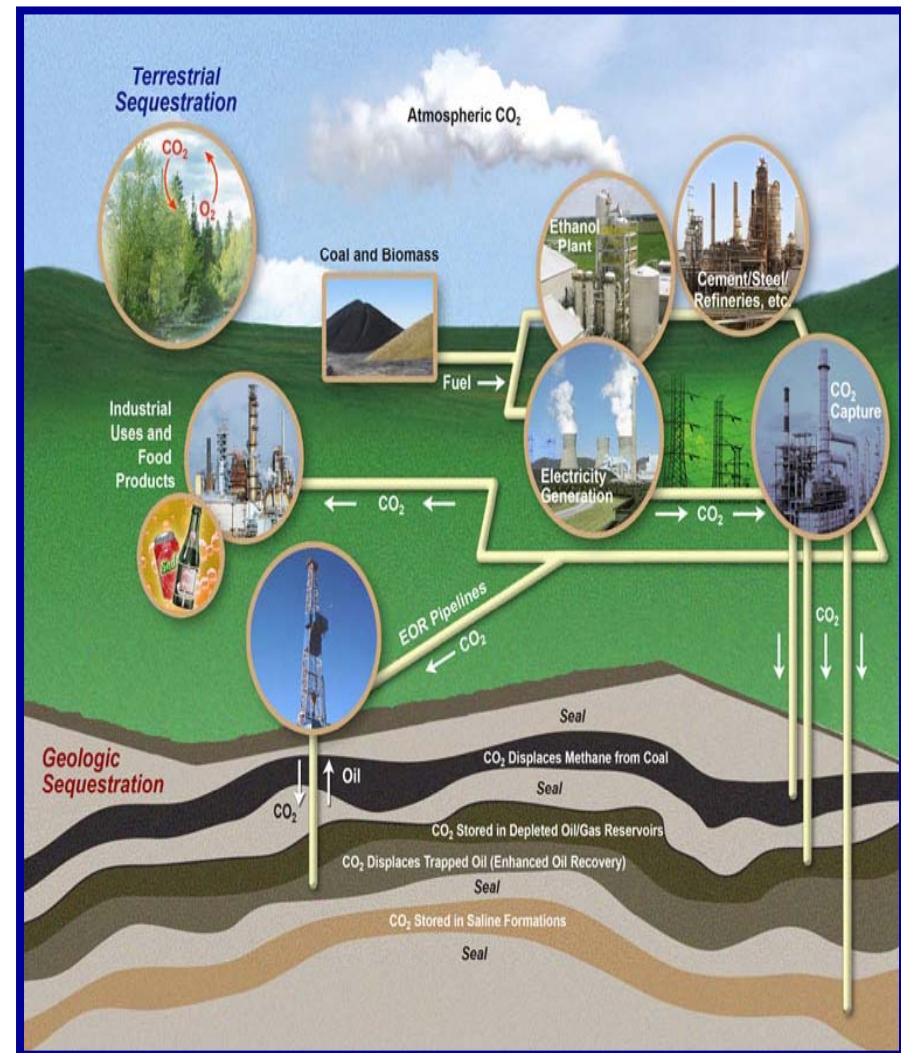
Protein structure alignment



X-ray crystallography



CO₂ capture and sequestration



<http://www.fossil.energy.gov/programs/sequestration/overview.html>

GLOBAL/MINLP SOFTWARE

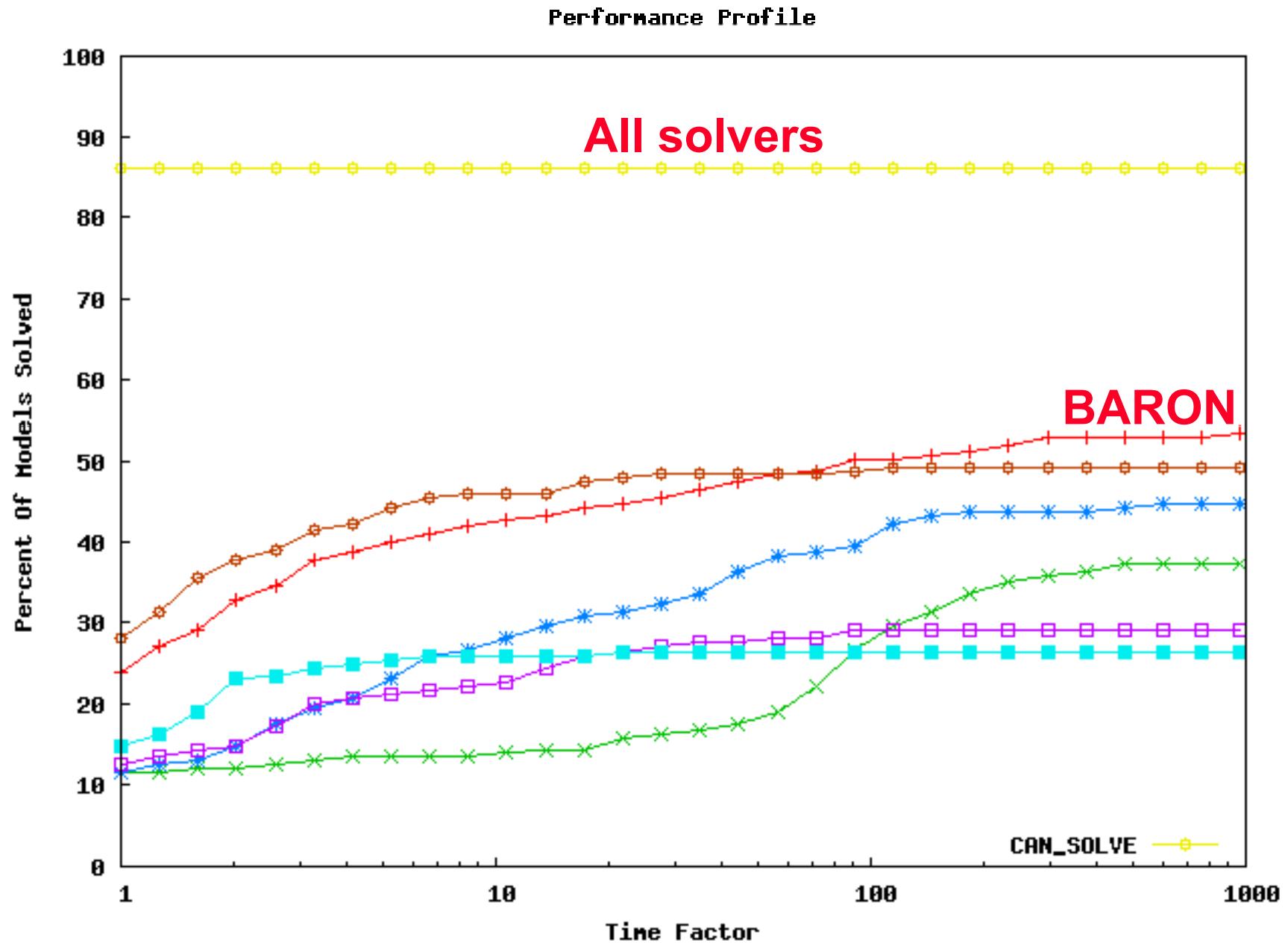
- **AlphaECP**—Exploits pseudoconvexity
- **BARON**—Branch-And-Reduce
- **BONMIN**—Integer programming technology (CMU/IBM)
- **Couenne**—factorable relaxations; trigonometric functions
- **DICOPT**—Decomposition
- **GlobSol**—Interval arithmetic
- **Interval Solver (Frontline)**—Interval solver; Excel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

NLP/MINLP

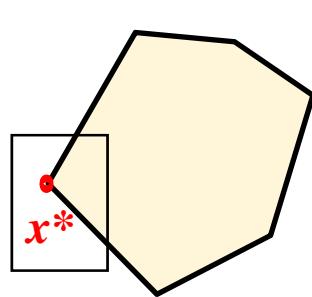
NLP

MINLP

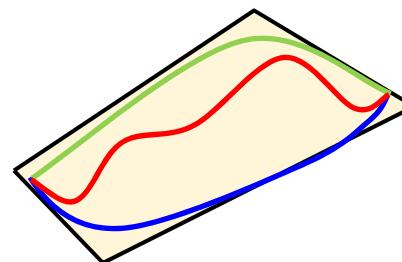
COMPARISONS ON MINLPLIB



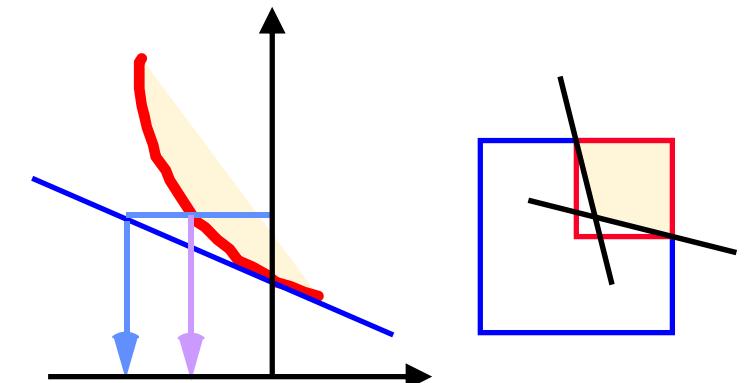
Finiteness



Convexification



Range Reduction



BRANCH-AND-REDUCE

**Engineering
design**

**Management
and Finance**

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