# Global Optimization and Constraint Satisfaction:

# THE BRANCH-AND-REDUCE APPROACH

**Nick Sahinidis**

**University of Illinois at Urbana-Champaign**

**Chemical and Biomolecular Eng.**

# ACKNOWLEDGMENTS

- **Shabbir Ahmed: Georgia Tech**
- **Hong Ryoo: University of Illinois at Chicago**
- **Joe Shectman: Boston**
- **Mohit Tawarmalani: Purdue**

- **DuPont, ExxonMobil, Lucent, Mitsubishi, NSF, PRF, TAPPI**

- **GAMS Development Corporation**

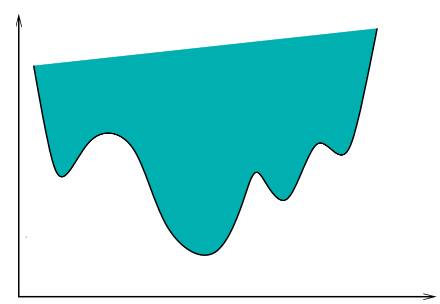
- **Tawarmalani, M. and N. V. Sahinidis, *Convexification and Global Optimization in Continuous and Mixed-Integer Nonlinear Programming,* Kluwer Academic Publishers, 2002.**

# MIXED-INTEGER NONLINEAR PROGRAMMING

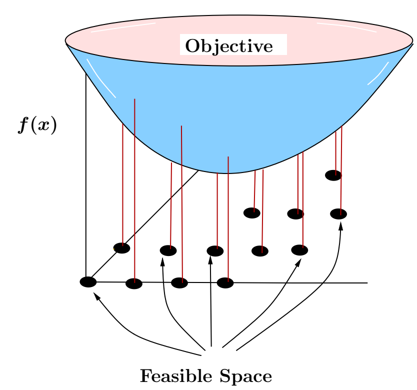
$$
\begin{array}{llll}
(\mathrm{P}) & \min & f(x,y) & \text{Objective Function} \\
 & \text{s.t.} & g(x,y) \leq 0 & \text{Constraints} \\
 & & x \in \mathbb{R}^n & \text{Continuous Variables} \\
 & & y \in \mathbb{Z}^p & \text{Integrality Restrictions}
\end{array}
$$

**Challenges:**

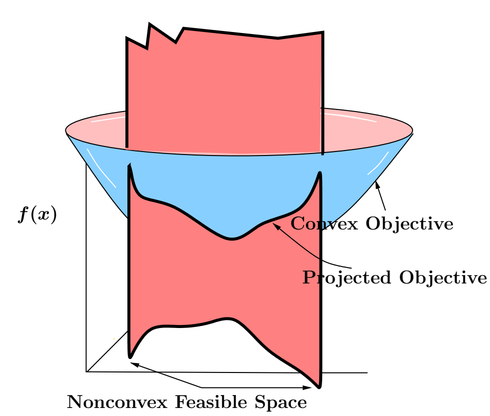
- Multimodal Objective



- Integrality




- Nonconvex Constraints



# MOTIVATION FOR AN ALGORITHM

- **Diverse Application Areas**
  - **Combinatorial Chemistry**
  - **Molecular Biology**
  - **Finance**
  - **Parameter Estimation**
    - » **Design of Experiments**
  - **Engineering Design**
    - » **Process Synthesis**
    - » **CAD**
    - » **Layout Design**

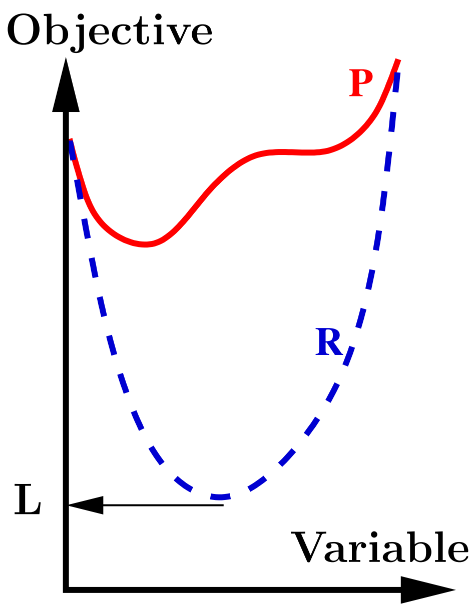
- **Theoretical Challenges**
- **Important Subclasses**
  - **Mixed-Integer Linear Programming**
  - **Continuous Nonlinear Programming**
  - **Nonlinear 0-1 Programming**
- **NP-hard Problem**
  - **Murty and Kabadi (1987)**

# MINLP ALGORITHMS

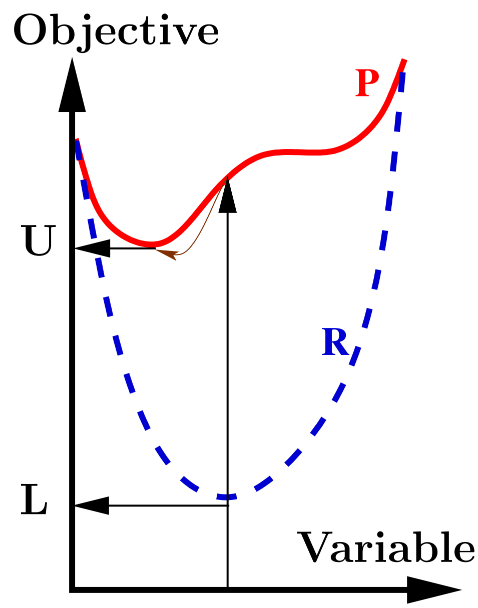
- **Branch and Bound**
  - Bound problem over successively refined partitions
    - » Falk and Soland, 1969
    - » Gupta and Ravindran, 1985
- **Convexification**
  - Outer-approximate with increasingly tighter convex programs
  - Tuy, 1964
  - Sherali and Adams, 1994
- **Decomposition**
  - Project out some variables by solving subproblem
    - » Duran and Grossmann, 1986
    - » Visweswaran and Floudas, 1990

- **Our approach**
  - Branch and Bound
    - » Ryoo and Sahinidis, 1995, 1996
    - » Shectman and Sahinidis, 1998
  - Convexification
    - » Tawarmalani and Sahinidis, 2001, 2002
  - Constraint Propagation & Duality-Based Reduction
    - » Ryoo and Sahinidis, 1995, 1996
    - » Tawarmalani and Sahinidis, 2002

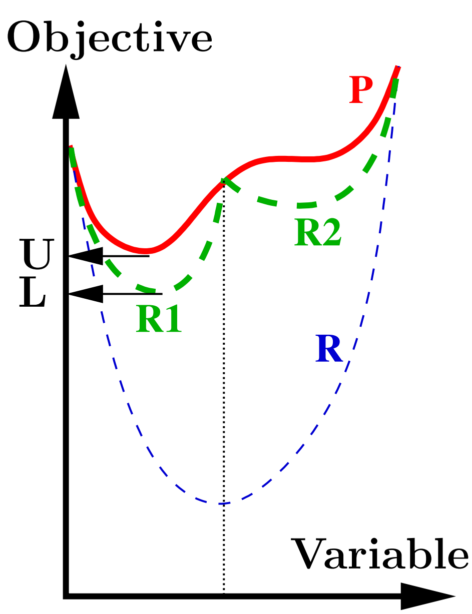
# Branch and Bound Algorithm



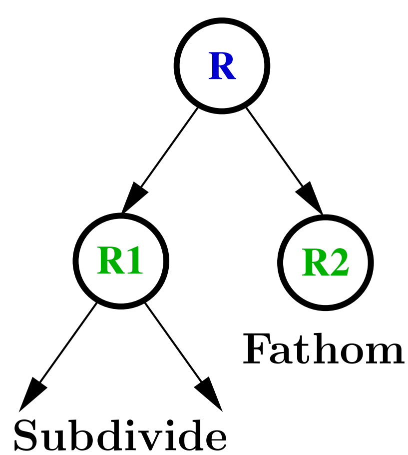

a. Lower Bounding




b. Upper Bounding




c. Domain Subdivision




d. Search Tree

# COMPUTATIONAL RESULTS WITH 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)

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

# CHALLENGES

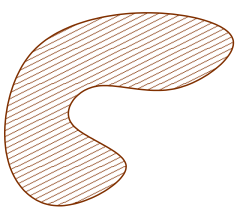
- Standard Global Optimization Converges Slowly

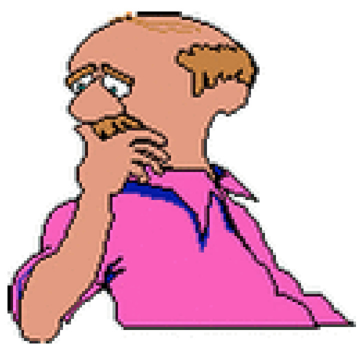
- Algorithmic Issues
  - Reduce domain by automatically identifying sub-optimal regions
  - Develop finite instead of merely convergent algorithms
  - Build tight relaxations

- Implementation Issues
  - Existing NLP solves are often unreliable
  - Numerical instabilities are common with nonlinear terms
  - Ease of use
  - Capability to sole problems of industrial-scale magnitude

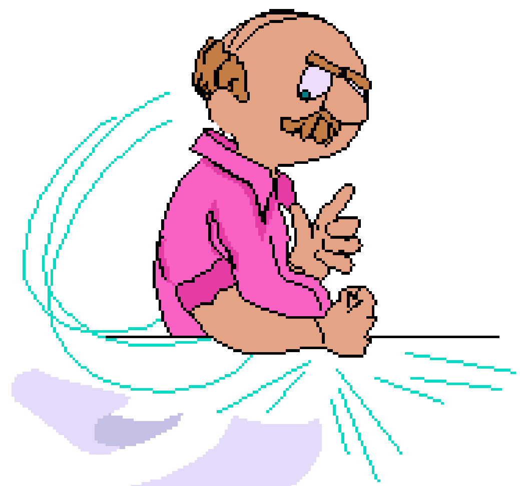
# What is Domain Reduction?

Do I have to look at the whole feasible region?

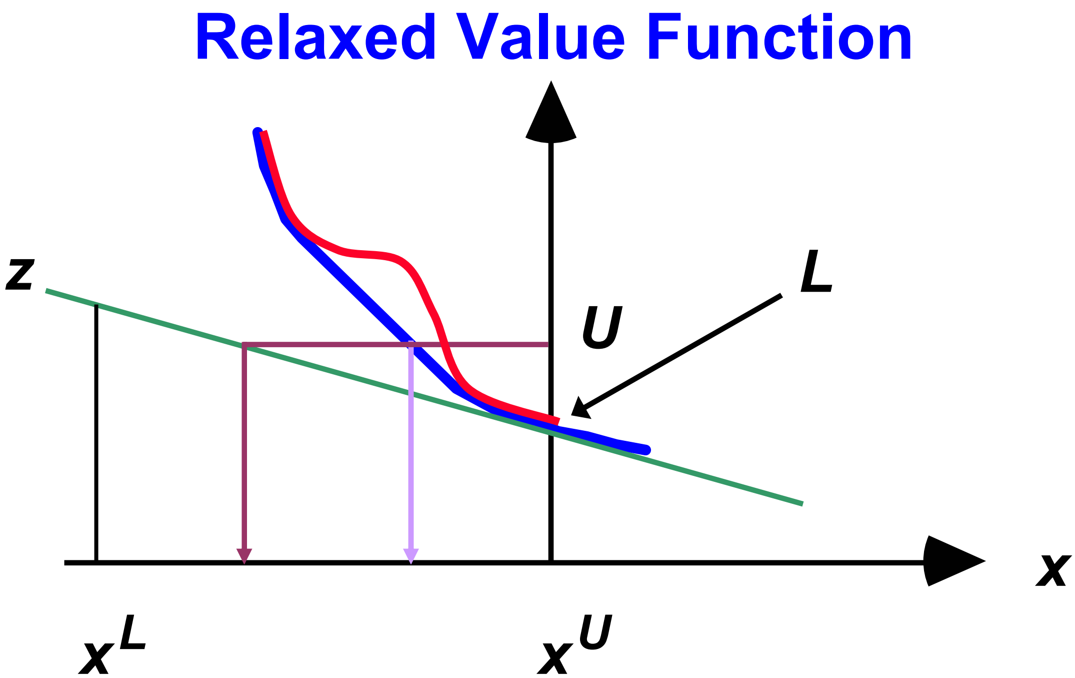




No, part of the region is provably not optimal



# RANGE REDUCTION



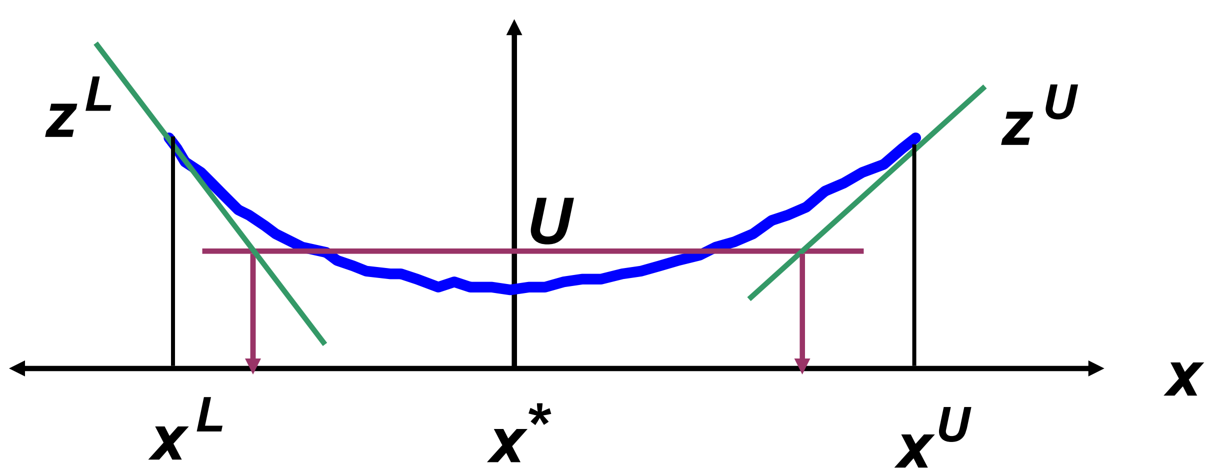

- **If a variable goes to its upper bound at the relaxed problem solution, this variable's lower bound can be improved**

# PROBING

**Q.** **What if a variable does not go to a bound?**

**A.** **Use probing: temporarily fix variable at a bound.**

## Relaxed Value Function



# The Value Function

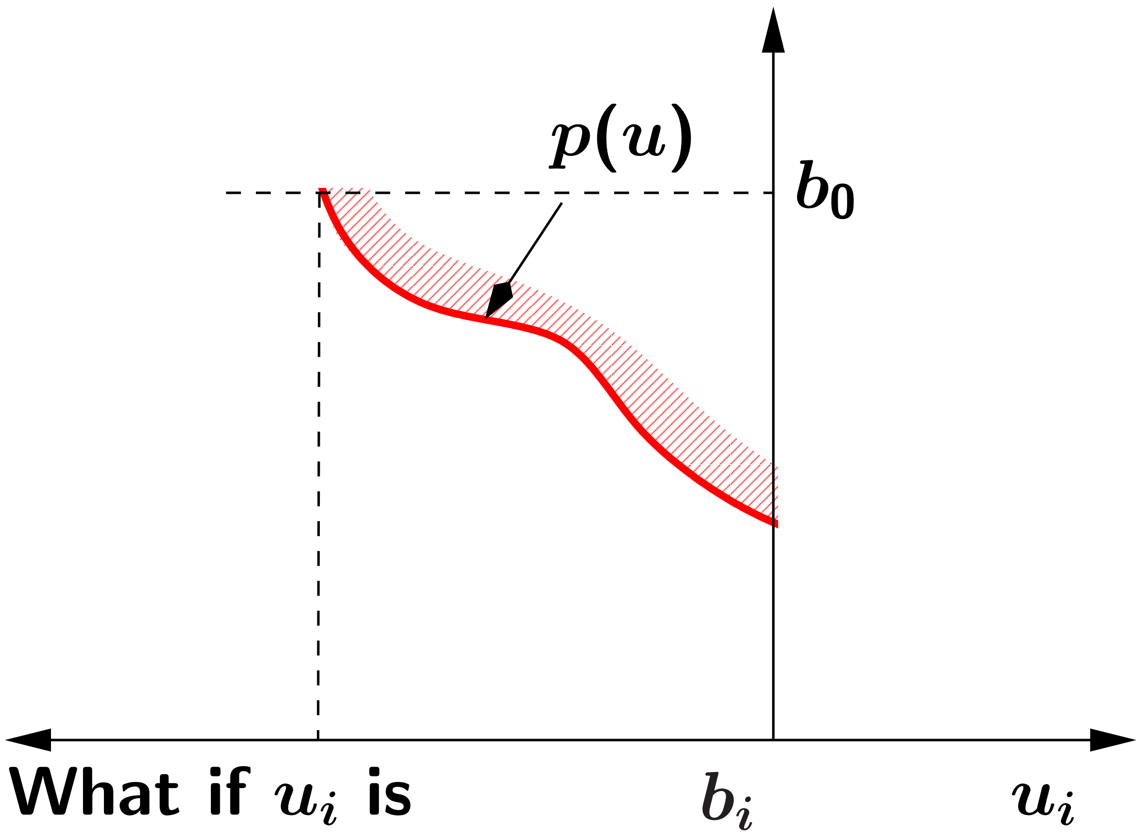
## Mathematical program:

$$
\begin{array}{lll}
\min & f(x) & \\
\text{s.t.} & g_i(x) \leq b_i & i = 1, \ldots, m \\
& x \in X \subseteq \mathbb{R}^n &
\end{array}
$$

## Perturbation Function:

$$
\begin{array}{lll}
p(u) = \min & f(x) & \\
\text{s.t.} & g_i(x) \leq u_i \leq b & i = 1, \ldots, m \\
& f(x) \leq u_0 \leq b_0 & \\
& x \in X \subseteq \mathbb{R}^n & \\
& u_0, u_1, \ldots, u_m \in \mathbb{R} &
\end{array}
$$

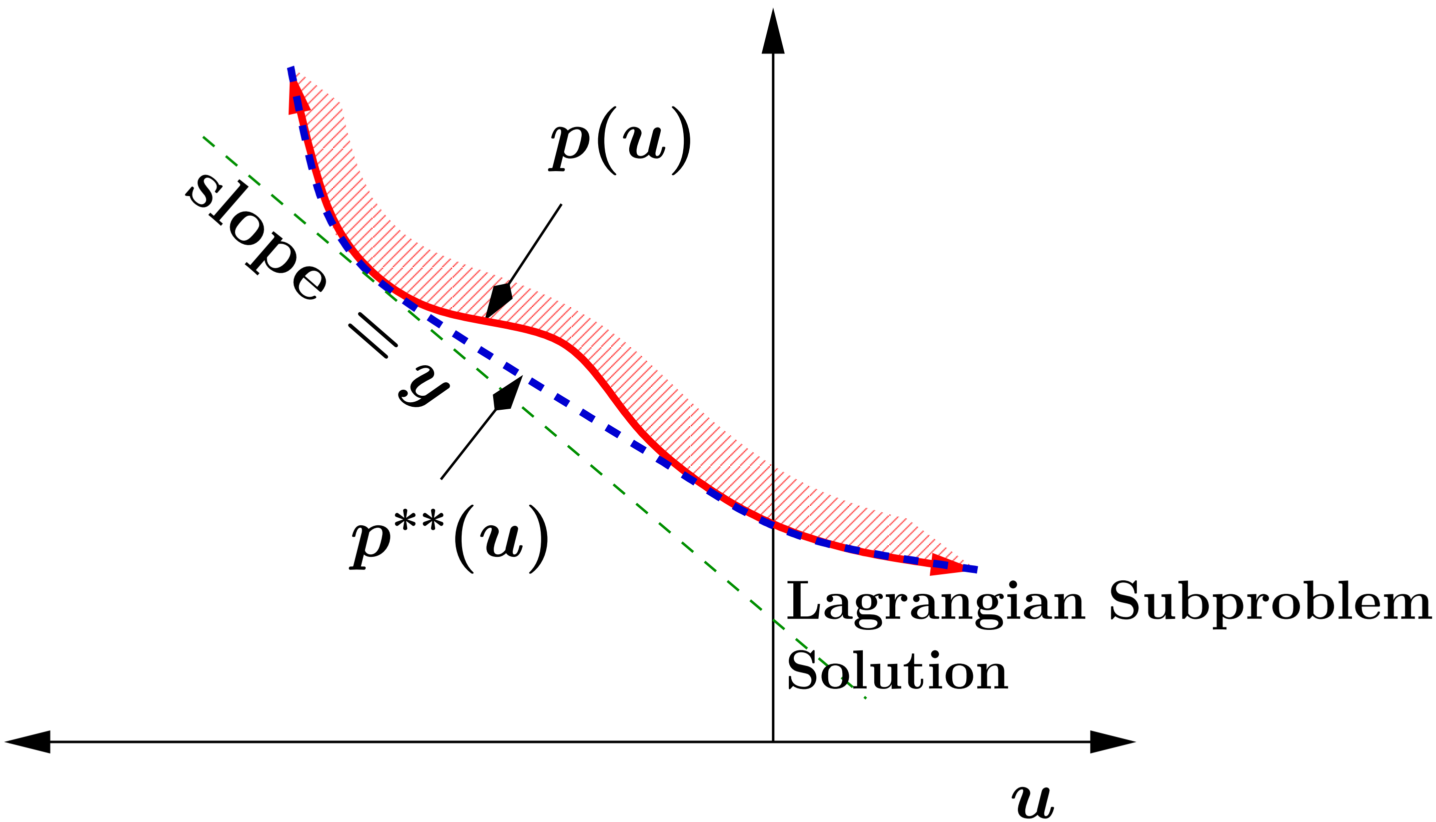
# Domain Reduction in the $u$ space



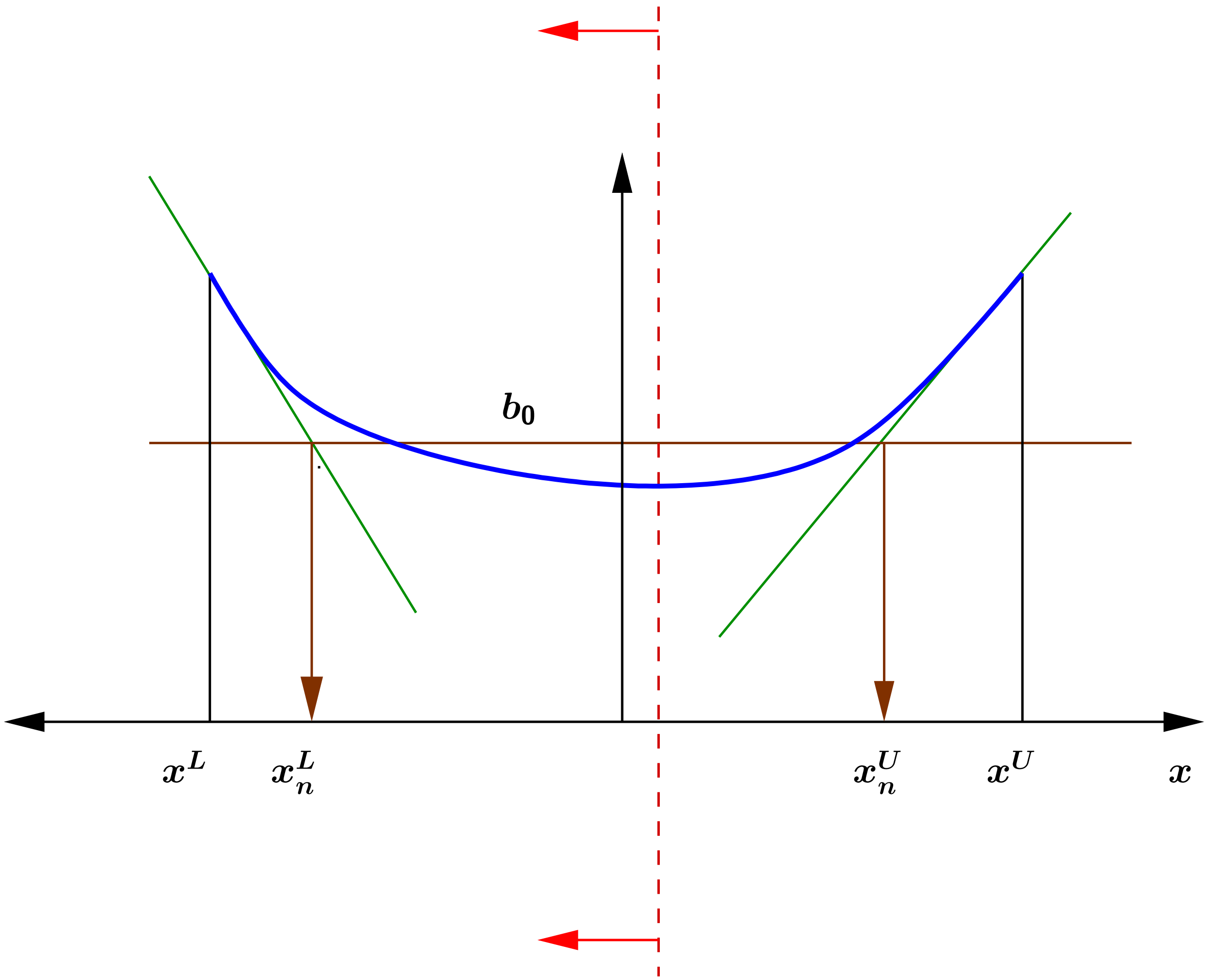

**What if $u_i$ is smaller than this?**

# An Important Property of the Lagrangian Subproblem

**Theorem**: $p^*(y) = \boxed{-\inf_x l(x,y)} \rightarrow$ Lagrangian Subproblem

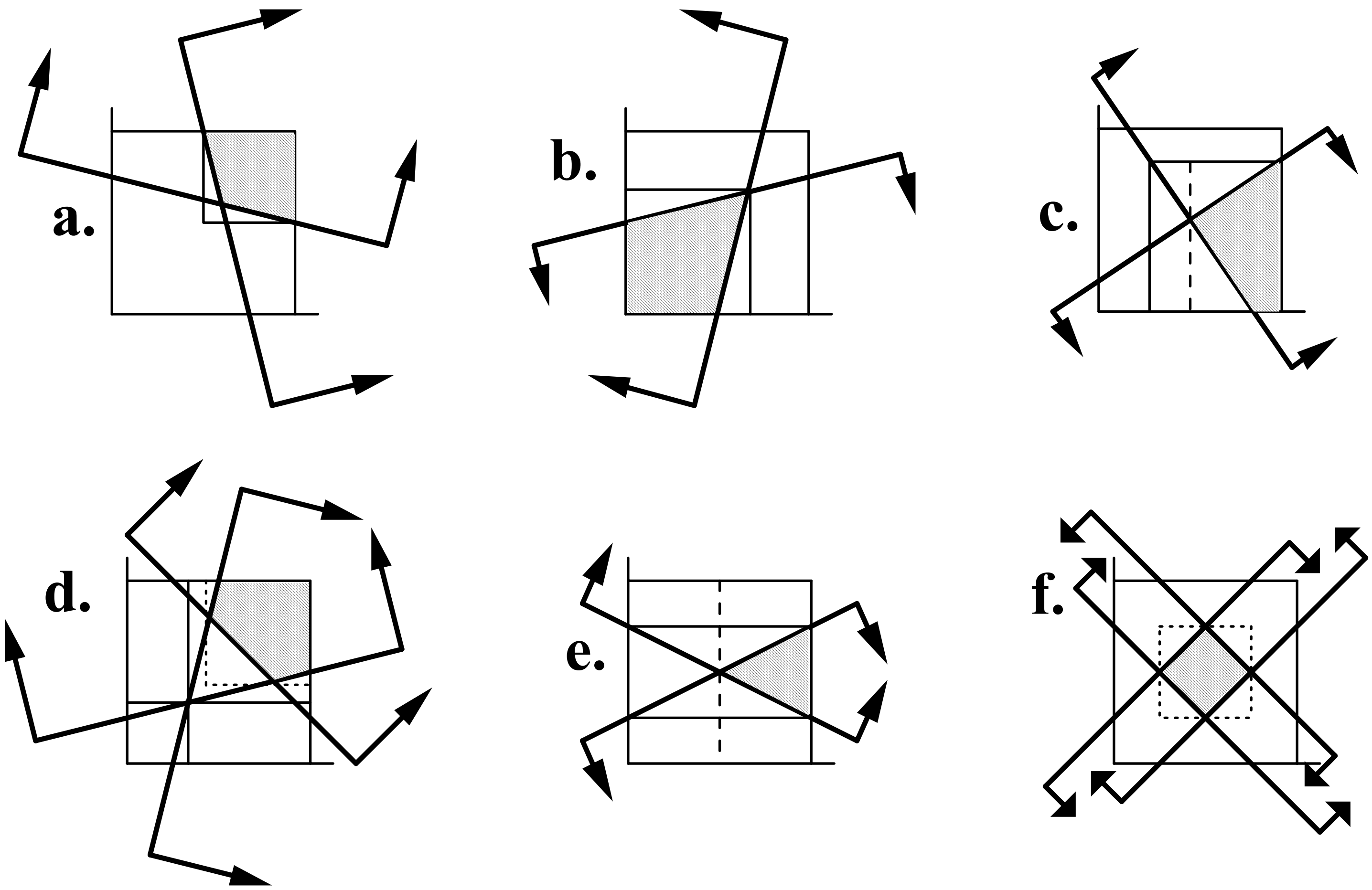


# Probing and Extensions




Ryoo and Sahinidis, 1996

# “POOR MAN’S LPs”



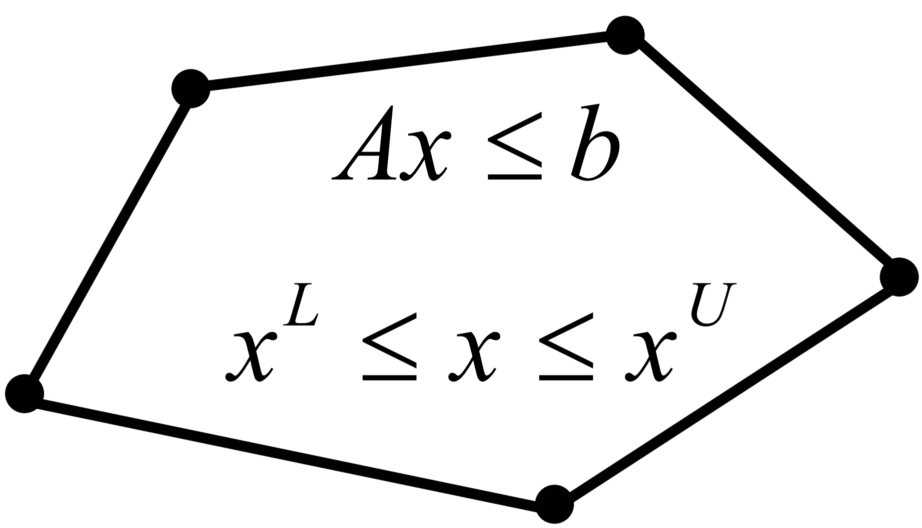
# Other Implied Results

- **Monotone Complementarity Bounds for Convex Programs**
  - **Mangasarian and McLinden (Math. Prog., 1985)**
- **Linearity Based Tightening**
  - **For example, Andersen and Andersen, (Math. Prog., 1995)**
- **Marginals Based Range Reduction**
  - **Ryoo and Sahinidis (JOGO, 1996)**
- **Branch and Contract**
  - **Zamora and Grossmann (JOGO, 1999)**

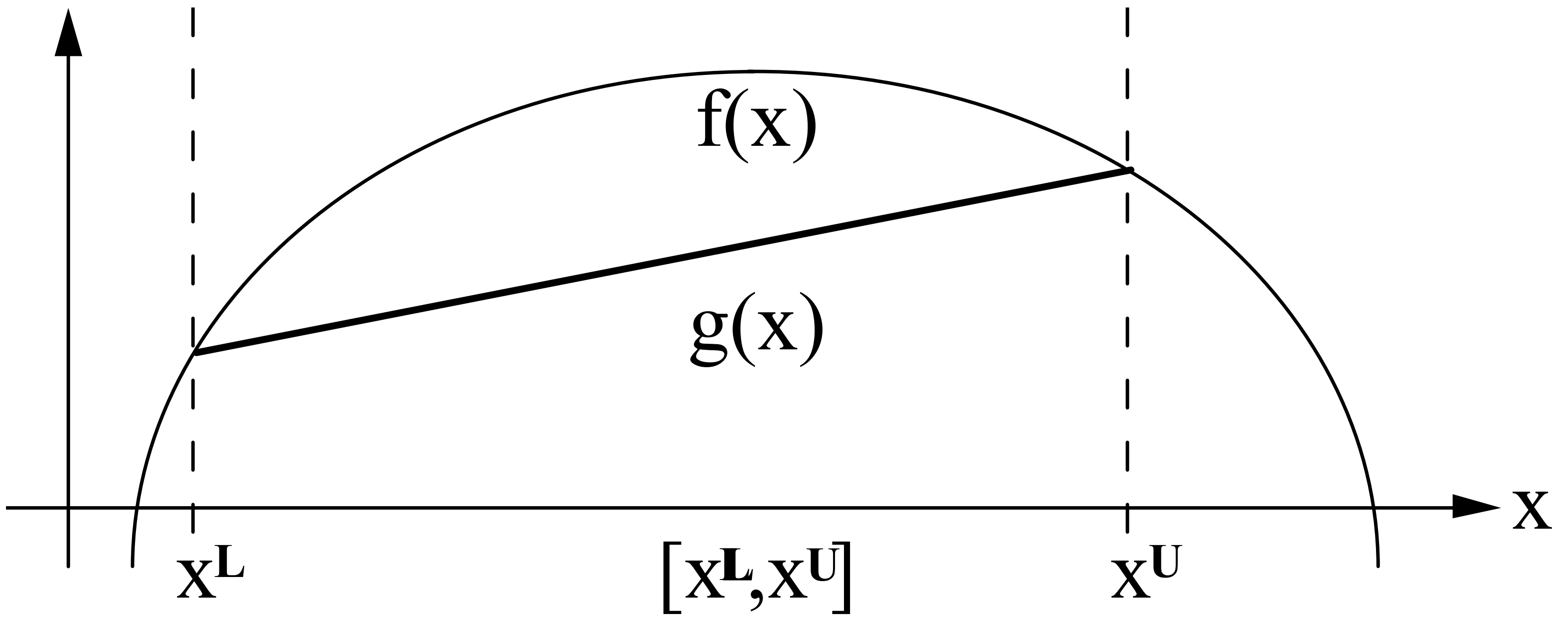
# SEPARABLE CONCAVE MINIMIZATION

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

$$f_k(x_k) \text{ concave, } \forall k.$$



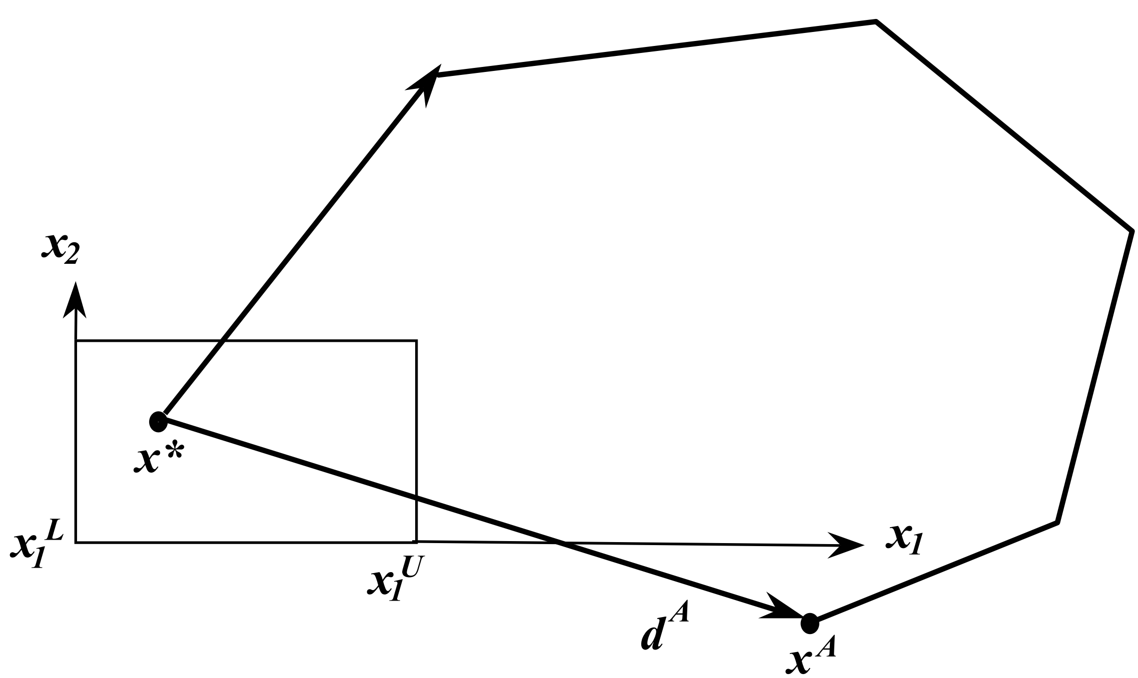
# LOWER BOUNDING



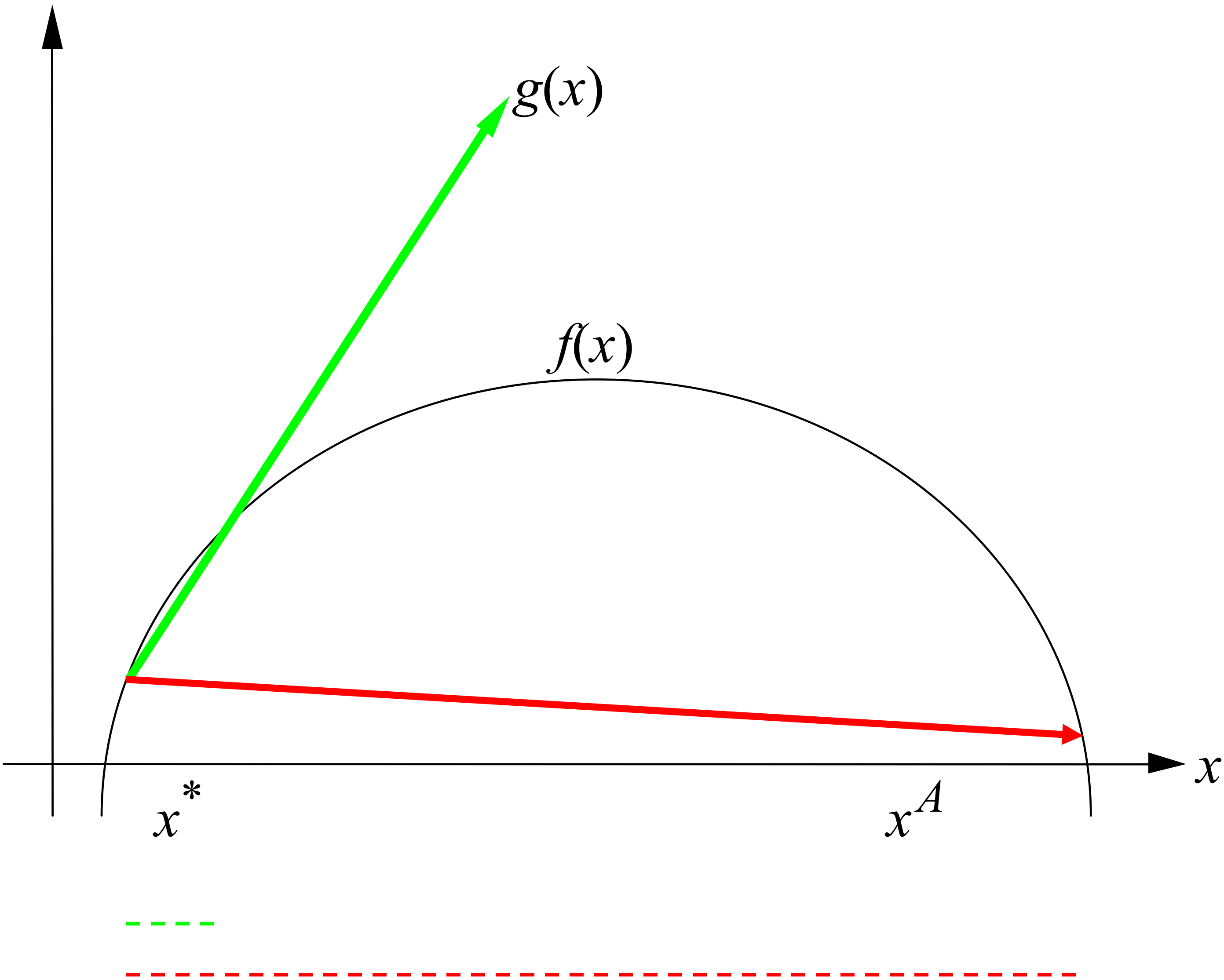

**CONVEX ENVELOPE IS LINEAR**

# FINITE BRANCHING RULE

- **Variable selection:**
  - Typically, select variable with largest underestimating gap
  - Occasionally, select variable corresponding to largest edge
- **Locating partition:**
  - 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**



# PROOF OF FINITENESS




- **Ascent directions of the concave program (*f*) are also ascent directions for the relaxation (*g*).**
- **Once global optimum found, all open nodes are finitely deleted.**

# TWO-STAGE STOCHASTIC INTEGER PROGRAMMING

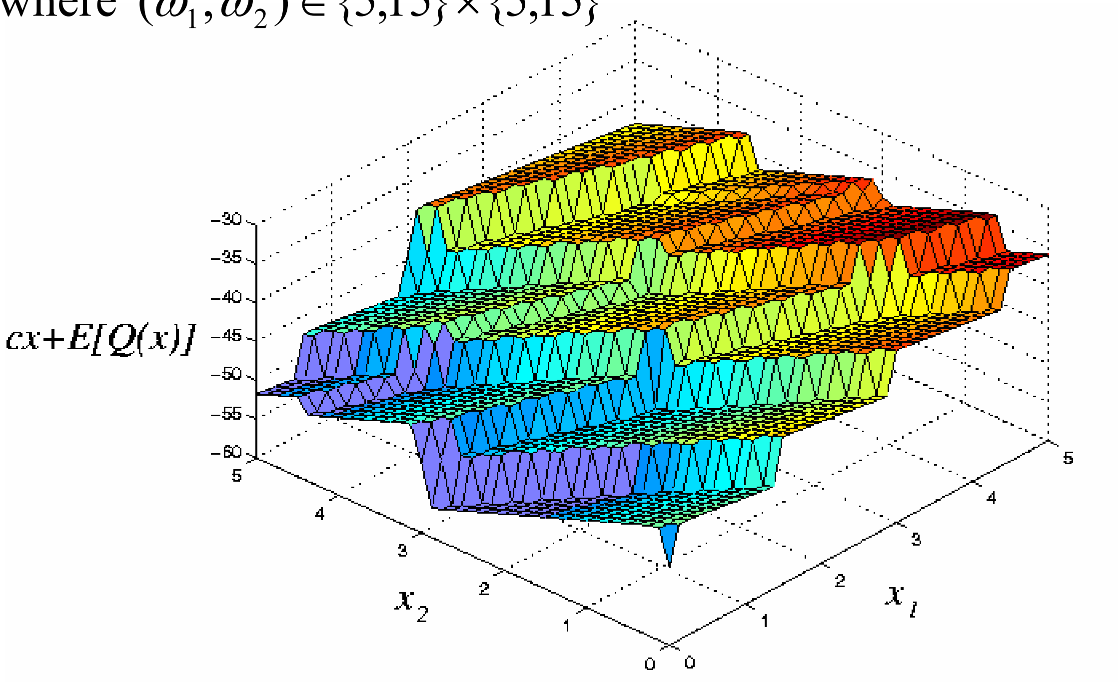
$$\min_{x \in X} cx + E[Q(x,\omega)]$$

where,

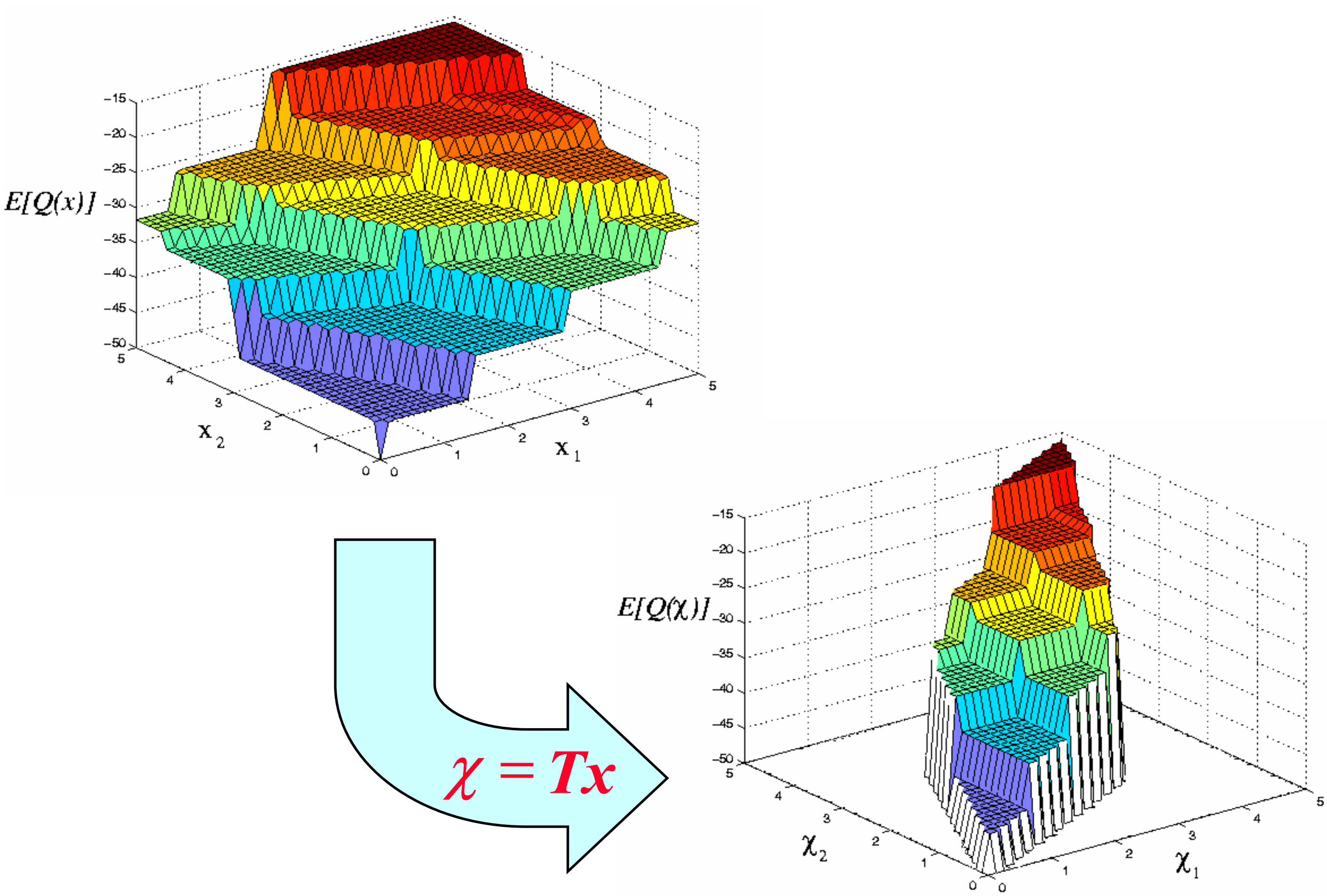
$$Q(x,\omega) := \min_{y \in \{0,1\}} fy \text{ s.t. } D(\omega)y \geq h(\omega) - Tx$$

$$\begin{aligned}
\min \quad & f(x_1,x_2) = -1.5x_1 - 4x_2 + \sum_{s=1}^{4} \frac{1}{4} Q^s(x_1,x_2) \\
s.t. \quad & 0 \leq x_1, x_2 \leq 5 \\
& Q^s(x_1,x_2) := \quad \min \quad -16y_1 - 19y_2 - 23y_3 - 28y_4 \\
& \qquad\qquad\qquad\quad s.t. \quad 2y_1 + 3y_2 + 4y_3 + 5y_4 \leq \omega_1^s - \frac{1}{2}x_1 - \frac{2}{3}x_2 \\
& \qquad\qquad\qquad\qquad\quad\;\; 6y_1 + y_2 + 3y_3 + 2y_4 \leq \omega_2^s - \frac{2}{3}x_1 - \frac{1}{3}x_2 \\
& \qquad\qquad\qquad\qquad\quad\;\; y_i \in \{0,1\} \quad \text{for } i = 1,\ldots,4
\end{aligned}$$

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

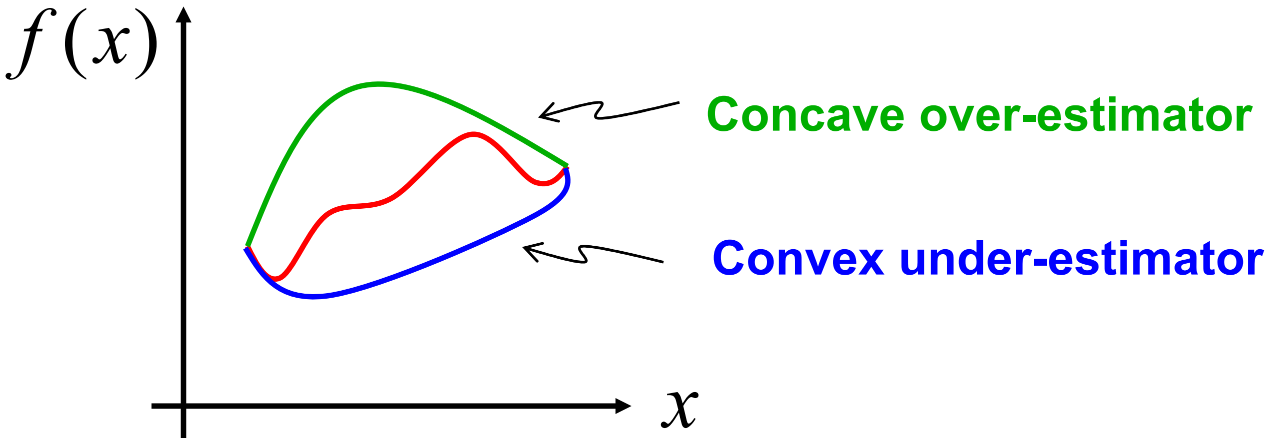


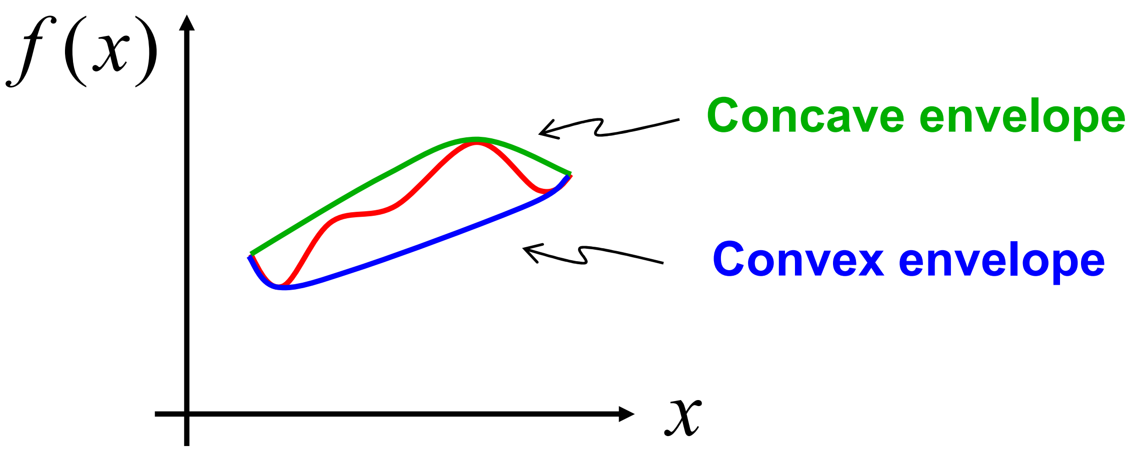
# A FINITE B&B ALGORITHM

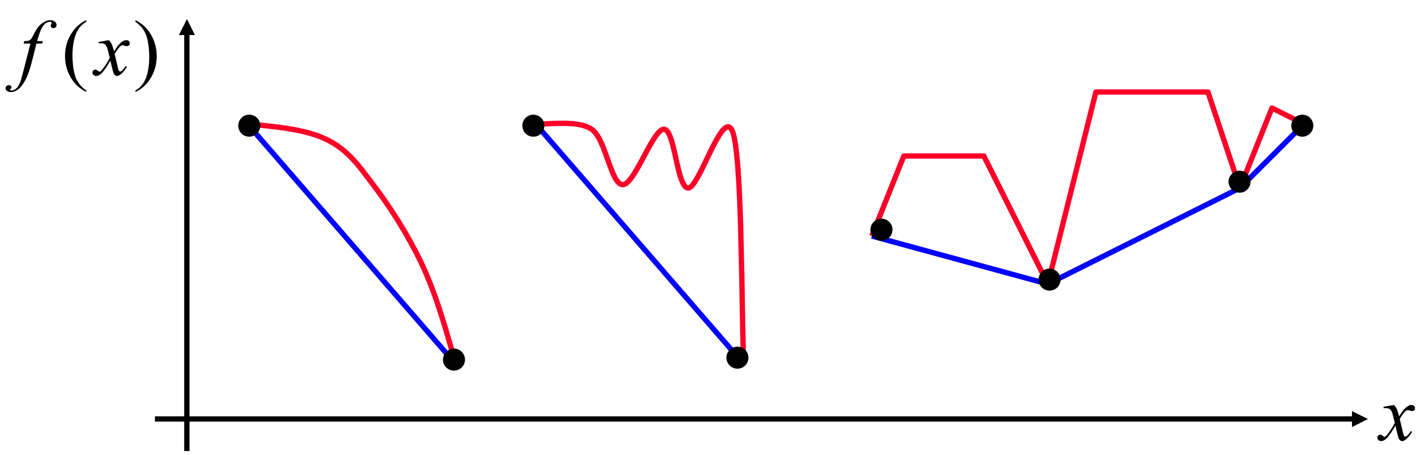



- **Previous algorithms were infinite or explicitly enumerative (Shultz et al., Math. Progr. 1998).**
- **Variable transformation aligns discontinuities orthogonal to variable axes.**
- **Rectangular partitioning of the search space along with integer cuts isolates the discontinuous pieces.**

# TIGHT RELAXATIONS



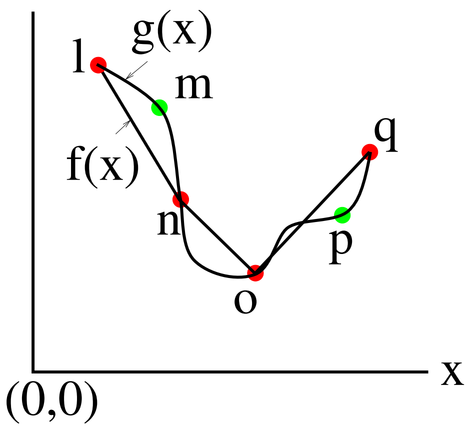

**Convex/concave envelopes often finitely generated**

# Convex Extensions of l.s.c. functions

**Definition:** A function $f(x)$ is a convex extension of $g(x) : C \mapsto R$ restricted to $X \subseteq C$ if

- $f(x)$ is convex on conv $(X)$,
- $f(x) = g(x)$ for all $x \in X$.

**Example: The Univariate Case**




- $f(x)$ is a convex extension of $g(x)$ restricted to $\{l, n, o, q\}$
- Convex extension of $g(x)$ restricted to $\{l, m, n, o, p, q\}$ cannot be constructed

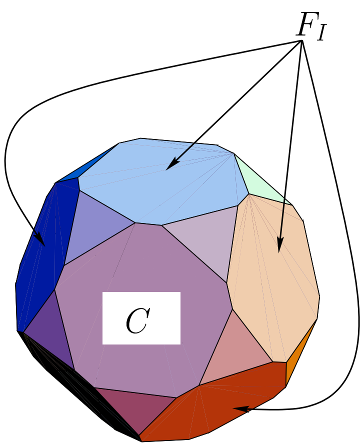
# Constructibility of Convex Extensions

**Theorem:** A convex extension of $g(x) : X \mapsto R$ over a convex set $C \supseteq X$ may be constructed if and only if

$$g(x) \leq \min \left\{ \sum_i \lambda_i g(x_i) \mid \sum_i \lambda_i x_i = x; \sum_i \lambda_i = 1, \lambda_i \in (0,1), x_i \in X \right\} \quad \text{for all } x \in X$$

where the above summations consist of finite terms.

An interesting sufficient condition




If $F_I$ is an arbitrary collection of faces of a convex set $C$, and we are interested in the convex extension of $g(x)$ restricted to $F_I$ over $C$,

Convex Extension constructible over $F_I$ $\xleftrightarrow{\text{Equivalence}}$ $g(x)$ is convex over each face in $F_I$

# The Generating Set of a Function

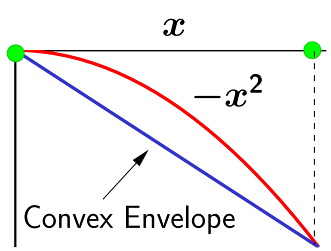
**Definition:*** The generating set of the epigraph of a function $g(x)$ over a compact convex set $C$ is defined as

$$G_C^{\text{epi}}(g) = \left\{ x \;\middle|\; (x,y) \in \text{vert}\Big(\text{epi conv}\,\big(g(x)\big)\Big) \right\},$$

where vert$(\cdot)$ is the set of extreme points of $(\cdot)$.

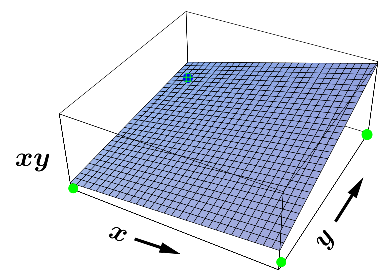
**Examples:**

$g(x) = -x^2$




$G_{[0,6]}^{\text{epi}}(g) = \{0\} \cup \{6\}$

$g(x) = xy$



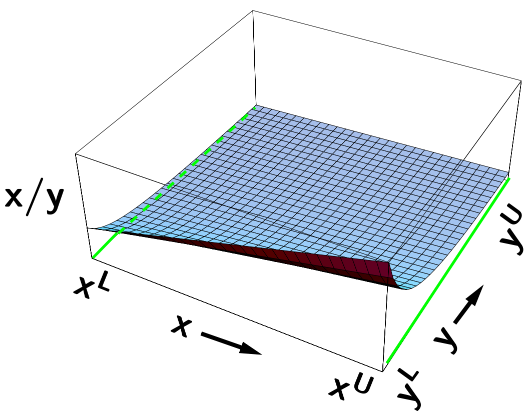

$G_{[1,4]^2}^{\text{epi}}(g) = \{1,1\} \cup \{1,4\} \cup \{4,1\} \cup \{4,4\}$

Similar in vein to that for polyhedral convex functions in Rikun (1997)

# Identifying the Generating Set

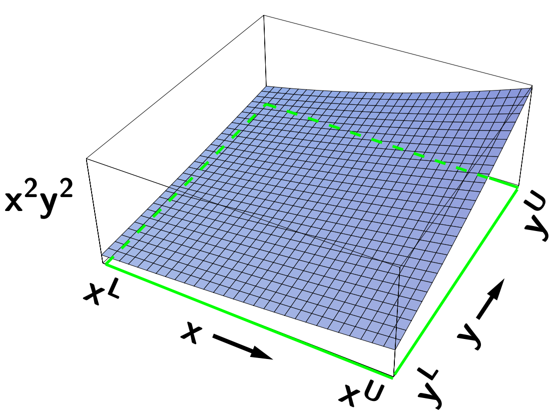
**Characterization:** $x_0 \notin G_C^{\text{epi}}(g)$ if and only if there exists $X \subseteq C$ and $x_0 \notin G_X^{\text{epi}}(g)$.

**Example I:** $X$ is linear joining $(x^L, y^0)$ and $(x^U, y^0)$



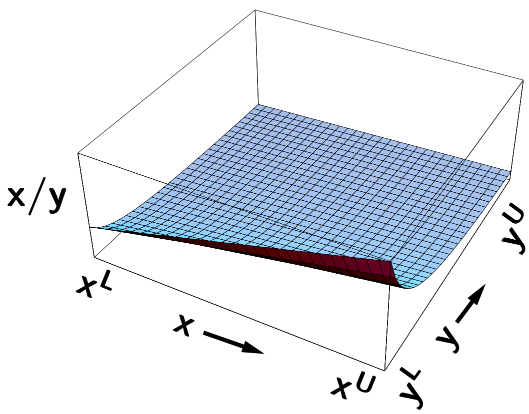

$$G^{\text{epi}}(x/y) = \{(x, y) \mid x \in \{x^L, x^U\}\}$$

**Example II:** $X$ is $\epsilon$ neighborhood of $(x^0, y^0)$




$$G^{\text{epi}}(x^2y^2) = \{(x, y) \mid x \in \{x^L, x^U\}\} \cup \{(x, y) \mid y \in \{y^L, y^U\}\}$$

# Ratio: The 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

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

# Properties: Envelope of $x/y$

## Second Order Cone Representation:

$$\left\| \begin{pmatrix} 2(1-\lambda)\sqrt{x^L} \\ z_p - y_p \end{pmatrix} \right\| \le z_p + y_p$$

$$\left\| \begin{pmatrix} 2\lambda\sqrt{x^U} \\ z - z_p - y + y_p \end{pmatrix} \right\| \le z - z_p + y - y_p$$

$$y_p \ge y^L(1-\lambda), y_p \ge y - y^U\lambda$$

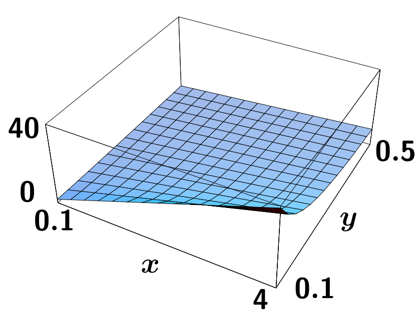
$$y_p \le y^U(1-\lambda), y_p \le y - y^L\lambda$$

$$x = (1-\lambda)x^L + \lambda x^U$$

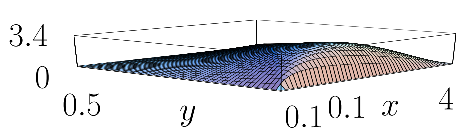
$$z_p, u, v \ge 0, z_c - z_p \ge 0$$

$$0 \le \lambda \le 1$$

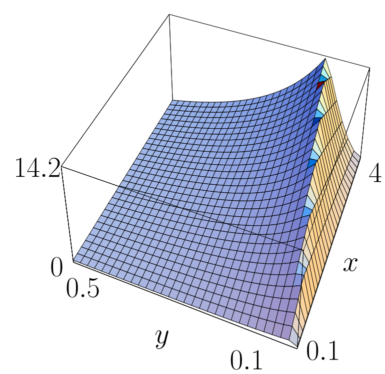
## Comparison of Tightness:




Ratio: $x/y$




$x/y$ − Envelope




$x/y$ − Factorable

## Maximum Gap: Envelope and Factorable Relaxation:

**Point:** $$\left(x^U, y^L + \frac{y^L(y^U - y^L)(x^U y^U - x^L y^L)}{x^U {y^U}^2 - x^L {y^L}^2}\right)$$

**Gap:** $$\frac{x^U(y^U - y^L)^2(x^U y^U - x^L y^L)^2}{y^L y^U(2x^U y^U - x^L y^L - x^U y^L)(x^U {y^U}^2 - x^L {y^L}^2)}$$

## Proof relies on Convex Extensions

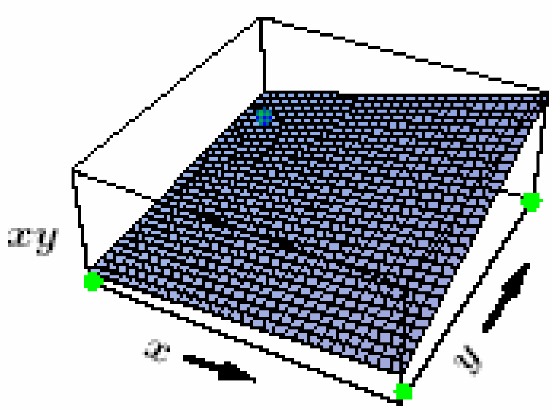
# ENVELOPES FOR SIMPLE MONOMIALS

$$\prod_{i=1}^{p} x_i$$

$$\sum_t a_t \prod_{i=1}^{p_t} x_i$$

- Sherali, Acta Mathematica Vietnamica (1997)
- Tawarmalani and Sahinidis, *Math. Programming* (2002)

$$g(x) = xy$$




$$G^{\text{epi}}_{[1,4]^2}(g) = \{1,1\} \cup \{1,4\} \cup \{4,1\} \cup \{4,4\}$$

# Further Applications . . .

$$M(x_1, x_2, \cdots x_n)/(y_1^{a_1} y_2^{a_2} \ldots y_m^{a_m})$$

where

$M(\cdot)$ is a multilinear expression

$y_1, \ldots, y_m \neq 0$

$a_1, \ldots, a_m \geq 0$

**Example:** $(x_1 x_2 + x_3 x_2)/(y_1 y_2 y_3)$

$$f(x) \sum_{i=1}^{n} \sum_{j=-p}^{k} a_{ij} y_i^j$$

where

$f$ is concave

$a_{ij} \geq 0$ for $i = 1, \ldots, n$; $j = -p, \ldots, k$

$y_i > 0$

**Example:** $x/y + 3x + 4xy + 2xy^2$

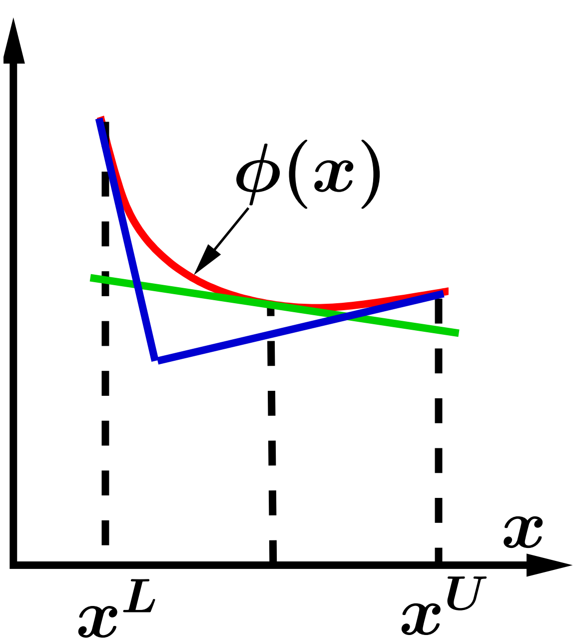
# Outer Approximation

**Motivation:**

- Convex Programming Solvers are not robust
- Linear programs can be solved efficiently

**Outer-Approximation:**

Convex Functions are underestimated by tangent lines



# Quadratic Convergence with Projective Error Rule

**Theorem:**

- Let $\phi(x_j)$ be a convex function over $[x_j^l, x_j^u]$ and $\epsilon_p$ the desired projective approximation error
- Outer-approximate $\phi(x_j)$ at the end-points
- At every iteration of the Sandwich Algorithm construct an underestimator at the point that maximizes the projective error of function with current outer-approximation.
- Let $k = (x_j^u - x_j^l)(x_j^{u*} - x_j^{l*})/\epsilon_p$
- Then, the algorithm needs at most

$$N(k) = \begin{cases} 0 & k \leq 4 \\ \lceil \sqrt{k} - 2 \rceil, & k > 4 \end{cases}$$

iterations

# Branch And Reduce Optimization Navigator

**BARON CORE**

- Preprocessor
- Data Organizer
- Range Reduction
- Solver Links
- I/O Handler
- Debugging Facilities
- Sparse Matrix Utilities
- Heuristics

**USER MODULE**

- Relaxation
- Local Search
- Range Reduction
- Heuristics

**Core Module:** Global Optimization Library

- expandable, application-independent

**Application Modules:** Special Problem Classes

- factorable nonlinear, linear multiplicative, bilinear, concave, fixed-charge, integer, fractional programming
- solve convex relaxations using CPLEX, OSL, MINOS, SNOPT, SDPA

# BARON MODELING LANGUAGE

```
// Design of an insulated tank

OPTIONS{
nlpdolin: 1;
dolocal: 0; numloc: 3;
brstra: 7; nodesel: 0;
nlpsol: 4; lpsol: 3;
pdo: 1; pxdo: 1; mdo: 1;
}
MODULE: NLP;
```

Relaxation Strategy

Local Search Options

B&B options

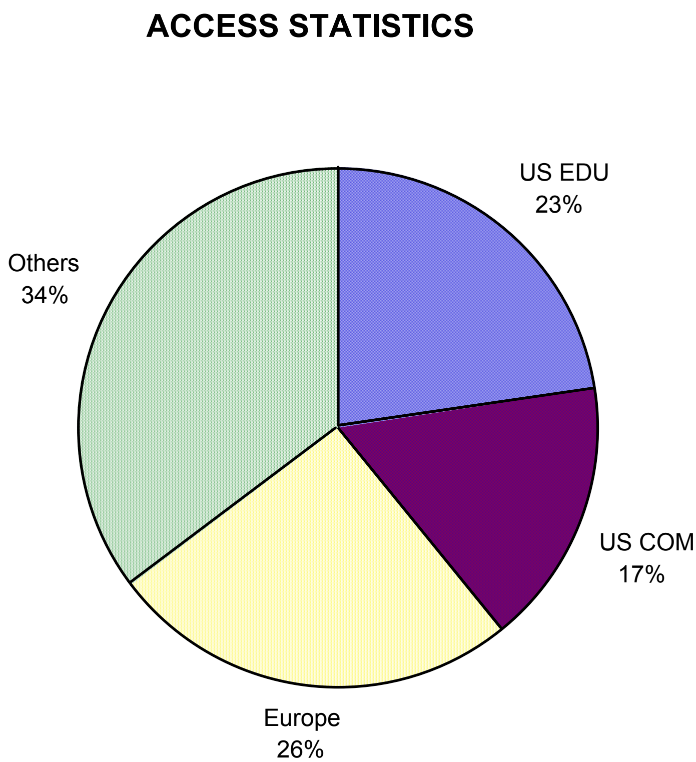
Solver Links

Domain Reduction Options

```
// INTEGER_VARIABLE y1;
POSITIVE_VARIABLES x1, x2, x4;
VARIABLE x3;

LOWER_BOUNDS{x2:14.7;  x3:-459.67;}

UPPER_BOUNDS{
x1:   15.1;  x2:   94.2;
x3:   80.0;  x4: 5371.0;
}

EQUATIONS e1, e2;
e1: x4*x1 - 144*(80-x3) >= 0;
e2: x2-exp(-3950/(x3+460)+11.86) == 0 ;
OBJ: minimize 400*x1^0.9 + 1000
    + 22*(x2-14.7)^1.2+x4;
```

# BARON ACCESS

- On the internet since March 1995
- http://archimedes.scs.uiuc.edu
- Accessed from over 44 countries
- 10 accesses per day




- Web interface since October 1999
- Password-accessible online runs
- Used by 165 research groups
- Over 6100 problems solved

# COMPUTATIONAL RESULTS

| | BRANCH-AND-BOUND | | | | BRANCH-AND-REDUCE | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | No probing | | | | With Probing | | | |
| Ex. | $N_{tot}$ | $N_{opt}$ | $N_{mem}$ | 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 |

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

**COMPUTER: SUN Sparc Station 2**

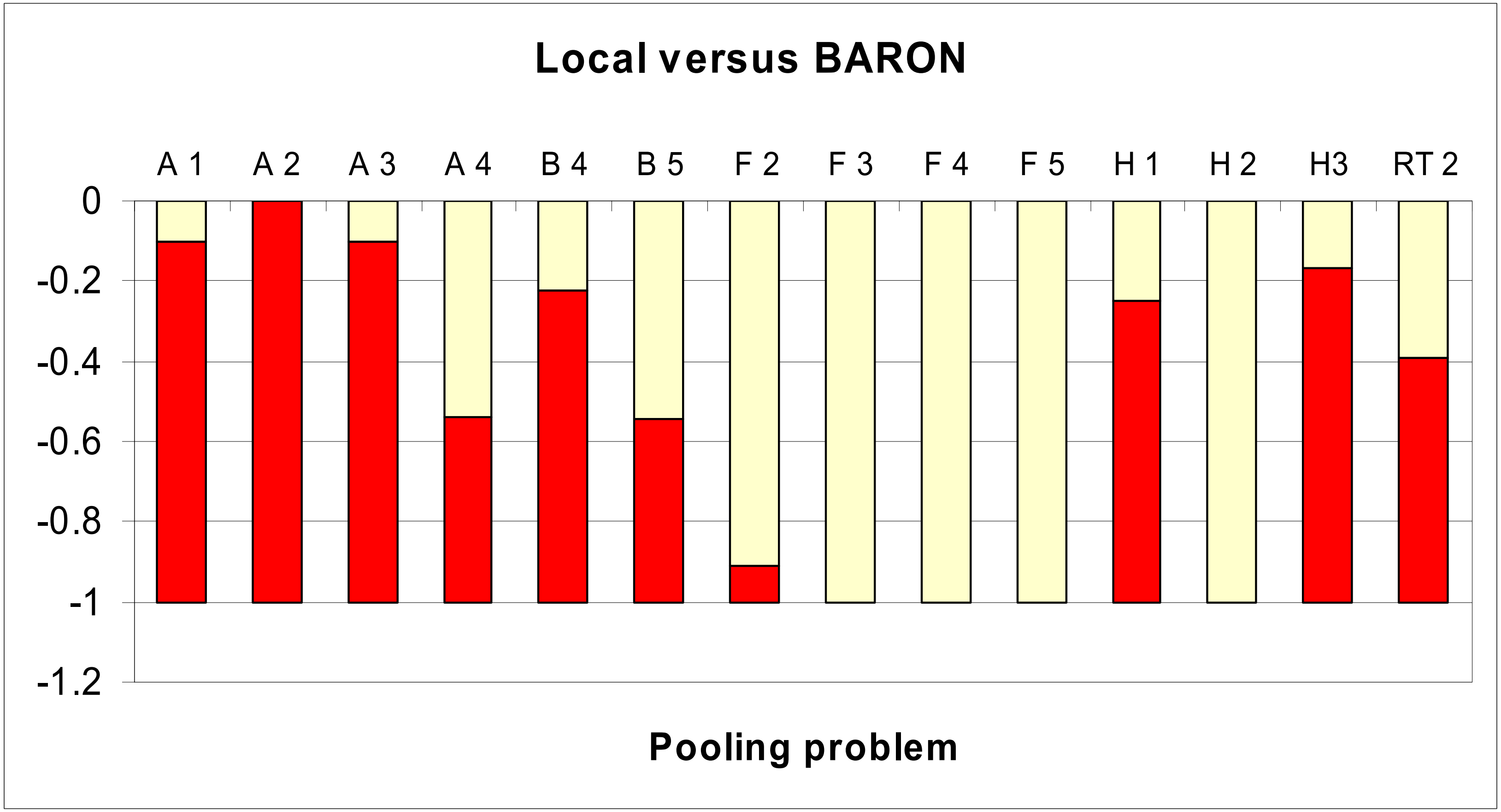
# Pooling Problems in Literature

| Algorithm | Foulds '92 | | Ben-Tal '94 | | GOP '96 | | BARON '99 | | BARON '01 | |
|---|---|---|---|---|---|---|---|---|---|---|
| Computer* | CDC 4340 | | | | HP9000/730 | | RS6000/43P | | RS6000/43P | |
| Linpack | $> 3.5$ | | | | 49 | | 59.9 | | 59.9 | |
| Tolerance* | | | | | ** | | $10^{-6}$ | | $10^{-6}$ | |
| Problem | $N_{\text{tot}}$ | $T_{\text{tot}}$ | $N_{\text{tot}}$ | $T_{\text{tot}}$ | $N_{\text{tot}}$ | $T_{\text{tot}}$ | $N_{\text{tot}}$ | $T_{\text{tot}}$ | $N_{\text{tot}}$ | $T_{\text{tot}}$ |
| Haverly 1 | 5 | 0.7 | 3 | - | 12 | 0.22 | 3 | 0.09 | 1 | 0.09 |
| Haverly 2 | | | 3 | - | 12 | 0.21 | 9 | 0.09 | 1 | 0.13 |
| Haverly 3 | | | 3 | - | 14 | 0.26 | 5 | 0.13 | 1 | 0.07 |
| Foulds 2 | 9 | 3.0 | | | | | 1 | 0.10 | 1 | 0.04 |
| Foulds 3 | 1 | 10.5 | | | | | 1 | 2.33 | 1 | 1.70 |
| Foulds 4 | 25 | 125.0 | | | | | 1 | 2.59 | 1 | 0.38 |
| Foulds 5 | 125 | 163.6 | | | | | 1 | 0.86 | 1 | 0.10 |
| Ben-Tal 4 | | | 25 | - | 7 | 0.95 | 3 | 0.11 | 1 | 0.13 |
| Ben-Tal 5 | | | 283 | - | 41 | 5.80 | 1 | 1.12 | 1 | 1.22 |
| Adhya 1 | | | | | | | 6174 | 425 | 15 | 4.00 |
| Adhya 2 | | | | | | | 10743 | 1115 | 19 | 4.48 |
| Adhya 3 | | | | | | | 79944 | 19314 | 5 | 3.16 |
| Adhya 4 | | | | | | | 1980 | 182 | 1 | 0.97 |

* Blank indicates problem not reported or not solved

** 0.05% for Haverly 1, 2, 3, 0.05% for Ben-Tal 4 and 1% for Ben-Tal 5

# LOCAL vs. GLOBAL SEARCH



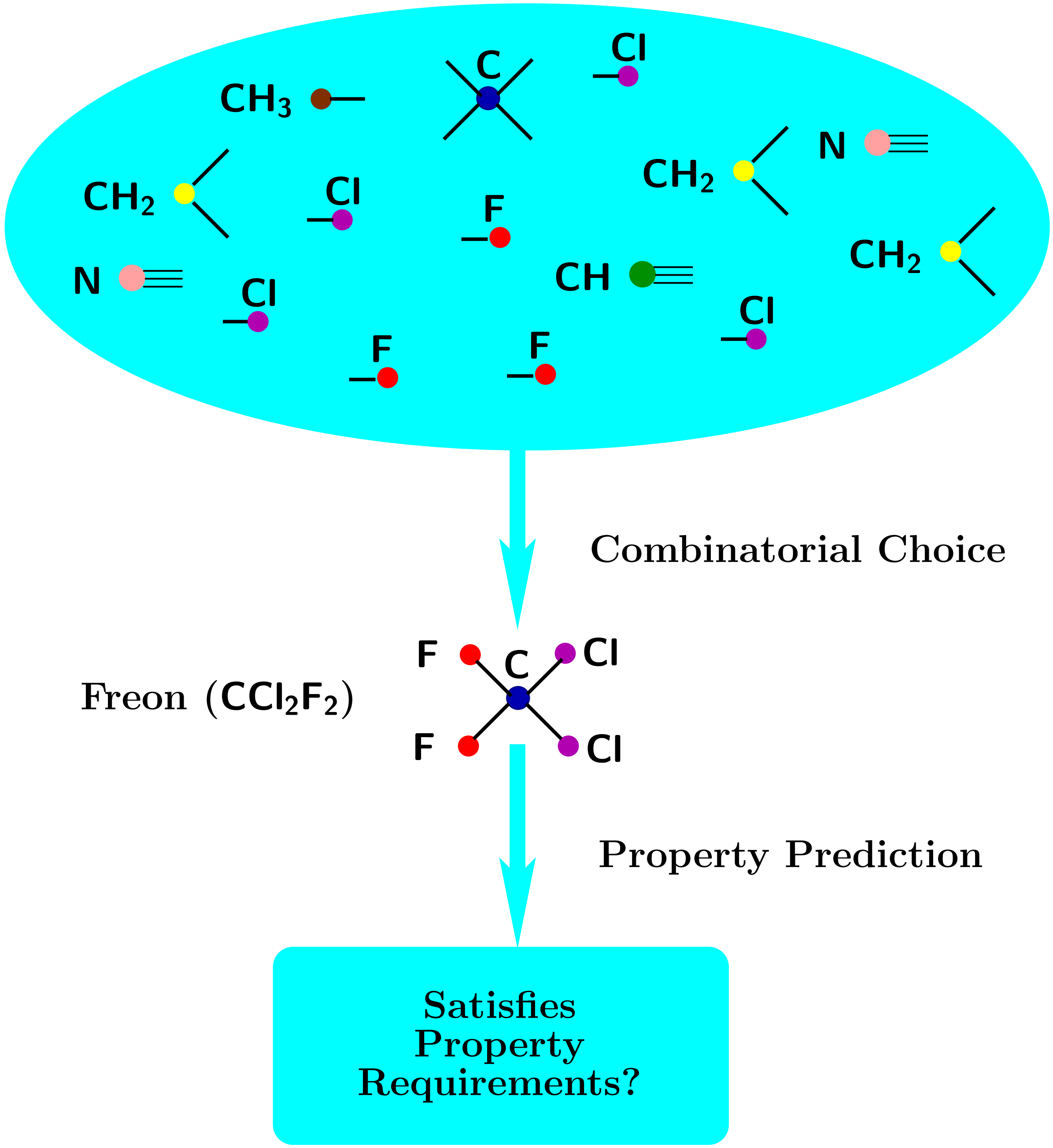
# Gupta Problems

| Problem | | Obj. | $T_{tot}$ | $N_{tot}$ | $N_{mem}$ |
|---|---|---|---|---|---|
| 1 | | 12.47 | 0.11 | 22 | 4 |
| 2 | * | 5.96 | 0.03 | 7 | 4 |
| 3 | | 16.00 | 0.03 | 3 | 2 |
| 4 | | 0.72 | 0.01 | 1 | 1 |
| 5 | | 5.47 | 4.48 | 232 | 22 |
| 6 | | 1.77 | 0.06 | 11 | 5 |
| 7 | | 4.00 | 0.03 | 3 | 2 |
| 8 | | 23.45 | 0.40 | 7 | 2 |
| 9 | | -43.13 | 0.58 | 37 | 7 |
| 10 | | -310.80 | 0.06 | 12 | 4 |
| 11 | | -431.00 | 0.12 | 34 | 8 |
| 12 | | -481.20 | 0.29 | 67 | 12 |

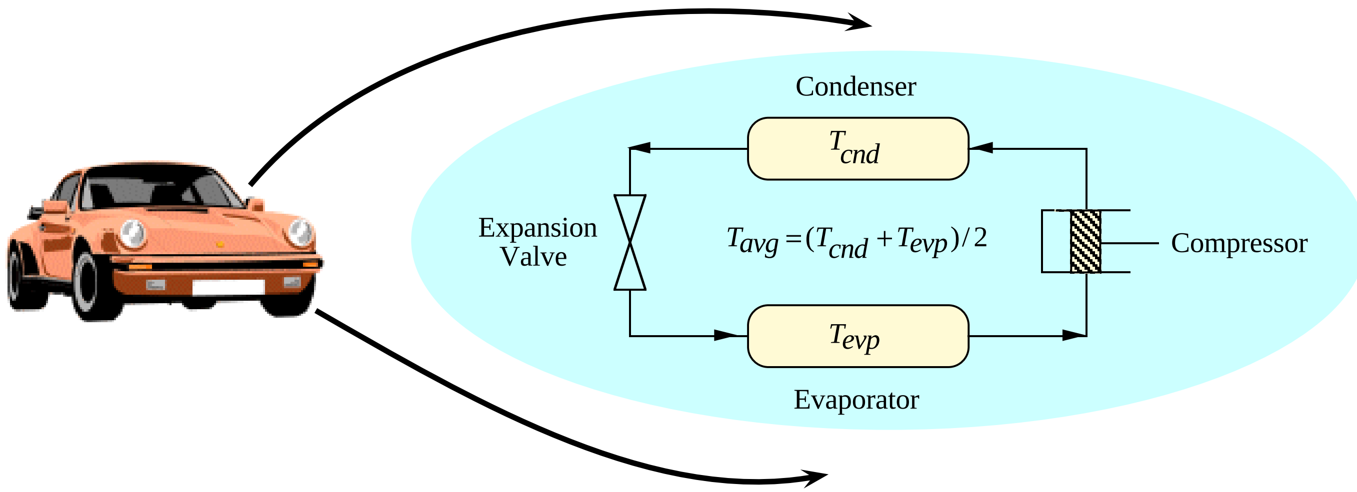
| Problem | | Obj. | $T_{tot}$ | $N_{tot}$ | $N_{mem}$ |
|---|---|---|---|---|---|
| 13 | | -585.20 | 1.13 | 197 | 28 |
| 14 | * | -40358.20 | 0.05 | 7 | 4 |
| 15 | | 1.00 | 0.05 | 11 | 3 |
| 16 | | 0.70 | 0.05 | 23 | 12 |
| 17 | | -1100.40 | 42.2 | 3489 | 399 |
| 18 | | -778.40 | 8.85 | 993 | 121 |
| 19 | | -1098.40 | 133 | 6814 | 833 |
| 20 | * | 230.92 | 6.58 | 143 | 18 |
| 21 | * | -5.68 | 0.21 | 54 | 5 |
| 22 | | 6.06 | 2.36 | 171 | 39 |
| 23 | | -1125.20 | 1152 | 39918 | 4678 |
| 24 | | -1033.20 | 4404 | 124282 | 15652 |

* Indicates that a better solution was found than reported in Gupta and Ravindran, 1985.

# MOLECULAR DESIGN



# AUTOMOTIVE REFRIGERANT DESIGN




- Higher enthalpy of vaporization reduces the amount of refrigerant
- Lower liquid heat capacity reduces amount of vapor generated in expansion valve

# Functional Groups Considered

| Acyclic Groups | Cyclic Groups | Halogen Groups | Oxygen Groups | Nitrogen Groups | Sulfur Groups |
|---|---|---|---|---|---|
| $-\mathrm{CH_3}$ | ${}^{r} - \mathrm{CH_2} - {}^{r}$ | $-\mathrm{F}$ | $-\mathrm{OH}$ | $-\mathrm{NH_2}$ | $-\mathrm{SH}$ |
| $-\mathrm{CH_2}-$ | ${}^{r}_{r} > \mathrm{CH} - {}^{r}$ | $-\mathrm{Cl}$ | $-\mathrm{O}-$ | $>\mathrm{NH}$ | $-\mathrm{S}-$ |
| $>\mathrm{CH}-$ | ${}_{r} > \mathrm{CH} - {}^{r}$ | $-\mathrm{Br}$ | ${}^{r} - \mathrm{O} - {}^{r}$ | ${}^{r}_{r} > \mathrm{NH}$ | ${}^{r} - \mathrm{S} - {}^{r}$ |
| $>\mathrm{C}<$ | ${}^{r}_{r} > \mathrm{C} < {}^{r}_{r}$ | $-\mathrm{I}$ | $>\mathrm{CO}$ | $>\mathrm{N}-$ | |
| $=\mathrm{CH_2}$ | ${}_{r} > \mathrm{C} < {}^{r}_{r}$ | | ${}^{r}_{r} > \mathrm{CO}$ | $=\mathrm{N}-$ | |
| $=\mathrm{CH}-$ | $> \mathrm{C} < {}^{r}_{r}$ | | $-\mathrm{CHO}$ | ${}^{r} = \mathrm{N} - {}^{r}$ | |
| $=\mathrm{C}<$ | ${}^{r} = \mathrm{CH} - {}^{r}$ | | $-\mathrm{COOH}$ | $-\mathrm{CN}$ | |
| $=\mathrm{C}=$ | ${}^{r} = \mathrm{C} < {}^{r}_{r}$ | | $-\mathrm{COO}-$ | $-\mathrm{NO_2}$ | |
| $\equiv \mathrm{CH}$ | ${}^{r} = \mathrm{C} < {}_{r}$ | | $=\mathrm{O}$ | | |
| $\equiv \mathrm{C}-$ | $= \mathrm{C} < {}^{r}_{r}$ | | | | |

**Number of Groups $= 44$**

**Maximum Selection Size $= 15$**

**Candidates $= 39,895,566,894,524$**

# Property Prediction Constraints

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

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

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

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

$$T_{\mathrm{br}} = \frac{T_{\mathrm{b}}}{T_c}$$

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

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

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

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

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

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

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

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

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

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

$$G = 0.4835 + 0.4605h$$

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

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

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

$n_i$ integer

# Structure Feasibility Constraints

$$\sum_{i=1}^{N} n_i \geq 2$$

$$Y_A \leq \sum_{i\in\mathcal{A}} n_i \leq N_{max} Y_A \|\mathcal{A}\|$$

$$Y_C \leq \sum_{i\in\mathcal{C}} n_i \leq N_{max} Y_C \|\mathcal{C}\|$$

$$Y_M \leq \sum_{i\in\mathcal{M}} n_i \leq N_{max} Y_M \|\mathcal{M}\|$$

$$Y_A + Y_C - 1 \leq Y_M \leq Y_A + Y_C$$

$$3Y_R \leq \sum_{i\in\mathcal{R}} n_i \leq N_{max} Y_R \|\mathcal{R}\|$$

$$\sum_{i=1}^{N} n_i b_i \geq 2(\sum_{i=1}^{N} n_i - 1);$$

$$\sum_{i=1}^{N} n_i b_i \leq \left(\sum_{i=1}^{N} n_i\right)\left(\sum_{i=1}^{N} n_i - 1\right)$$

$$\sum_{i\in\mathcal{SD}} n_i \geq 1 \text{ if } \sum_{i\in\mathcal{S}/\mathcal{D}} n_i \geq 1 \text{ and } \sum_{i\in\mathcal{D}/\mathcal{S}} n_i \geq 1$$

$$\sum_{i\in\mathcal{ST}} n_i \geq 1 \text{ if } \sum_{i\in\mathcal{S}/\mathcal{T}} n_i \geq 1 \text{ and } \sum_{i\in\mathcal{T}/\mathcal{S}} n_i \geq 1$$

$$\sum_{i\in\mathcal{SSR}} n_i \geq 1 \text{ if } \sum_{i\in\mathcal{S}/\mathcal{SR}} n_i \geq 1 \text{ and } \sum_{i\in\mathcal{SR}/\mathcal{S}} n_i \geq 1$$

$$\sum_{i\in\mathcal{SDR}} n_i \geq 1 \text{ if } \sum_{i\in\mathcal{S}/\mathcal{DR}} n_i \geq 1 \text{ and } \sum_{i\in\mathcal{DR}/\mathcal{S}} n_i \geq 1$$

$$\sum_{i\in\mathcal{DSR}} n_i \geq 1 \text{ if } \sum_{i\in\mathcal{D}/\mathcal{SR}} n_i \geq 1 \text{ and } \sum_{i\in\mathcal{SR}/\mathcal{D}} n_i \geq 1$$

$$\sum_{i\in\mathcal{B}} n_i = 2Z_B; \quad \sum_{i\in\mathcal{S}} n_i = 2Z_S; \quad \sum_{i\in\mathcal{SR}} n_i = 2Z_{SR}$$

$$\sum_{i\in\mathcal{D}} n_i = 2Z_D$$

$$\sum_{i\in\mathcal{DR}} n_i = 2Z_{DR}$$

$$\sum_{i\in\mathcal{T}} n_i = 2Z_T$$

$$\sum_{i} n_i(2 - b_i) = 2m$$

$$\sum_{i=1}^{N} n_i \geq n_j(b_j - 1) + 2 \quad j = 1, \ldots, N$$

$$\sum_{\substack{i\in\mathcal{O}, \\ \text{single-bonded}}} n_i \leq \sum_{i\in\mathcal{H}} n_i S_{ai} \text{ if } \sum_{i\in\mathcal{H}} n_i \neq 0$$

$$\sum_{\substack{i\in\mathcal{O}, \\ \text{double-bonded}}} n_i \leq \sum_{i\in\mathcal{H}} n_i D_{ai} \text{ if } \sum_{i\in\mathcal{H}} n_i \neq 0$$

$$\sum_{\substack{i\in\mathcal{O}, \\ \text{triple-bonded}}} n_i \leq \sum_{i\in\mathcal{H}} n_i T_{ai} \text{ if } \sum_{i\in\mathcal{H}} n_i \neq 0$$

$$\sum_{i\in\mathcal{H}} n_i(S_{ai} + D_{ai} + T_{ai}) - \sum_{i\in\mathcal{O}} n_i \leq 2(\sum_{i\in\mathcal{H}} n_i - 1)$$

# MOLECULAR STRUCTURES

| | Molecular Structure | $\frac{\Delta H_{ve}}{C_{pla}}$ |
|---|---|---|
| FNO | $F - N = O$ | 1.2880 |
| FSH | $F - SH$ | 1.1697 |
| $CH_3Cl$ | $CH_3 - Cl$ | 1.1219 |
| ClFO | $(Cl-)(-O-)(-F)$ | 0.9822 |
| $C_2HClO_2$ | $O = C < (-CH = O)(-Cl)$ | 1.1207 |
| $C_3H_40$ | $CH_3 - CH = C = O$ | 0.9619 |
| $C_3H_4$ | $CH_3 - C \equiv CH$ | 0.9278 |
| $C_2F_2$ | $F - C \equiv C - F$ | 0.9229 |
| $CH_2ClF$ | $F - CH2 - Cl$ | 0.9202 |
| $C_2HO_2F$ | $F - O - CH = C = O$ | 0.8705 |
| $C_3H_4$ | $CH_2 = C = CH_2$ | 0.8656 |
| $C_2H_6$ | $CH_3 - CH_3$ | 0.8632 |
| $C_3H_3FO$ | $(F-)(CH3-) > C = C = O$ | 0.8531 |
| $NHF_2$ | $F - NH - F$ | 0.8468 |
| $C_2HOF$ | $CH \equiv C - O - F$ | 0.8263 |

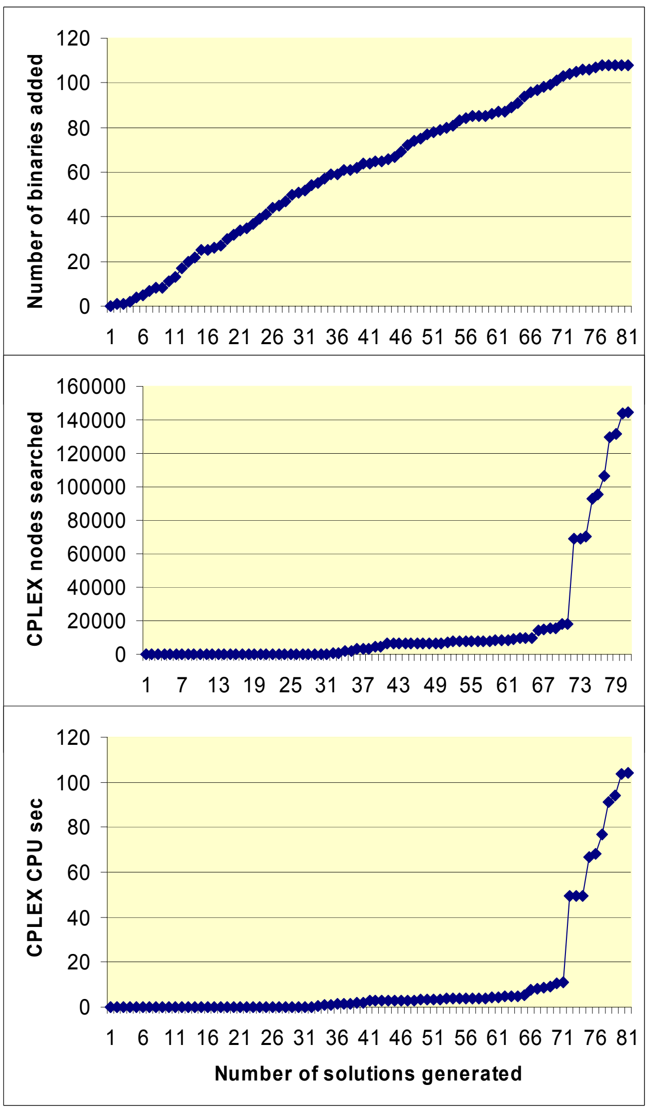
| | Molecular Structure | $\frac{\Delta H_{ve}}{C_{pla}}$ |
|---|---|---|
| $C_3H_3F$ | $CH \equiv C - CH_2 - F$ | 0.7802 |
| $CHF_2Cl$ | $(F-)(F-) > CH - Cl$ | 0.7770 |
| $C_2H_3OF$ | $CH_2 = CH - O - F$ | 0.7685 |
| $NF_2Cl$ | $(F-)(F-) > N - Cl$ | 0.7658 |
| $C_2H_6NF$ | $(CH3-)(CH3-) > N - F$ | 0.6817 |
| $N_2HF_3$ | $(F-)(F-) > N - NH - F$ | 0.6711 |
| $C_2H_2OF_2$ | $CH2 = C < (-O - F)(-F)$ | 0.6705 |
| $C_3H_2F_2$ | $(F-)(F-) > CH - C \equiv CH$ | 0.6686 |
| $C_2HNF_2$ | $CH \equiv C - N < (-F)(-F)$ | 0.6587 |
| $C_3H_4F_2$ | $(F-)(F - CH_2-) > C = CH_2$ | 0.6377 |
| $C_3H_4F_2$ | $(F-)(F-) > CH - CH = CH_2$ | 0.6263 |
| $C_2H_3NF_2$ | $CH2 = CH - N < (-F)(-F)$ | 0.6176 |
| $CH_3NOF_2$ | $(F-)(CH_3-) > N - O - F$ | 0.6139 |
| $C_3H_3F_3$ | (r> CH– ')₃(–F)₃ | 0.5977 |

**For $CCl_2F_2$, $\Delta H_{ve}/C_{pla} \approx 0.57$**

**In 30 CPU minutes**

# FINDING ALL or the K-BEST SOLUTIONS

**Typically found through repetitive applications of branch-and-bound and generation of cutting planes**

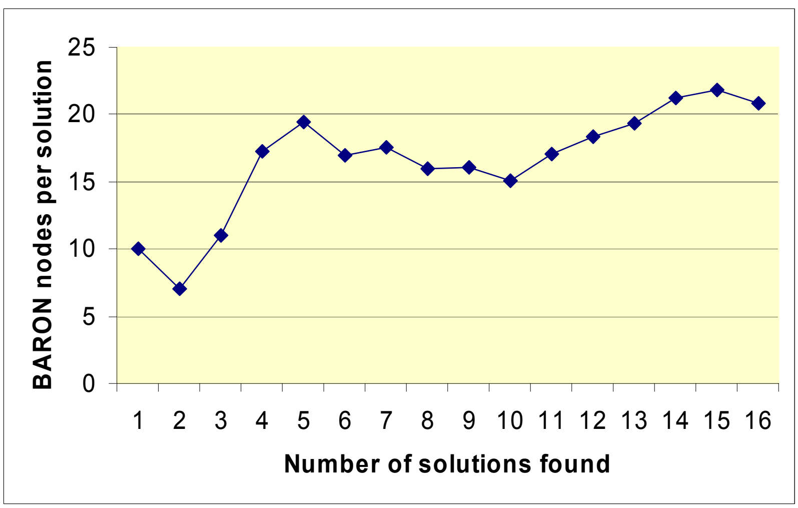


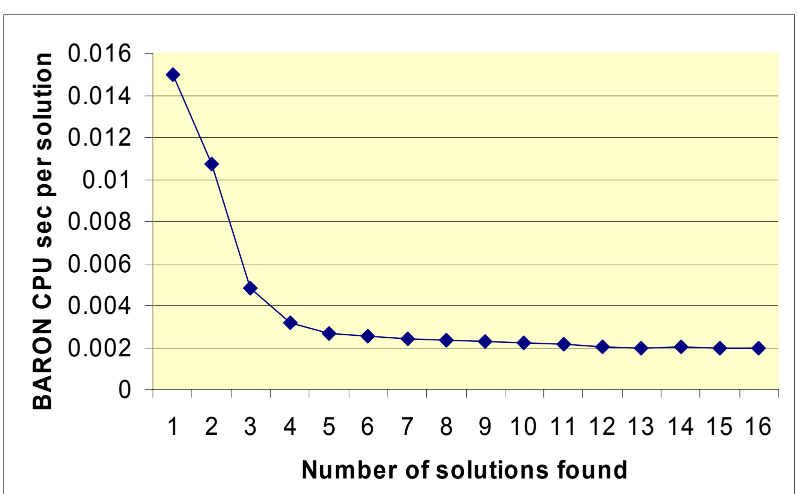

$$\begin{aligned}
\min \quad & \sum_{i=1}^{4} 10^{4-i} x_i \\
s.t. \quad & 2 \le x_i \le 4, \qquad i = 1,\dots,4 \\
& x \quad \text{integer}
\end{aligned}$$

**BARON finds all solutions:**
- **No cuts**
- **Single search tree**
- **511 nodes**
- **0.56 seconds**

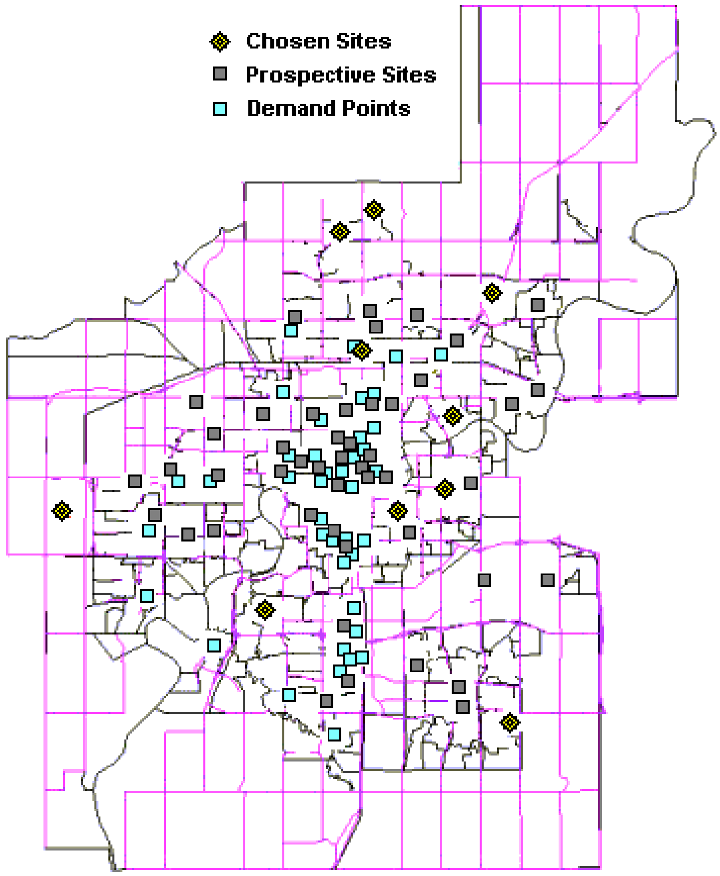
# FINDING ALL or the K-BEST SOLUTIONS for CONTINUOUS PROBLEMS

- Boon problem: 8 solutions (3.1 sec)
- Robot problem: 16 solutions (0.03 sec)



# Discrete Location Problems



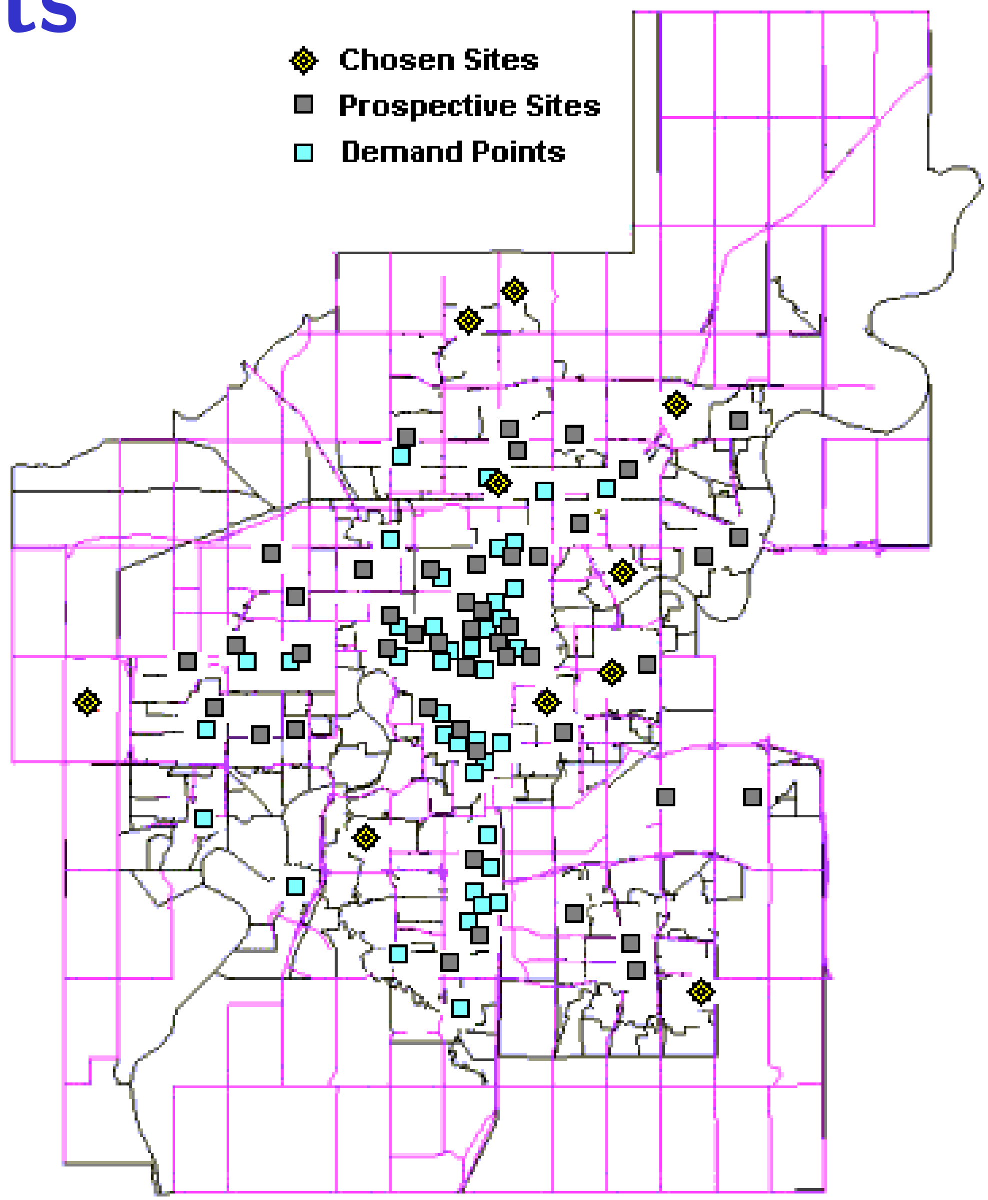

Restaurants in Edmonton

$$\textbf{p-choice Utility} = \sum_{\text{location: } j} w_j \sum_{\text{customer: } i} \overbrace{\frac{U_{ij} x_j}{\sum_k U_{ik} x_k}}^{\text{Utility Ratio}} d_i$$

| | |
|---|---|
| $U_{ij}$ | **Utility of location $j$ for customer $i$** |
| $x_j$ | **decision variable for locating facility $j$** |
| $d_i$ | **demand by customer $i$** |
| $w_j$ | **preferential weight of site $j$** |

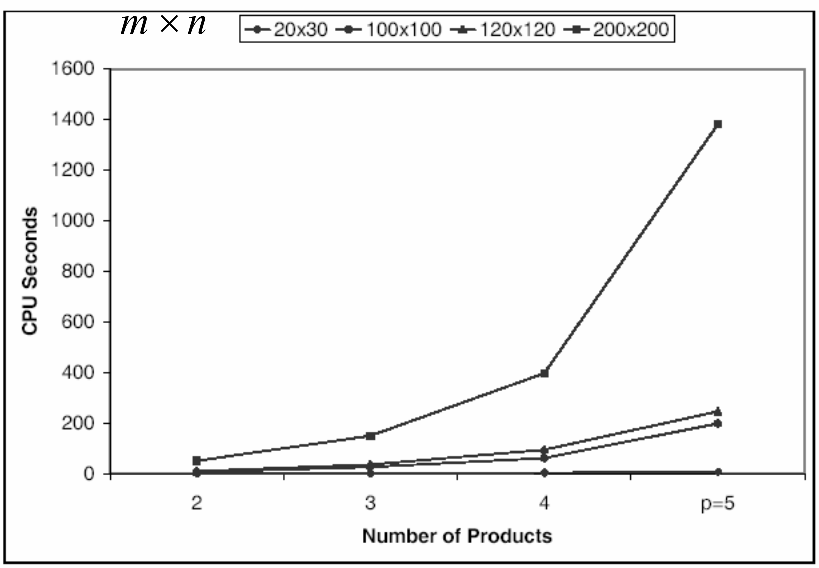
# Located Restaurants

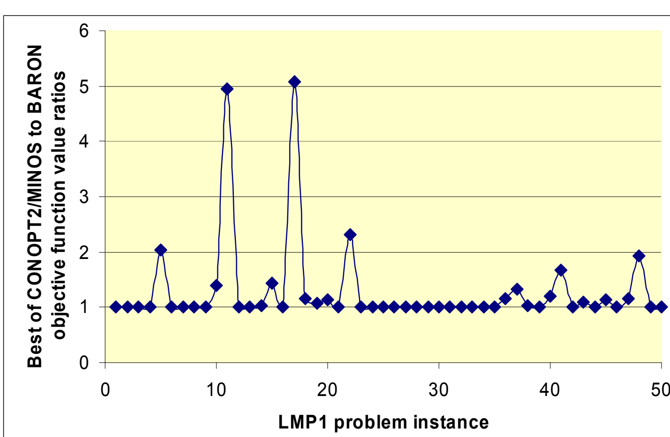
- IBM SP/2 Single Processor
- Time: 5.5 hours
- Relaxations take 95% time
- Iterations: 79
- Nodes in Memory: 9

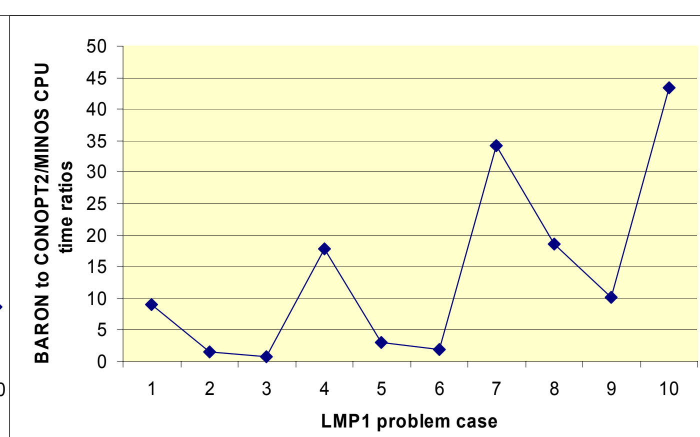


# LINEAR MULTIPLICATIVE PROGRAMS

$$\min \prod_{i=1}^{p} f_i(x) = \prod_{i=1}^{p} \left( c_i^t x + c_{i0} \right)$$
$$s.t. \quad Ax \le b$$
$$x \in \Re_+^n, A \in \Re^{m \times n}$$

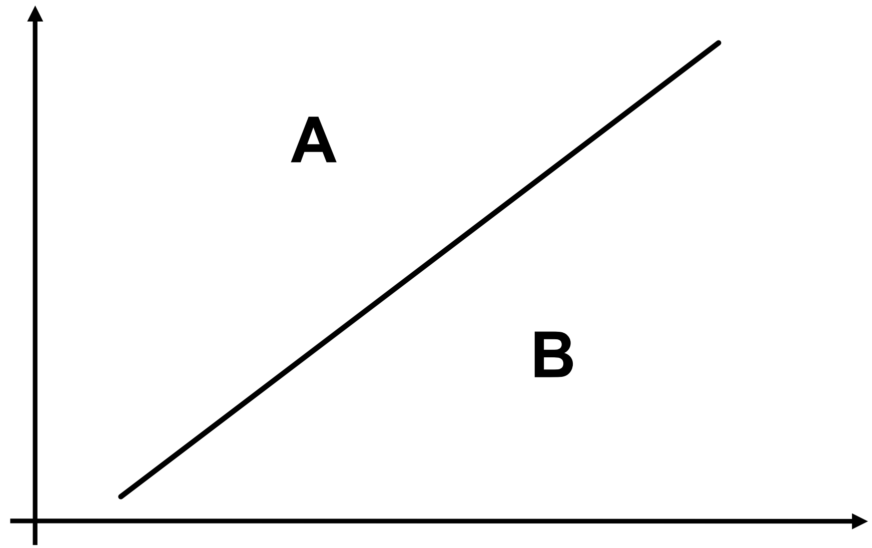


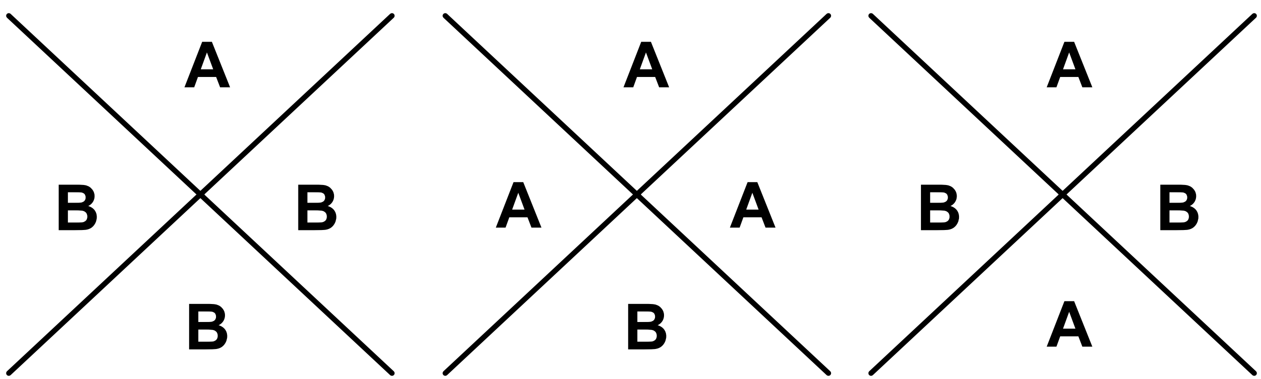



# MEDICAL DIAGNOSIS & PROGNOSIS

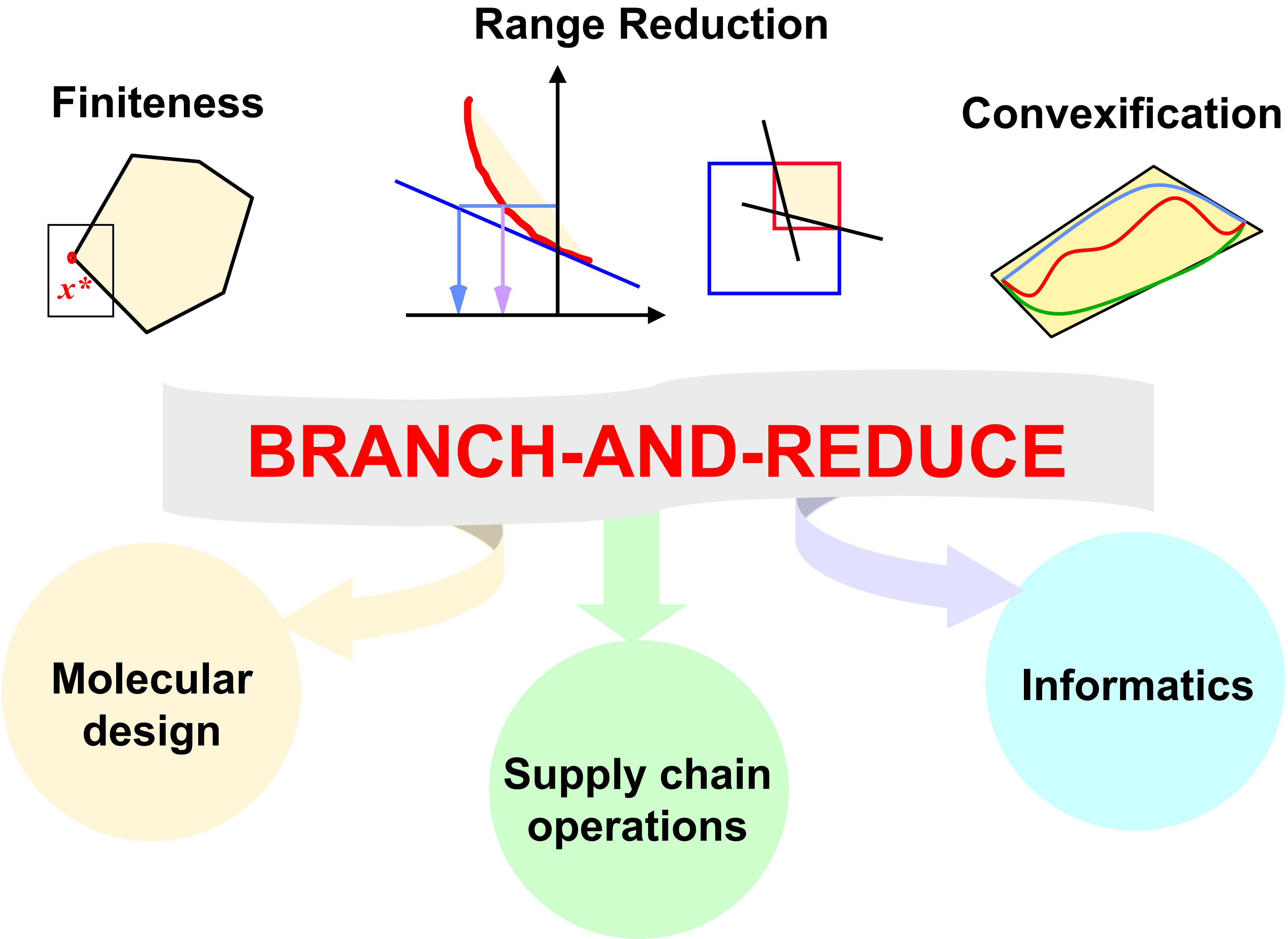
- **Linear Separation of Sets:**




- **Bilinear Separation of Sets:**




- **Wisconsin breast cancer diagnosis: 99% vs. 95%**


Range Reduction
Finiteness
Convexification
x*
BRANCH-AND-REDUCE
Molecular design
Supply chain operations
Informatics