# CONVEXIFICATION AND GLOBAL OPTIMIZATION

**Nick Sahinidis**

University of Illinois
at Urbana-Champaign

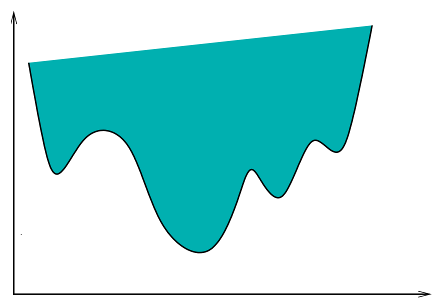
Chemical and Biomolecular Engineering

# MIXED-INTEGER NONLINEAR PROGRAMMING

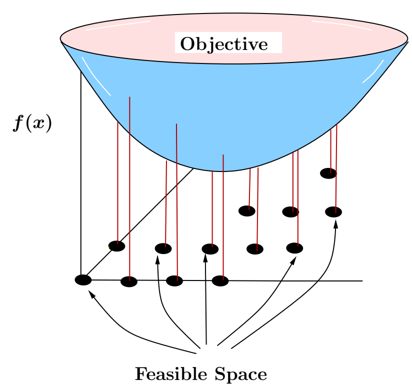
| | | | |
|---|---|---|---|
| (P) | min | $f(x, y)$ | Objective Function |
| | s.t. | $g(x, y) \leq 0$ | Constraints |
| | | $x \in \mathbb{R}^n$ | Continuous Variables |
| | | $y \in \mathbb{Z}^p$ | Integrality Restrictions |

**Challenges:**

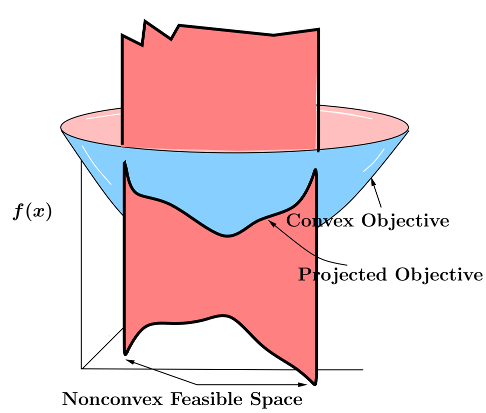
- Multimodal Objective



- Integrality



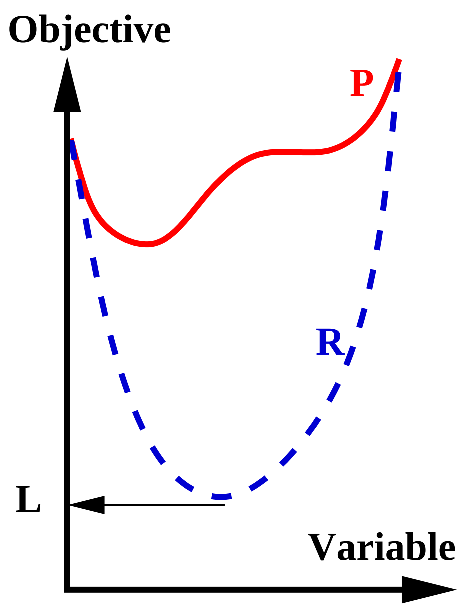

- Nonconvex Constraints



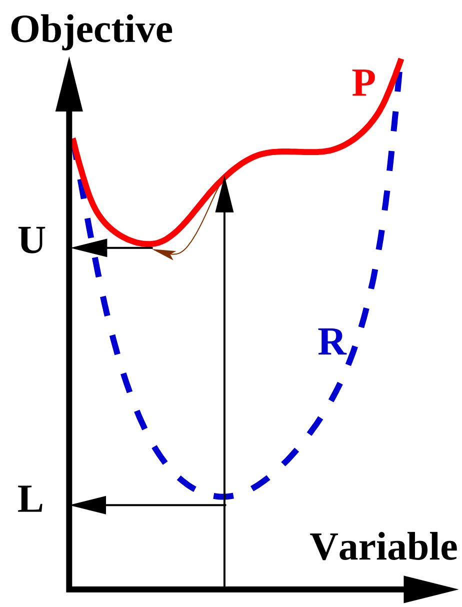
# MINLP ALGORITHMS

- 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
- Decomposition
  - Project out some variables by solving subproblem
    - » Duran and Grossmann, 1986
    - » Visweswaran and Floudas, 1990
- 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
- Tawarmalani, M. and N. V. Sahinidis, *Convexification and Global Optimization in Continuous and Mixed-Integer Nonlinear Programming,* Kluwer Academic Publishers, Nov. 2002.

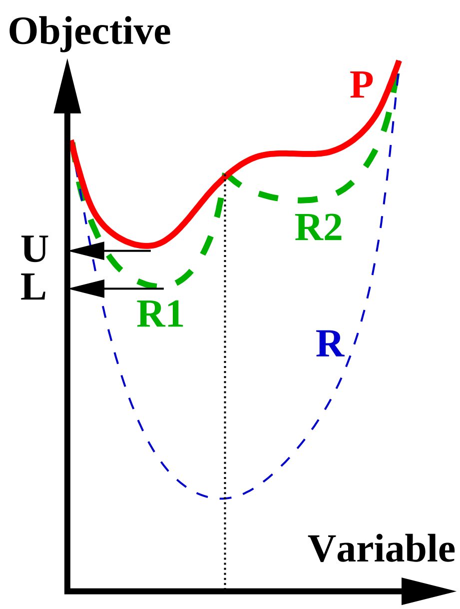
# BRANCH-AND-BOUND



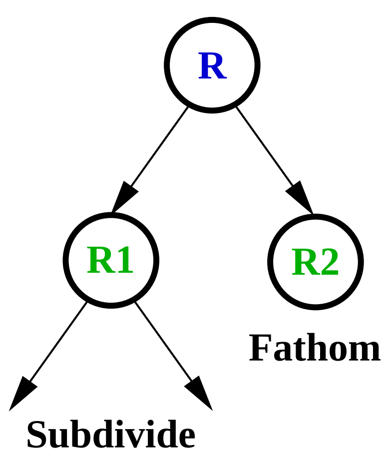

a. Lower Bounding




b. Upper Bounding




c. Domain Subdivision




d. Search Tree

# FACTORABLE FUNCTIONS
## (McCormick, 1976)

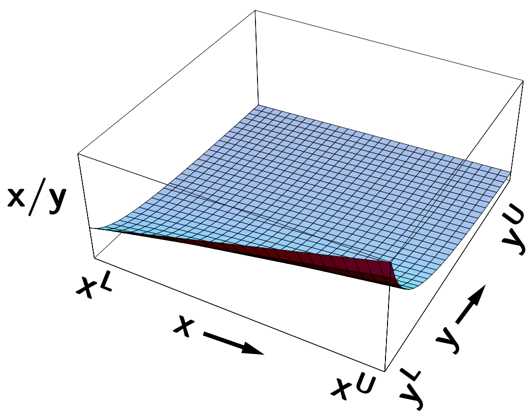
**Definition:** Factorable functions are recursive compositions of sums and products of functions of single variables.

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

$$\overbrace{\Big(\underbrace{\overbrace{\exp(\underbrace{\underbrace{xy}_{x_1} + \overbrace{z\,\underbrace{\ln w}_{x_2}}^{x_3}}_{x_4})}^{x_5}\;\overbrace{z^3}^{x_6}}_{x_7}\Big)^{0.5}}^{f}$$

$$x_1 = xy$$
$$x_2 = \ln(w)$$
$$x_3 = z x_2$$
$$x_4 = x_1 + x_3$$
$$x_5 = \exp(x_4)$$
$$x_6 = z^3$$
$$x_7 = x_5 x_6$$
$$f = \sqrt{x_7}$$

# RATIO: THE FACTORABLE RELAXATION




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

$$z \geq x/y, \quad x^L \leq x \leq x^U, \quad y^L \leq y \leq y^U$$

**cross-multiplying** →

$$zy \geq x, \quad y^L \leq y \leq y^U, \quad x^L/y^U \leq z \leq x^U/y^L, \quad x^L \leq x \leq x^U$$

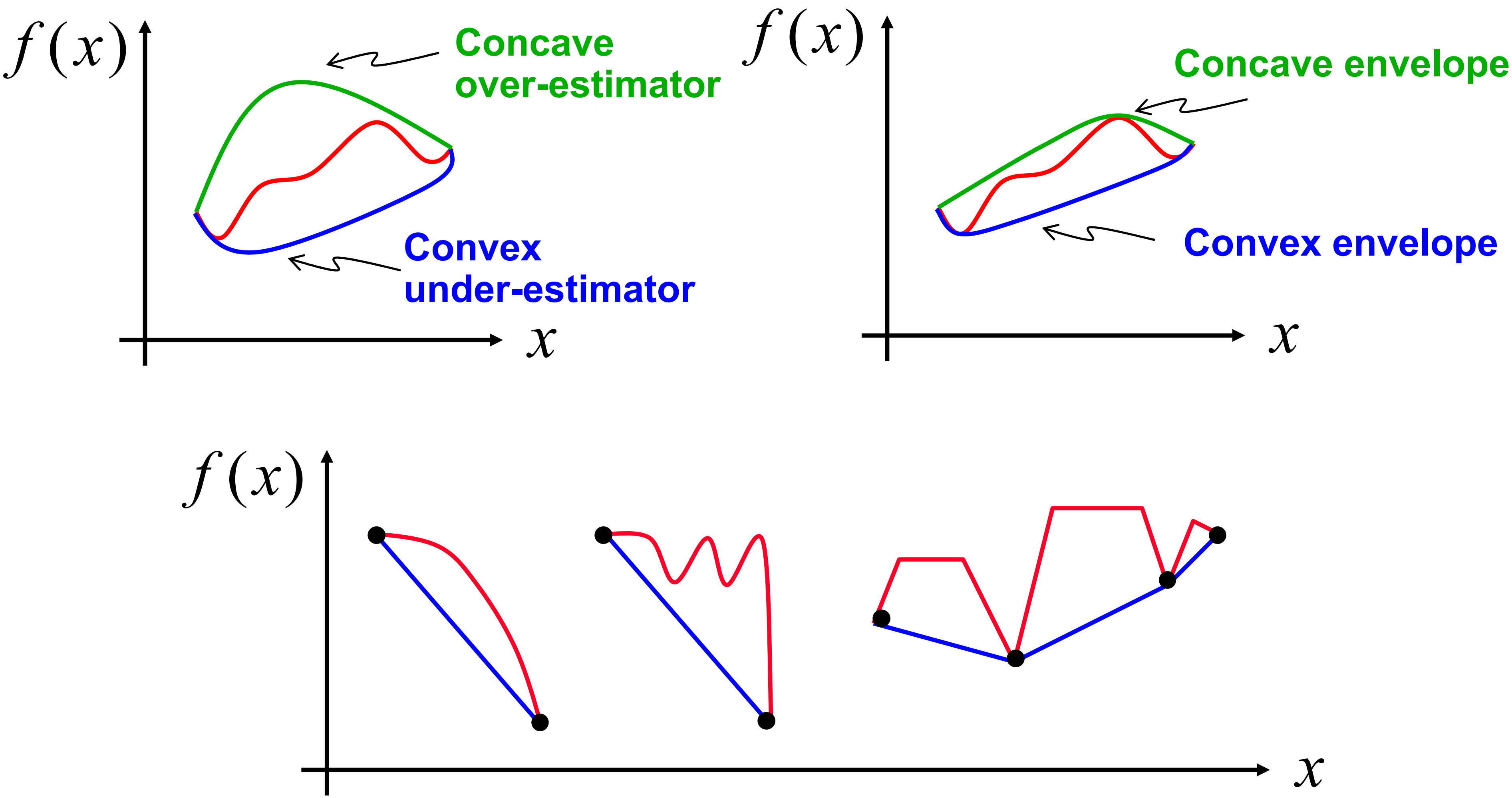
**Relaxing** ↓

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

← **Simplifying**

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

# TIGHT RELAXATIONS



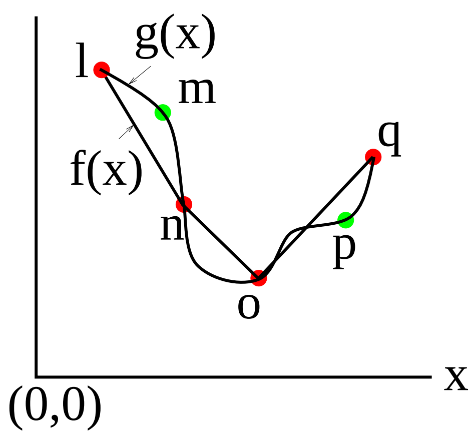

**Convex/concave envelopes often finitely generated**

# 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

# THE GENERATING SET OF A FUNCTION

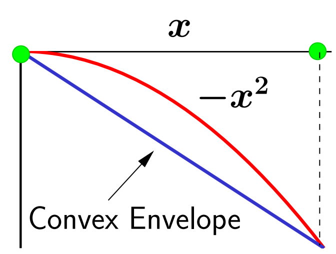
**Definition:** The generating set of the epigraph of a function $g(x)$ over a compact convex set $C$ is defined as

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

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

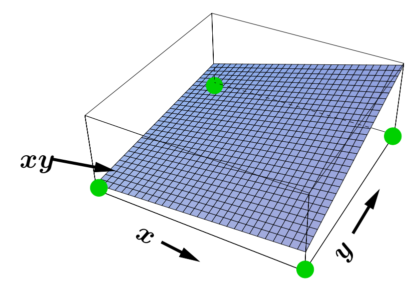
**Examples:**

$g(x) = -x^2$




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

$g(x) = xy$




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

# TWO-STEP CONVEX ENVELOPE CONSTRUCTION

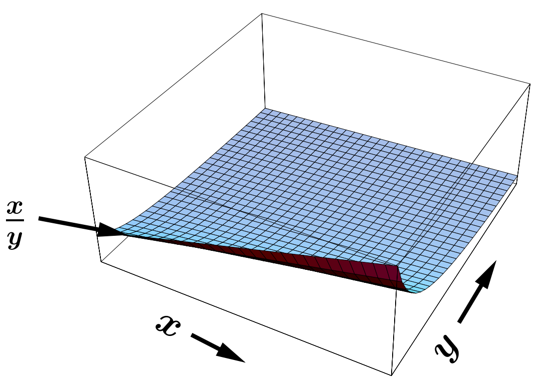
1. **Identify generating set**
   - **Key result:** **A point in set X is *not* in the generating set if it is not in the generating set over a neighborhood of X that contains it**

2. **Use disjunctive programming techniques to construct epigraph over the generating set**
   - **Rockafellar (1970)**
   - **Balas (1974)**

# IDENTIFYING THE GENERATING SET

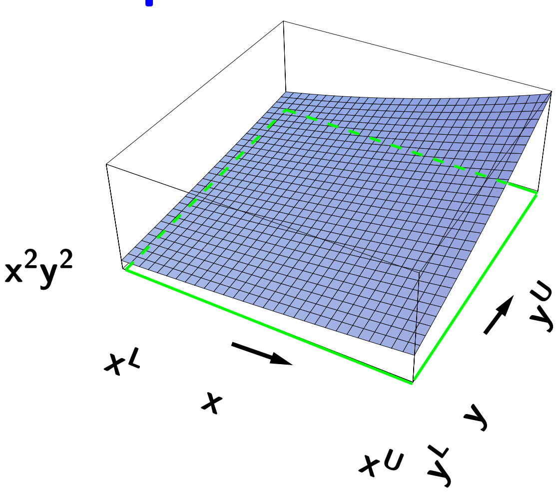
**Characterization:** $x_0 \notin G_C^{\text{epi}}(g)$ if and only if there exists $X \subseteq C$ and $x_0 \notin G_X^{\text{epi}}(g)$.

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




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

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




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

# CONVEX ENVELOPE OF $x/y$

## Second Order Cone Representation:

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

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

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

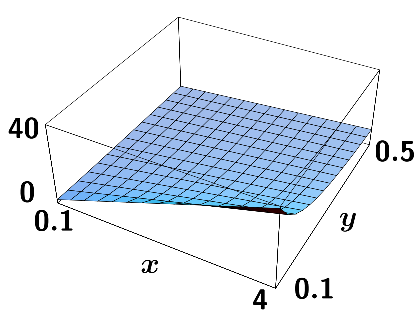
$$y_p \le y^U(1-\lambda), y_p \le y - y^L\lambda$$

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

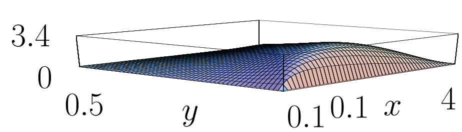
$$z_p, u, v \ge 0, z_c - z_p \ge 0$$

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

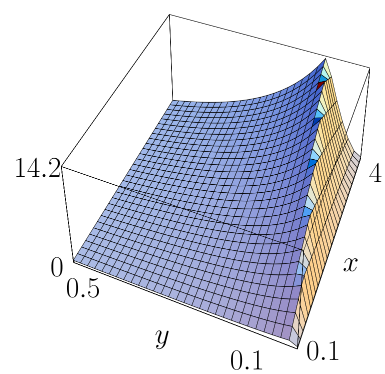
## Comparison of Tightness:




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

# ENVELOPES OF MULTILINEAR FUNCTIONS

- **Multilinear function over a box**

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

- **Generating set**

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

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

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

# PRODUCT DISAGGREGATION

**Consider the function:**

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

**Let**

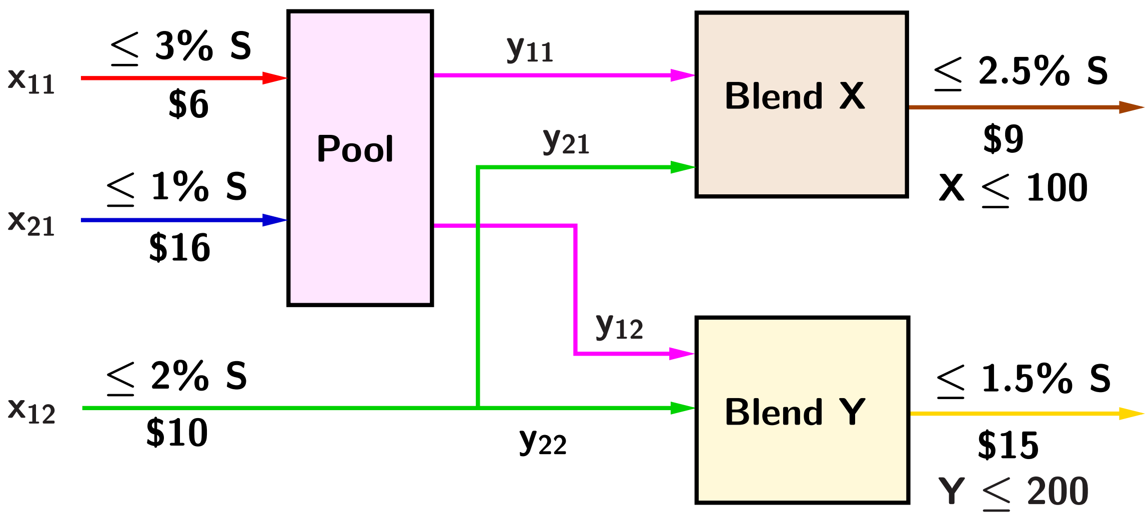
$$H = [x^L, x^U] \times \prod_{k=1}^{n} [y_k^L, y_k^U]$$

**Then**

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

**Disaggregated formulations are tighter**

# POOLING: p FORMULATION




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

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

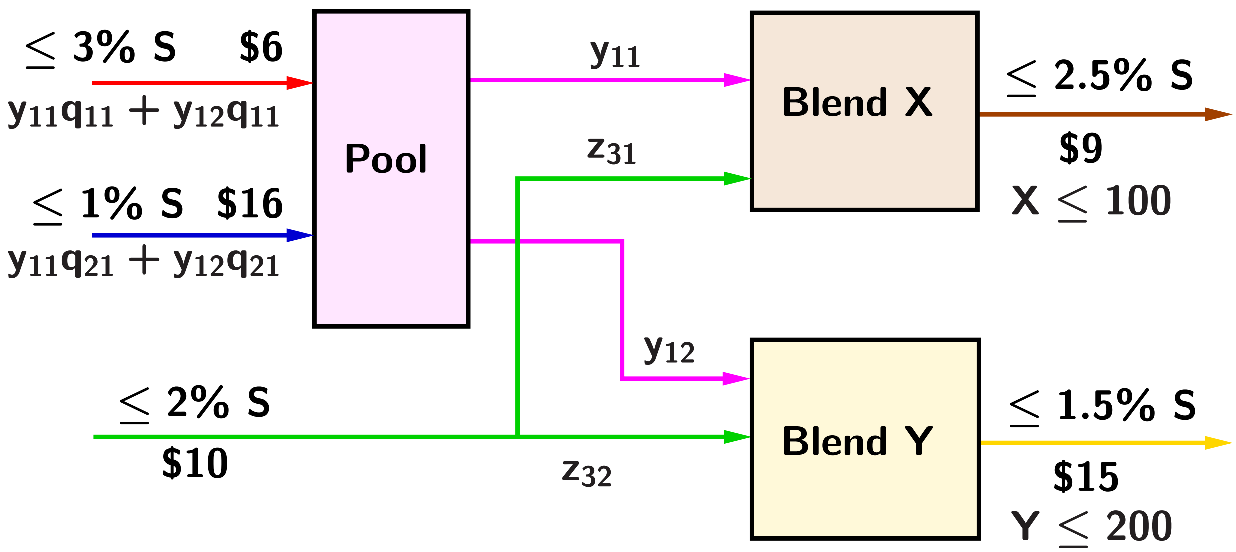
$$x_{11} + x_{21} = y_{11} + y_{12}$$
$$x_{12} = y_{21} + y_{22}$$
Mass balance

$$\frac{qy_{11} + 2y_{21}}{y_{11} + y_{21}} \leq 2.5$$
$$\frac{qy_{12} + 2y_{22}}{y_{12} + y_{22}} \leq 1.5$$
Quality Requirements

$$y_{11} + y_{21} \leq 100$$
$$y_{12} + y_{22} \leq 200$$
Demands

Haverly 1978

# POOLING: q FORMULATION




$$\min \quad \overbrace{6\,(y_{11}q_{11} + y_{12}q_{11}) + 16\,(y_{11}q_{21} + y_{12}q_{21}) + 10\,(z_{31} + z_{32})}^{\text{cost}}$$

$$- \overbrace{9(y_{11} + y_{21})}^{X\text{-revenue}} - \overbrace{15(x_{12} + x_{22})}^{Y\text{-revenue}}$$

s.t. $\quad q_{11} + q_{21} = 1$ **Mass Balance**

$$-0.5z_{31} + 3y_{11}q_{11} + y_{11}q_{21} \le 2.5y_{11}$$
$$0.5z_{32} + 3y_{12}q_{11} + y_{12}q_{21} \le 1.5y_{12}$$

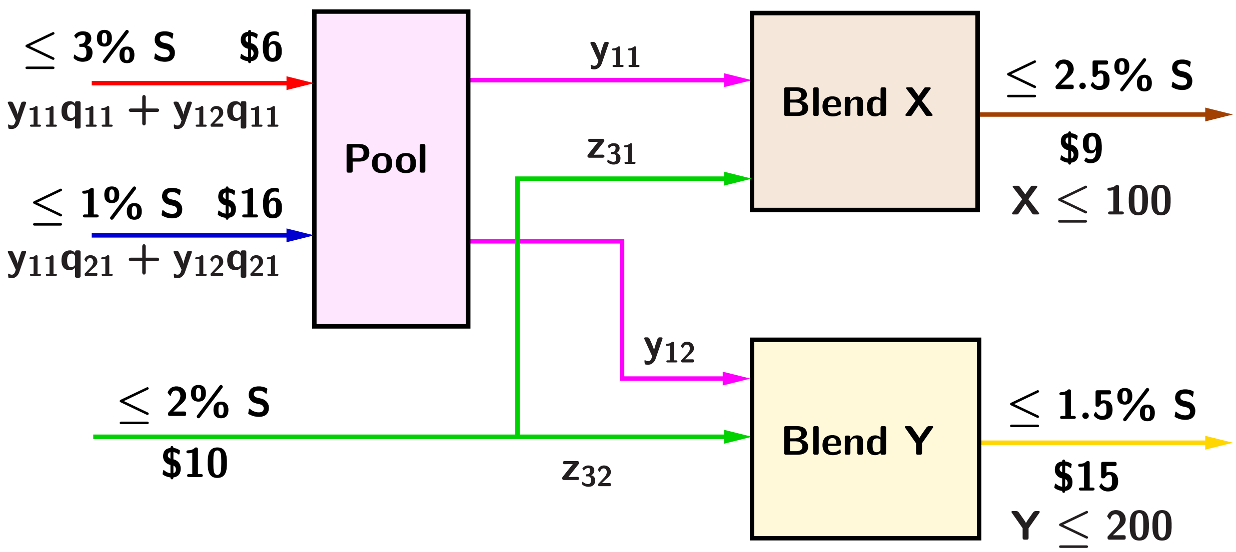
**Quality Requirements**

$$y_{11} + z_{31} \le 100$$
$$y_{12} + z_{32} \le 200$$

**Demands**

Ben-Tal et al. 1994

# POOLING: $pq$ FORMULATION




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

s.t.

$$q_{11} + q_{21} = 1 \qquad \text{Mass Balance}$$

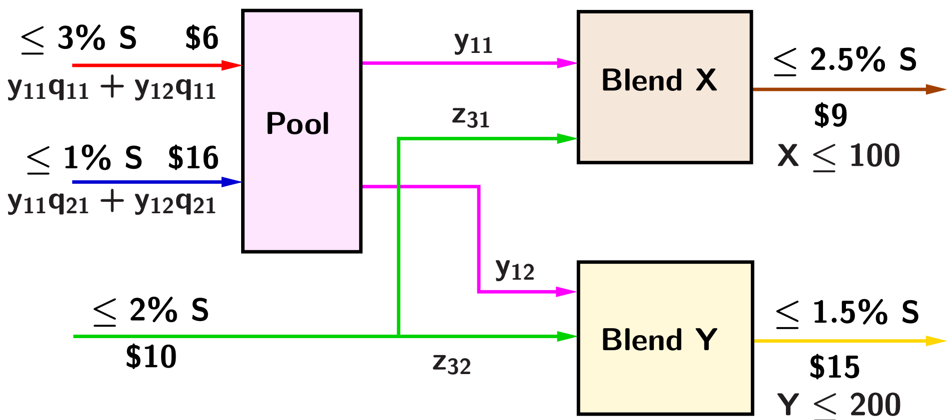
$$\begin{aligned} -0.5z_{31} + 3y_{11}q_{11} + y_{11}q_{21} &\le 2.5y_{11} \\ 0.5z_{32} + 3y_{12}q_{11} + y_{12}q_{21} &\le 1.5y_{12} \end{aligned} \qquad \text{Quality Requirements}$$

$$\begin{aligned} y_{11} + z_{31} &\le 100 \\ y_{12} + z_{32} &\le 200 \end{aligned} \qquad \text{Demands}$$

$$\begin{aligned} y_{11}q_{11} + y_{11}q_{21} &= y_{11} \\ y_{12}q_{11} + y_{12}q_{21} &= y_{12} \end{aligned} \qquad \text{Convexification Constraints}$$

**Proof relies on Convex Extensions**

# PROOF VIA CONVEX EXTENSIONS




**With Convexification Constraints, the convex envelope of**

$$\sum_{i=1}^{I} C_{ik} q_{il} y_{lj}$$

**over**

$$\sum_{i=1}^{I} q_{il} = 1$$
$$q_{il} \in [0, 1]$$
$$y_{lj} \in [y_{lj}^L, y_{lj}^U]$$

**is included. In the example, the convex envelopes of**

$$3q_{11}y_{11} + q_{21}y_{11} \text{ and}$$
$$3q_{11}y_{12} + q_{21}y_{12}$$

**over**

$$q_{11} + q_{12} = 1$$
$$q_{11}, q_{12} \in [0, 1]$$
$$y_{11} \in [0, 100], y_{12} \in [0, 200]$$

**are generated in this way.**

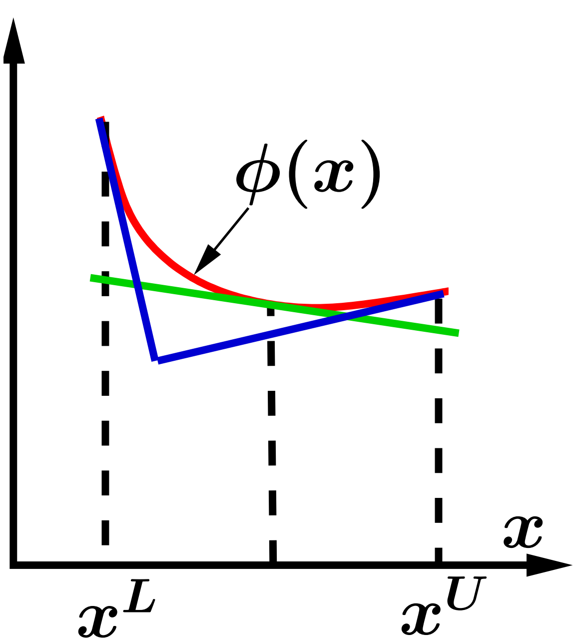
# OUTER APPROXIMATION

**Motivation:**

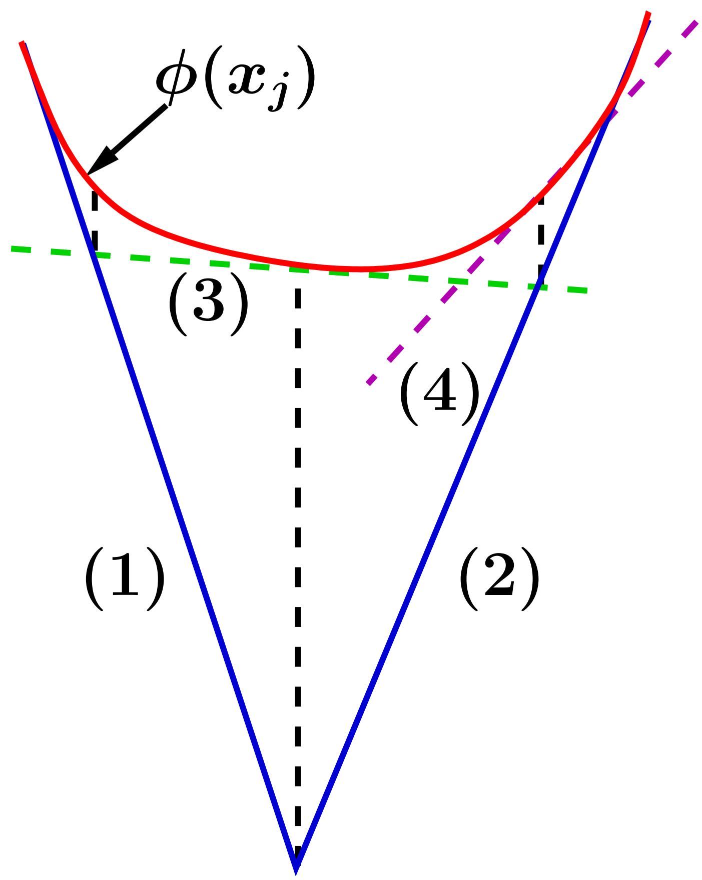
- Convex NLP solvers are not as robust as LP solvers
- Linear programs can be solved efficiently

**Outer-Approximation:**

Convex Functions are underestimated by tangent lines



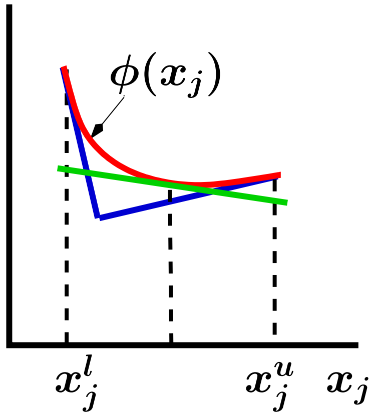
# THE SANDWICH ALGORITHM



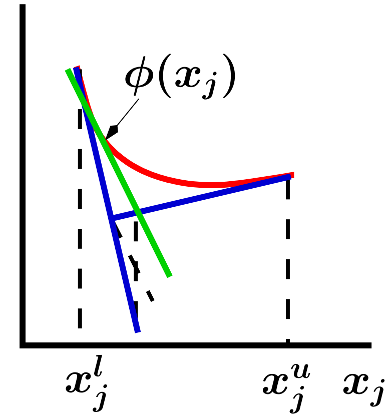

**An adaptive strategy**

- **Assume an initial outer-approximation**
- **Find point maximizing an error measure**
- **Construct underestimator at located point**

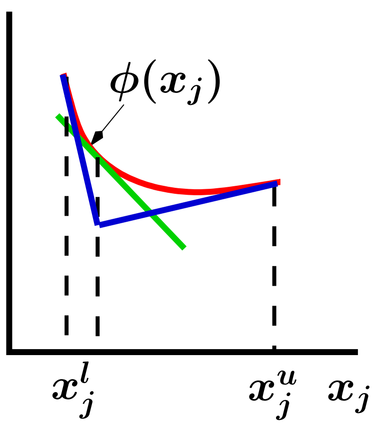
# TANGENT LOCATION RULES



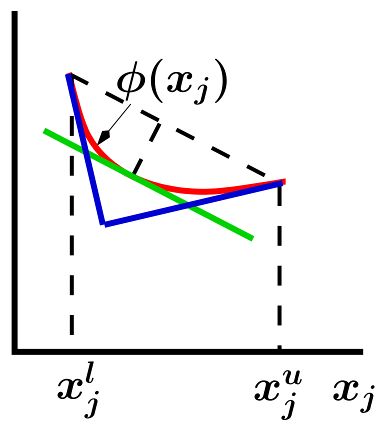

Interval bisection



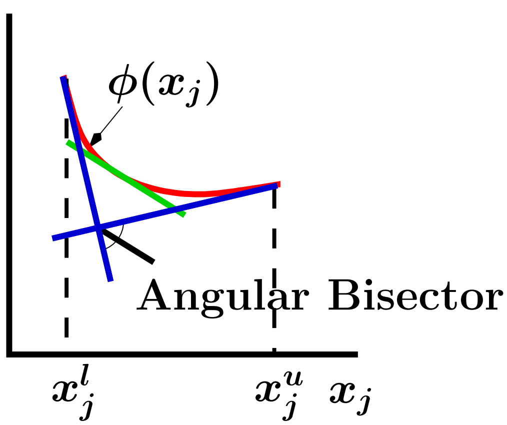

Slope Bisection



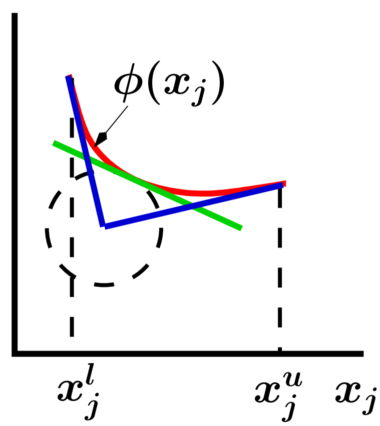

Maximum error rule




Chord rule




Angle bisection




Maximum projective error

# QUADRATIC CONVERGENCE OF PROJECTIVE ERROR RULE

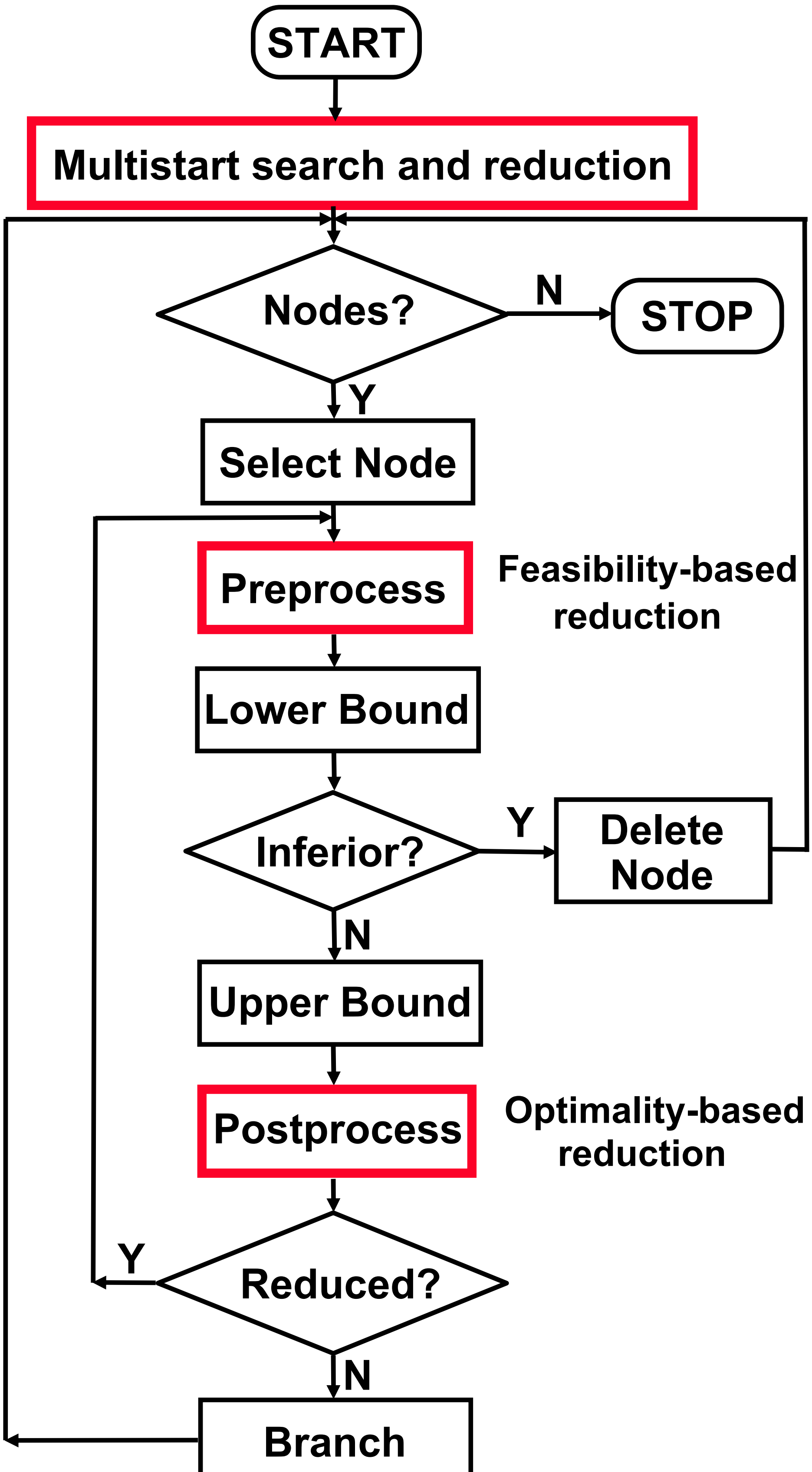
**Theorem:**

- 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



# Branch-And-Reduce Optimization Navigator

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

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

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

# 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;
```

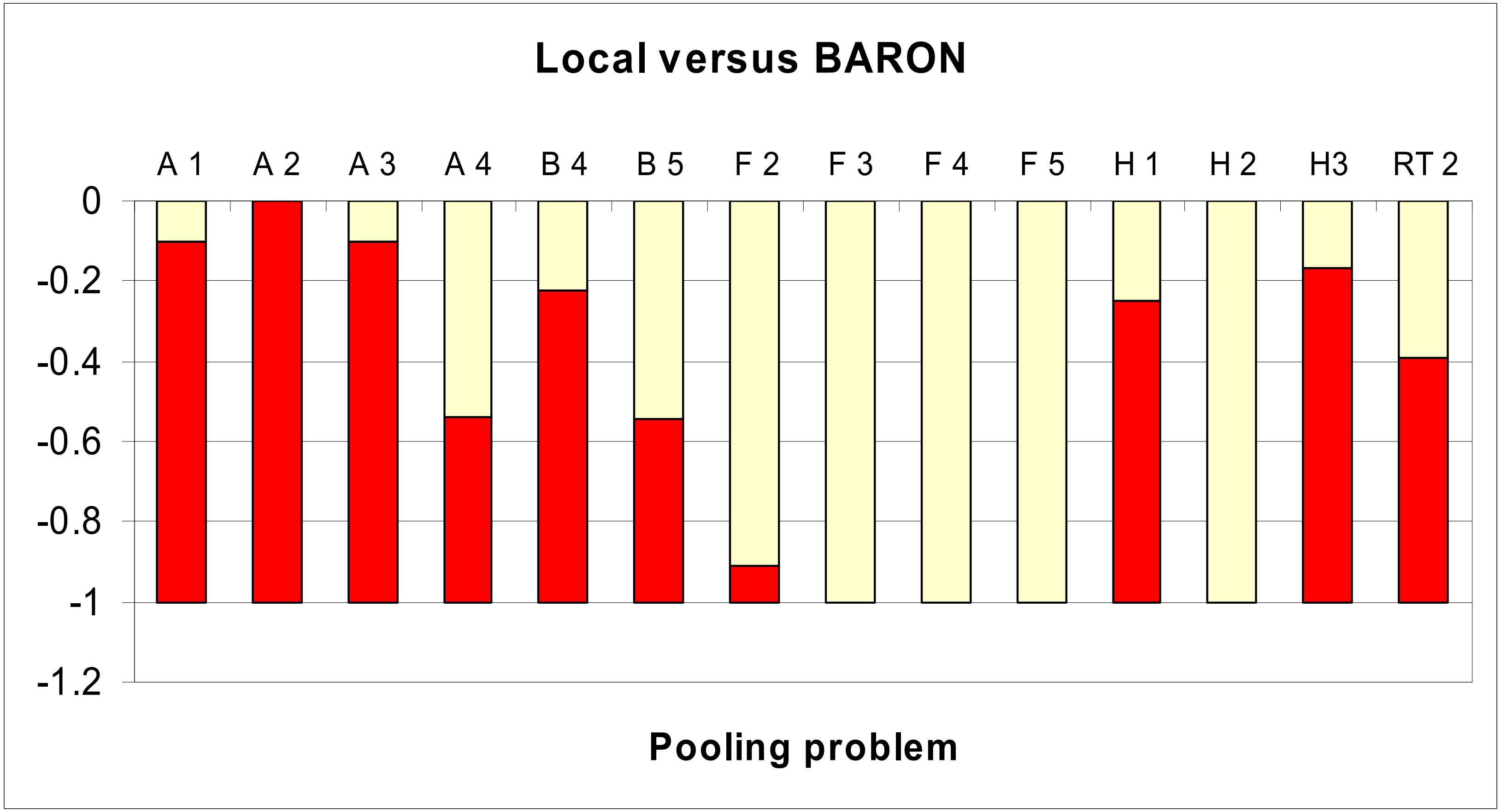
# POOLING PROBLEMS

| 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



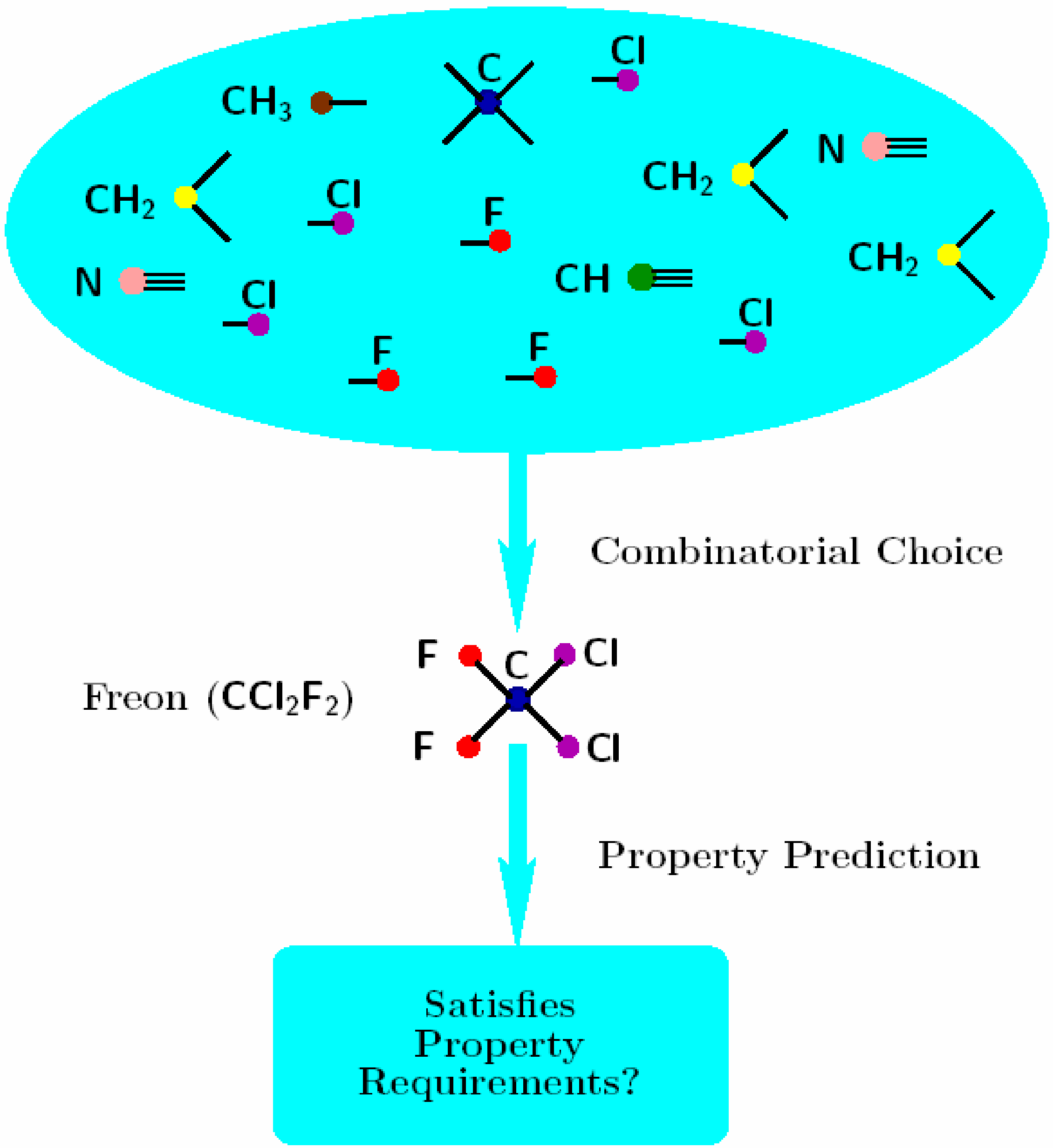
# GUPTA-RAVINDRAN MINLPs

| 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 |

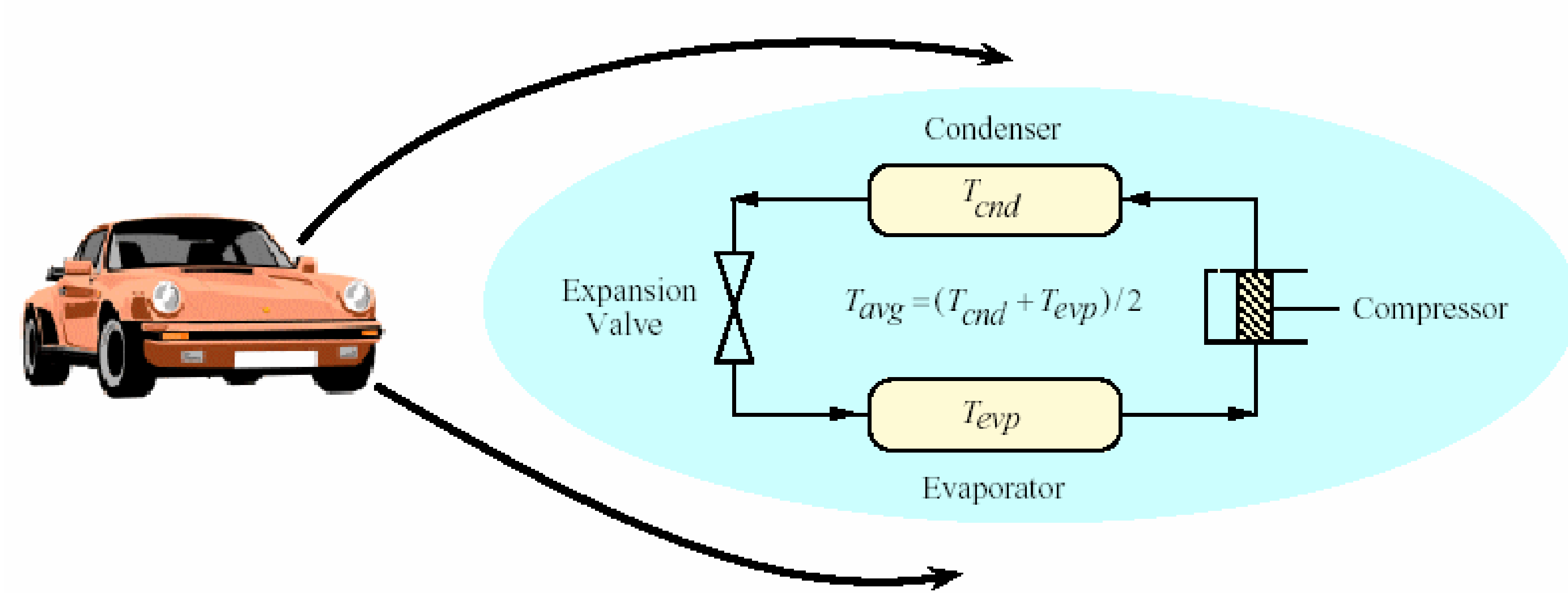
| Problem | | Obj. | $T_{tot}$ | $N_{tot}$ | $N_{mem}$ |
|---|---|---|---|---|---|
| 13 | | -585.20 | 1.13 | 197 | 28 |
| 14 | * | -40358.20 | 0.05 | 7 | 4 |
| 15 | | 1.00 | 0.05 | 11 | 3 |
| 16 | | 0.70 | 0.05 | 23 | 12 |
| 17 | | -1100.40 | 42.2 | 3489 | 399 |
| 18 | | -778.40 | 8.85 | 993 | 121 |
| 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, Man. Sci., 1985.

# MOLECULAR DESIGN



# AUTOMOTIVE REFRIGERANT DESIGN
# (Joback and Stephanopoulos, 1990)




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

# FUNCTIONAL GROUPS CONSIDERED

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

Number of Groups $= 44$

Maximum Selection Size $= 15$

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

# PROPERTY PREDICTION

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$G = 0.4835 + 0.4605 h$$

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

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

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

$n_i$ integer

# MOLECULAR STRUCTURES

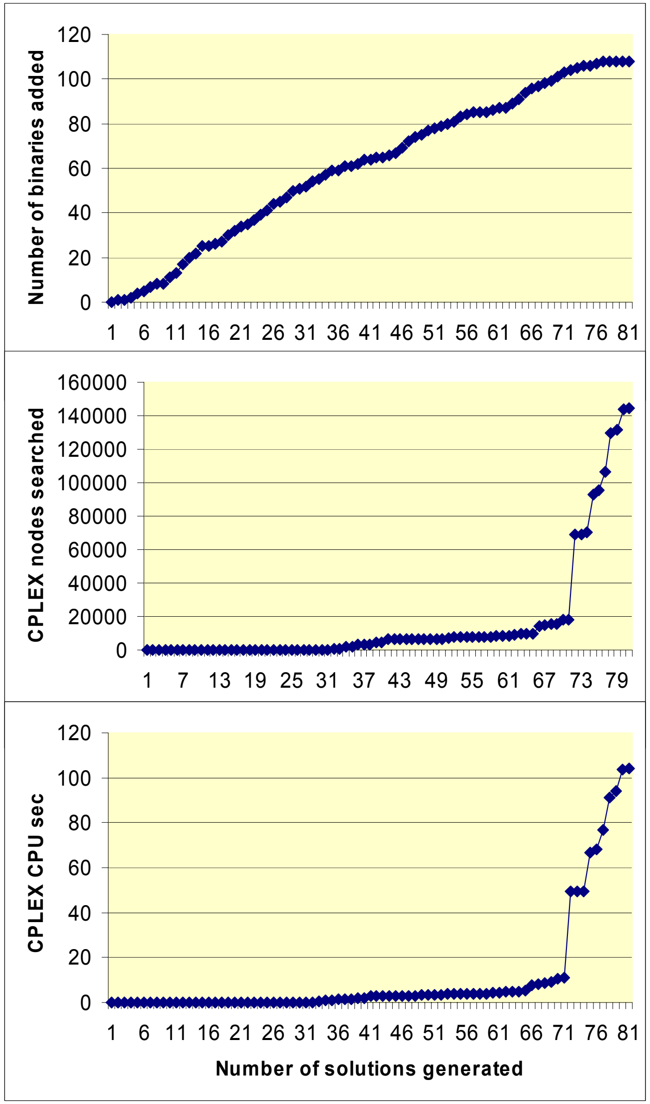
| | Molecular Structure | $\frac{\Delta H_{ve}}{C_{pla}}$ |
|---|---|---|
| FNO | $F - N = O$ | 1.2880 |
| FSH | $F - SH$ | 1.1697 |
| $CH_3Cl$ | $CH_3 - Cl$ | 1.1219 |
| ClFO | $(Cl-)(-O-)(-F)$ | 0.9822 |
| $C_2HClO_2$ | $O = C < (-CH = O)(-Cl)$ | 1.1207 |
| $C_3H_40$ | $CH_3 - CH = C = O$ | 0.9619 |
| $C_3H_4$ | $CH_3 - C \equiv CH$ | 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 THE *K*-BEST OR ALL FEASIBLE SOLUTIONS




**Typically found through repetitive applications of branch-and-bound and generation of "integer cuts"**

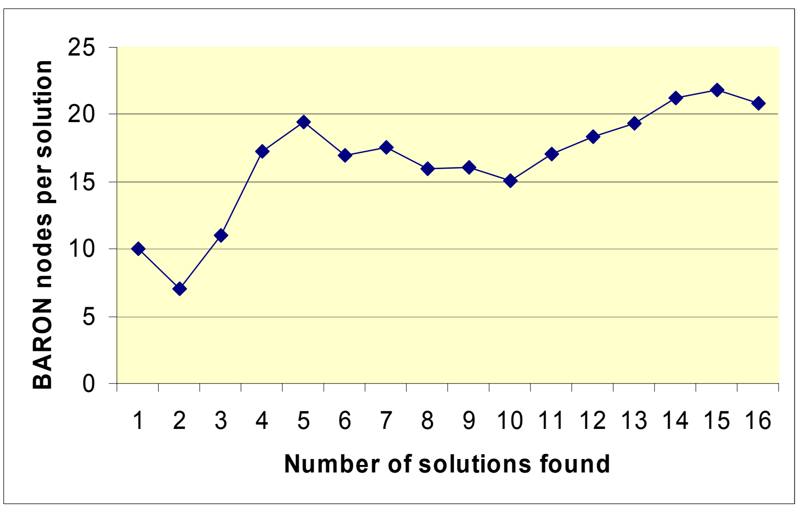
$$
\begin{aligned}
\min \quad & \sum_{i=1}^{4} 10^{4-i} x_i \\
\text{s.t.} \quad & 2 \le x_i \le 4, \qquad i = 1,\ldots,4 \\
& x \quad \text{integer}
\end{aligned}
$$

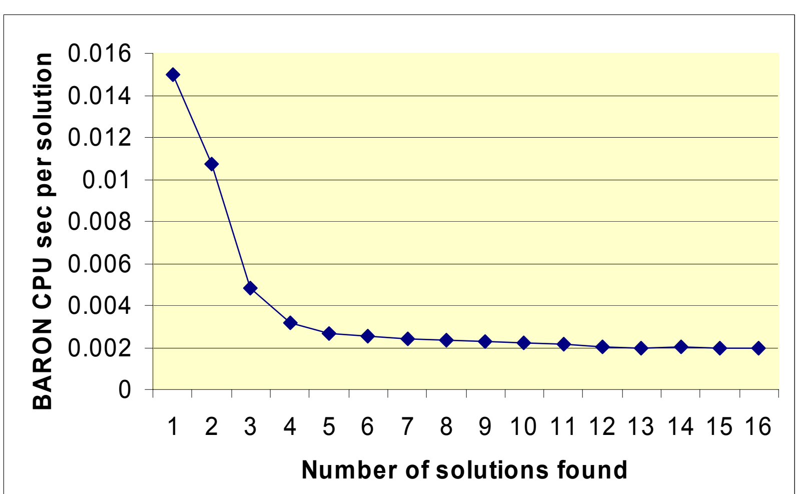
**BARON finds all solutions:**

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

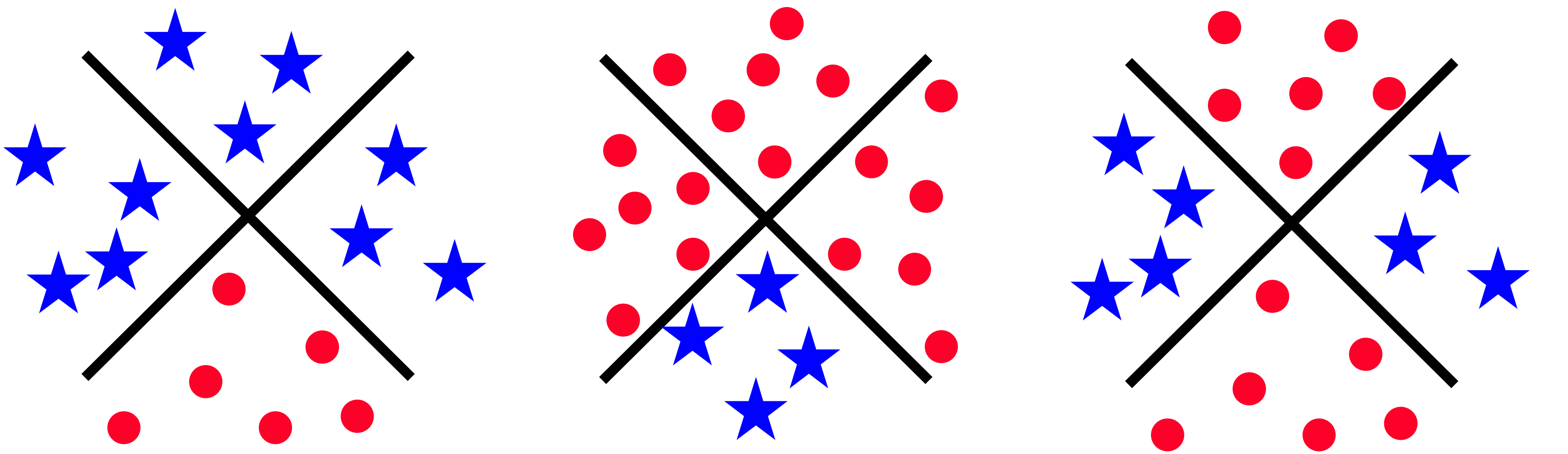
# FINDING ALL or the K-BEST SOLUTIONS for CONTINUOUS PROBLEMS

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



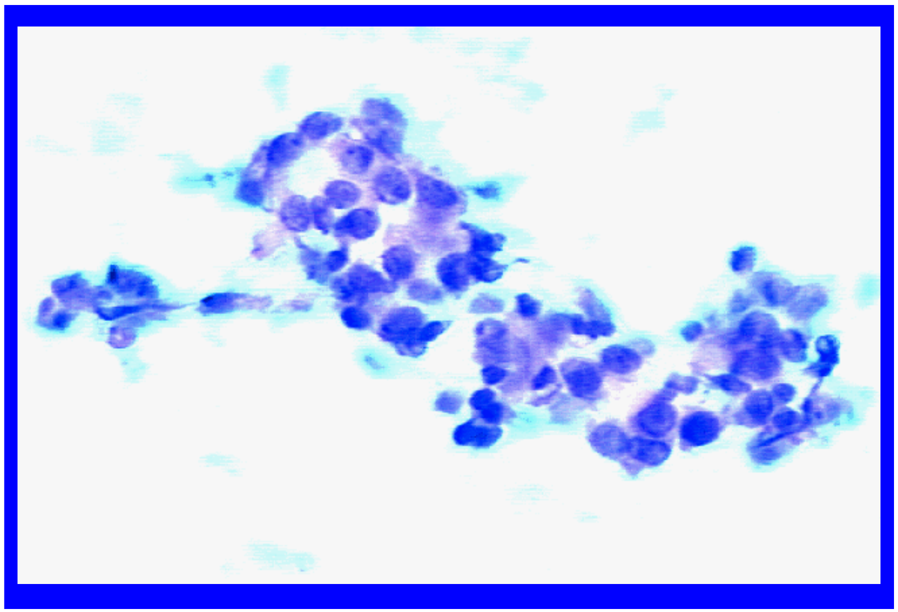



# BILINEAR (IN-)SEPARABILITY OF TWO SETS IN $R^n$



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

# WISCONSIN DIAGNOSTIC BREAST CANCER (WDBC) DATABASE



From Wolberg, Street, & Mangasarian, 1993

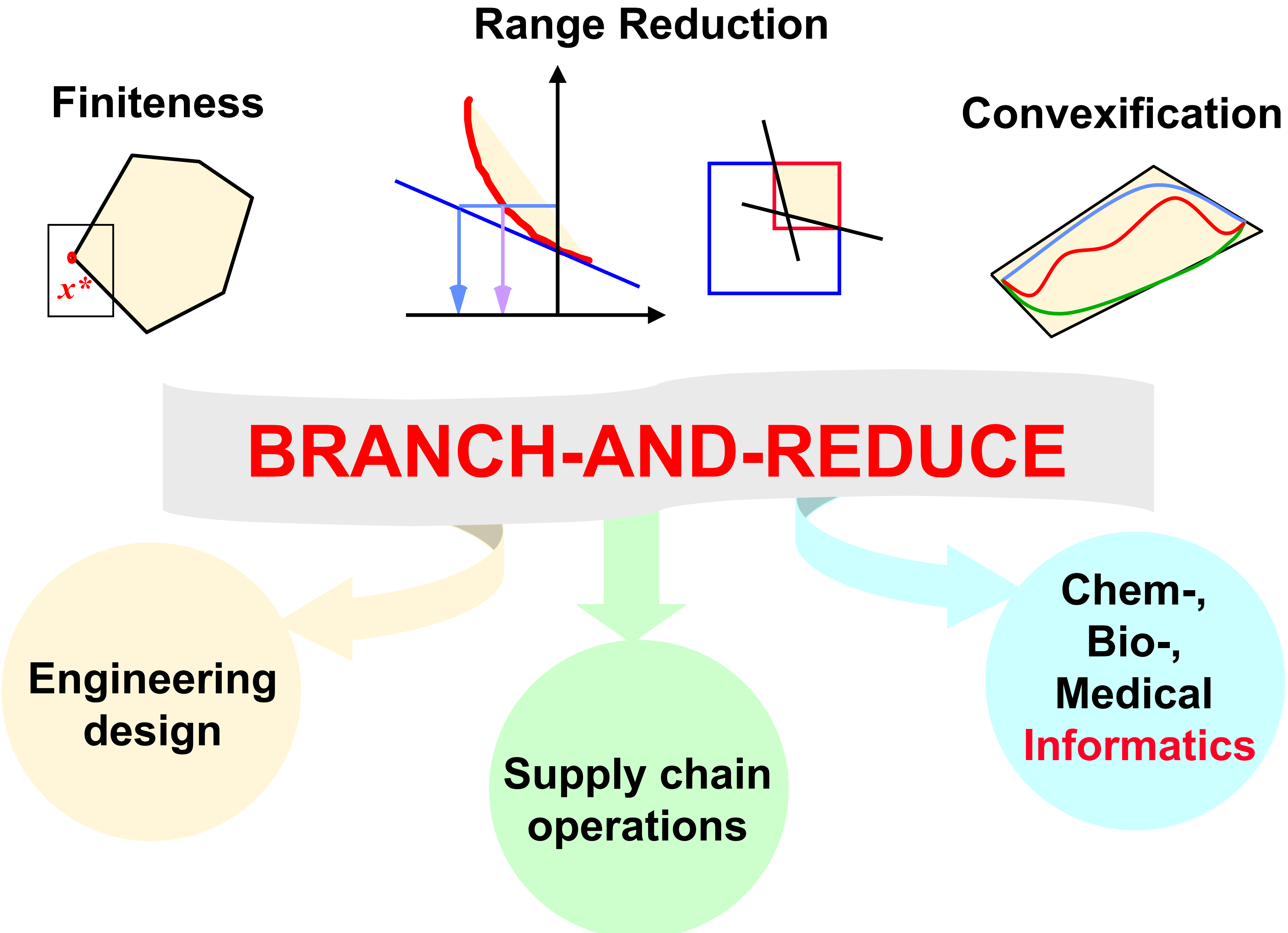
- 353 FNAs (Group 1)
  - 2 Classes:
    - » 188 Benign
    - » 165 Malignant
- 9 Cytological Characteristics:
  - Clump Thickness
  - Uniformity of Cell Size
  - Uniformity of Cell Shape
  - Marginal Adhesion
  - Single Epithelial Cell Size
  - Bare Nuclei
  - Bland Chromatin
  - Normal Nucleoli
  - Mitoses
- 300 FNAs (Groups 2-8)
  - Used for testing

# RESULTS ON WDBC DATABASE

| | Rows | Columns | Bilinear Terms | CPU sec |
|---|---|---|---|---|
| BLP1 | 706 | 350 | 165 | 11 |
| BLP2 | 706 | 396 | 188 | 27 |
| BLP3 | 1412 | 1432 | 1412 | 460 |

**99% accuracy on testing set**

- LP-based method has 95% accuracy
- Millions of women screened every year


Range Reduction
Finiteness
Convexification
x*
BRANCH-AND-REDUCE
Engineering design
Supply chain operations
Chem-,
Bio-,
Medical
Informatics

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