# GLOBAL OPTIMIZATION WITH GAMS/BARON

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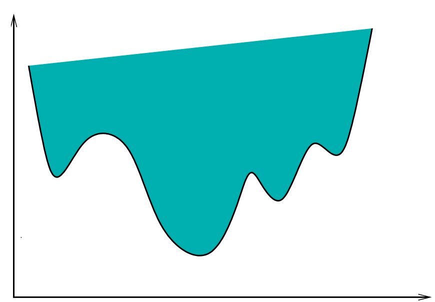
# MIXED-INTEGER NONLINEAR PROGRAMMING

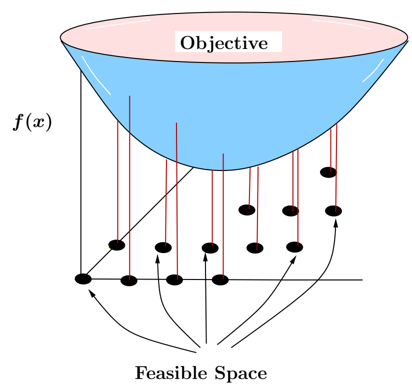
$$
\begin{array}{llll}
\text{(P)} & \min & f(x,y) & \text{Objective Function} \\
& \text{s.t.} & g(x,y) \leq 0 & \text{Constraints} \\
& & x \in \mathbb{R}^n & \text{Continuous Variables} \\
& & y \in \mathbb{Z}^p & \text{Integrality Restrictions}
\end{array}
$$

**Challenges:**

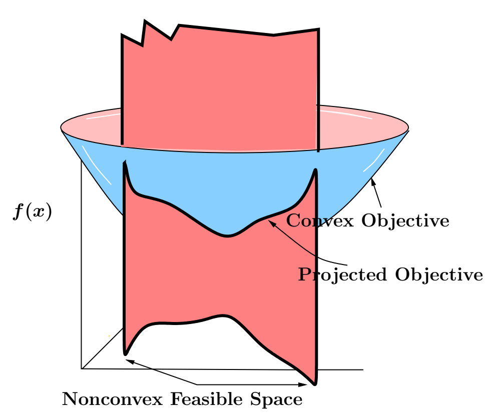
- Multimodal Objective



- Integrality



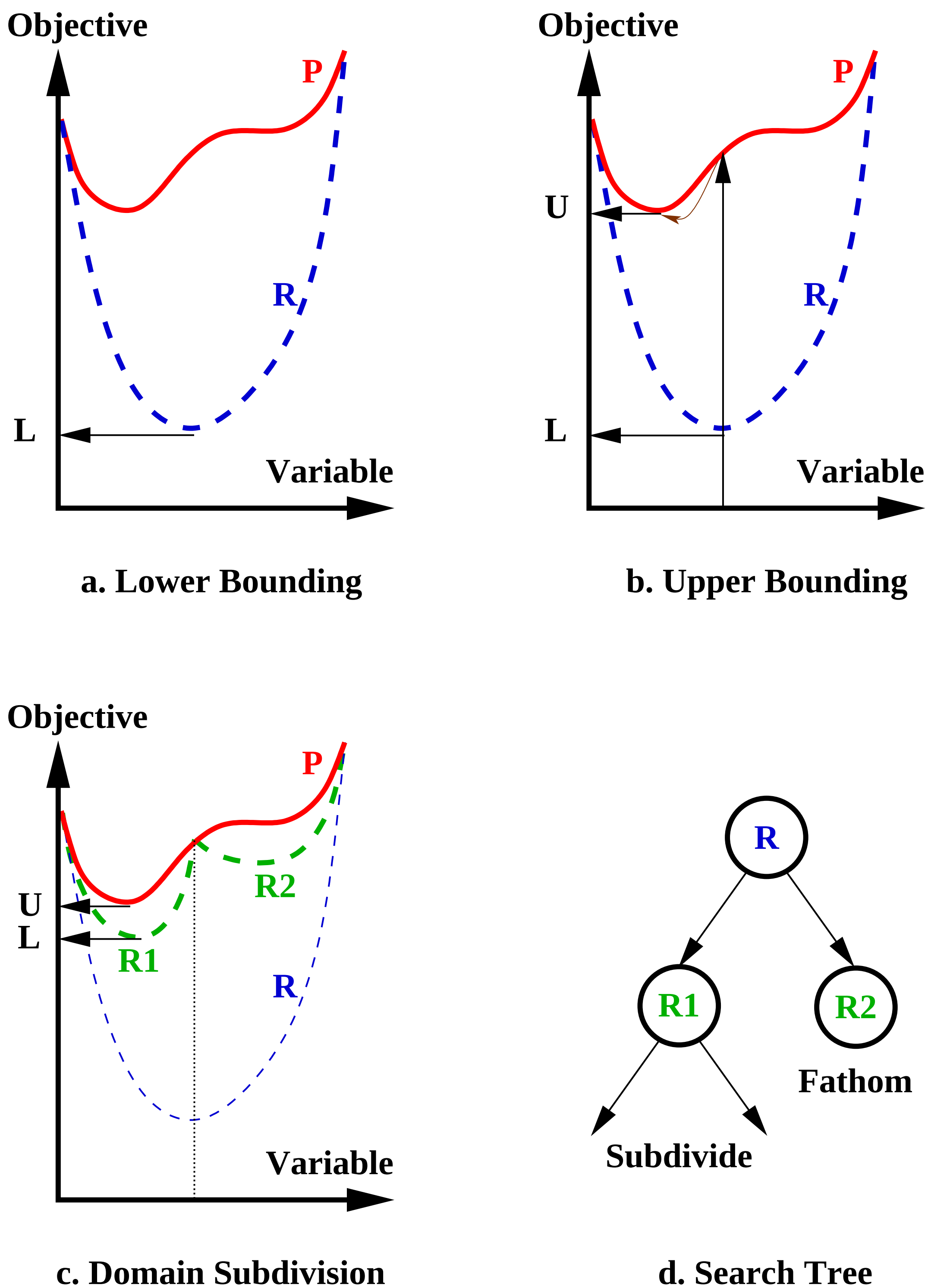

- Nonconvex Constraints



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

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

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

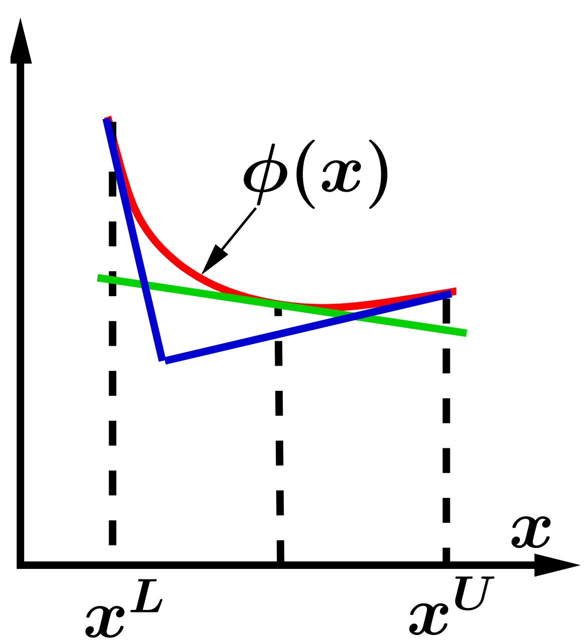
# OUTER APPROXIMATION

**Motivation:**

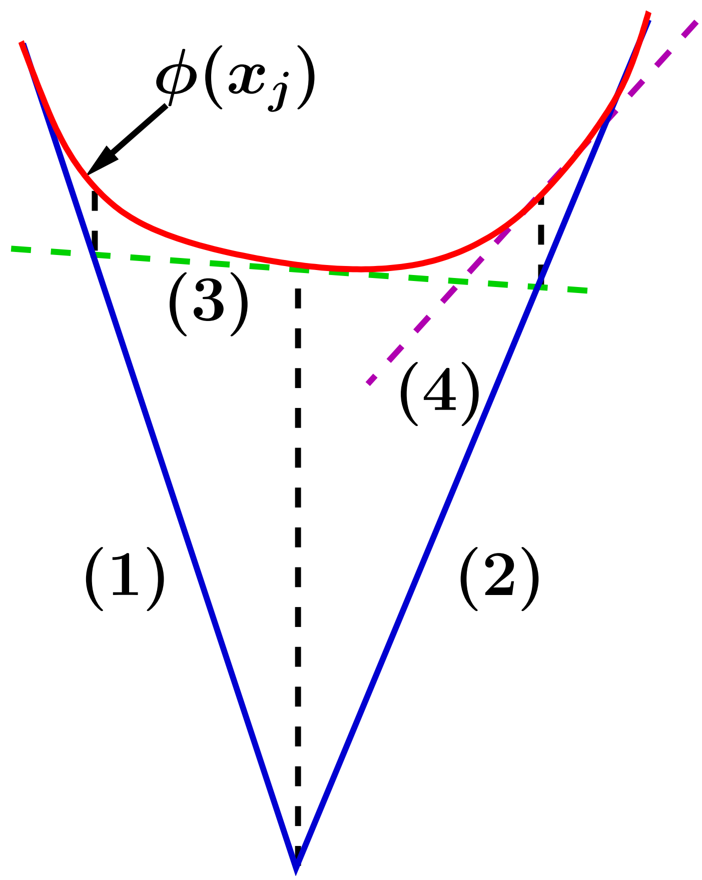
- **Convex NLP solvers are not as robust as LP solvers**
- **Linear programs can be solved efficiently**

**Outer-Approximation:**

**Convex Functions are underestimated by tangent lines**



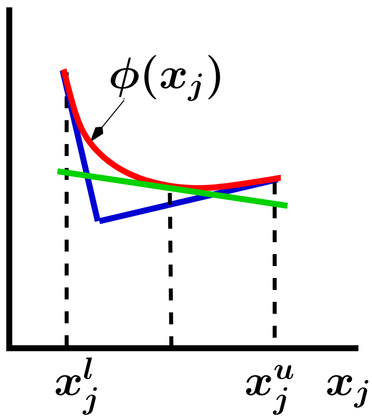
# THE SANDWICH ALGORITHM



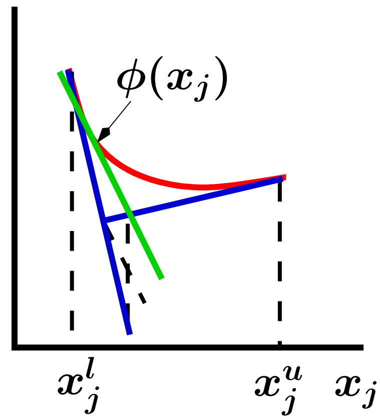

**An adaptive strategy**

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

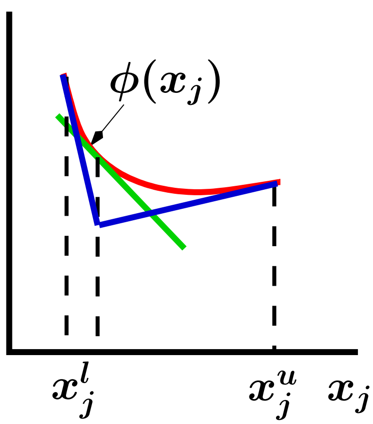
# TANGENT LOCATION RULES



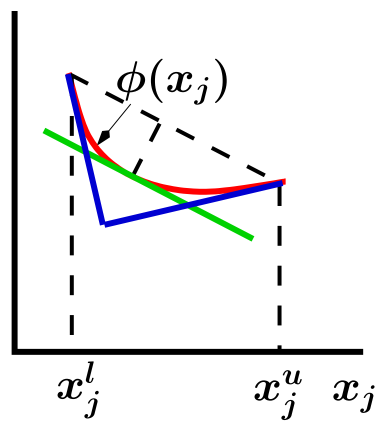

Interval bisection



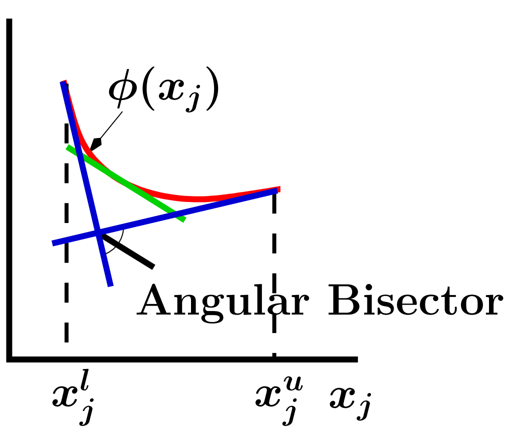

Slope Bisection



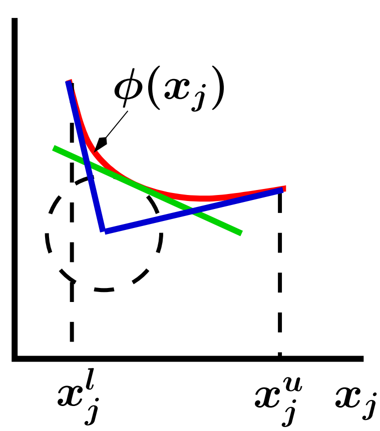

Maximum error rule




Chord rule



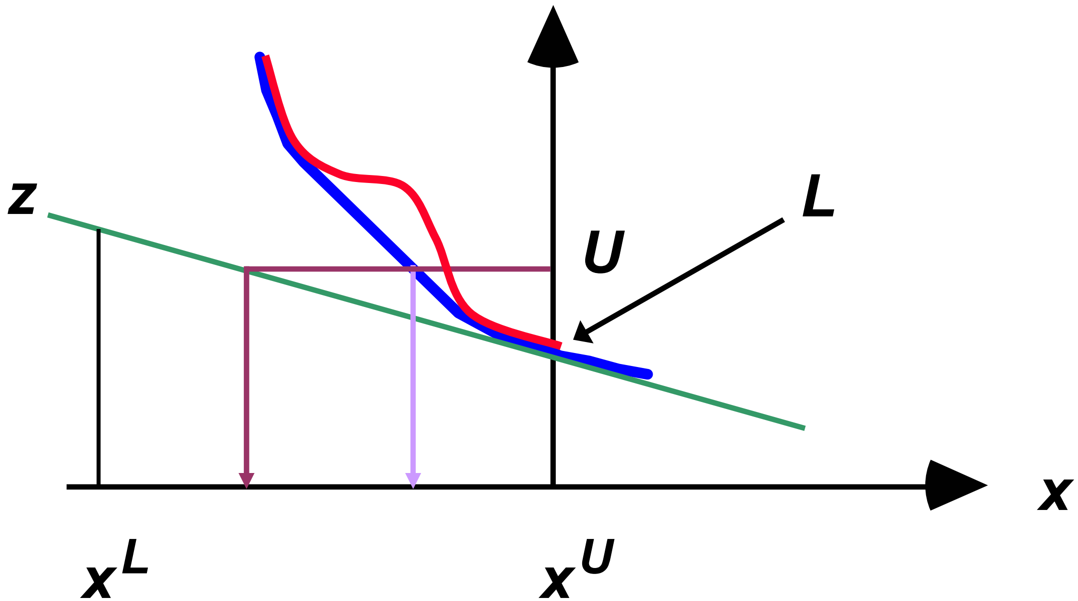

Angle bisection




Maximum projective error

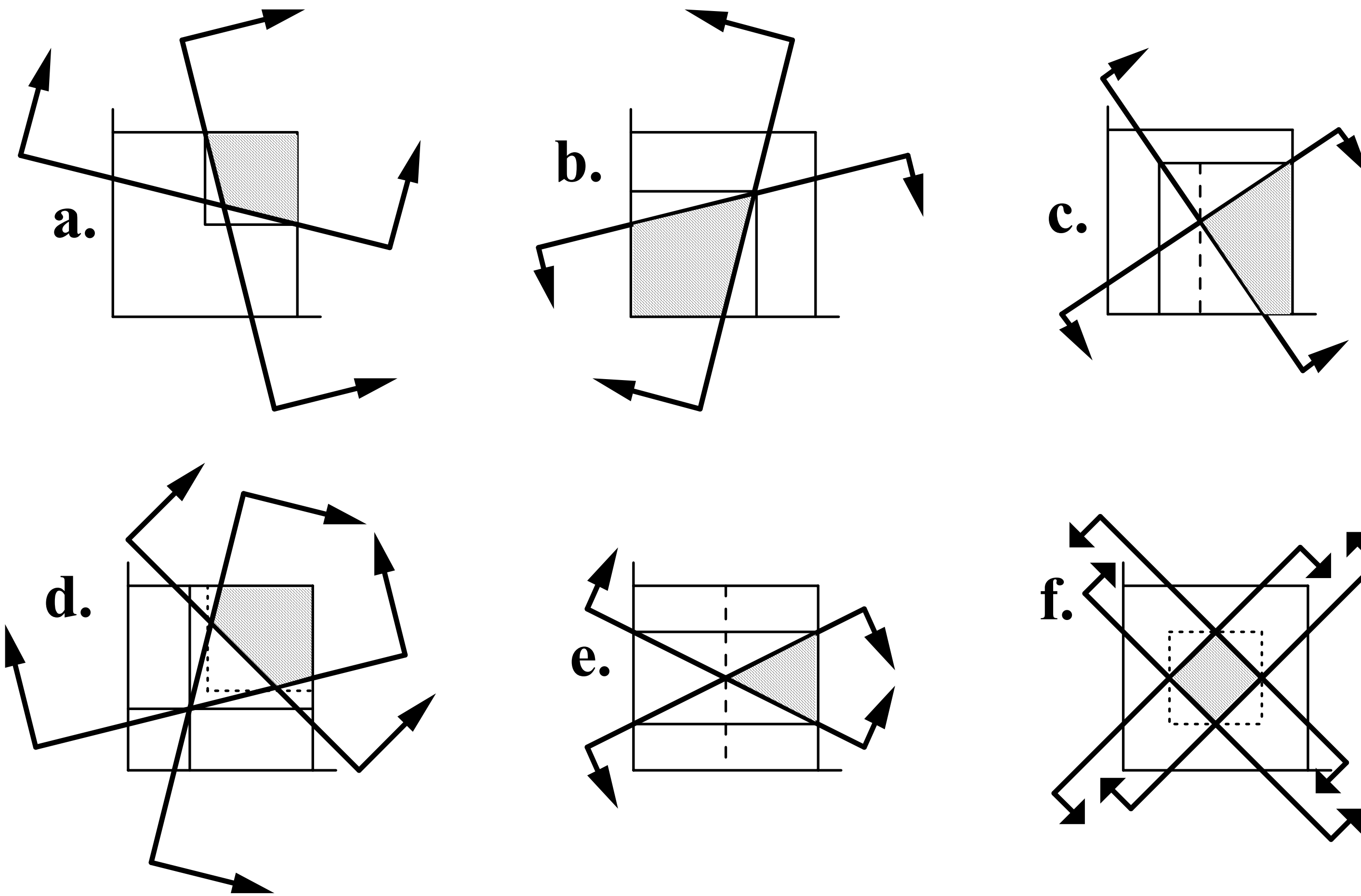
# MARGINALS-BASED RANGE REDUCTION

## Relaxed Value Function



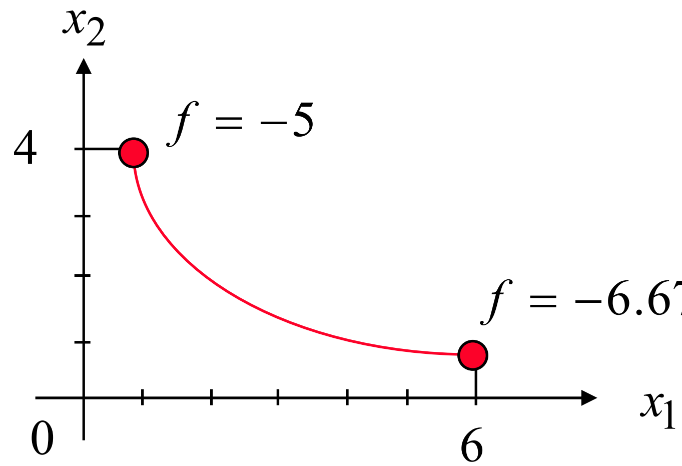

**If a variable goes to its upper bound at the relaxed problem solution, this variable's lower bound can be improved**

# “POOR MAN’S LPs AND NLPs”



# ILLUSTRATIVE EXAMPLE

$$\left.\begin{array}{ll} \min & f = -x_1 - x_2 \\ s.t. & x_1 x_2 \le 4 \\ & 0 \le x_1 \le 6 \\ & 0 \le x_2 \le 4 \end{array}\right\} \quad (P)$$




**Reformulation :**

$$\begin{array}{ll} \min & f = -x_1 - x_2 \\ s.t. & x_3^2 - x_1^2 - x_2^2 \le 8 \\ & x_3 = x_1 + x_2 \\ & 0 \le x_1 \le 6 \\ & 0 \le x_2 \le 4 \\ & 0 \le x_3 \le 10 \end{array}$$

**Relaxation :**

$$\left.\begin{array}{ll} \min & -x_1 - x_2 \\ s.t. & x_3^2 - 6x_1 - 4x_2 \le 8 \\ & x_3 = x_1 + x_2 \\ & 0 \le x_1 \le 6 \\ & 0 \le x_2 \le 4 \\ & 0 \le x_3 \le 10 \end{array}\right\} \quad (R)$$

**Solution of** $R$ **:** $x_1 = 6, x_2 = 0.89, L = -6.89, \lambda_1 = 0.2$

**Local Solution of** $P$ **with MINOS :** $U = -6.67$

**Range reduction :** $x_1^L \leftarrow x_1^U - (U - L)/\lambda_1 = 4.86$

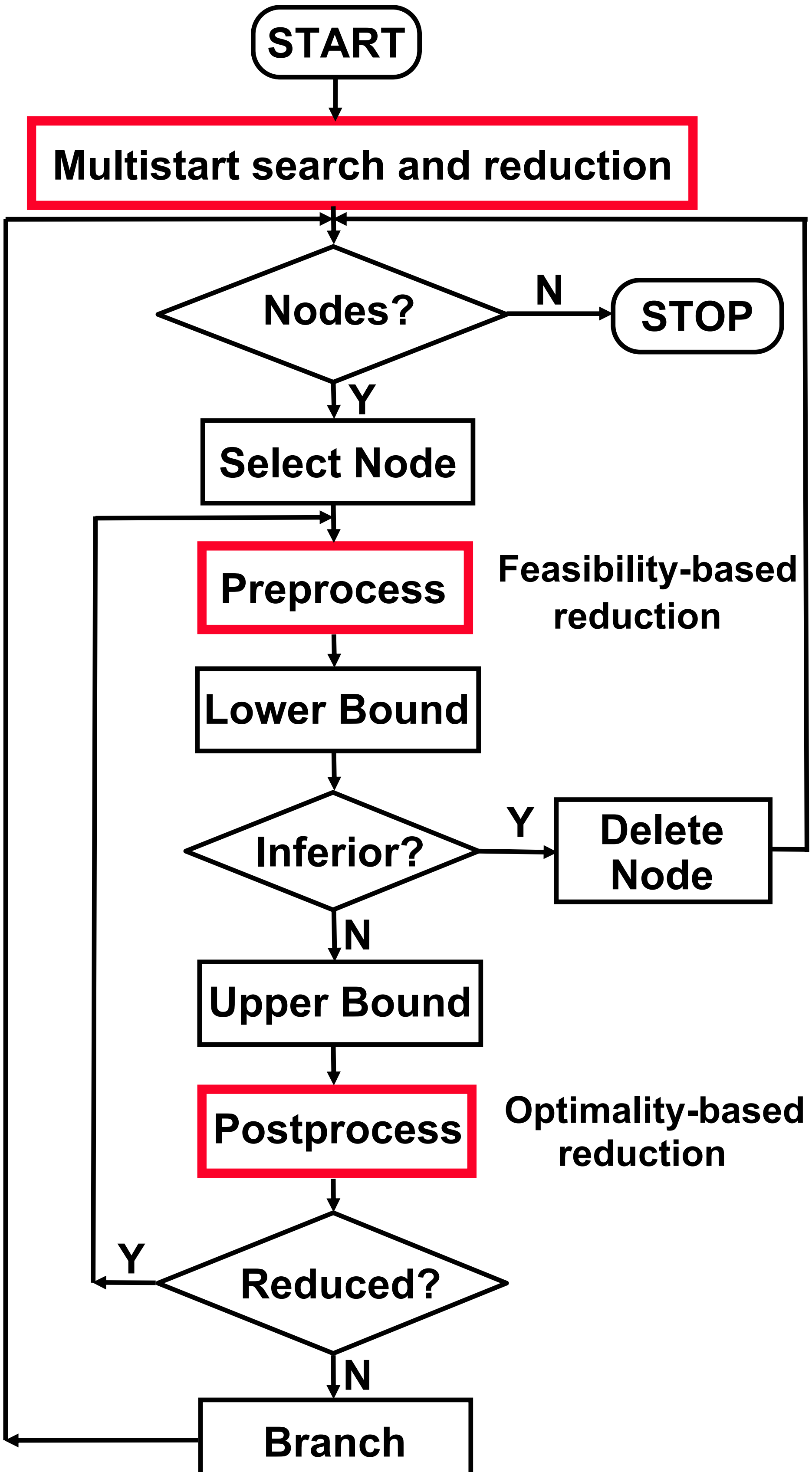
**Probing** (Solve $R$ with $x_2 \le 0$) : $L = -6, \lambda_2 = 1 \Rightarrow x_2^L = 0.67$

**Update** $R$ with $x_1 \ge 4.86, x_2 \ge 0.67$

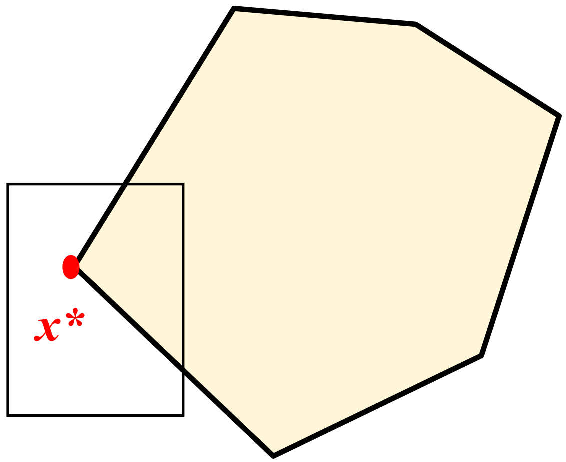
**Solution** is : $L = -6.67$

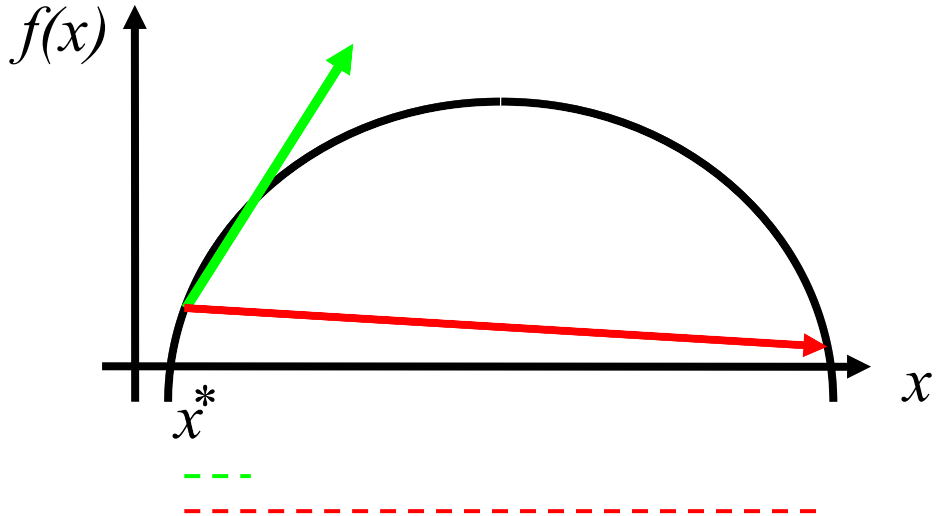
$\therefore$ **Proof of globality with NO Branching!!**

# Branch-and-REDUCE



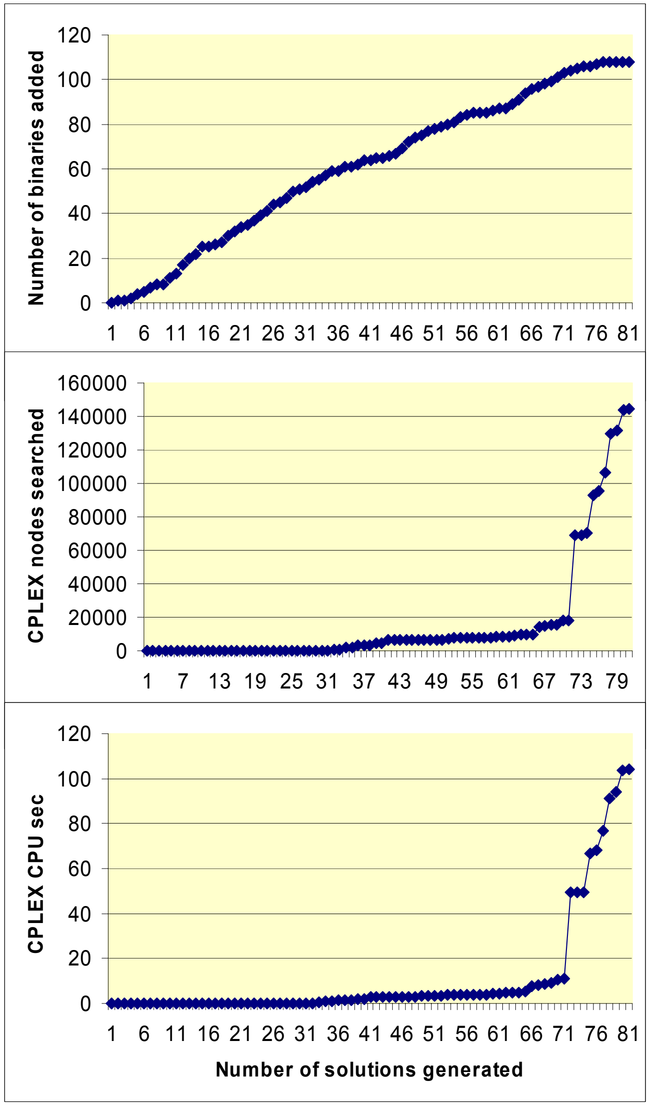
# FINITE BRANCHING RULE




- **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**
- **Finite termination in many cases**

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




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

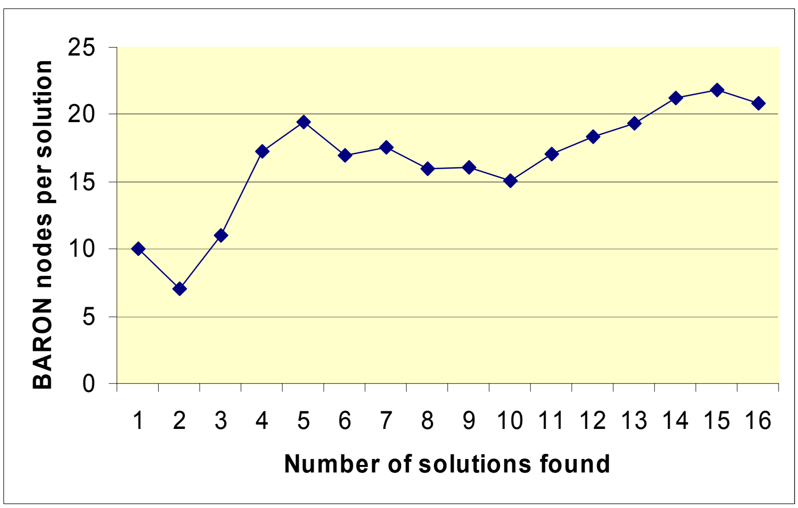
$$\begin{aligned} \min \quad & \sum_{i=1}^{4} 10^{4-i} x_i \\ \text{s.t.} \quad & 2 \le x_i \le 4, \quad i = 1,\ldots,4 \\ & x \ \ \text{integer} \end{aligned}$$

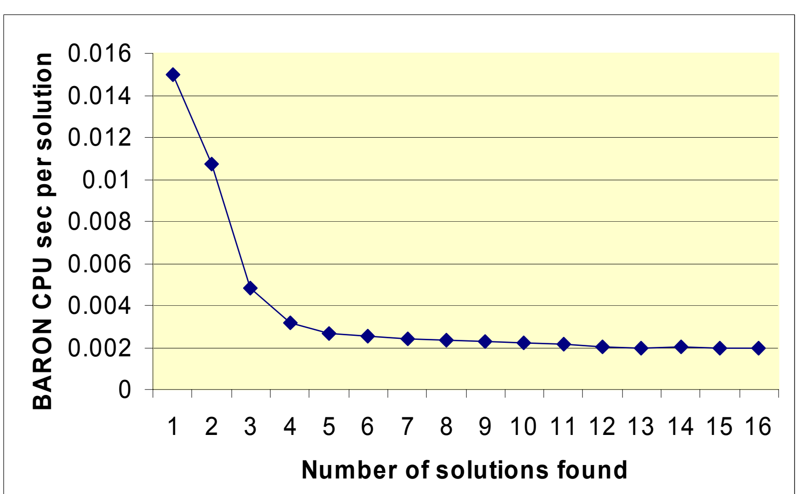
**BARON finds all solutions:**

- **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)



# 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
- GAMS link since November 2000

# 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.

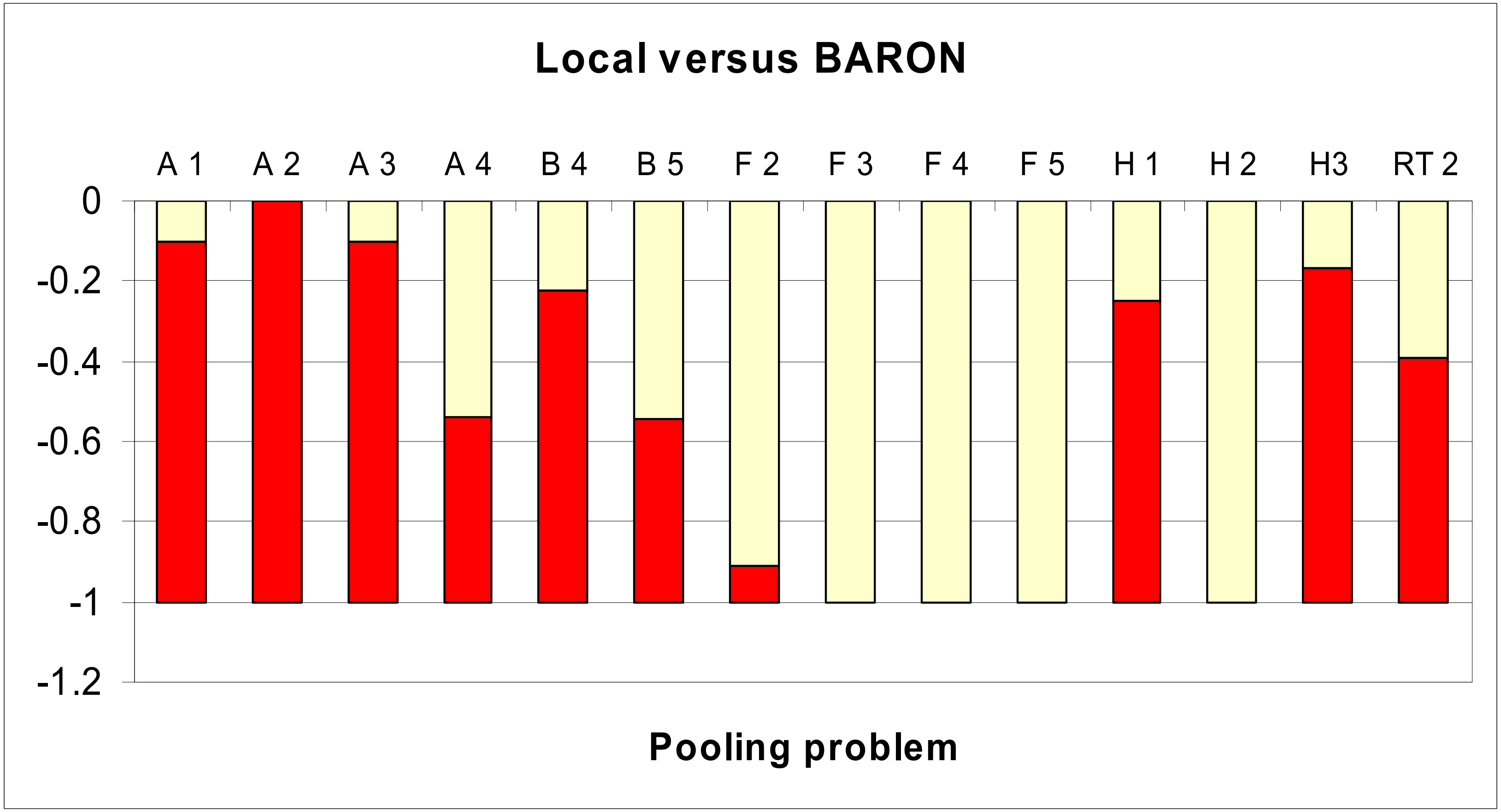
# POOLING PROBLEMS

| 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 | $N_{tot}$ | $T_{tot}$ | $N_{tot}$ | $T_{tot}$ | $N_{tot}$ | $T_{tot}$ | $N_{tot}$ | $T_{tot}$ | $N_{tot}$ | $T_{tot}$ |
| 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

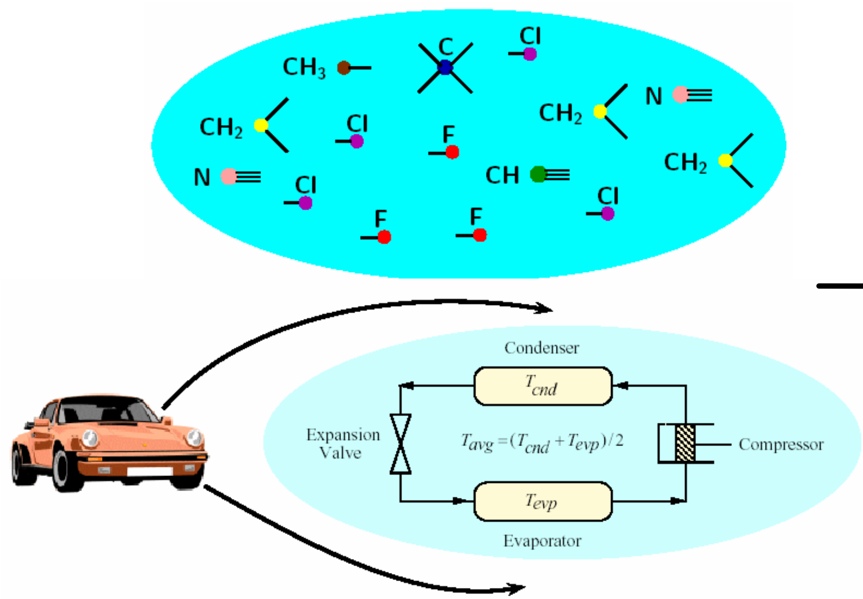
** 0.05% for Haverly 1, 2, 3, 0.05% for Ben-Tal 4 and 1% for Ben-Tal 5

# LOCAL vs. GLOBAL SEARCH

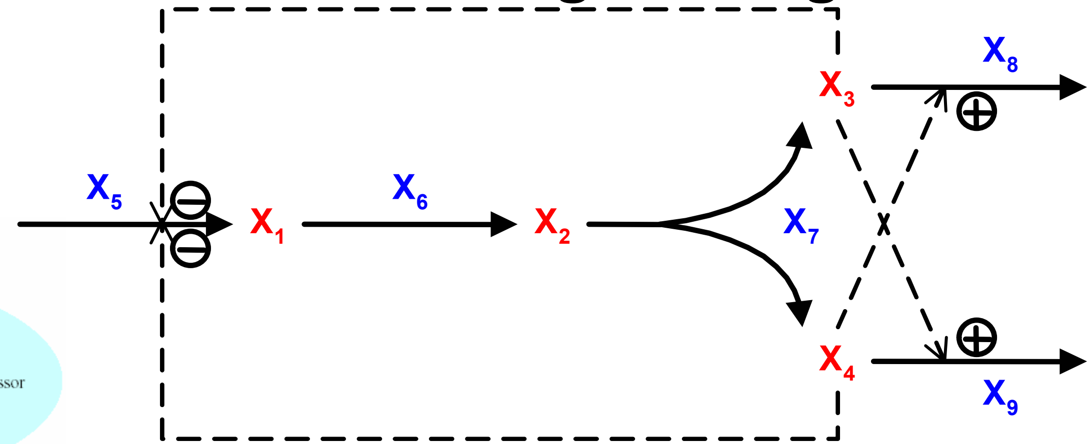


# CHEMICAL- AND BIO-INFORMATICS

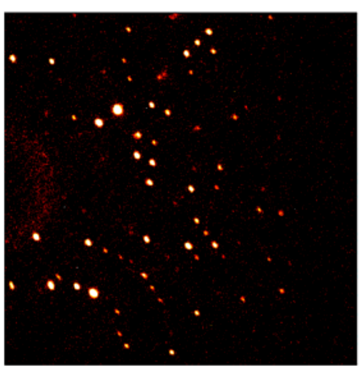
## Molecular design




## Metabolic engineering



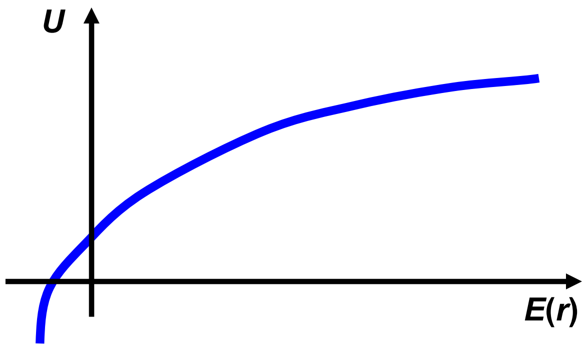

## X-ray imaging



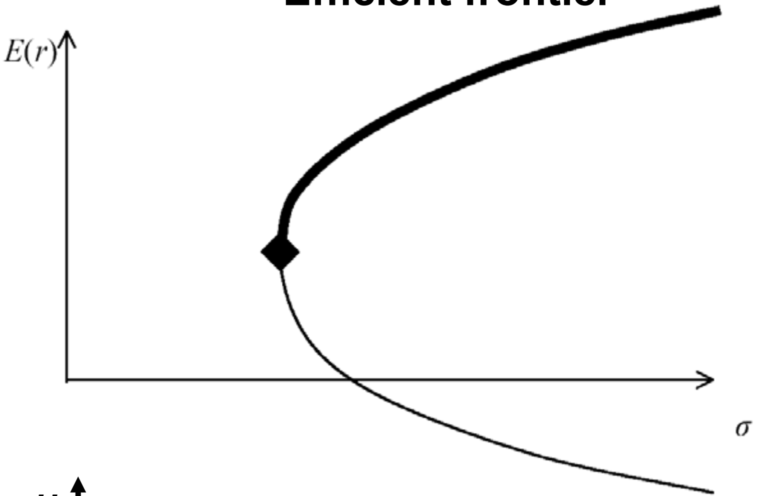
## Bioinformatics

# PORTFOLIO OPTIMIZATION FOR WEALTH-DEPENDENT PREFERENCES

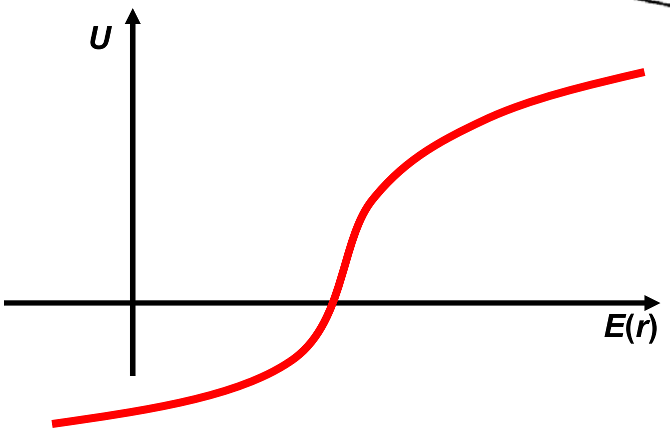
- **Markowitz model:**
  - variance vs. expected return
  - quadratic programming
  - risk-averse individuals




Efficient frontier




- **Empirical studies:**
  - Individuals have utility with two segments




M. L. Rios and N. V. Sahinidis, paper TD31.4

# NEW IN GAMS/BARON 6.0

- More decimals in solution, accurate timing of NLP sub-solvers, new branching and probing options, minimize and maximize, …
- Provide dual solution
- Report lower bounds independent of tolerances
- Bug fixes
  - Infinite loops
    - Local search
    - numsol > 1
  - Power relaxations
  - *x* and 1/*x*
  - *Thanks to:* Arne Drud, Oleg Shcherbina, Arnold Neumaier
- New options defaults
  - Reduced memory requirements
  - Faster convergence

# COMPUTATIONAL RESULTS

- **Collection of 102 NLP and MINLP problems from globallib and gamslib**
- **Average of 40.2 variables**

| | version 5 | version 6 | % Improvement |
|---|---|---|---|
| Nodes | 2,187,512 | 76,112 | 96 |
| Nodes to optimum | 438,269 | 15,825 | 96 |
| Nodes in memory | 65,765 | 4,179 | 94 |
| CPU sec | 4,381 | 1,975 | 55 |

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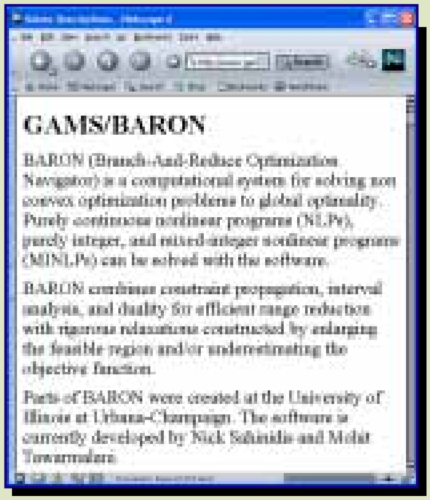
## Global Optimization Solver BARON



GAMS/BARON

BARON (Branch-And-Reduce Optimization Navigator) is a computational system for solving non convex optimization problems to global optimality. Purely continuous nonlinear programs (NLPs), purely integer, and mixed-integer nonlinear programs (MINLPs) can be solved with the software.

BARON combines constraint propagation, interval analysis, and duality for efficient range reduction with rigorous relaxations constructed by enlarging the feasible region and/or underestimating the objective function.

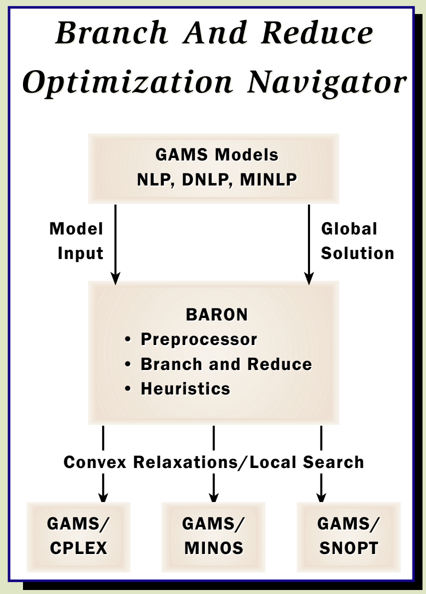
Parts of BARON were created at the University of Illinois at Urbana-Champaign. The software is currently developed by Nick Sahinidis and Mohit Tawarmalani.

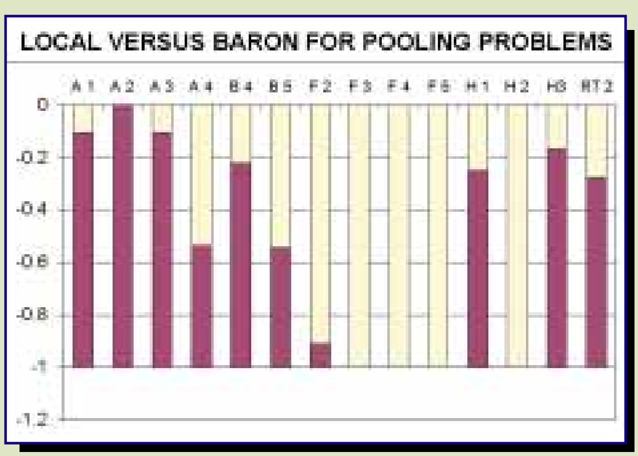
High performance and reliability of solvers come as a result of technological and theoretical developments in solution technology and modeling systems.

BARON combines constraint propagation, interval analysis, and duality for efficient range reduction while rigorous relaxations are constructed by enlarging the feasible region and/or underestimating the objective function.

### Important Application Areas for Global Optimization:

- Reliability
- Parameter Estimation
- Engineering Design
- Economics
- Finance
- Supply Chain Design and Operation
- Molecular Design and Bioinformatics




The darker area of each box is proportional to the difference between the global solution and the best local solution obtained using two local solvers for 14 pooling problems from the literature.

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