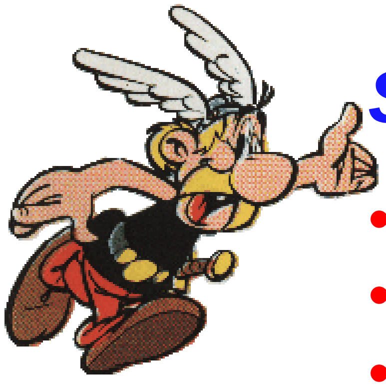
Introduction: Models, Model Building and Mathematical Optimization
The Importance of Modeling Langauges for Solving Real World Problems

Josef Kallrath

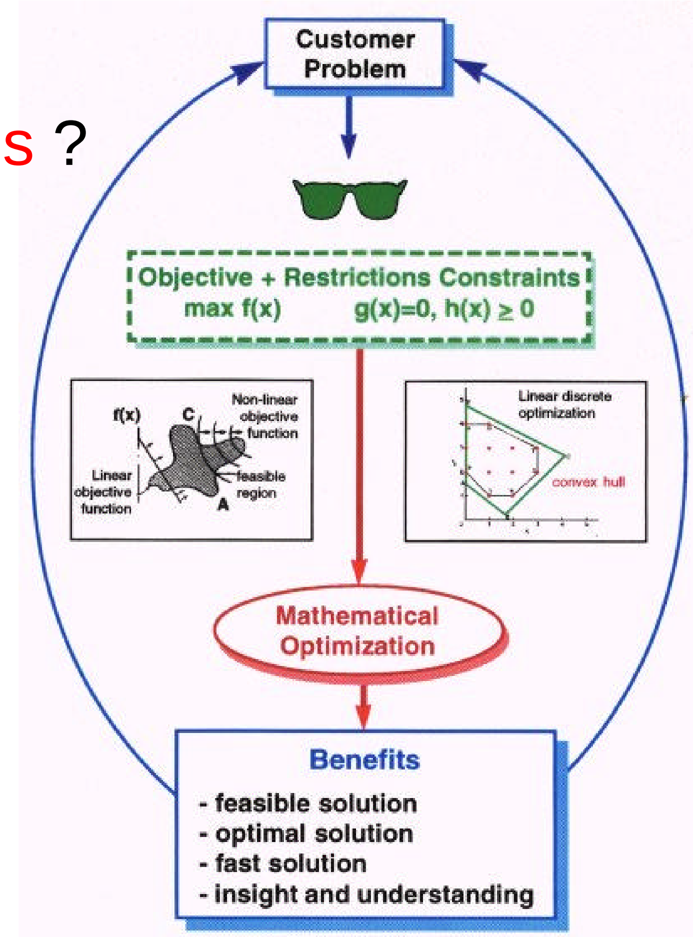


Structure of the Lecture:

- the Modeling Process
- survey of Real World Problems
- mathematical background (solution algorithms)
- efficient problem solving & good modeling practice
- mathematical modeling & optimization in practice
- practioners‘s requirements towards modeling languages

Introduction

- what is mathematical optimization ?
  what are (MIP) optimization problems ?
- what do we need to solve real world problems as optimization problems:
  data, model, algorithms (solver)
  modeling language/system
- simulation versus optimization
- commerical potential in optimization

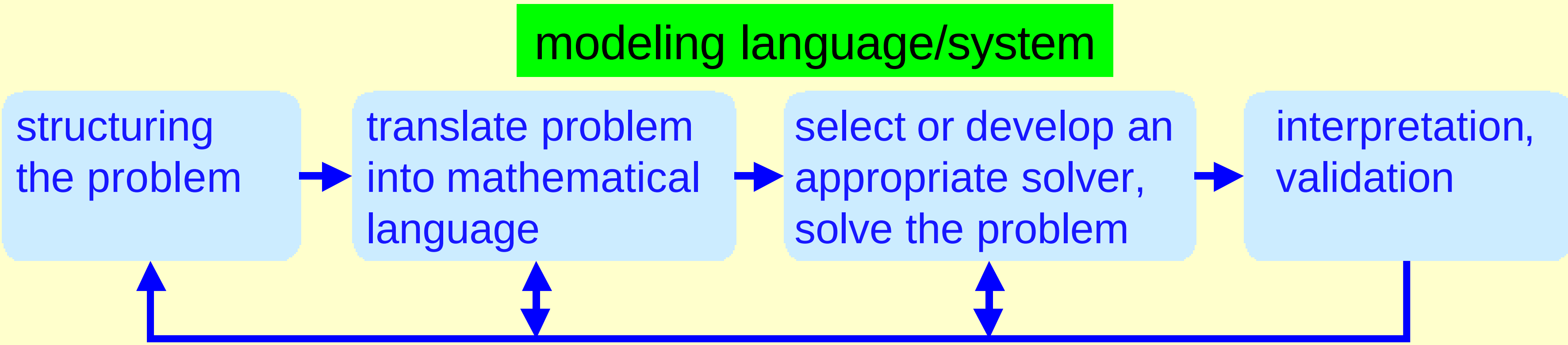


How Does MIP-Modeling Work?

strong focus on
methods & know-how

computer based

interdisciplinary



theory- & model building
- no tool, no standard

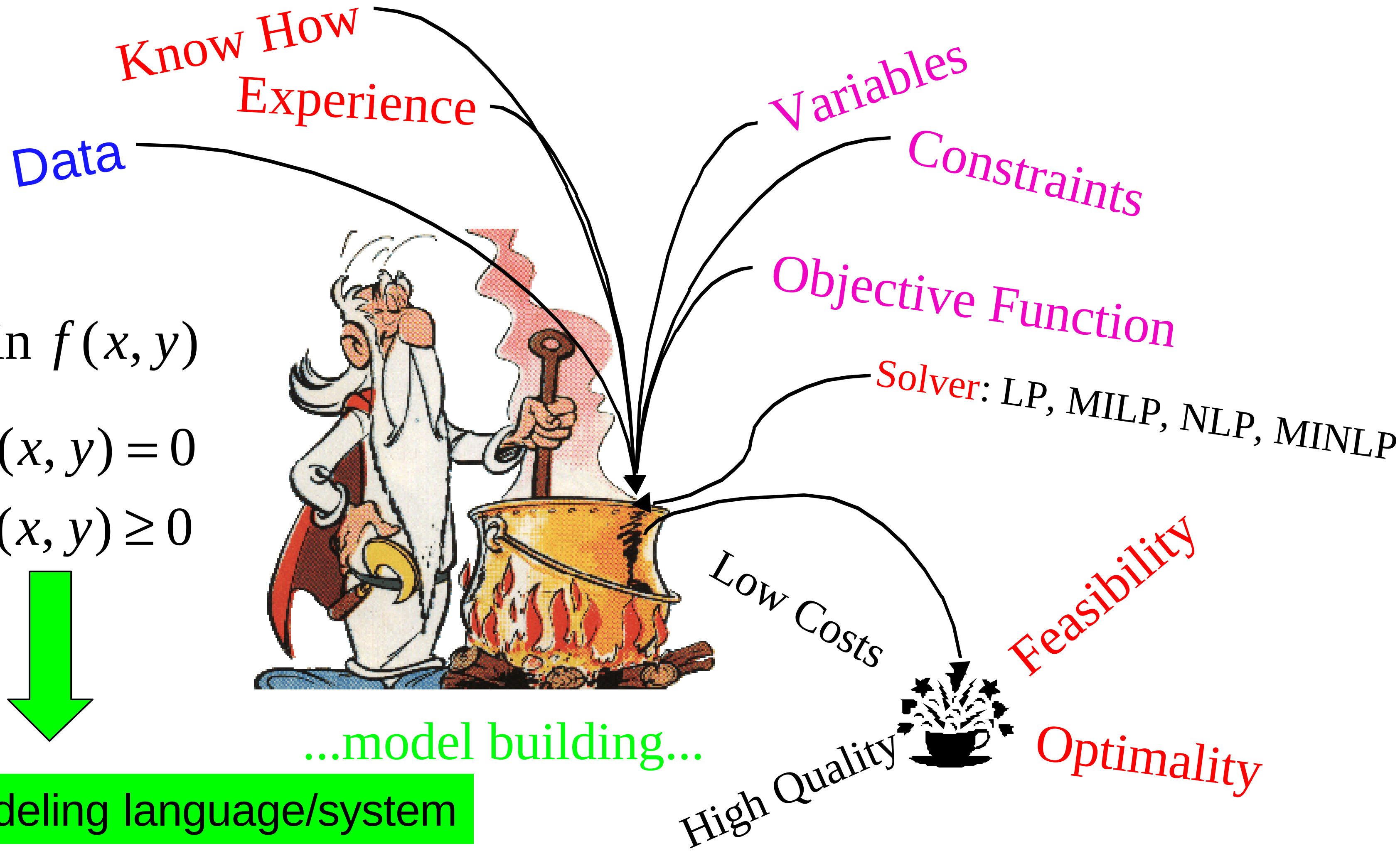
mathematical Algorithms
numeric mathematics
- no standard approach

The Ingredients of Mathematical Optimization

$$\min \ f(x,y)$$

$$g(x,y) = 0$$

$$h(x,y) \geq 0$$



modeling language/system

Mathematical Modeling and Optimization
Building Blocks

- data (Actual Situation and Requirements, Control Parameters)

  e.g., number of sites, unit capacities, demand forecasts, avaliable resources

- model (variables, constraints, objective function)

  e.g., how much to produce, how much to ship, (decision variables, unknowns)

  e.g., mass balances, network flow preservation, capacity constraints

  e.g., max. contribution margin, min. costs, yield maximization

- optimization algorithm and solver

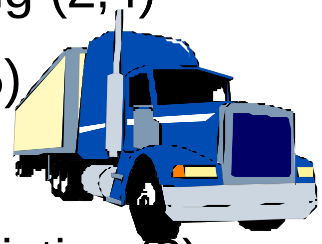
  e.g., simplex algorithm, B&B algorithm, SQP, outer approximation...

- optimal solution (Suggested Values of the Variables)

  e.g., production plan, unit-connectivity, feed concentrations...

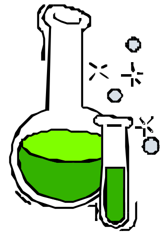
Survey of Real World Problems

- production planning (2,4)
- sequencing (2)
- man power planning (2,4)
- scheduling (2,3,4,5)

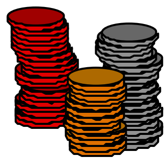


- allocation (2)
- distribution and logistics (2)

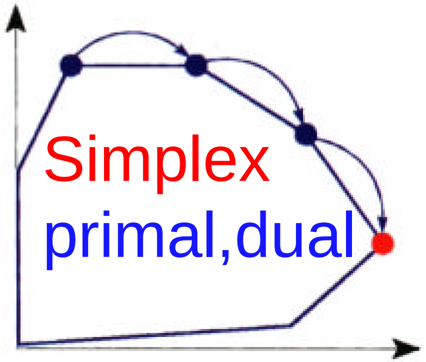
1 LP : Linear Programming
2 MILP : Mixed Integer LP
3 NLP : Nonlinear Programming
4 MINLP : Mixed Integer NLP
5 CP : Constraint Programming

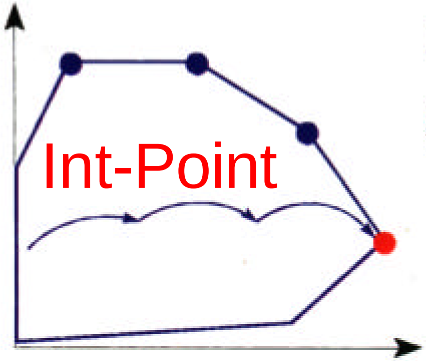


- blending (1,2,3,4)
- refinery optimization (3,4)
- process design (4)
- engineering design (3,4)
- selection & depot location (2)
- investment / de-investment (2,4)
- network design (2,4)
- financial optimization (2,4)



Revised Simplex & Interior Point Methods





PreSolve, algorithms   hardware

LP:

$$\min c^t x \quad \text{s.t.} \quad Ax = b, \quad x \geq 0,\ x \in \mathrm{IR}^n_+$$

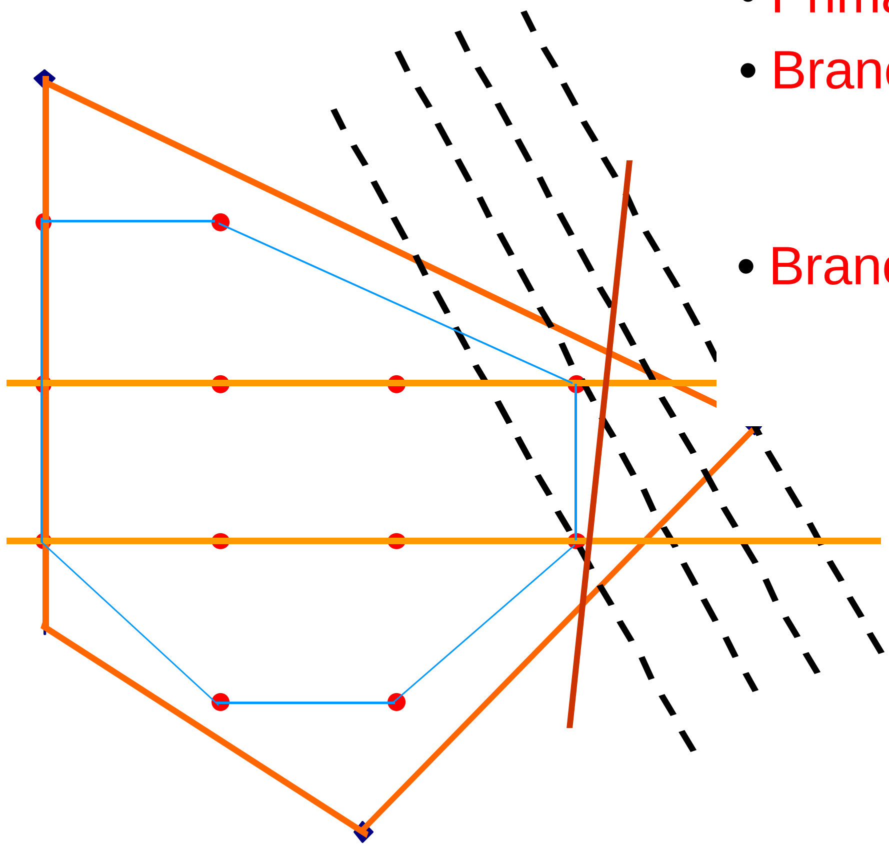
sequence of NLP problems P(k):

$$\min c^t x - \mu^k \sum_{i=1}^{n} \ln x_i \quad \text{s.t.} \quad Ax = b, \quad (x \geq 0),\ x \in \mathrm{IR}^n_+$$

Remarks:

- feasible point required
- IPMs are originally made for NLPs
- P(k) is a equality constrained NLP
- choose homotopy parameter such
- that lim argmin(LP)=argmin(P(k))

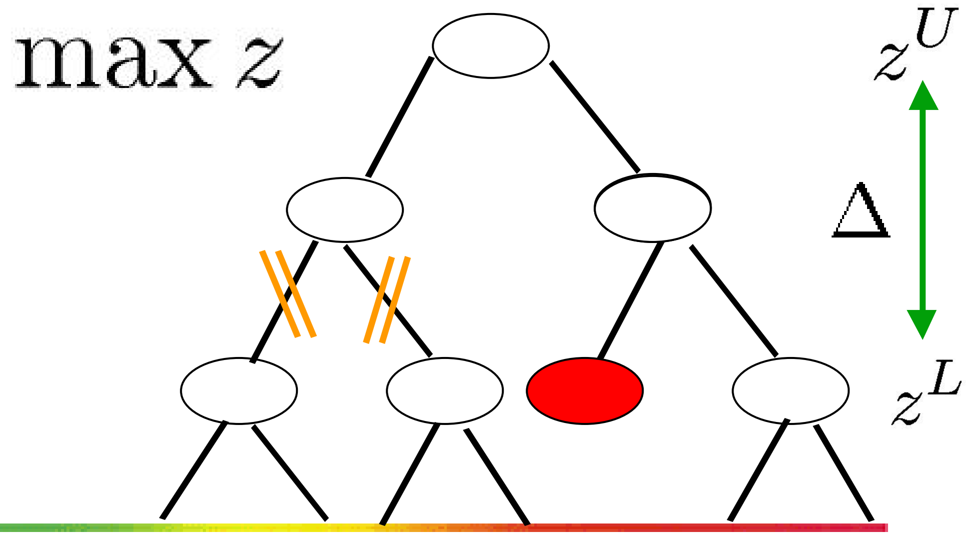
Mixed Integer Linear Programming
Branch & Bound - Branch & Cut



- Primal & Dual Simplex for relaxed LP problems
- Branch and Bound - implicit enumeration

  solve relaxed LP problem
  with additional bounds for integer variables
- Branch and Cut

  solve relaxed LP problem
  with additional valid constraints



B&B is a proof techniques !!!

MILP Algorithms

- Branch & Bound

  [Land&Doig (1960), Dakin(1964), Beale (1967)]

- Benders Decomposition [Benders (1962)]
- Cutting Plane [Gomory (1960)]
- Branch & Cut

  [Crowder, Johnson & Padberg (1983)

  van Roy & Wolsey (1987), Balas, Ceria & Cornuejols (1993)]

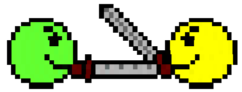
Good Modeling Practice

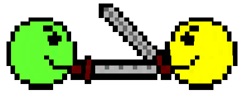
- pre-processing
- modeling techniques
- scaling (User&Software)

- inequality relaxation of equations

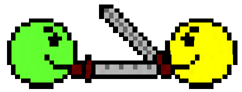
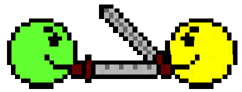
  flow_out = flow_in 

  --> flow_out <= flow_in

- introduce auxiliary variables for  branching

- choice of branch in integer programming 

  entity choice, choice of branch or node, priorities

- branching for special ordered sets 
- branching on semi-continuous variables 

MILP formulations for MINLP problems

- nonlinear convex objective functions or inequalities
- products of one continous and k binary variables
- linear constraints & nonlinear separable objective functions
- products of one integer and two continuous variables

Modeling Product Terms
One Continuous & Several Binary Variables

given K binary variables δ_k and

assume that

$$0 \leq x \leq X^+$$

$$y := x \cdot \Pi_{k=1}^{K} \delta_k \quad ; \quad \delta_k \in \{0,1\} \quad ; \quad x \in \mathbb{R}$$

equivalent representation of y by set of linear inequalities

$$\forall k : y \leq X^+ \delta_k \quad , \quad y \leq x \qquad (*)$$

$$y \geq x - X^+ \left(K - \sum_{k=1}^{K} \delta_k \right) \qquad (**)$$

Model Cuts
Cuts for Integer Variables

given

$$x + A\alpha \geq B \quad ; \quad \alpha \in \mathbb{N} \quad ; \quad x \in \mathbb{R}$$

define

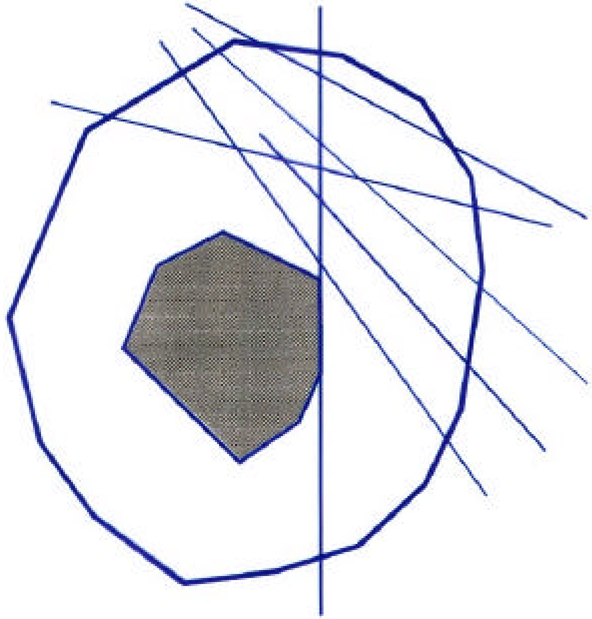
$$\eta := \left\lceil \frac{B}{A} \right\rceil = ceil\left(\frac{B}{A}\right)$$

$\Rightarrow$ valid inequality (cut)

$$x \geq [B - (\eta - 1)A]\,(\eta - \alpha)$$

Cutting Plane Approach

- general mixed-integer cuts (!)
  - Gomory Mixed Cuts
  - Flow Cover Cuts
  - Knapsack Cuts
  - others ....
- problem specific cuts

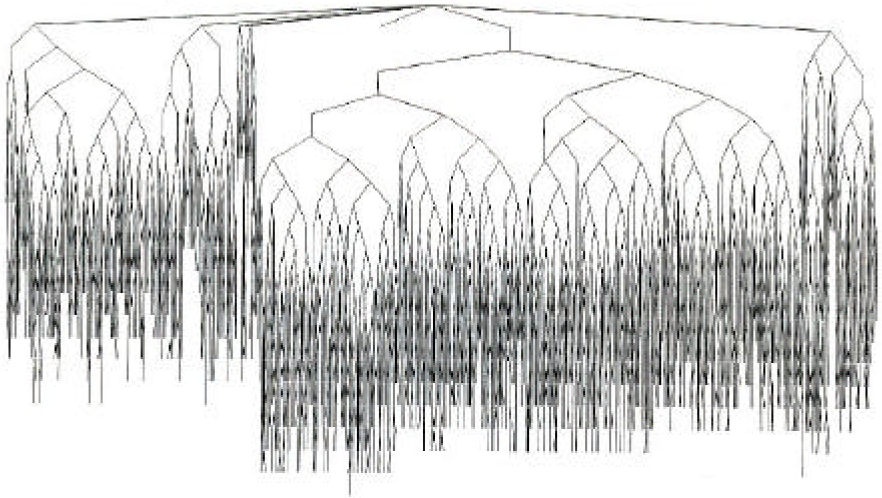


Example: cuts for semi-continuous variables

$$x + A\sigma \geq B \quad ; \quad \sigma = 0 \vee \sigma \geq 1 \quad ; \quad x \in \mathbb{R}$$

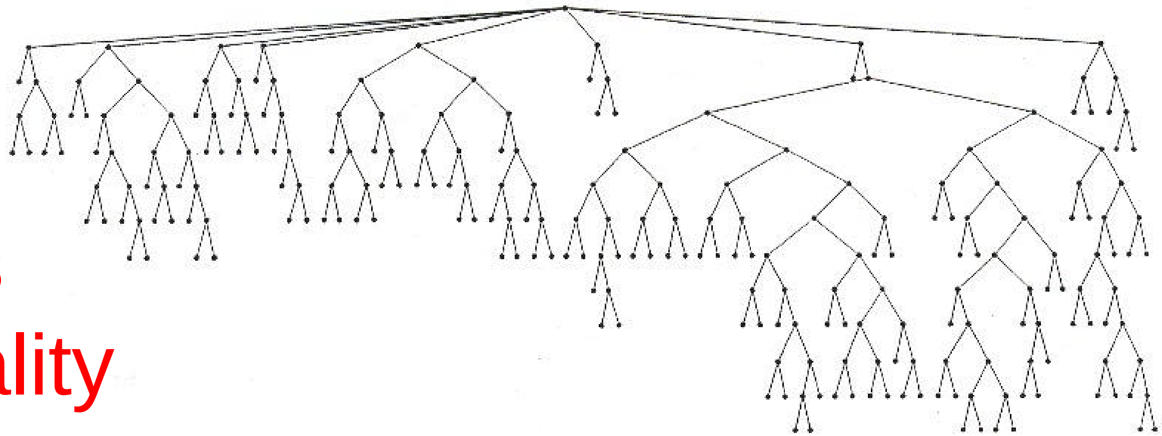
$\Rightarrow$ valid inequality (cut) $\quad \frac{1}{B}x + \sigma \geq 1$

Cutting Plane Approach



without cuts
8388 nodes

with cuts
only 240 nodes
to prove optimality



Mixed Integer Nonlinear Programming Applications

- petrochemical network problem

  several steamcrackers, plants at two sites

- tanker and refinery scheduling problem

  production schedule and storage model, medium size refinery

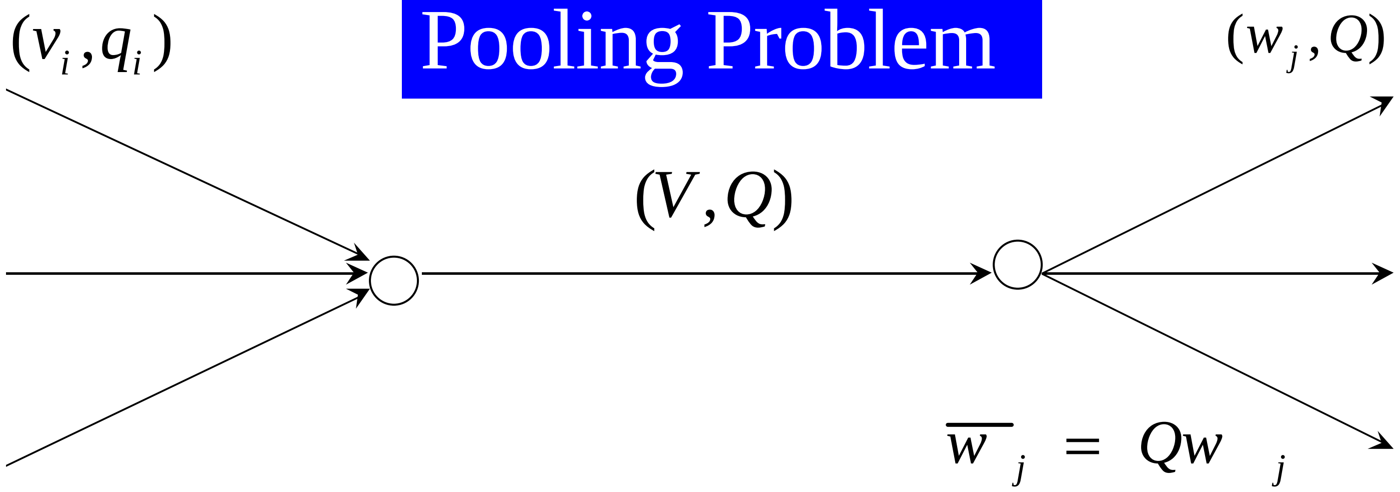
- network design problem

  pooling problems, large number of binary variables

- process design problem

  non-linear reaction kinetics, pooling problems

Pooling Problem



explicit pooling

$$V = \sum_i v_i$$

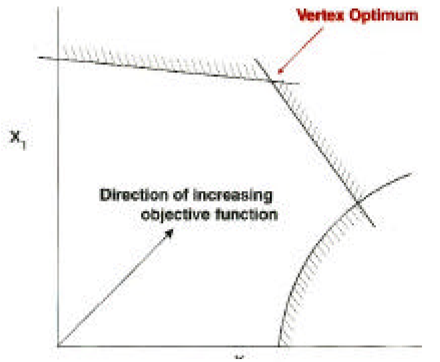
$$V \cdot Q = \sum_i v_i \cdot q_i$$

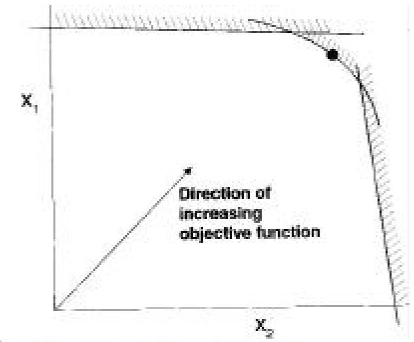
implicit pooling

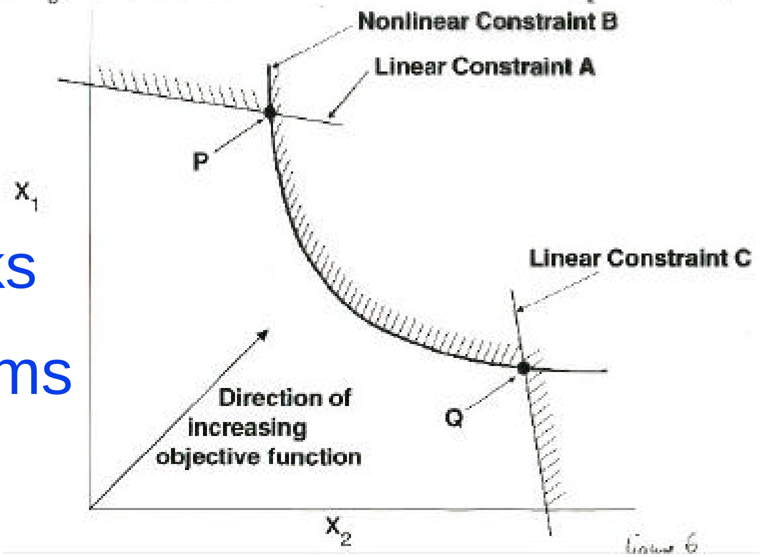
$$Q = \frac{\overline{w}_{j_1}}{w_{j_1}} = \frac{\overline{w}_{j_2}}{w_{j_2}}, \; j_1 \neq j_2$$

Definition of MINLP Problems (Mixed Integer Nonlinear Programming)

$$
\begin{aligned}
\min_{\mathbf{x}\in\mathbb{R}^{n_x},\mathbf{y}\in\mathbb{N}^{n_y}} \quad & \mathbf{f}(\mathbf{x},\mathbf{y}) \\
\mathbf{g}(\mathbf{x},\mathbf{y}) & = 0 \\
\mathbf{h}(\mathbf{x},\mathbf{y}) & \geq 0
\end{aligned}
$$

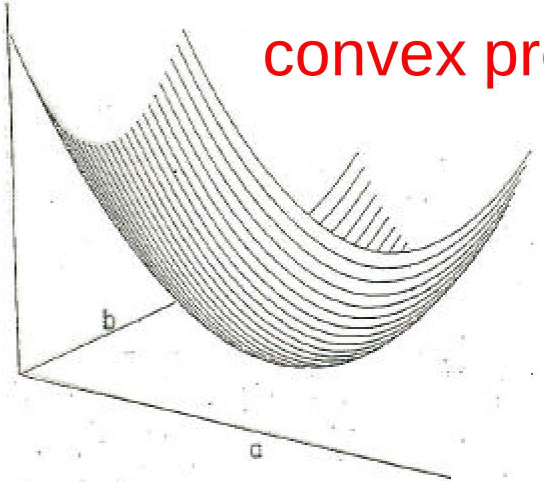




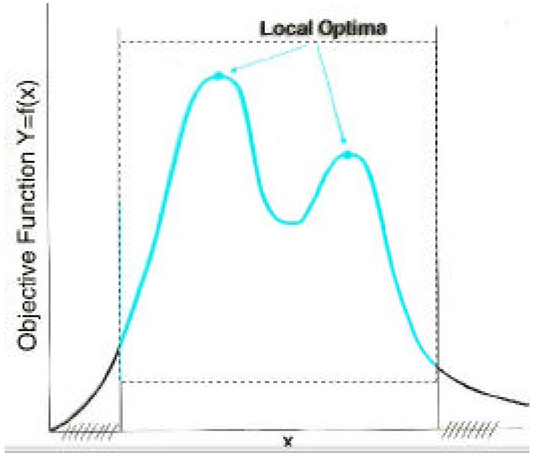


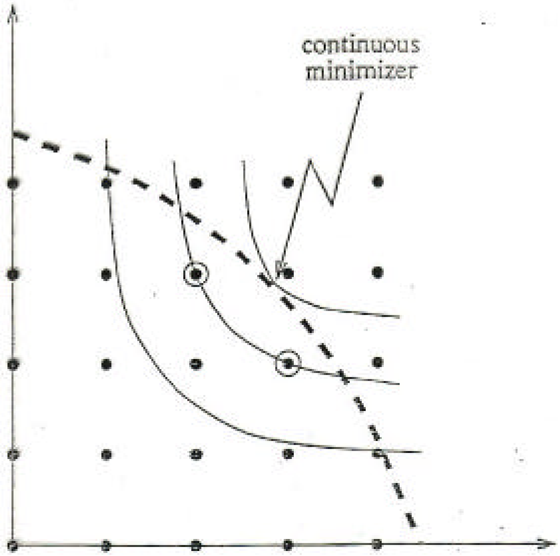
- Petrochemical Production Networks
- Process & Network Design Problems
- Financial Service Industry

Remarks on NLP & MINLP Problems

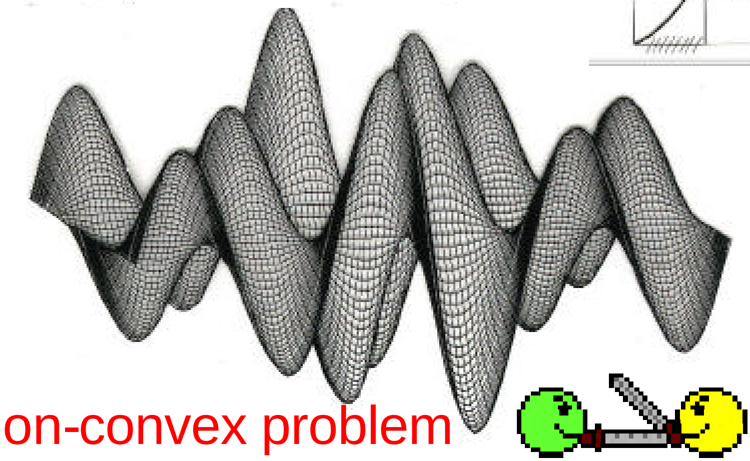


convex problem





multiple optima for a strictly convex problem



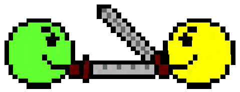
non-convex problem

Remarks:

- MINLP have all the difficulties of MILP and NLP
- MINLPs have new special features

MINLP Algorithms & Global Optimization

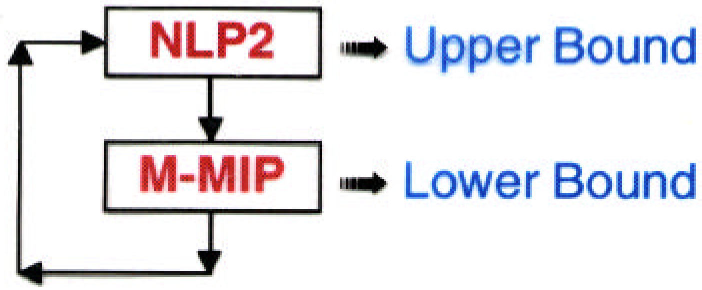
- Branch& Bound (BB) Gupta and Ravindran (1985),
  Nabar and Schrage (1991), Borchers and Mitchell (1992)
- Generalized Benders Decomposition [Benders (1962)]
- Outer-Approximation [Grossmann and Duran (1986)]
- LP/NLP based Branch&Bound [van Roy & Wolsey (1987)]
- Extended Cutting Plane Method [Westerlund and Petterson (1992)]
- *Convex Under Estimation Techniques (Floudas, Neumaier, Sahinides)*



Outer-Approximation

NLP2

$$\min \; Z_U^k = f(x, y^k)$$
$$s.t. \; g_j(x, y^k) \le 0 \quad j \in J$$
$$x \in X$$



M-MIP

$$\min \; Z_L^K = \alpha$$

$$s.t \quad \left.\begin{array}{l} \alpha \ge f(x^k, y^k) + \nabla f(x^k, y^k)^T \begin{bmatrix} x - x^k \\ y - y^k \end{bmatrix} \\ g(x^k, y^k) + \nabla g_j(x^k, y^k)^T \begin{bmatrix} x - x^k \\ y - y^k \end{bmatrix} \le 0 \quad j \in J^k \end{array}\right\} k = 1..K$$

$$x \in X, \; y \in Y, \; \alpha \in R^1$$

Remarks:

- only 1 iteration if linear
- exclude infeasible points by integer cuts (binary v.)

$$\sum_{i \in B^k} y_i - \sum_{i \in N^k} y_i \le \left|B^k\right| - 1 \quad k = 1,\ldots K$$

The Idea of Outer Approximation

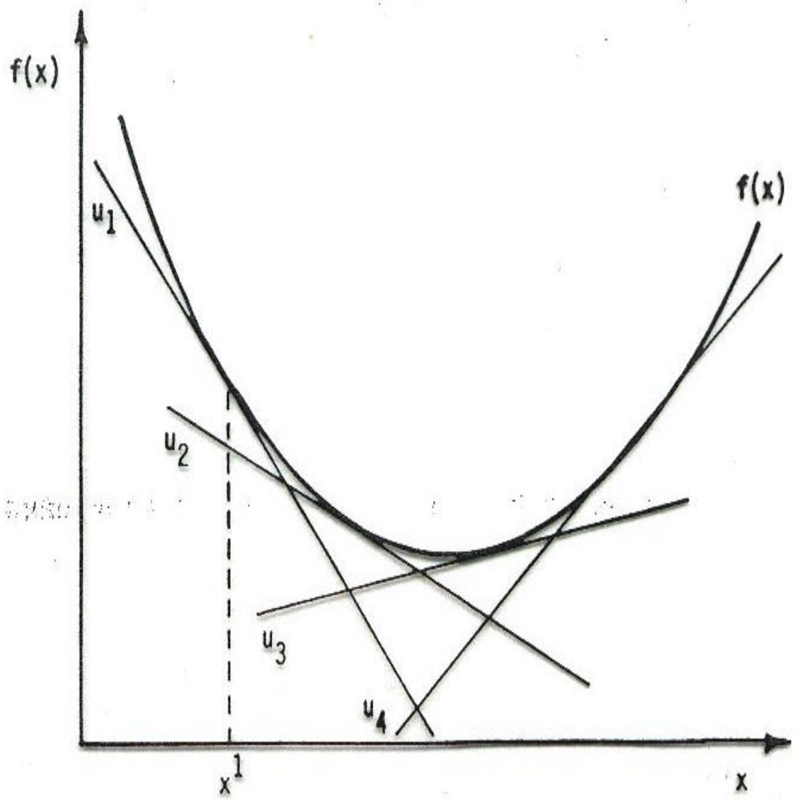
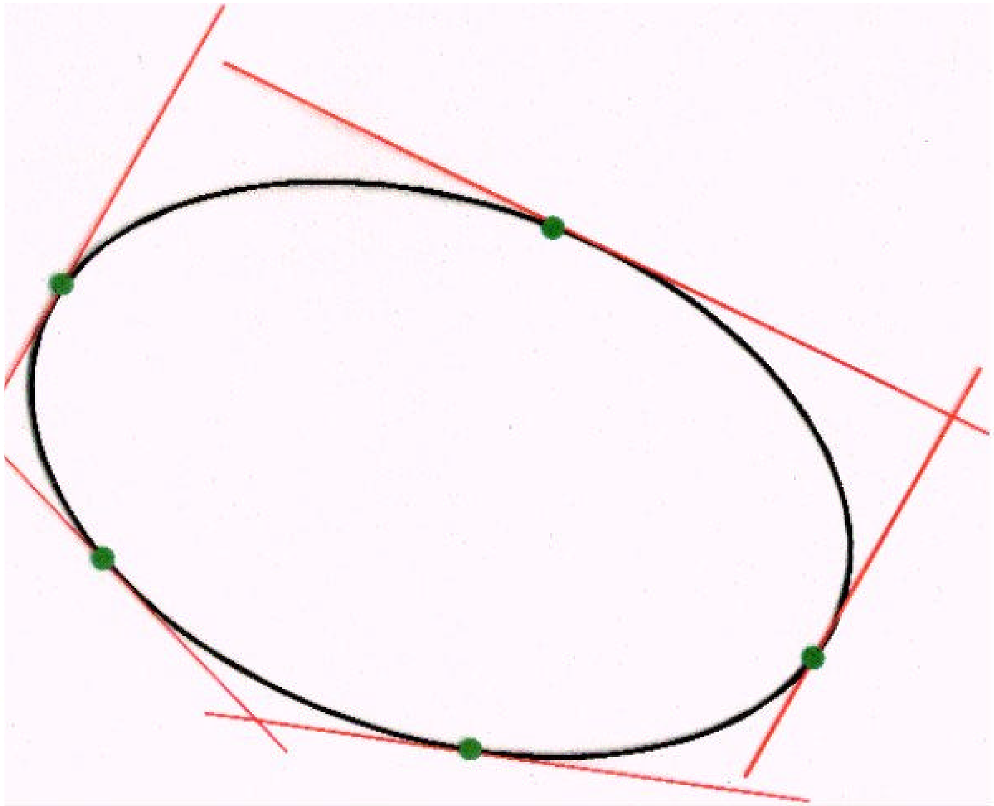
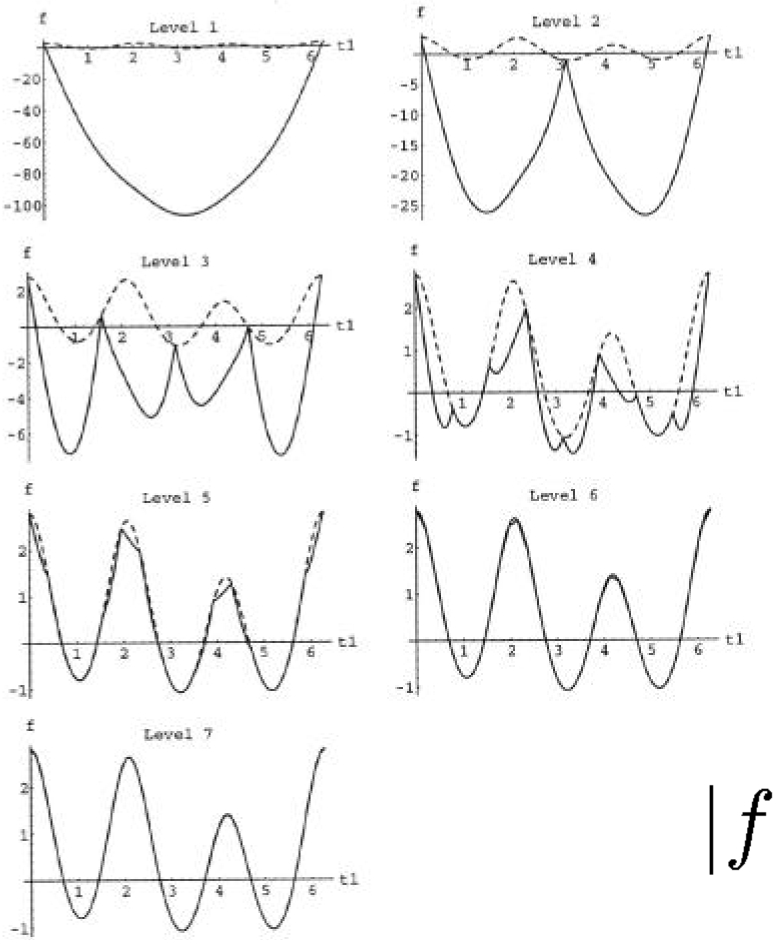
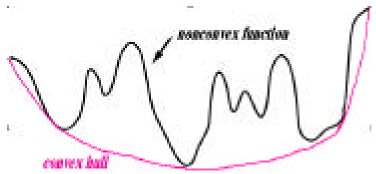


Fig. 2. Outer-approximation (at four points) of a convex function in R^1.



The Idea of Global Optimization





Algebraic Models

- convex underestimators
- branch & bound method
- interval arithmetic

Black-Box Models

- use local Lipschitz constants

$$|f(x_1) - f(x_2)| \leq L\,|x_1 - x_2|$$

A Wider Class of Models: Integro-Differential-Algebraic

- PCOMP (embedded in Easy-Fit) [Klaus Schittkowski]
- MINOPT [Chris Floudas and Carl Schweiger]
- gPROMS [Imperial College]

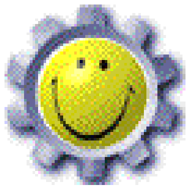
- Remark: process industry

Scheduling - The Real Challenge

- production plan -----------> schedule (daily business)
- Rem 1: SP are rather feasibility problems
- Rem 2: SP contain many details

  MILP/MINLP time-indexed formulations

  have many binary variables



What can be done ?

- Good modelling practice
- parallel MIL/MINLP
- problem-specific heuristics
- Constraint Programming

- Rem 3: poor LP relaxation, weak bounds
- Example: Modeling and Solving Train Timetabling Problems

  MILP + Lagrangian Relaxation & Multipliers, Dual Information,

  Caprara, Fischetti & Toth, *Operations Research* **50**, 851-861

Mathematial Modeling & Optimization in Practice

- Benefits to Users of Mathematical Optimization
- The Profile of the Client
- Relaxation of Constraints
- Structured Situations
- Consistent & Obtainable Data
- User Interface
- Communication
- Implementation &
- Validating Solutions
- Keeping a Model Alive

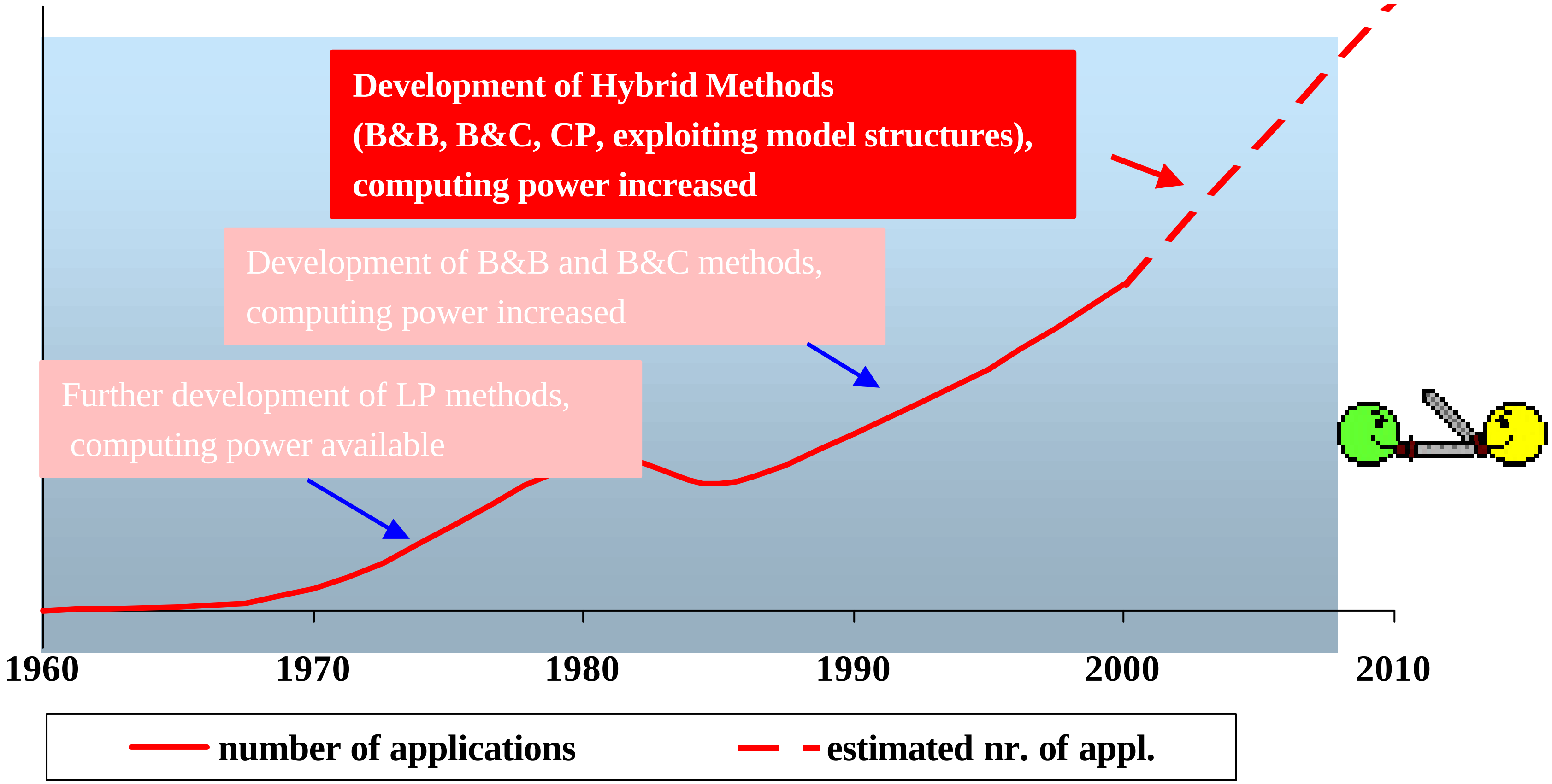
Trends

- Parallelism
- Online Optimization (car rental, (hotel: yield management)
- Integrated Systems

Barriers

- Technological Barriers (Data Aquisition)
- Explicit Representation of Know-How
- Social Barriers (men-machine relation)
- Psychological Barriers (influence, acknowl

Mathematical Optimization Development



Future Paths of Mixed Integer Optimization

- Solving Scheduling Problems Efficiently 

  complexity, bad LP relaxations, constraint programming often help

- Hybrid Approaches: (Scheduling,Man Power Planning,....)

  The Happy Marriage of MIP and CP 

- Solving Design/Strategic and Operative Planning (SCM,...)

  ... Problems Simultaneously

- MINLP & Global Optimization (Financial Opt, Chem. Eng.)

  commericial software is available now

- MINLP + ODE + PDE + Optimal Control + Global Optimiz

  ... system such as MINOPT go in this direction 

MINLP Algorithms & Global Optimization

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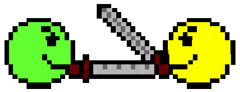

Requirements from Practioners towards Modeling Languages & Modeling Systems

- Modeling Language [complete, easy-to-learn, easy-to-read]
- Advanced Macros, Aliases [repeated structures]
- Multi-Criteria Optimization [goal programming]
- Solver Suite [LP, MILP, NLP, MINLP, GO, CP, metaheurist]
- Infeasibilty Tracing [identify infeasibilities, IIS]
- Multiple Platforms [Windows, UNIX, LINUX, Mac]
- Open Design [multiple solvers/database]
- Indexing [powerful sparse index and data handling]
- Scalabilty [millions of rows/columns]

Requirements from Practioners towards Modeling Languages & Modeling Systems

- Memory Management [keep all in memory]
- Speed [10 Million in nonzeros in less than a minute]
- Robustness [very stable codes, years of testing]
- Deployment [embed into applications]
- Synchronism [keeping up with the state-of-the-art solvers]
- Optimization under Uncertainty [robust opt, multi-stage opt]
  support new data types: Interval Data
- Exploiting Structure of MINLPs [convex underestimators]
- Embedding of own Solvers [Fortran, C, C++]

Summary

Summary

- MILP/MINLP is a promising approach to solve real world problems
- modeling is very important (needs mathematical-algebraic reformulations)
- algebraic modeling language
- modeler-client interaction
- GUIs !!!
- increasing importance

Advantages

- deeper understanding
  - better interpretation
  - satisfying all constraints
  - developing new ideas
  - focused „experiments“
- consistency
- decisions based on quantitative reasoning
- what-if-when analyses
- documentation
- maintenance