Progress and Challenges in Discrete and Continuous Optimization for Process Systems Engineering

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Center for Advanced Process Decision-making

Faculty

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PhD Students: 26  MS Students: 7
Post Docs: 5  Visitors: 7

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Center for Advanced Process Decision-making

Goals:

1. Do basic research in Process Systems Engineering
2. Produce students with unique skills in PSE
3. Interact with industry through mutually beneficial projects

Basic methodologies
Process modeling
Mathematical programming
Systems Engineering
Process control
Advanced computing

Areas of application
Process and product synthesis
Energy Systems
Supply chain optimization
Molecular Design
Systems Biology
## CAPD
Center for Advanced Process Decision-making

### Industrial Partners

<table>
<thead>
<tr>
<th>ABB</th>
<th>GAMS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air Liquide</td>
<td>NETL</td>
</tr>
<tr>
<td>Air Products</td>
<td>Neste Engineering Oy</td>
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<tr>
<td>Bayer</td>
<td>Nova Chemicals</td>
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<tr>
<td>Braskem</td>
<td>Paragon Decision</td>
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<tr>
<td>Cognizant</td>
<td>Petrobras</td>
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<tr>
<td>Dow Chemical</td>
<td>Pfizer</td>
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<tr>
<td>Eastman Chemical</td>
<td>PPG</td>
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<tr>
<td>Ecopetrol</td>
<td>Praxair</td>
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<tr>
<td>ExxonMobil</td>
<td>Total</td>
</tr>
<tr>
<td>FICO</td>
<td>Unilever</td>
</tr>
</tbody>
</table>
Research Ignacio Grossmann

Mixed-Integer Programming
Global Optimization of Bilinear GDP Problems Juan Ruiz, Francisco Trespalacios
Global Optimization of Multiperiod Blending Scott Kolodziej ExxonMobil
Cyber-MINLP Virtual Environment Biegler, Margot, Ruiz, Sahinidis IBM-Lee, Waechter
LOGMIP- Aldo Vecchietti, INGAR, Argentina
GAMS based interfaces Rosanna Franco

Process Synthesis/Energy
Optimal Design of IGCC Plants Ravi Kamath NETL*
Simultaneous Optimization, Heat Integration and Water Management Linlin Yang NETL
Optimal Design of Biofuel Plants Mariano Martin
Optimal Integrated Water Process Networks in Biofuel Plants Elvis Ahmetovic
Modeling and Optimization of Water Treatment Systems Berta Galan

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Research Ignacio Grossmann (cont)

Planning and Scheduling

**Enterprise-wide Optimization** Biegler, Grossmann, Hooker, Secomandi, Snyder
ABB, Air Products, Air Liquide, Dow Chemical, ExxonMobil, PPG, Praxair, NOVA, TOTAL, Unilever

Multistage Stochastic Optimization of Offshore Facilities **Vijay Gupta** ExxonMobil
Design of Responsive and Uncertain Supply Chains **Fengqi You**
Optimal Capacity Planning under Uncertain Electricity Prices **Sumit Mitra**, Praxair
Optimal Design of Reliable Integrated Sites **Sebastian Terrazas Pablo Garcia Herrero** Dow Chemical
Optimal Multisite Planning and Scheduling **Bruno Calfa** Dow Chemical
Optimal Scheduling of Crude Oil Operations **Sylvain Mouret** TOTAL
Optimal Model-Based Refinery Planning **Abdulah Alattas** BP
Planning and long-term scheduling for PPG glass production **Ricardo Lima** PPG
Batch Process Scheduling under Electricity Price Constraints **Pedro Castro** ABB

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Motivation discrete and continuous optimization

Cost and inventory reductions, reducing energy, water consumption, and investment in energy systems, improving responsiveness, global optimization of energy potentials

Discrete and continuous optimization models

Provide a powerful framework for modeling selection of:

a) Structure of system
b) Design parameters

Models

a) Mixed-integer linear programming (MILP)
b) Mixed-integer nonlinear programming (MINLP)
c) Generalized Disjunctive Programming (GDP/linear-nonlinear)

Goal: Overview state-of-art, progress and future directions:

a) What tools are available for effectively solving linear and nonlinear discrete/continuous models?
b) What are major challenges for global optimality and handling uncertainty?
MINLP: Mixed-integer nonlinear programming

\[
\begin{align*}
\text{min } Z &= f(x, y) \\
\text{s.t. } h(x, y) &= 0 \\
&\quad g(x, y) \leq 0 \\
&\quad x \in \mathbb{R}^n, \ y \in \{0,1\}^m
\end{align*}
\]

\[
\begin{align*}
f(x):\mathbb{R}^n &\rightarrow \mathbb{R}^1, h(x):\mathbb{R}^n &\rightarrow \mathbb{R}^m, g(x):\mathbb{R}^n &\rightarrow \mathbb{R}^q
\end{align*}
\]

**MILP:** \(f, h, g\) linear

**LP:** \(f, h, g\) linear, only \(x\)

**NLP:** \(f, h, g\) nonlinear, only \(x\)

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Evolution of Mathematical Programming

**LP: Linear Programming** Kantorovich (1939), Dantzig (1947)

**NLP: Nonlinear Programming** Karush (1939); Kuhn, A.W.Tucker (1951)

**IP: Integer Programming** R. E. Gomory (1958)
Major developments in last 20 years

- **Interior Point Method for LP** Karmarkar (1984)

- **Convexification of Mixed-Integer Linear Programs**
  Lovacz & Schrijver (1989), Sherali & Adams (1990),
  Balas, Ceria, Cornuejols (1993)

- **Modeling Systems** GAMS, AMPL, AIMMS

- **MILP codes**: CPLEX, GUROBI, XPRESS

- **NLP codes**: MINOS, CONOPT, SNOPT, IPOPT

- **MINLP** Duran & Grossmann (1986)

- **Global Optimization** Floudas (1990), Sahinidis (1996)

- **Logic-based optimization** Hooker (1991), Raman & Grossmann (1994)

Applications of Mathematical Programming in Chemical Engineering

Process Design

Process Synthesis

Production Planning

Process Scheduling

Supply Chain Management

Process Control

Parameter Estimation

LP, MILP, NLP, MINLP, Optimal Control

Major contribution: new problem representations and models

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**MILP**

\[
\begin{align*}
\min \; Z &= a^T y + b^T x \\
\text{st} \quad Ay + Bx &\leq d \\
y \in \{0,1\}^m, \quad x \geq 0
\end{align*}
\]

**Objective function**

**Constraints**

**Cutting planes**

Gomory (1959)

**Branch and Bound**

Beale (1958), Balas (1962), Dakin (1965)

**Theory for Convexification**

Lovacz & Schrijver (1989), Sherali & Adams (1990),

Balas, Ceria, Cornuejols (1993)

**Branch and cut**

Johnson, Nemhauser & Savelsbergh (2000)

Combine Branch and Bound with Cutting Planes

**Codes:** CPLEX, XPRESS, GUROBI

**Algorithmic features:** Cuts, presolve, heuristics, multithread
Progress in Mixed-Integer Linear Programming

Bixby, Rothberg and Gu (2009)

MIP Performance Improvements 1991–2010

=> 80,000 speed-up!!

CPLEX 1.2 to Gurobi 3.0

Unit-Commitment Model: California 7-Day Model
2,856 0-1 vars, 22,899 cont vars, 48,939 constr.

1999 CPLEX 7.0: 1 hr initial LP, unfinished after 8 hours
2010 Gurobi 3.0: ~3 min (195 secs) to optimality!
Which Single Feature Helps Most?
(After CPLEX 6.5 < 1000 seconds, Before CPLEX 6.5 unsolvable)

- Cuts: 53.7x
- Presolve: 10.8x
- Variable selection: 2.9x
- No heuristics: 1.4x
- No node presolve: 1.3x
State Task Network (STN) (Kondili, Pantelides, Sargent, 1993)
Classical Kondili Example

STN

MILP
72 0-1 variables
179 continuous variables
250 constraints

Optimal Schedule

1987 Kondili’s B&B: 908 sec, 1466 nodes, Vax-8600

1992 Shah’s B&B: 119 sec, 419 nodes, SUN Sparc

2011 CPLEX 12.1: 0.2 sec!! 14 nodes!! Lenovo-T60
Tank Farm Optimization Problem
Terrazas-Moreno, Wassick, Grossmann (2011)

Given
- A set of orders
- A set of production lines
- A set of tanks
- Release and due dates for production orders
- A set of shipping resources
- Intervals where those shipping resources are available

Determine:
- Schedule of production orders
- Assignment of products to tanks

With the objective of:
- Maximizing allocated product

Multi-operation Sequencing (MOS) model for scheduling of production orders:
- Slot-based continuous time model

2 lines, 10 tanks, 21 orders (8 products) 4 weeks
MILP: 1,340 0-1 vars, 16,561 cont vars, 40,261 constraints 530 s CPUtime Gurobi 4.0

Nonlinear Programming

NLP: Algorithms (variants of Newton's method)
- Successive quadratic programming (SQP) (Han 1976; Powell)
- Reduced gradient
- Interior Point Methods
Nonlinear CDU Models in Refinery Planning Optimization

Alattas, Palou-Rivera, Grossmann (2010)

Typical Refinery Configuration

(Adapted from Aronofsky, 1978)
Planning Model Example Results

<table>
<thead>
<tr>
<th>Crude</th>
<th>Type</th>
<th>Location</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Crude1</td>
<td>Louisiana</td>
<td>Sweet</td>
<td>Lightest</td>
</tr>
<tr>
<td>Crude2</td>
<td>Texas</td>
<td>Sweet</td>
<td></td>
</tr>
<tr>
<td>Crude3</td>
<td>Louisiana</td>
<td>Sour</td>
<td></td>
</tr>
<tr>
<td>Crude4</td>
<td>Texas</td>
<td>Sour</td>
<td>Heaviest</td>
</tr>
</tbody>
</table>

- Comparison of *nonlinear fractionation index* (FI) with *linear* fixed yield (FY) and swing cut (SC) models
- Economics
  - FI calculates the maximum profit scenario

<table>
<thead>
<tr>
<th>Model</th>
<th>Case1</th>
<th>Case2</th>
<th>Case3</th>
</tr>
</thead>
<tbody>
<tr>
<td>FI</td>
<td>245</td>
<td>249</td>
<td>247</td>
</tr>
<tr>
<td>SC</td>
<td>195</td>
<td>195</td>
<td>191</td>
</tr>
<tr>
<td>FY</td>
<td>51</td>
<td>62</td>
<td>59</td>
</tr>
</tbody>
</table>
MINLP

Mixed-Integer Nonlinear Programming

\[
\begin{align*}
\text{min } Z &= f(x, y) \\
\text{s.t. } h(x, y) &= 0 \\
&\quad g(x, y) \leq 0 \\
&\quad x \in X, \; y \in Y
\end{align*}
\]

\[X = \{x \mid x \in R^n, x^L \leq x \leq x^U, Bx \leq b\}\]

\[Y = \{y \mid y \in \{0,1\}^m, Ay \leq a\}\]

\[f(x) : R^n \rightarrow R^1, h(x) : R^n \rightarrow R^m, g(x) : R^n \rightarrow R^q\]

**Remarks**

1. Basic MINLP algorithms rely on convexity assumptions
2. When applied to nonconvex problems suboptimal solutions may be obtained
Mixed-integer Nonlinear Programming

Algorithms

**Branch and Bound (BB)** Ravindran and Gupta (1985),
Stubbs, Mehrotra (1999), Leyffer (2001)

**Generalized Benders Decomposition (GBD)** Geoffrion (1972)

**Outer-Approximation (OA)** Duran and Grossmann (1986),
Fletcher and Leyffer (1994)

**LP/NLP based Branch and Bound** Quesada, Grossmann (1994)

**Extended Cutting Plane (ECP)** Westerlund and Pettersson (1992)
High-Level Modeling

The General Algebraic Modeling System (GAMS) is a high-level modeling system for mathematical programming problems. GAMS is tailored for complex, large-scale modeling applications, and allows you to build large maintainable models that can be adapted quickly to new situations. Models are fully portable from one computer platform to another.

Wide Range of Model Types

GAMS allows the formulation of models in many different problem classes, including:

- Linear (LP) and Mixed Integer Linear (MILP)
- Quadratic Programming (QCP)
- and Mixed Integer QCP (MIQCP)
- Nonlinear (NLP) and Mixed Integer Nonlinear Programming (MINLP)
- Generalized Reduced-Index Systems (GRS)
- Nonlinear Complementarity (NCP)
- Programs with Equilibrium Constraints (MEPC)
- Convex Programming Problems
- Stochastic Linear Programs

MINLP and Global Solvers in GAMS

The area of Mixed Integer Nonlinear Programming (MINLP) and Global Optimization has experienced significant growth in industry and academia over the last years. More and more general purpose solution algorithms have been implemented and have matured into reliable solution systems:

- AlphaECP®: Extended cutting plane method from Argonne National Laboratory
- BARON: Branch-and-Reduce Optimization Navigator for proven global solutions from the Optimization Firm
- Bonmin®: Hybrid outer-approximation based branch-and-cut algorithm jointly developed by a collaboration between Carnegie Mellon University and the IBM Corporation and distributed from COIN-OR
- DICOPT: Outer approximation framework from Carnegie Mellon University
- LINDO®: Lisztél global optimizer from LINDO Systems, Inc.
- MINLP/OCPLib-Model start method for global optimization from Optimal Methods, Inc.
- SBB: Branch-and-Bound algorithm from Argonne National Laboratory

* New in GAMS 22.5.
http://www.minlp.org

CMU-IBM Cyber-Infrastructure for MINLP collaborative site

This collaborative site has as a major goal to promote the optimization of linear and nonlinear models with one or several alternative model formulations involving discrete and continuous variables through mixed integer nonlinear programming (MINLP), or generalized disjunctive programming (GDP). Three major objectives are:

- Create a library of optimization problems that can be generally formulated as MINLP/GDP models.
- Provide high level descriptions of the problems with one or several model formulations with corresponding input files for one or several instances.
- Allow users to pose open problems that are unsolved and with unknown or tentative formulations.

min Z = f(x, y)

s.t.  g(x, y) ≤ 0

x ∈ X, y ∈ Y

We invite researchers and practitioners to contribute to the library of problems and models, and to participate in the discussions on these problems. We look forward to collaborating with you!

About us

Goals of our project
Participants of the project

Contribute

Create an account
Learn how to contribute problems
Contribute solved problems, models, and instances to our library
Post open unsolved problems

Our library

View our library of problems
Discuss problems in the forums

Resources

Conferences
Lectures and Tutorials
Optimization of Number of Trays

Viswanathan & Grossmann (1993)

Discrete variables: Number of trays, feed tray location.
Continuous variables: reflux ratio, heat loads, exchanger areas, column diameter.

Acetone-acetonitrile-water, max 25 trays, Virial-UNIQUAC
MINLP: 22 0-1 vars, 891 cont. vars, 957 const. ~ 40 min
Synthesis of Heat Exchanger Networks
Yee and Grossmann (1990)

Multiple stages with potential heat exchangers  \( z_{ijk} = 0,1 \)

7 hot, 3 cold streams
MINLP 115 0-1, 447 cont vars, 476 constr. 26s CPU-time (DICOPT-2011)
Optimal Development of Oil Fields \textit{(deepwater)}

Offshore field having several reservoirs (oil, gas, water)

Decisions:
- Number and capacity of FPSO facilities
- Installation schedule for facilities
- Number of sub-seawells to drill
- Oil/gas production profile over time

Objective:
- Maximize the Net Present Value (NPV) of the project

\textbf{MINLP model}
- Nonlinear reservoir behavior
- Three components (oil, water, gas)
- Lead times for FPSO construction
- FPSO Capacity expansion
- Well Drilling Schedule
Optimal NPV = $30.946 billion

Example

20 Year Time Horizon
10 Fields
3 FPSOs
23 Wells
3 Yr lead time FPSO
1 Yr lead time expansion

Oil Flowrate

Total Oil/Gas Production

FPSO-1

FPSO-2

FPSO-3

Field-1

Field-7

Field-6

Field-4

Field-2

Field-3

Field-5

Field-10

Field-9

Field-8

Yr 1

Yr 2

Yr 3

Yr 4

Yr 5

Yr 6

Yr 7

Yr 8

Yr 9

Yr 10

Yr 11

Yr 12

Yr 13

Yr 14

Yr 15

Yr 16

Yr 17

Yr 18

Yr 19

Yr 20

Time

x (kstb/d)

0

50

100

150

200

250

300

350

400

450

fpso1

fpso2

fpso3
MINLP can be reformulated as MILP using exact linearization and piece-wise linearization approximation

<table>
<thead>
<tr>
<th>MINLP</th>
<th></th>
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<tbody>
<tr>
<td></td>
<td>Discrete Var.</td>
</tr>
<tr>
<td></td>
<td>SOS1 Var.</td>
</tr>
<tr>
<td></td>
<td>Continuous Var.</td>
</tr>
<tr>
<td></td>
<td>Constraints</td>
</tr>
<tr>
<td>Solver</td>
<td>DICOPT 2x-C</td>
</tr>
<tr>
<td>NPV (billion dollars)</td>
<td>30.946</td>
</tr>
<tr>
<td>CPU time(s)</td>
<td>67</td>
</tr>
</tbody>
</table>

*Solved in GAMS 23.6.3 on an Intel Core i7 machine with 4 GB of RAM

=> MINLP model basis for Stochastic Programming
Simultaneous Cyclic Scheduling and Control of a Multiproduct CSTR Reactor

Antonio Flores (U. Iberoamericana)

Given is a CSTR reactor
- N products
- Lower bounds demand rates
- Dynamic model for reactions

Determine cyclic schedule
- Cycle time
- Sequence
- Amounts to produce
- Lenghts transitions and their dynamic profile

Objective: Maximize total profit
Basic ideas MIDO model

\[ y_{il} = \begin{cases} 
1 & \text{product } i \text{ assigned slot } l \\ 
0 & \text{otherwise} 
\end{cases} \]

Requires guessing transition times

Use orthogonal collocation for converting dynamic eqtns into algebraic eqtns.

Discretized DAE solved as MINLP (DICOPT)
MIDO Optimization model

\[
\begin{align*}
\text{max} & \quad \left\{ \sum_{i=1}^{N_P} \frac{C_i^W W_i}{T_e} - \sum_{i=1}^{N_P} \frac{C_i^a (G_i - W_i)}{2\Theta_i T_e} - \sum_{k=1}^{N_s} \sum_{f=1}^{N_f} \sum_{e=1}^{N_{\xi}} \frac{C_r t_{fck} \Omega e_{cN_{\xi}}}{T_e} \left( (x_{fck}^1 - \bar{x}_k^1)^2 \right. \\
& \quad + \left. \ldots + (x_{fck}^N - \bar{x}_k^n)^2 + (u_{fck}^1 - \bar{u}_k^1)^2 + \ldots + (u_{fck}^m - \bar{u}_k^m)^2 \right) \right\}
\end{align*}
\]

s.t. Scheduling constraints:
- Product assignments
- Amounts manufactured
- Processing times
- Transition constraints
- Timing relations

**Dynamic and control optimization**
- Dynamic mathematical model discretization
- Continuity constraint between finite elements
- Model behavior at each collocation point

**Reformulated as MINLP**
Example: 5 products

Results

<table>
<thead>
<tr>
<th>Slot</th>
<th>Product</th>
<th>Process time [h]</th>
<th>Production rate [Kg/h]</th>
<th>( w ) [Kg]</th>
<th>Transition Time [h]</th>
<th>T start [h]</th>
<th>T end [h]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>A</td>
<td>41.5</td>
<td>9.033</td>
<td>374.31</td>
<td>5</td>
<td>0</td>
<td>46.4</td>
</tr>
<tr>
<td>2</td>
<td>D</td>
<td>2.06</td>
<td>607</td>
<td>1249.4</td>
<td>5</td>
<td>46.4</td>
<td>53.6</td>
</tr>
<tr>
<td>3</td>
<td>E</td>
<td>23.4</td>
<td>1250</td>
<td>29270.4</td>
<td>5</td>
<td>53.6</td>
<td>82</td>
</tr>
<tr>
<td>4</td>
<td>C</td>
<td>4.48</td>
<td>278.72</td>
<td>1249.4</td>
<td>5</td>
<td>82</td>
<td>91.5</td>
</tr>
<tr>
<td>5</td>
<td>B</td>
<td>12.48</td>
<td>80</td>
<td>999.5</td>
<td>21</td>
<td>91.5</td>
<td>125</td>
</tr>
</tbody>
</table>

Optimal sequence
A → E → C → D → B →

Cycle time = 124.8 h
Profit = $7889/h
Generalized Disjunctive Programming (GDP)

Raman and Grossmann (1994)  (Extension Balas, 1979)

Motivation: Facilitate modeling discrete/continuous problems

Objective Function
\[
\min \ Z = \sum_k c_k + f(x)
\]

Common Constraints
\[
s.t. \quad r(x) \leq 0
\]

Disjunction
\[
k \in K
\]

Constraints
\[
g_{jk}(x) \leq 0
\]

Fixed Charges
\[
c_k = \gamma_{jk}
\]

Logic Propositions
\[
\Omega(Y) = \text{true}
\]

Continuous Variables
\[
x \in R^n, c_k \in R^1
\]

Boolean Variables
\[
Y_{jk} \in \{ \text{true, false} \}
\]

Properties: a) Every GDP can be transformed into an MINLP
b) Every bounded MINLP can be transformed into GDP
Methods Generalized Disjunctive Programming

GDP

Logic based methods

- Branch and bound
  
  (Lee & Grossmann, 2000)

- Decomposition
  
  Outer-Approximation
  Generalized Benders
  
  (Turkay & Grossmann, 1997)

Reformulation MINLP

- Outer-Approximation
  Generalized Benders
  Extended Cutting Plane

- Convex-hull
  Cutting plane
  
  (Sawaya & Grossmann, 2004)

- Big-M
  
  (Lee & Grossmann, 2000)
Big-M MINLP (BM)

• MINLP reformulation of GDP

\[
\begin{align*}
\min Z &= \sum_{k \in K} \sum_{j \in J_k} \gamma_{jk} \lambda_{jk} + f(x) \\
\text{s.t.} \quad r(x) &\leq 0 \\
g_{jk}(x) &\leq M_{jk} (1 - \lambda_{jk}) \quad j \in J_k, k \in K \\
\sum_{j \in J_k} \lambda_{jk} &= 1, \quad k \in K \\
A\lambda &\leq a \\
x &\geq 0,
\end{align*}
\]

**Big-M Parameter**

**Logic constraints**

*Williams (1990)*

**NLP Relaxation** \[ 0 \leq \lambda_{jk} \leq 1 \quad \Rightarrow \quad \text{Lower bound to optimum of GDP} \]
Hull Relaxation Problem (HRP)

\[ \text{HRP:} \quad \min \ Z = \sum_{k \in K} \sum_{j \in J_k} \gamma_{jk} \lambda_{jk} + f(x) \]

\[ \text{s.t.} \quad r(x) \leq 0 \]

\[ x = \sum_{j \in J_k} \nu_{jk}, \ k \in K \]

\[ 0 \leq \nu_{jk} \leq \lambda_{jk} U_{jk}, \ j \in J_k, \ k \in K \]

\[ \sum_{j \in J_k} \lambda_{jk} = 1, \ k \in K \]

\[ \lambda_{jk} g_{jk} \left( \nu_{jk} / \lambda_{jk} \right) \leq 0, \ j \in J_k, \ k \in K \]

\[ A \lambda \leq a \]

\[ x, \nu_{jk} \geq 0, \ 0 \leq \lambda_{jk} \leq 1, \ j \in J_k, \ k \in K \]

\[ \text{Property:} \quad \text{The NLP (HRP) yields a lower bound to optimum of (GDP).} \]

\[ \text{Carnegie Mellon} \]
**Strength Lower Bounds**

- **Theorem 1:** The relaxation of (HRP) yields a lower bound that is greater than or equal to the lower bound that is obtained from the relaxation of problem (BM).
  

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**Convex hull relaxation**

Convex Hull of a set of disjunctions is smallest convex set that includes set of disjunctions. Projected relaxation of (CH) onto the space of (BM) is as tight or tighter than that of (BM).
Multiperiod Production Planning LP Model

Max PROFIT = \sum_{j \in J} \sum_{t \in T} \psi_{jt} S_{jt} - \sum_{j \in J} \sum_{t \in T} \phi_{jt} P_{jt}

- \sum_{i \in I} \sum_{j \in JM_i} \sum_{t \in T} \delta_{it} W_{ijt} - \sum_{j \in J} \sum_{t \in T} \xi_{jt} V_{jt} - \sum_{j \in J} \sum_{t \in T} \theta_{jt} SF_{jt}

Fixed price purchases

Mass balance process
\[ W_{ijt} = \mu_{ij} W_{ij't} \quad i \in I, j \in J_i, j' \in JM_i, t \in T \]

Capacity
\[ W_{ijt} \leq Q_{it} \quad i \in I, j \in JM_i, t \in T \]

Mass balance chemicals
\[ V_{j,t-1} + \sum_{i \in O_j} W_{ijt} + P_{jt} = V_{jt} + \sum_{i \in I_j} W_{ijt} + S_{jt} \quad j \in J, t \in T \]

Shortfalls
\[ SF_{jt} \geq d_{jt}^U - S_{jt} \quad j \in J, t \in T \]

Purchases
\[ a_{jt}^L \leq P_{jt} \leq a_{jt}^U \quad j \in J, t \in T \]

Sales
\[ d_{jt}^L \leq S_{jt} \leq d_{jt}^U \quad j \in J, t \in T \]

Limit inventory
\[ V_{jt} \leq V_{jt}^U \quad j \in J, t \in T \]

What if prices not fixed but given by contracts?

\[ 0 \leq SF_{jt} \leq SF_{jt}^U \quad j \in J, t \in T \]

\[ S_{jt}, P_{jt}, W_{it}, V_{jt} \geq 0 \]
Modeling of Contracts with MILP

Discount after $\sigma^d_{jt}$ amount.

Bulk discount

Disjunctive constraints $\Rightarrow$ MILP constraints (hull relaxation)
## Computational Results

38 processes, 25 chemicals 10 time periods

<table>
<thead>
<tr>
<th>Case</th>
<th>0-1 variables</th>
<th>Cont. variables</th>
<th>Constraints</th>
<th>CPU time [s]</th>
<th>Time periods</th>
<th>Solution [10^5 $]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fixed prices</td>
<td>0</td>
<td>12,606</td>
<td>13,416</td>
<td>0.18</td>
<td>10</td>
<td>18,085.95</td>
</tr>
<tr>
<td>Contracts</td>
<td>6,160</td>
<td>40,606</td>
<td>46,002</td>
<td>0.95</td>
<td>10</td>
<td>22,073.06</td>
</tr>
</tbody>
</table>

ILOG CPLEX Dec 1, 2008 22.9.2 LNX 7311.8080 LX3 x86/Linux
Cplex 11.2.0, GAMS Link 34

MIP Presolve eliminated 44425 rows and 38571 columns.
Reduced MIP has 909 rows, 1367 columns, and 3267 nonzeros.
Reduced MIP has 270 binaries, 0 generals, 0 SOSs, and 0 indicators.

Implied bound cuts applied: 3
Flow cuts applied: 40
Gomory fractional cuts applied: 15
MIP Solution: 22073.060039 (959 iterations, 21 nodes)

### Synergy between CPLEX (presolve) and GDP (tight bounds)!
Superstructure Separations Olefins Plant

(Lee, Foral, Logsdon, Grossmann, 2003)

25 states
53 separation tasks

Feed

A- H$_2$
B- CH$_4$
C- C$_2$H$_4$
D- C$_3$H$_6$
E- C$_3$H$_6$
F- C$_3$H$_8$
G- C$_4$
H- C$_5$

GDP→big-M MINLP: 5,800 0-1 vars, 24,500 cont. vars., 52,700 constraints ~3hrs CPU-time
MINLP optimal solution

Dephlegmator first process
7 separation units

20M$/yr cost saving

1 dephlegmator
1 absorber
4 distillation columns
1 cold box
1 heat exchange

Total cost: 110.82 MM$/yr

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Global Optimization Algorithms

Algorithms based on spatial branch and bound method and use of underestimators/convex envelopes (Horst & Tuy, 1996)

• Nonconvex NLP/MINLP
  - αBB (Adjiman, Androulakis & Floudas, 1997; 2000)
  - BARON (Branch and Reduce) (Ryoo & Sahinidis, 1995, Tawarmalani and Sahinidis, 2002)
  - Branch and cut (Kesavan, Allgor, Gatzke and Barton, 2004)
  - Branch and Contract (Zamora & Grossmann, 1999)
  - Transformation signomials (Bjoerk, Lindberg, Westerlund, 2002)
  - Couenne (COIN-OR) (Belotti & Margot, 2008)

• Nonconvex GDP
  - Two-level Branch and Bound (Lee & Grossmann, 2001)
  - Bound strengthening (Ruiz, Grossmann, 2010)
Spatial Branch and Bound to obtain the Global Optimum

- Guaranteed to converge to global optimum given a certain tolerance between lower and upper bounds

Global optimum search

Branch and bound tree
Progress BARON 1998-2006  
Sahinidis (2008)

26 problems from *globallib* and *minlplib*

<table>
<thead>
<tr>
<th></th>
<th>Minimum</th>
<th>Maximum</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>Constraints</td>
<td>2</td>
<td>513</td>
<td>76</td>
</tr>
<tr>
<td>Variables</td>
<td>4</td>
<td>1030</td>
<td>115</td>
</tr>
<tr>
<td>Discrete variables</td>
<td>0</td>
<td>432</td>
<td>63</td>
</tr>
</tbody>
</table>

**Impact of Algorithmic Improvements**

<table>
<thead>
<tr>
<th></th>
<th>BARON 1998</th>
<th>BARON 2006</th>
</tr>
</thead>
<tbody>
<tr>
<td># Nodes</td>
<td>23,031,434</td>
<td>253,754</td>
</tr>
<tr>
<td>CPU sec</td>
<td>275,163</td>
<td>20,430</td>
</tr>
</tbody>
</table>

# Nodes reduction factor 100!  
CPU-time reduction factor > 10!
Large scale water network problem

4 feeds, 6 process units, 4 treatment units, 3 contaminants  

Ahmetovic, Grossmann (2011)

Optimal Freshwater Consumption

40 t/h

VS

390 t/h

conventional

NLP: 232 variables, 121 constraints  
BARON: 2 secs

1.5 vs 3.4
Lowest Reported!
De Novo Protein Design (Floudas)

Define target template
Backbone coordinates for N,Ca,C,O and possibly Ca-Cb vectors from PDB

Design folded protein
Which amino acid sequences will stabilize this target structure?

In silico sequence selection => MILP
Fold specificity => Global optimization

=> New improved inhibitors (Klapeis, Floudas, Lambris, Morikis, 2004)

Human b-Defensin-2 hbd-2 (PDB: 1fqq)

Full sequence design
Global Sourcing Project with Uncertainties

You, Wassick, Grossmann (2009)

• Given
  ♦ Minimum and initial inventory
  ♦ Inventory holding cost and throughput cost
  ♦ Single sourcing and minimum sourcing
  ♦ Transport times of all the transport links
  ♦ Uncertain production reliability and demands

• Determine
  ♦ Inventory level, transportation and sale amounts

• Objective: Minimize Cost
Simulation results to assess benefits stochastic model

Average cost saving 5.70±0.03%
Supply Chain Design with Single-Stage Stochastic Inventory

Given: A supply chain superstructure (single-product)  

- Including fixed suppliers, markets and potential DC locations
- Each market has uncertain demand, only DCs hold inventory with \((Q, r)\) policy
- Assume all DCs have identical lead time \(L\) (lumped to one supplier)

Determine: Network: number of DCs and their locations, assignments between retailers and DCs (single sourcing), shipping amounts  

Inventory: number of replenishments, order quantity, safety stock

\[ 150 \text{ DC, 150 markets: Lagrangean Relaxation: decomposition by Distribution Centers} \]
\[ \text{MINLP: 150 0-1 var., 22,800 cont. var., 22,800 constr. 3061s CPU-time) (<1% gap)} \]
Conclusions

1. Discrete/continuous optimization methods have had
   - tremendous progress in MILP
   - very significant progress in MINLP/GDP
   - good progress in global MINLP/GDP

2. Theory has contributed to progress:
   - sequential convexification for MILP
   - concepts of disjunctive programming => MINLP and GDP
   Complemented by algorithmic implementations/new computer architectures

3. Many of models/algorithms used increasingly by industry
Major remaining challenges:

- Improvement of relaxations for MILP and MINLP
- Improvement of relaxations for global optimization
- Large-scale computations for nonconvex MINLP/GDP
- Effective algorithms for Mixed-Integer Dynamic Optimization
- Effective extension to stochastic programming, parametric programming
Conclusions

1. Enterprise-wide Optimization area of great industrial interest
   Great economic impact for effectively managing complex supply chains
   and complex manufacturing facilities

2. Two key components: Planning and Scheduling
   Modeling challenge:
   Multi-scale modeling (temporal and spatial integration)

3. Computational challenges lie in:
   a) Large-scale optimization models (decomposition, advanced computing)
   b) Handling uncertainty (stochastic programming)

Scope for significant economic savings

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Future challenges

1. Logic-based Optimization
   Facilitate modeling
   Exploit logic for more efficient solution

2. Global Optimization
   Effectively solve nonconvex MINLP problems

3. Stochastic Mixed-integer Programming
   Reduce computational times by order of magnitude
Generalized Disjunctive Programming (GDP) Model

\[
\min Z = \sum_i (IC_i + CC_i + UC_i)
\]

s.t. \( Ax = 0 \)
\( f_{eq}(P_i, T_i), \quad \forall i \in I \)
\[
YS_{i,s}
\]
\[
x_i^{\text{top}} = RT_i x_i^{\text{feed}}
\]
\[
x_i^{\text{btm}} = RB_i x_i^{\text{feed}}
\]

\[
\begin{bmatrix}
\forall s \in S_i \\
\forall st \in ST_i
\end{bmatrix}
\]
\[
\begin{bmatrix}
\text{mass balance: } f_m(x_i) = 0 \\
\text{energy balance: } f_e(x_i, T_i, P_i, Q_i) = 0 \\
\text{cost function: } (IC_i, UC_i) = f_c(x_i, T_i, P_i, Q_i)
\end{bmatrix}
\]

\[
\begin{bmatrix}
YZ_{i,k} \\
T_i^C \geq T_k^R + EMAT \\
QEX_{i,k} \geq 0
\end{bmatrix}
\]

\[
\begin{bmatrix}
\forall i \in I, \forall k \in K
\end{bmatrix}
\]

\[
\begin{bmatrix}
\neg YZ_{i,k} \\
QEX_{i,k} = 0
\end{bmatrix}
\]

\[
\begin{bmatrix}
Y_i C_i \\
(T_i, P_i)_{out} = fP_1(T_i, P_i)_{in} \\
CR_L \leq P_i^{out} / P_i^{in} \leq CR_U \\
CC_i = fP_2(x_i, T_i, P_i)
\end{bmatrix}
\]

\[
\begin{bmatrix}
\forall i \in I
\end{bmatrix}
\]

\[
\begin{bmatrix}
\neg YC_i \\
(T_i, P_i)_{out} = (T_i, P_i)_{in} \\
CC_i = 0
\end{bmatrix}
\]

Cost
Mass balances
Equilibrium Eqtns.
Separation choice
Heat exchange
Compression
Can we obtain stronger relaxations?

**Regular Form (RF):** Form represented by the intersection of the unions of convex sets.

\[ F = \bigcap_{t \in T} S_t \quad \text{where} \quad S_t = \bigcup_{i \in Q} P_i \quad t \in T \quad \text{and} \quad P_i \quad \text{is a convex set} \]

**Basic Step:** Intersect a pair of disjunctions & bring into DNF

\[ S_r \cap S_s = S_{rs} = \bigcup_{i \in Q_r, t \in Q_s} (P_i \cap P_t) \]

**Example:**

\[ F = S_1 \cap S_2 \]

\[ S_1 = (P_{11} \cup P_{21}) \quad S_2 = (P_{12} \cup P_{22}) \]

Apply Basic Step to:

\[ S_1 \cap S_2 = (P_{11} \cup P_{21}) \cap (P_{12} \cup P_{22}) \]

\[ \Rightarrow S_{12} = (P_{11} \cap P_{12}) \cup (P_{11} \cap P_{22}) \cup (P_{21} \cap P_{12}) \cup (P_{21} \cap P_{22}) \]

*Balas (1974, 1979, 1985) addressed linear disjunctive programs*
Hierarchy of relaxations for nonlinear convex GDP

**Theorem 2:** For $i = 0, 1, 2, \ldots, t$ let $F_i = \bigcap_{j \in T_i} S_j$ be a sequence of regular forms of a disjunctive set such that $F_i$ is obtained from $F_{i-1}$ by the application of a basic step, then:

$$h - \text{rel}(F_i) \subseteq h - \text{rel}(F_{i-1})$$

Tighter region!
GDP Example

- Find \( x \geq 0, \ (x \in S_1) \lor (x \in S_2) \lor (x \in S_3) \)

  to minimize \( Z = (x_1 - 3)^2 + (x_2 - 2)^2 + c \)

![Diagram showing contour plots and local solutions]
**Hull Relaxation (one basic step)**

**Apply basic step:** Intersect inequality objective with disjunction

\[
\begin{align*}
\min & \quad Z \\
\text{s.t.} & \quad \begin{bmatrix}
Y_1 \\
x_1^2 + x_2^2 \leq 1 \\
c = 2 \\
Z \geq (x_1 - 3)^2 + (x_2 - 2)^2 + c
\end{bmatrix} \lor \\
& \quad \begin{bmatrix}
Y_2 \\
(x_1 - 4)^2 + (x_2 - 1)^2 \leq 1 \\
c = 1 \\
Z \geq (x_1 - 3)^2 + (x_2 - 2)^2 + c
\end{bmatrix} \lor \\
& \quad \begin{bmatrix}
Y_1 \\
(x_1 - 2)^2 + (x_2 - 4)^2 \leq 1 \\
c = 2 \\
Z \geq (x_1 - 3)^2 + (x_2 - 2)^2 + c
\end{bmatrix}
\end{align*}
\]

\( Y_1 \lor Y_2 \lor Y_3 = \text{True} \)

Relaxation of convex hull MINLP reformulations yields optimal solution!

\[ Z^{rel} = 1.172 \]

Solves as an NLP!
GDP Model (continued)

Logic Propositions

\( \forall YS_{i,s} \quad \forall i \in I \)
\( YS_{i,s} \Rightarrow \forall YT_{s, st} \quad \forall st \in ST_s, \forall s \in S_i, \forall i \in I \)
\( \neg YS_{s, st} \Rightarrow \neg YZ_{i, k} \quad \forall st \in ST_s, \forall s \in S_i, \forall i \in I, \forall k \in K \)

Variable Bounds

\( 0 \leq x_i \leq x_{UP} ; T_{LO} \leq T_i \leq T_{UP} ; P_{LO} \leq P_i \leq P_{UP} , \forall i \)
\( 0 \leq RT_i , RB_i \leq 1 \quad \forall i \)
\( 0 \leq IC_i , CC_i , UC_i \quad \forall i \)
\( YS_{i,s} , YT_{s, st} , YZ_{i,k} , YC_i \in \{true, false\} \quad \forall i, s, st, k \)
\( 0 \leq Q_i , QEX_{i,k} \quad \forall i, k \)
\( T_{LO} \leq T_{C_i} , T_{R_k} \leq T_{UP} \quad \forall i, k \)
MINLP Model

- GDP reformulated as a MINLP

**Problem Size**
- No. of 0-1 variables = 5,800
- No. of variables = 24,500
- No. of constraints = 52,700

**GAMS/DICOPT**
- NLP solver: CONOPT2/ MIP solver: CPLEX
- CPU time ~ 3 hrs on Pentium III PC
Optimized base case design

Depropanizer first process
8 separation units

Total cost: 131.74MM$/yr

7 distillation columns
1 cold box
2 heat exchange
Continuous multistage plants

Pinto, Grossmann (1996)

Cyclic schedules (constant demand rates, infinite horizon)

Intermediate storage

Given:

N Products
Transition times (sequence dependent)
Demand rates

Determine:

PLANNING

Amount of products to be produced
Inventory levels

SCHEDULING

Cyclic production schedule
Sequencing
Lengths of production
Cycle time

Objective:

Maximize Profit = + Sales of products - inventory costs - transition costs
MINLP Model

Basic ideas:

a. NP products
b. NP time slots at each stage

Binary variables for assignments
\[ y_{ik} = \begin{cases} 1 & \text{product } i \text{ assigned to slot } k \\ 0 & \text{otherwise} \end{cases} \]

- Assignments of products to slots
- Definition of transition variables
- Processing rates, mass balances and amounts produced => Linear Constraints
- Timing constraints
- Inventory levels for intermediates
- Demand constraints

Objective function: Maximize Profit (Nonlinear)
Example 3 stages, 8 products

MINLP model
448 binary 0-1 variables, 2050 continuous variables, 3010 constraints

DICOP (CONOPT/Cplex): 38.2 secs

Optimal solution  Profit = $6609/h  -  47% improvement

stage 1  A  C  B E F H D  G

stage 2  

stage 3  

cycle time = 675 hrs

Intermediate storage (ton) Stages 1-2

Intermediate storage (ton) Stages 2-3

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Simultaneous Cyclic Scheduling and Control of a Multiproduct CSTR Reactor

(MIDO) Mixed-integer Dynamic Optimization Problem

Flores, Grossmann (2008)

\[
y_{il} = \begin{cases} 
1 & \text{product } i \text{ assigned slot } l \\
0 & \text{otherwise}
\end{cases}
\]

Slot 1  Slot 2  Slot N

Cycle time

Requires determining transition times

Dynamic system behaviour

(b) Time

Requires determining transition times

Use orthogonal collocation for converting dynamic eqtns into algebraic eqtns.

Mixed-Integer Dynamic Optimization solved as MINLP \((DICOPT\ or\ SBB)\)
Outline

1. Historical Evolution of Mathematical Programming

2. Progress in Mixed-integer Linear Programming
   Impact on batch scheduling

3. Progress in Mixed-integer Nonlinear Programming
   Impact on optimal process operations

4. Future challenges
Motivation MINLP in PSE
Math Programming Approach to Process Synthesis


1. Develop a superstructure of alternative designs

2. Develop an MINLP model to select topology and parameters of design

3. Solve MINLP to extract optimum design embedded in superstructure
Hull Relaxation Formulation

• Consider Disjunction \( k \in K \)

\[
\bigvee_{j \in J_k} \begin{bmatrix}
Y_{jk} \\
g_{jk}(x) \leq 0 \\
c = \gamma_{jk}
\end{bmatrix}
\]

▶ Theorem: Convex Hull of Disjunction \( k \)  

- Disaggregated variables \( \nu^j \)

\[
\{(x, c) \mid x = \sum_{j \in J_k} \nu_{jk}, \quad c = \sum_{j \in J} \lambda_{jk} \gamma_{jk}, \\
0 \leq \nu_{jk} \leq \lambda_{jk} U^*, j \in J_k \\
\sum_{j \in J_k} \lambda_{jk} = 1, \quad 0 < \lambda_{jk} \leq 1, \\
\lambda_{jk} g_{jk}(\nu_{jk} / \lambda_{jk}) \leq 0, j \in J_k \}
\]

- \( \lambda_j \) - weights for linear combination

- Generalization of Balas (1979)
- Stubbs and Mehrotra (1999)

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Hull relaxation: intersection of convex hull of each disjunction
Olefin Separation System  (BP)

(Lee, Foral, Logsdon, Grossmann, 2003)

Goal: Synthesize optimal separation system

Input

Feed
Ethane C2H6
Propane C3H8
Butane C4H10
Naphtha C8–C12

RXN System

Pyrolysis Furnaces

Components

Mixture
Hydrogen H2
Fuel gas CH4
Acetylene C2H2
Ethylene C2H4
Ethane C2H6
MAPD C3H4
Propylene C3H6
Propane C3H8
C4 Mixture
C5 Mixture
C6+ Mixture

Separation Tasks

Output

Hydrogen H2
Fuel gas CH4
Ethylene C2H4
Propylene C3H6
C4 Mixture
C5 Mixture
C6+ Mixture
# Alternative Separation Schemes

## Separation Technologies

<table>
<thead>
<tr>
<th>T1</th>
<th>Distillation column</th>
</tr>
</thead>
<tbody>
<tr>
<td>T2</td>
<td>Physical absorption</td>
</tr>
<tr>
<td>T3</td>
<td>Membrane separator</td>
</tr>
<tr>
<td>T4</td>
<td>Dephlegmator</td>
</tr>
<tr>
<td>T5</td>
<td>Pressure swing adsorption (PSA)</td>
</tr>
<tr>
<td>T6</td>
<td>Cold box</td>
</tr>
<tr>
<td>T7</td>
<td>Chemical absorption</td>
</tr>
</tbody>
</table>

## Feed Components

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>H&lt;sub&gt;2&lt;/sub&gt;</td>
<td>E</td>
<td>C&lt;sub&gt;3&lt;/sub&gt;H&lt;sub&gt;6&lt;/sub&gt;</td>
</tr>
<tr>
<td>B</td>
<td>CH&lt;sub&gt;4&lt;/sub&gt;</td>
<td>F</td>
<td>C&lt;sub&gt;3&lt;/sub&gt;H&lt;sub&gt;8&lt;/sub&gt;</td>
</tr>
<tr>
<td>C</td>
<td>C&lt;sub&gt;2&lt;/sub&gt;H&lt;sub&gt;4&lt;/sub&gt;</td>
<td>G</td>
<td>C&lt;sub&gt;4&lt;/sub&gt;</td>
</tr>
<tr>
<td>D</td>
<td>C&lt;sub&gt;2&lt;/sub&gt;H&lt;sub&gt;6&lt;/sub&gt;</td>
<td>H</td>
<td>C&lt;sub&gt;5&lt;/sub&gt;</td>
</tr>
</tbody>
</table>
Example: convex hull

Convex hull = \text{conv}(\bigcup S_j)
Example: CRP solution

Convex hull = \text{conv}(\cup S_j)

Convex combination of \( z_j \)

\[ z_j = \frac{\psi}{\lambda_j} \]

Local solution point

Convex hull optimum, \( Z^L = 1.154 \) Lower Bound

\( x^L = (3.159, 1.797) \)

Infeasible for GDP

\[ \lambda_1 = 0.016 \]
\[ \lambda_2 = 0.955 \]
\[ \lambda_3 = 0.029 \]
Example: branch and bound

First Node: $S_2$
Optimal solution: $Z^* = 1.172$

Optimal Solution
(3.293, 1.707)
$Z^* = 1.172$
Example: branch and bound

Second Node: \( \text{conv}(S_1 \cup S_3) \)
Optimal solution: \( Z^L = 3.327 \)

Lower Bound \( Z^L = 3.327 \)

Upper Bound \( Z^U = 1.172 \)
Example: Search Tree

- **Branching Rule:** $\lambda_j$ - the “weight” of disjunction
  - Fix $Y_j$ as true: fix $\lambda_j$ as 1.

Root Node
Convex hull of all $S_i$
$Z = 1.154$
$\lambda = [0.016, 0.955, 0.029]$

First Node
Fix $\lambda_2 = 1$, $Z = 1.172$
$[x_1, x_2] = [3.293, 1.707]$
$\lambda = [0, 1, 0]$
$Z^U = 1.172$
Backtrack

$\neg Y_2$

$Z^L = 1.154$
Branch on $Y_2$

Second Node
Convex hull of $S_1$ and $S_3$
$Z = 3.327$
$\lambda = [0.337, 0, 0.623]$
$Z^L = 3.327 > Z^U$
Stop
GDP Example Revisited

- Find $x \geq 0, (x \in S_1) \lor (x \in S_2) \lor (x \in S_3)$ to minimize $Z$

  Transfer objective as inequality

  $$Z \geq (x_1 - 3)^2 + (x_2 - 2)^2 + c$$

![Diagram showing contour of $f(x)$, local solutions, and global optimum at $(3.293, 1.707)$ with $Z^* = 1.172$.]
Applications of Mathematical Programming in Chemical Engineering

**Process Design**

**Process Synthesis**

**Production Planning**

**Process Scheduling**

**Supply Chain Management**

**Process Control**

**Parameter Estimation**

*Models: LP, MILP, NLP, MINLP*

*new problem representations and models*
Progress in Linear Programming

Increases in computational speed 1987-2002

For 50,000 row LP model

Bixby-ILOG (2002)

Algorithms
Primal simplex in 1987 (XMP) versus
Best (primal,dual,barrier) 2002 (CPLEX 7.1) 2400x

Machines
Sun 3/150
Pentium 4, 1.7GHz 800x

Net increase: Algorithm * Machine ~ 1,900,000x

Two million-fold increase in speed!!
Proposed framework to obtain stronger relaxations for nonconvex GDP

*(Bilinear and Concave GDP)*

Ruiz, Grossmann (2009)

---

**Basic idea:**
Based on relaxation of the nonconvex GDP as a linear GDP exploit the theory behind DP to obtain stronger relaxations.

---

The **framework** consists of **two main phases**:

1- Generate a **valid Linear Generalized Disjunctive Program relaxation for the nonconvex GDP problem** (e.g. convex envelopes bilinear and concave).

2- Strengthen the **continuous relaxation of the linear GDP** obtained in phase 1 by applying a set of basic steps

---

The **hierarchy of relaxations** obtained by the application of basic steps is **valid for the original nonconvex GDP** problem
Big-M and HR vs. Proposed strengthening

All problems were solved using \textit{NLP branch-and-bound SBB/CONOPT 3.14 (GAMS)}

Table: Performance using different reformulation strategies

<table>
<thead>
<tr>
<th>Example</th>
<th>Opt.</th>
<th>BM Approach</th>
<th>IIR Approach</th>
<th>Proposed Approach</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>LB</td>
<td>Nds</td>
<td>T(s)</td>
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<td>Circles2D3</td>
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<td>4</td>
<td>1.0</td>
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<td>0.00</td>
<td>70</td>
<td>7.8</td>
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<td>Circles3D36</td>
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<td>0.44</td>
<td>70</td>
<td>7.3</td>
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<td>27.7</td>
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<td>Flay02</td>
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<td>6</td>
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</table>

Proposed vs BM: faster 10 out of 12
Proposed vs HR: faster 8 out of 12

Improved lower bounds 100% prods
Disjunctive Model using EMP-LOGMIP

LOGIC EQUATION IMP8; IMP8.. Y('6') -> Y('4')
LOGIC EQUATION IMP9; IMP9.. Y('7') -> Y('4')

* Initialization
Y.L('1') = 1;
Y.L('2') = 0;
Y.L('3') = 1;
Y.L('4') = 0;
Y.L('5') = 0;
Y.L('6') = 0;
Y.L('7') = 0;
Y.L('8') = 1;

$ONECHO > '%LM.INFO%'

**DISJUNCTION bigM 50 Y('1') INOUT11 INOUT14 ELSE INOUT12 INOUT13
DISJUNCTION Y('2') INOUT21 INOUT24 ELSE INOUT22 INOUT23
DISJUNCTION Y('3') INOUT31 INOUT34 ELSE INOUT32
DISJUNCTION Y('4') INOUT41 INOUT44 ELSE INOUT42 INOUT43 INOUT44
DISJUNCTION Y('5') INOUT51 INOUT54 ELSE INOUT52 INOUT53
DISJUNCTION Y('6') INOUT61 INOUT64 ELSE INOUT62 INOUT63
DISJUNCTION Y('7') INOUT71 INOUT74 ELSE INOUT72 INOUT73
DISJUNCTION Y('8') INOUT81 INOUT84 ELSE INOUT82 INOUT83 INOUT84 INOUT85

* optional, if not set LOGMIP will find the modeltype suitable
MODELTYPE MINLP
$OFFECHO

OPTION OPTCR = 0, LIMCOL = 0, LIMROW = 0, EMP = LOGMIP;

MODR1 EXAMPLES3 / ALL /;

SOLVE EXAMPLES3 USING EMP MINIMIZING PROF;
Hierarchy of Relaxations for Convex Disjunctive Programs

**Theorem 2.4.** For $i = 1, 2, \ldots, k$ let $F_i = \bigcap_{k \in K} S_k$ be a sequence of regular forms of a disjunctive set such that $F_i$ is obtained from $F_{i-1}$ by the application of a basic step, then:

$$h\text{-}rel(F_i) \subseteq h\text{-}rel(F_{i-1})$$

**Illustration:** 

$$F_0 = (P_{11} \cup P_{12}) \cap (P_{21} \cup P_{22})$$

$$F_1 = (P_{11} \cap P_{21}) \cup (P_{11} \cap P_{22}) \cup (P_{12} \cap P_{21}) \cup (P_{21} \cap P_{22})$$

No Basic Step Applied $\Rightarrow$ HR

Basic Step Applied $\Rightarrow$ CH

Tighter relaxation!
Can we obtain stronger relaxations for MINLP/GDP?

Assume *convexity and relate GDP to Disjunctive Programming (DP)* \cite{saway2007, ruiz2011}

**GDP**

\[
\begin{align*}
\min & \quad Z = f(x) + \sum_{k \in K} c_k \\
\text{s.t.} & \quad r(x) \leq 0 \\
& \quad \bigvee_{i \in D_k} \begin{bmatrix} Y_{ik} \\ g_{ik}(x) \leq 0 \\ c_k = \gamma_{ik} \end{bmatrix} \quad k \in K \\
& \quad \Omega(Y) = \text{True} \\
& \quad x_{lo} \leq x \leq x_{up} \\
& \quad x \in \mathbb{R}^n, c_k \in \mathbb{R}, Y_{ik} \in \{\text{True, False}\}
\end{align*}
\]
Can we obtain stronger relaxations for MINLP/GDP?

Assume convexity and relate GDP to Disjunctive Programming (DP) \cite{Sawaya2007, Ruiz2011}

\[ \text{GDP} \]

\[ \begin{align*}
\min & \quad Z = f(x) + \sum_{k \in K} c_k \\
\text{s.t.} & \quad r(x) \leq 0 \\
& \quad \bigvee_{i \in D_k} \begin{cases} 
Y_{ik} \\
g_{ik}(x) \leq 0 \\
\lambda_k = \gamma_{ik}
\end{cases} \\
& \quad \Omega(Y) = True 
\end{align*} \]

\[ x^{lo} \leq x \leq x^{up} \]

\[ x \in \mathbb{R}^n, \ c_k \in \mathbb{R}^1, \ Y_{ik} \in \{True, False\} \]

\[ \text{DP} \]

\[ \begin{align*}
\min & \quad Z = f(x) + \sum_{k \in K} c_k \\
\text{s.t.} & \quad r(x) \leq 0 \\
& \quad \bigvee_{i \in D_k} \begin{cases} 
\lambda_{ik} = 1 \\
g_{ik}(x) \leq 0 \\
\lambda_k = \gamma_{ik}
\end{cases} \\
& \quad A\lambda \geq a \\
& \quad \sum_{i \in D} \lambda_i = 1, \\
& \quad x^{lo} \leq x \leq x^{up} \\
\end{align*} \]

\[ x \in \mathbb{R}^n, \ c_k \in \mathbb{R}^1, \lambda_{ik} \geq 0 \]

The integrality of \( \lambda \) is guaranteed

Proposition: GDP and DP have equivalent solutions.