New Optimization Paradigms for Formulation, Solution, Data and Uncertainty Integration, and Results Interpretation

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2040 Visions of Process Systems Engineering

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Giant and Intellectual Leader in Process Systems Engineering

NAE Citation:
For contributions to the research, industrial practice, and education of process systems engineering, and for international intellectual and professional leadership.

Mathematical Programming

MINLP: Mixed-integer nonlinear programming

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

\[f(x): \mathbb{R}^n \to \mathbb{R}, h(x): \mathbb{R}^n \to \mathbb{R}^m, g(x): \mathbb{R}^n \to \mathbb{R}^q\]

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

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

NLP: \(f, h, g\) nonlinear, only \(x\)
Applications of Mathematical Programming in Chemical Engineering

Product Design

Process Synthesis

Production Planning

Process Scheduling

Supply Chain Management

Process Control

Parameter Estimation

LP, MILP, NLP, MINLP, Optimal Control

Major PSE contributions: theory, algorithms and software, new problem representations and models

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Predicting the future is difficult

Example Energy Crisis

1970s energy crisis - caused by the peaking of oil production in major industrial nations (Germany, United States, Canada, etc.) and embargoes from other producers

1973 oil crisis - caused by OAPEC oil export embargo by Arab oil-producing states, in response to Western support of Israel during the Yom Kippur War

1979 oil crisis - caused by the Iranian Revolution

Who would have thought in the 70’s about shale oil/gas, about the US becoming energy independent and rebirth of US chemical industry?
Visionary paper in 1967 on:

- Process design and integration with control, reliability
- Process models: steady state, dynamics
- Strategy of process calculations
- Computational methods for optimization

History Classical Optimization

\[ \min Z = f(x) \]
\[ x \in \mathbb{R}^n \]

Calculus

Newton (1673)  Leibniz (1673)

Lagrange multipliers

\[ \min Z = f(x) \]
\[ s.t. \quad h(x) = 0 \]
\[ x \in \mathbb{R}^n \]

Lagrange (1811)
Evolution of Mathematical Programming

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

\[
\min \phi = c^T x \\
\text{s.t.} \quad Ax \leq b \\
x \geq 0
\]

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

\[
\min \phi = f(x) \\
\text{s.t.} \quad g(x) \leq 0 \\
x \in \mathbb{R}^n
\]

**IP: Integer Programming** R. E. Gomory (1958)

\[
\min \phi = c^T y \\
\text{s.t.} \quad Ay \leq b \\
y \in \mathbb{Z}^m
\]
Major developments in last 30 years

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

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

- **Branch and Bound** Beale (1958), Balas (1962), Dakin (1965)

- **Cutting planes**
  Gomory (1959), Balas et al (1993)

- **Branch and cut**
  Johnson, Nemhauser & Savelsbergh (2000)

**NP-hard!**

- **MILP codes:** CPLEX, GUROBI, XPRESS
  Bob Bixby (1992)

- **Modeling Systems** GAMS, AMPL, AIMMS
  Kendrick, Meeraus (1988)

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MILP Electric Power Planning: ERCOT (Texas)

*Multiscale temporal/spatial*

- **30 year** time horizon
- Data from **ERCOT database**
- Regions:
  - Northeast (midpoint: Dallas)
  - West (midpoint: Glasscock County)
  - Coastal (midpoint: Houston)
  - South (midpoint: San Antonio)
  - Panhandle (midpoint: Amarillo)

**MILP Model**
- **Discrete variables:** 414,120
- **Continuous variables:** 682,471
- **Constraints:** 1,369,781
- **Solver:** CPLEX
- **CPU Time:** 3.4 hours
- **Objective value:** $223.93 billion
- **Optimality gap:** 0.4%

- **3330%** increase in **photo-voltaic (pv)** capacity
- **24%** increase in **wind** capacity
- **38%** increase in **natural gas combined-cycle (ng-cc)** capacity

**Generation capacity - total ERCOT**

Lara, Grossmann (2017)
- **NLP algorithms:**
  
  **Reduced gradient** *Murtagh, Saunders (1978)*
  
  **Successive quadratic programming (SQP)** *Han 1976; Powell, 1977*
  
  **Interior Point Methods** *Byrd, Hribar, Nocedal (1999)*
  
  *Wächter, Biegler (2002)*

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

- **Convex optimization:** *Rockefeller (1970)*
  
  *Boyd (2008) CVX*

- **MINLP algorithms**
  
  **Branch and Bound method (BB)** *Ravindran and Gupta (1985) Leyffer and Fletcher (2001)*
  
  **Generalized Benders Decomposition (GBD)** *Geoffrion (1972)*
  
  **Outer-Approximation (OA)**
  
  *Duran & Grossmann (1986), Fletcher & Leyffer (1994)*
  
  **Extended Cutting Plane (ECP)** *Westerlund and Pettersson (1995)*

- **MINLP codes:**
  
  DICPOPT, SBB, Bonmin, FilMINT

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- **Global Optimization Software**

  αBB *(Adjiman, Androulakis, Maranas & Floudas, 1996; 2000)*

  BARON *(Ryoo & Sahinidis, 1995, Tawarmalani and Sahinidis (2002))*

  OA for nonconvex MINLP *(Kesavan, Allgor, Gatzke, Barton (2001))*

  Couenne *(Belotti & Margot, 2008)*

  GLOMIQO, ANTIGONE *(Floudas and Misener (2011))*

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

- **Optimal Control** *(Cuthrell, Biegler (1987), Pantelides, Sargent, Vassiliadis (1994))*

- **Hybrid-systems** *(Barton & Pantelides (1994), Bemporad & Morari (1998))*
- **Stochastic programming** Birge & Louveaux (1997)
  
  A Ruszczyński, A Shapiro (2002)


  Bertsimas, Sim (2004)

- **Parametric Programming** Dua & Pistikopoulos (2000)

**Decomposition Techniques**

**Lagrangian decomposition**


*Complicating Constraints*

![Graph for Lagrangian decomposition]

**Benders decomposition**


*Complicating Variables*

![Graph for Benders decomposition]

Stephanopoulos, Westerberg (1974)

**Dynamic programming**

Bellman (1953), Bertsekas (1995)

*Multistage systems*
Rich History of Mathematical Programming

Challenges in mathematical programming and *existing paradigms*

1. **Formulation models:** *equation based*

2. **Solution models:**
   - Exponential complexity in combinatorial problems
   - Non-robust convergence in nonlinear problems

3. **Data handling:**
   - Interface of models with data
   - Uncertainty optimization

4. **Results interpretation:**
   - Limited indicators (active constraints, dual prices)
Challenge Formulation Models:

Equation based

Possible direction:

Develop higher level formulations, complex models (e.g. equations and logic)
Generalized Disjunctive Programming (GDP)

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

Motivation: Facilitate modeling discrete/continuous problems

\[
\begin{align*}
\text{min } & \quad Z = \sum_k c_k + f(x) \\
\text{s.t. } & \quad r(x) \leq 0 \\
& \quad \left[ \begin{array}{c}
Y_{jk} \\
g_{jk}(x) \leq 0 \\
c_k = \gamma_{jk}
\end{array} \right] \quad k \in K \\
& \quad \Omega(Y) = \text{true} \\
& \quad x \in R^n, c_k \in R^1 \\
& \quad Y_{jk} \in \{ \text{true, false}\}
\end{align*}
\]

Objective Function
Common Constraints
Disjunction
Constraints
Fixed Charges
Logic Propositions
Continuous Variables
Boolean Variables

\[f(x): R^n \to R^1, r(x): R^n \to R^m, g(x): R^n \to R^q\]
Strip-packing Problem

Problem statement: HiFi M. (1998) Fit a set of rectangles with width $w_i$ and length $l_i$ onto a large rectangular strip of fixed width $W$ and unknown length $L$. The objective is to fit all rectangles onto the strip without overlap and rotation while minimizing length $L$ of the strip.

$\begin{align*}
\text{Min } Z &= L \\
\text{s.t. } L &\geq x_i + l_i & i \in N \\
 Y^1_{ij} &\land (x_i + h_i \leq x_j \lor y_i - h_i \geq y_j) & i, j \in N, i < j \\
 Y^2_{ij} &\land (x_i + h_i \leq x_j \lor y_i - h_i \geq y_j) & i, j \in N, i < j \\
 Y^3_{ij} &\land (x_i + h_i \leq x_j \lor y_i - h_i \geq y_j) & i, j \in N, i < j \\
 0 &\leq x_i \leq u_i - l_i & i \in N \\
 h_i &\leq y_i \leq W & i \in N \\
x_{ip}, y_{ip} &\in \mathbb{R} & i \in N \\
 Y^1_{ij}, Y^2_{ij}, Y^3_{ij}, Y'^{i,j} &\in \{\text{True, False}\} & i, j \in N, i < j
\end{align*}$
Challenge Solution Models:

*Exponential complexity in combinatorial problems*
*Non-robust convergence in nonlinear problems*

Possible directions:

*Advances in computing*
*Towards polynomial complexity*
*New modeling frameworks with guaranteed convergence*
Quantum Computing \(10^8\) faster current chips!

Computation systems that use quantum-mechanics

Today’s implementations are very problem specific mainly in combinatorial optimization, but results are promising. e.g. evolutionary algorithm
New theory for combinatorial optimization?

Unsolved problem in theoretical computer science:  *is* $P = NP$?

If $P=NP$ integer programming and global optimization are solvable in *polynomial time*!
Canonical Primal-Dual Formulation for Process Models

Basic premise: physics not generic equations   Amundsen, Swaney (2008)

Macroscopic

Dissipation +
Couplings +
Reactions

Microscopic

LE
thermodynamics
transport
kinetics

<table>
<thead>
<tr>
<th>Conservation</th>
<th>Flux</th>
<th>Potential</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Transport $v^i$</td>
<td>Coupling $\sigma^i$</td>
</tr>
<tr>
<td>Species</td>
<td>$v^i = J^i + \rho^i v$</td>
<td>$\sigma^i$</td>
</tr>
<tr>
<td>Energy</td>
<td>$v^E = J^E + \rho^E v$</td>
<td>$\sigma^E$</td>
</tr>
<tr>
<td>Momentum</td>
<td>$v^p = J^p + \rho^p v$</td>
<td>$\sigma^p$</td>
</tr>
<tr>
<td>Strain</td>
<td>$v^V = J^V + \rho^V v$</td>
<td>$\sigma^V$</td>
</tr>
</tbody>
</table>

Euler-Lagrange eqns. variational formulation

\[
\begin{bmatrix}
\nu^i \\
\sigma^i \\
\gamma^k
\end{bmatrix} + Y \begin{bmatrix}
\nabla \lambda \\
-\lambda \\
-\nu^T \lambda
\end{bmatrix} = 0
\]

Solution composite model via homotopy

Primals are the fluxes and the duals are the adjoint potentials

Theoretical result: Theorem

Homotopy path points exist and remain bounded

$\Rightarrow$ Homotopy path guaranteed to converge to a solution

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Challenge Data handling:
*Interface of models with data*
*Uncertainty optimization*

Possible direction:
*Integration of Data Analytics and Decision Making*
How to anticipate effects of uncertainty?

Approaches to Optimization under Uncertainty

If deterministic uncertainty set

Robust Optimization: Ensure feasibility over uncertainty set


If probability distribution function

Stochastic Programming: Expected value, recourse actions

Birge & Louveaux, (1997)

Chance Constrained Optimization: Ensure feasibility with level confidence

Prékopa (1973)
Integration of Data Analytics and Decision Making

Calfa, Grossmann (2015)

Uncertainty

Variability

Data
- Historical
- Forecast

Predictive Analytics

Prescriptive Analytics

Decision-Making Model

max \( f(x) \)

s.t. \( h(x) = 0 \)

\( g(x) \leq 0 \)

- Stochastic
- Robust
- Reliable

Parameters
Functions

Statistical Models

Uncertainty Quantification
Challenge Interpretation Results:

*Limited indicators (active constraints, dual prices)*

Possible directions:

*AI/Constraint Programming techniques*
ANALYZE
A computer-assisted analysis system for mathematical programming models and solutions

For LP not only *What if?* but *Why?* (*Why solution value what it is*)

*Rule-based system (alla expert systems)*


Techniques for Integrating Qualitative Reasoning and Symbolic Computation in Engineering Optimization, A. M. AGOGINO, S. ALMGREN, 2007

*Irreducible infeasible sets (IISs)*
Identifying subset of constraints responsible for infeasible solutions
Applicable to linear programs (LPs), nonlinear programs (NLPs),
mixed-integer linear programs (MIPs), mixed-integer nonlinear programs (MINLPs)

*Bounds propagation based on BARON as in constraint programming*

Puranik, Y. and N. V. Sahinidis, *Deletion presolve for accelerating infeasibility diagnosis in optimization models*, INFORMS Journal on Computing, accepted, 2017
Future vision by 2040

Large-scale Global Multi-objective Nonconvex Nonlinear Discrete-Continuous Stochastic Dynamic Differential-Algebraic Optimization Problem

Easy to formulate, and solved reliably and efficiently,

Explanation of results that are easily understood with interactive input
Congratulations George for your 70th Birthday and for Outstanding Contributions!

We wish you Happy Retirement!