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

Ignacio E. Grossmann
Center for Advanced Process Decision-making
Department of Chemical Engineering
Carnegie Mellon University
Pittsburgh, PA 15213

2040 Visions of
Process Systems Engineering

Symposium on Occasion of the George Stephanopoulos's 70th Birthday and Retirement from MIT
June 1-2, 2017

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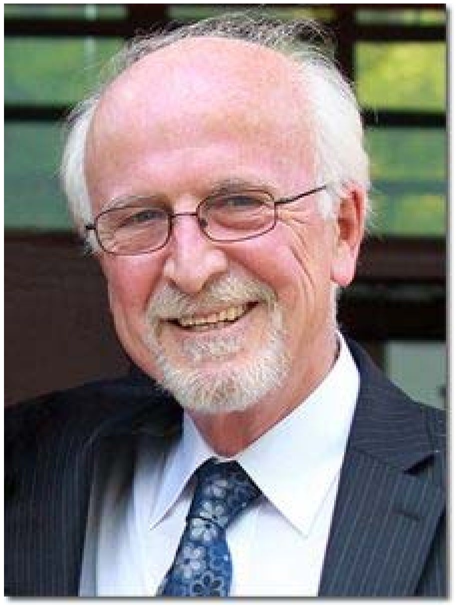
Professor George Stephanopoulos



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.

G. Stephanopoulos, A. W. Westerberg, „The use of Hestenes' method of multipliers to resolve dual gaps in engineering system optimization," *JOTA*, 15, 285–309 (1974)

Mathematical Programming

MINLP: *Mixed-integer nonlinear programming*

$$\min Z = f(x,y)$$
$$s.t. \quad h(x,y) = 0$$
$$g(x,y) \le 0$$
$$x \in R^n, \quad y \in \{0,1\}^m$$

$$f(x): R^n \to R^1, h(x): R^n \to R^m, g(x): R^n \to R^q$$

MILP: *f, h, g* linear

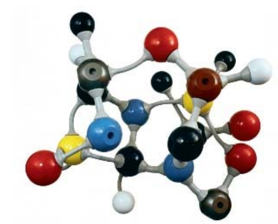
LP: *f, h, g* linear, only *x*

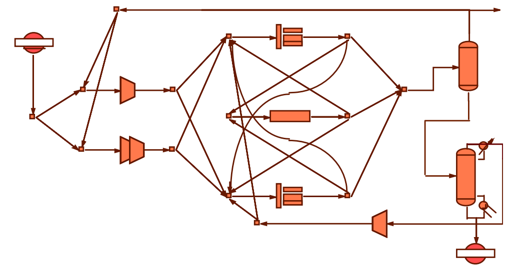
NLP: *f, h, g* nonlinear, only *x*

Applications of Mathematical Programming in Chemical Engineering

Product Design

Process Synthesis

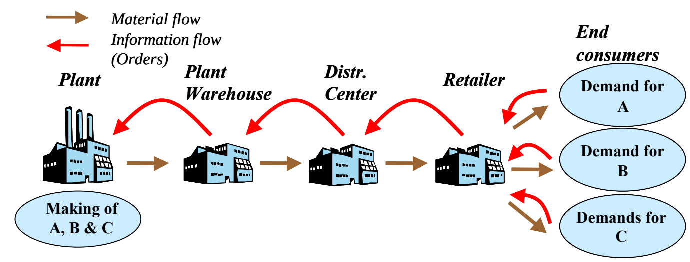




Production Planning

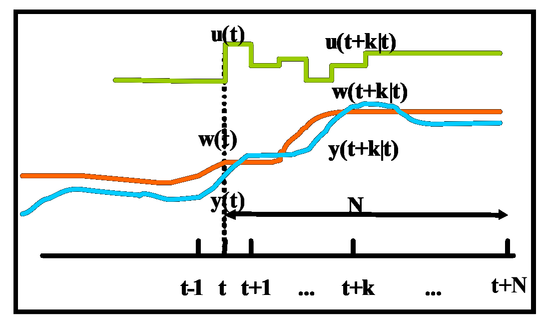
Process Scheduling

Supply Chain Management



Process Control

Parameter Estimation



LP, MILP, NLP, MINLP, Optimal Control

Major PSE contributions: <u>theory, algorithms and software, new problem representations and models</u>

Predicting the future is difficult

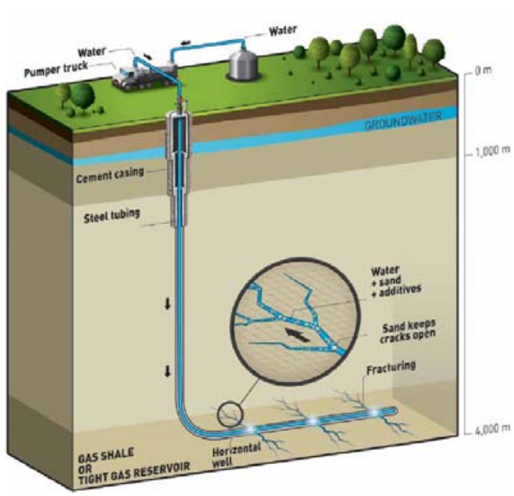
Example Energy Crisis

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?



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Roger W.H. Sargent

CEP review

Integrated Design and Optimization of Processes

Although we are in sight of a truly integrated approach to the design of complete processes, a great deal of work remains to be done. With the need for more sophisticated analysis of larger complexes, it is more than ever necessary to join hands with those working in the fields of control engineering, operational research, numerical analysis, and computer science.

R. W. H. Sargent
Imperial College of Science and Technology, University of London, London, England

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*

Sargent, R.W.H., "Integrated Design and Optimization of Processes," Chemical Engineering Progress, Volume: 63 Issue: 9, Pages: 71-78 (1967).

History Classical Optimization

$$\min Z = f(x)$$
$$x \in R^n$$

Calculus

Newton (1673)

Leibniz (1673)

Lagrange multipliers

$$\min Z = f(x)$$
$$s.t. \quad h(x) = 0$$
$$x \in R^n$$

Lagrange (1811)

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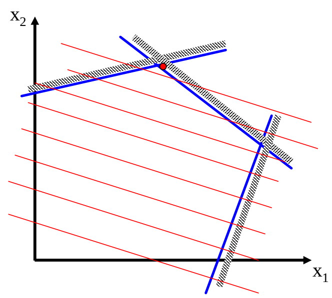
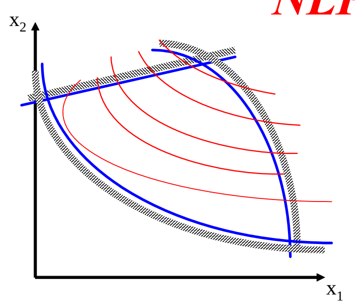
Evolution of Mathematical Programming



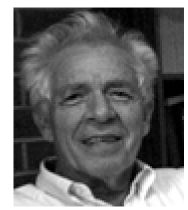
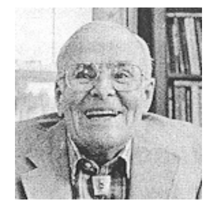
LP: Linear Programming ***Kantorovich (1939), Dantzig (1947)***

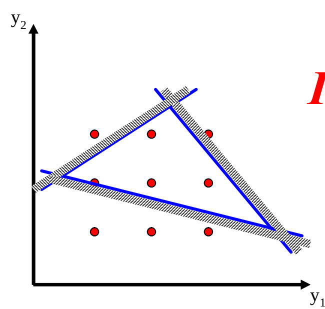
$$\min \phi = c^T x$$
$$s.t. \quad Ax \leq b$$
$$x \geq 0$$

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

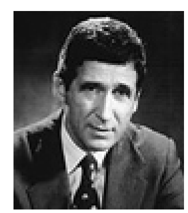
$$\min \phi = f(x)$$
$$s.t. \quad g(x) \leq 0$$
$$x \in R^n$$



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

$$\min \phi = c^T y$$
$$s.t. \quad Ay \leq b$$
$$y \in Z^m$$



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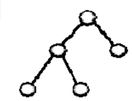
Major developments in last 30 years

- **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)***

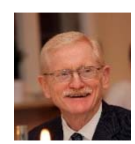
- **Cutting planes** ***Gomory (1959), Balas et al (1993)***
- **Branch and cut** ***Johnson, Nemhauser & Savelsbergh (2000)***



LP (simplex) based

NP-hard!

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



Bob Bixby (1992)

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

Kendrick, Meeraus (1988)

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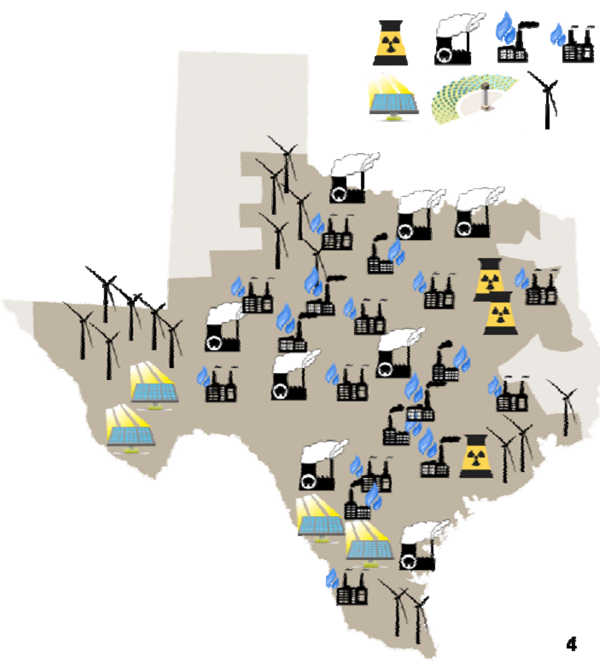
MILP Electric Power Planning: ERCOT (Texas)

Multiscale temporal/spatial

Lara, Grossmann (2017)

- **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)



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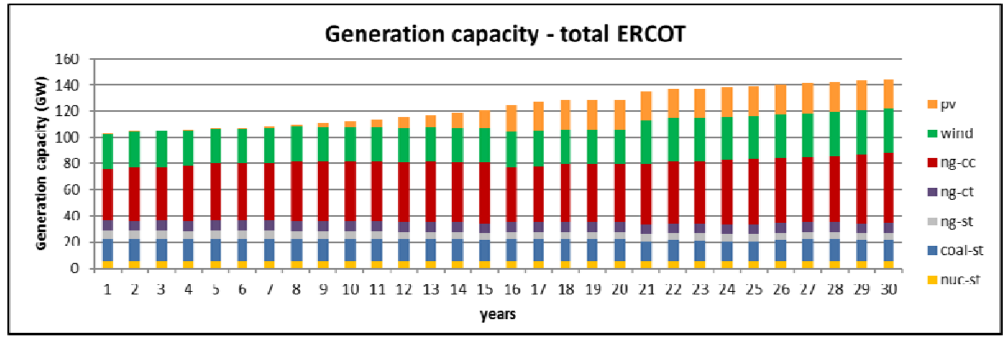


- 3330% increase in **photo-voltaic (pv)** capacity
- 24% increase in **wind** capacity
- 38% increase in **natural gas combined-cycle (ng-cc)** capacity

24

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%

- **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) 

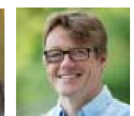
- **NLP codes:**

  MINOS, CONOPT, SNOPT, KNITRO, IPOPT

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

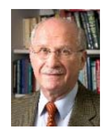
- **MINLP algorithms**

  Branch and Bound method (BB)

  Ravindran and Gupta (1985) Leyffer and Fletcher (2001)  

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

  Outer-Approximation (OA)

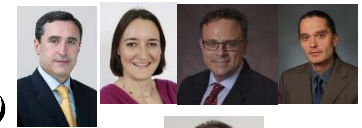
  Duran & Grossmann (1986), Fletcher & Leyffer (1994) 

  Extended Cutting Plane (ECP) *Westerlund and Pettersson (1995)* 

- **MINLP codes:**

  DICPOPT, SBB, Bonmin, FilMINT

- Global Optimization Software

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

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

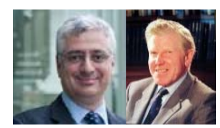
OA for nonconvex MINLP *(Kesavan, Allgor, Gatzke, Barton (2001)* 

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)

- **Robust optimization** *Rekalitis (1975), Ben-Tal, Nemirovski (1998)*

  Bertsimas, Sim (2004)

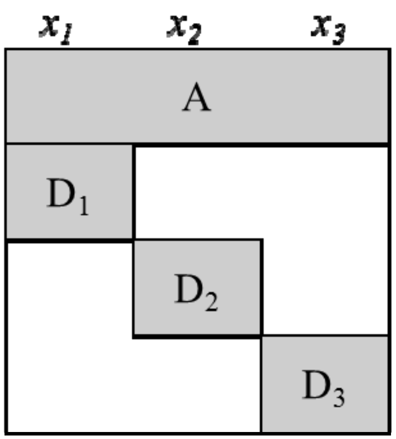
- **Parametric Programming** *Dua & Pistikopoulos (2000)*

- Decomposition Techniques

Lagrangean decomposition

Geoffrion (1972) Guinard (2003)

Complicating Constraints

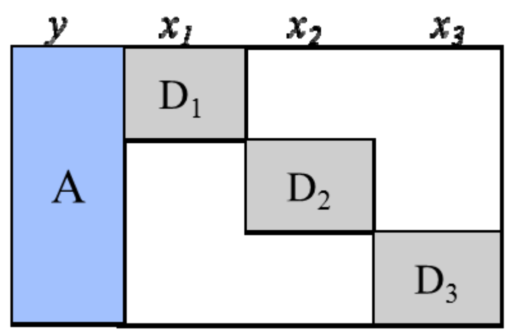


Stephanopoulos, Westerberg (1974)

Benders decomposition

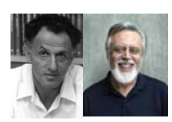
Benders (1962), Magnanti, Wong (1984)

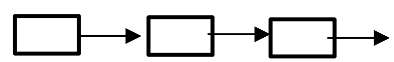
Complicating Variables



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

$$\min \; Z = \sum_k c_k + f(x)$$ **Objective Function**

$$s.t. \quad r(x) \le 0$$ **Common Constraints**

OR operator →

$$\bigvee_{j \in J_k} \begin{bmatrix} Y_{jk} \\ g_{jk}(x) \le 0 \\ c_k = \gamma_{jk} \end{bmatrix} \quad k \in K$$

Disjunction

Constraints

Fixed Charges

$$\Omega(Y) = true$$ **Logic Propositions**

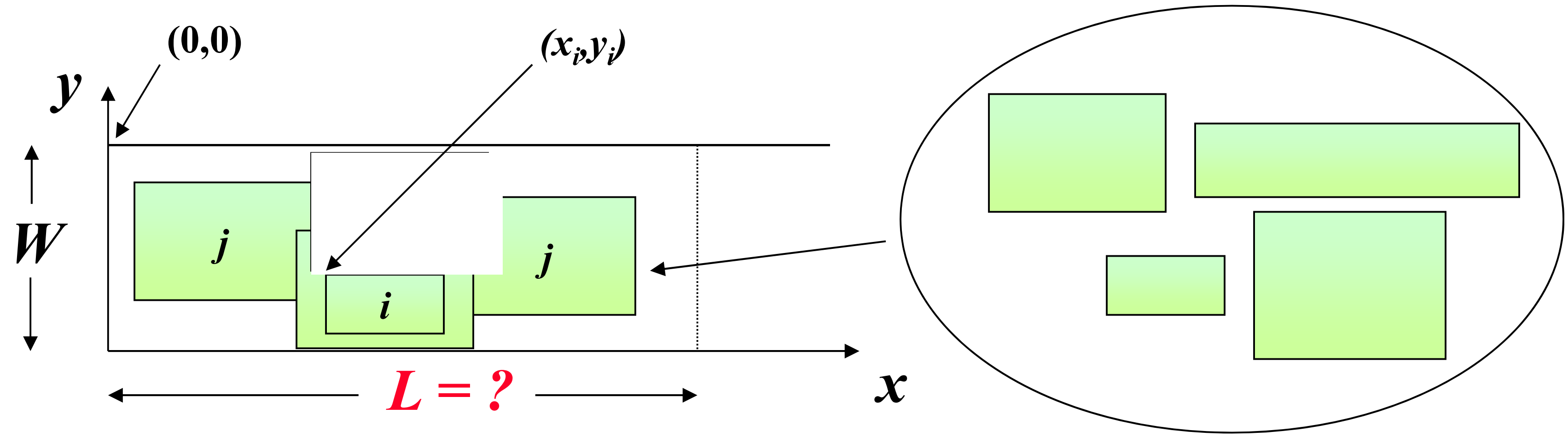
$$x \in R^n, c_k \in R^1$$ **Continuous Variables**

$$Y_{jk} \in \{ true, \; false \}$$ **Boolean Variables**

$$f(x): R^n \rightarrow R^1, r(x): R^n \rightarrow R^m, g(x): R^n \rightarrow R^q$$

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.*



Set of rectangles

$$\text{Min } Z = L \qquad \text{(SP-GDP)}$$

$$\text{s.t.} \quad L \ge x_i + l_i \qquad i \in N$$

$$\begin{bmatrix} Y^1_{ij} \\ x_i + l_i \le x_j \end{bmatrix} \vee \begin{bmatrix} Y^2_{ij} \\ x_j + l_j \le x_i \end{bmatrix} \vee \begin{bmatrix} Y^3_{ij} \\ y_i - h_i \ge y_j \end{bmatrix} \vee \begin{bmatrix} Y^4_{ij} \\ y_j - h_j \ge y_i \end{bmatrix} \qquad i,j \in N,\ i < j$$

$$0 \le x_i \le U_i - l_i \qquad i \in N$$

$$h_i \le y_i \le W \qquad i \in N$$

$$x_i, y_i \in R \qquad i \in N$$

$$Y^1_{ij}, Y^2_{ij}, Y^3_{ij}, Y^4_{ij} \in \{True, False\} \qquad i,j \in N,\ i < j$$

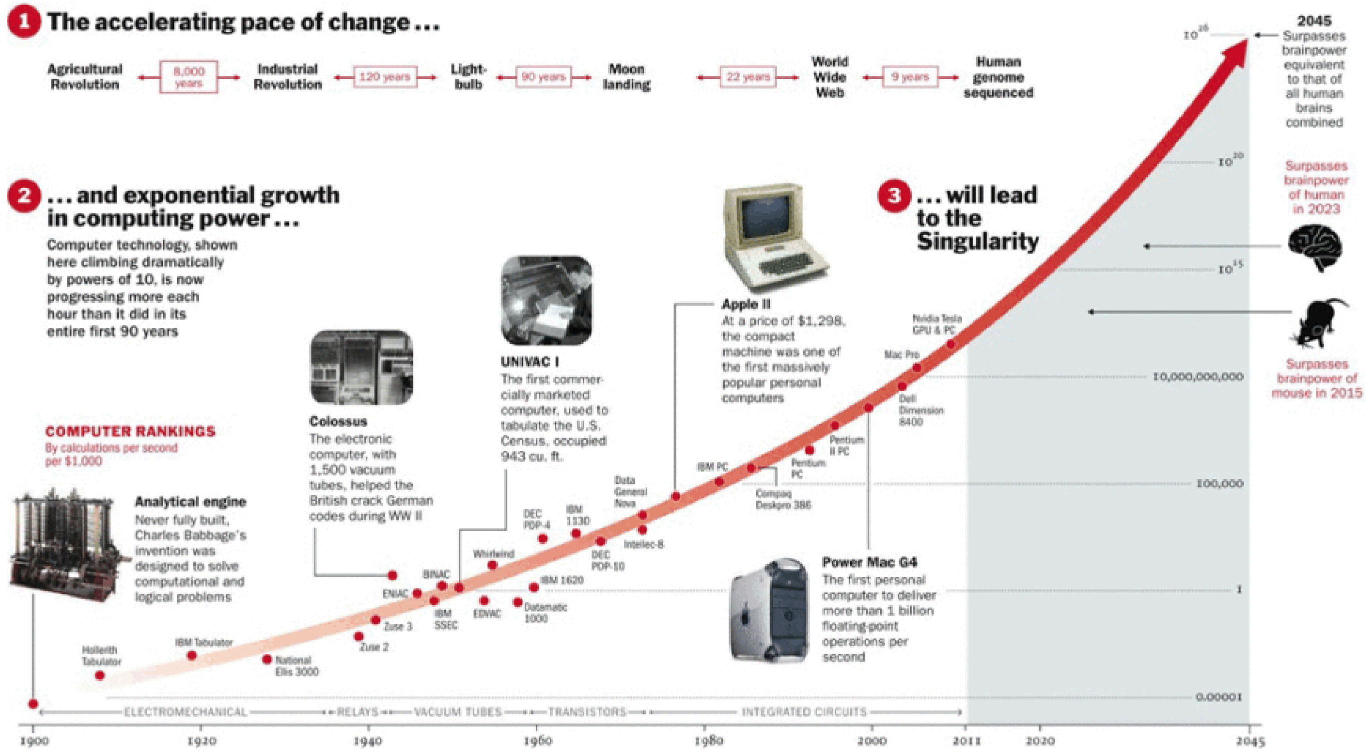
Challenge Solution Models:

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

Moore's Law: doubling processing power every two years

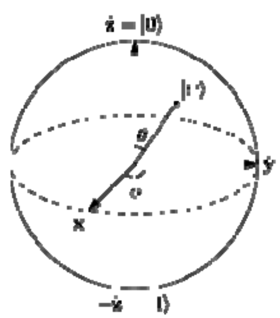


10^{20}

10^{10}

2011 2045

Quantum Computing *10^8 faster current chips!*



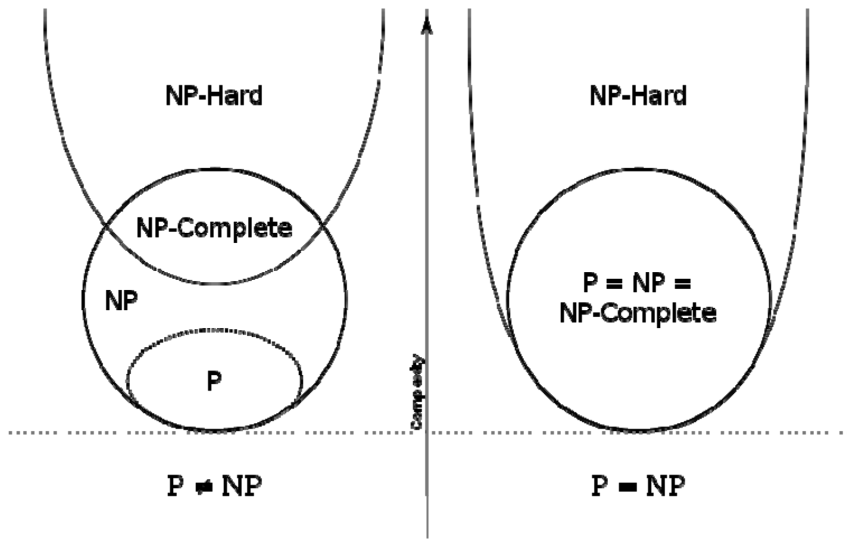
Computation systems that use quantum-mechanics

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	Microscopic
Dissipation + Couplings + Reactions	LE thermodynamics transport kinetics

Conservation	Flux			Potential
	Transport v^α	Coupling σ^α	Reaction r^k	
Species	$v^i = J^i + \rho^i \mathbf{v}$	-	$\sum_k \nu_i^k r^k$	λ^i
Energy	$v^E = J^E + \rho^E \mathbf{v}$	σ^E	-	λ^E
Momentum	$v^P = J^P + \rho^P \mathbf{v}$	σ^P	-	λ^P
Strain	$v^V = J^V + \rho^V \mathbf{v}$	σ^V	-	λ^V

Euler-Lagrange eqns.
variational formulation

$$\begin{bmatrix} v^\alpha \\ \sigma^\alpha \\ r^k \end{bmatrix} + Y \begin{bmatrix} \nabla\lambda \\ -\lambda \\ -\nu^T\lambda \end{bmatrix} = 0$$

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
=> Homotopy path *guaranteed to converge to a solution*

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Challenge Data handling:

Interface of models with data

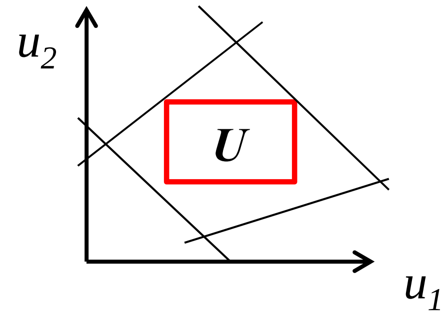
Uncertainty optimization

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 <u>feasibility</u> over uncertainty set**

Ben-Tal & Nemirowski. (2000)

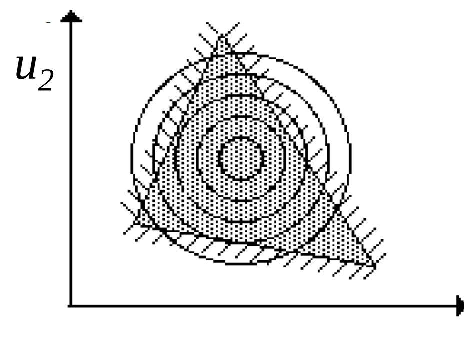
If probability distribution function

Stochastic Programming: **<u>Expected value, recourse actions</u>**

Birge & Louveaux, (1997)

Chance Constrained Optimization: **Ensure <u>feasibility with level confidence</u>**

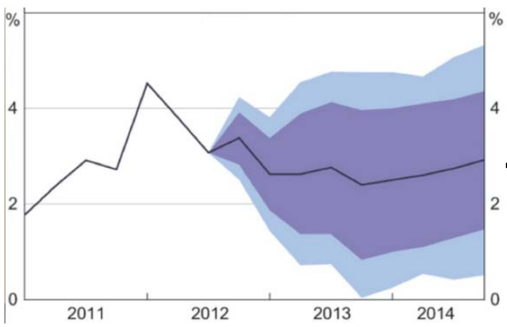
Prékopa (1973)



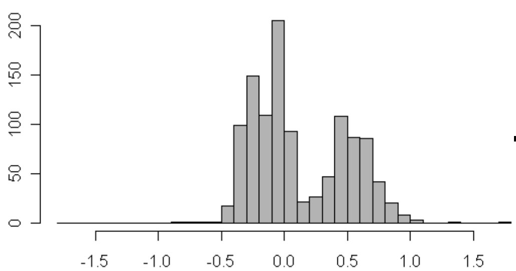
Integration of Data Analytics and Decision Making

Calfa, Grossmann (2015)

Uncertainty



Variability



Data
- **Historical**
- **Forecast**

Predictive Analytics

Statistical Models ?

Uncertainty Quantification

- **Parameters**
- **Functions**

Prescriptive Analytics

Decision-Making Model

$$\max_x \; f(x)$$
$$\text{s.t.} \quad h(x) = 0$$
$$g(x) \leq 0$$

- **Stochastic**
- **Robust**
- **Reliable**

Challenge Interpretation Results:

Limited indicators (active constraints, dual prices)

Possible directions:

AI/Constraint Programming techniques

AI/Constraint Propagation-based techniques for analysis results

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)

Greenberg, H., The ANALYZE rulebase for supporting LP analysis, Annals of Operations Research 65 (1996), 91-126.

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, I NFORMS Journal on Computing, accepted, 2017

Future vision by 2040

Large-scale Global Multi-objective Nonconvex Nonlinear

Discrete-Continuous Stochastic Dynamic Differential-Algebraic

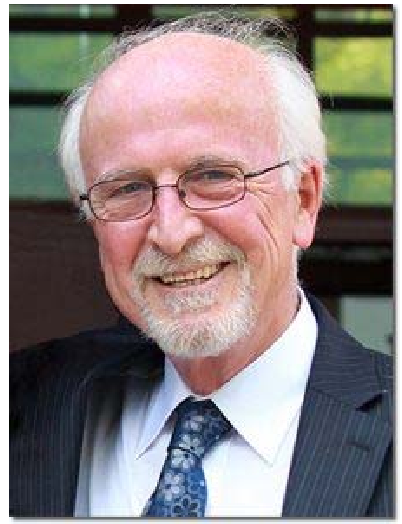
Optimization Problem

Easy to formulate, and solved reliably and efficiently,

Explanation of results that are easily understood with interactive input

Chemical ENGINEERING

CAPD CENTER



Congratulations George for your 70th Birthday and for Outstanding Contributions!

We wish you Happy Retirement!