Extended Mathematical Programming

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Extended Mathematical Programs

- Optimization models improve understanding of underlying systems and facilitate operational/strategic improvements under resource constraints
- Problem format is old/traditional

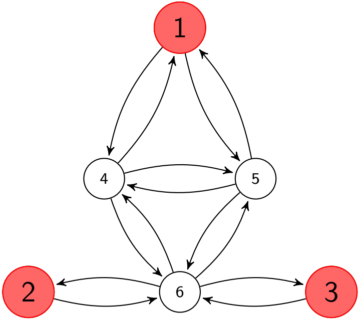
$$\min_x f(x) \text{ s.t. } g(x) \leq 0, h(x) = 0$$

- Extended Mathematical Programs allow annotations of constraint functions to augment this format.
- Give several examples of this: multi-agent competitive models, bilevel programming, variational inequalities

Model building with EMP

- Take one system of (nonlinear) relations and annotate them to:
  - form a simple nonlinear program (no annotations)
  - form a complementarity problem from an embedded optimization problem (nlp with side constraints outside of optimizers control)
  - form an equilibrium model consisting of optimality conditions of several nlp's along with equilibrium constraints (MOPEC)
  - form a bilevel program (an optimization problem with optimization problems as constraints)
  - Can assign multipliers (prices) from one sub-model as variables in another model (PIES)
  - Can reformulate nonsmooth models using duality (QS)
  - Can introduce random variables into a model
- The annotations essentially detail who controls which equations and variables

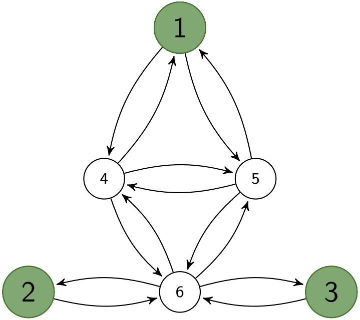
Spatial Price Equilibrium



$n \in \{1, 2, 3, 4, 5, 6\}$
$L \in \{1, 2, 3\}$

Supply quantity: S_L
Production cost: $\Psi(S_L) = ..$

Spatial Price Equilibrium



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Supply quantity: S_L
Production cost: $\Psi(S_L) = ..$
Demand: D_L
Unit demand price: $\theta(D_L) = ..$

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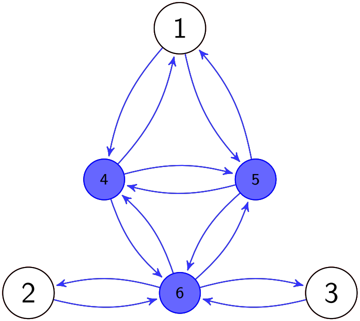

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Supply quantity: S_L
Production cost: $\Psi(S_L) = ..$
Demand: D_L
Unit demand price: $\theta(D_L) = ..$
Transport: T_{ij}
Unit transport cost: $c_{ij}(T_{ij}) = ..$

One large system of equations and inequalities to describe this (GAMS).

Nonlinear Program Model (Monopolist)

- One producer controlling all regions
- Full knowledge of demand system
- Full knowledge of transportation system

$$\max_{(D,S,T)\in\mathcal{F}} \quad \sum_{l\in L} \theta_l(D_l)D_l - \sum_{l\in L} \Psi_l(S_l) - \sum_{i,j} c_{ij}(T_{ij})T_{ij}$$

$$\text{s.t.} \quad S_l + \sum_{i,l} T_{il} = D_l + \sum_{l,j} T_{lj}, \quad \forall l \in L$$

EMP = NLP

2 agents: NLP + VI Model (Monopolist)

- One producer controlling all regions
- Full knowledge of demand system
- Price-taker in transportation system

$$\max_{(D,S,T)\in\mathcal{F}} \sum_{l\in L}\theta_l(D_l)D_l - \sum_{l\in L}\Psi_l(S_l) - \sum_{i,j}\overset{p_{ij}}{\cancel{c_{ij}(T_{ij})}}T_{ij} \qquad (1)$$

$$\text{s.t.} \quad S_l + \sum_{i,l} T_{il} = D_l + \sum_{l,j} T_{lj}, \quad \forall l \in L$$

$$p_{ij} = c_{ij}(T_{ij}) \qquad (2)$$

empinfo: equilibrium
vi tcDef tc

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EMP = MOPEC $\Longrightarrow$ MCP

EMP: MOPEC

- Model has the format:

$$\text{Agent o:} \quad \min_{x} \; f(x,y) \quad \text{s.t.} \; g(x,y) \le 0 \quad (\perp \lambda \ge 0)$$

$$\text{Agent v:} \quad H(x,y,\lambda) = 0 \qquad (\perp y \text{ free})$$

- Difficult to implement correctly (multiple optimization models)
- Can do automatically - simply annotate equations

  empinfo: equilibrium

  min f x defg

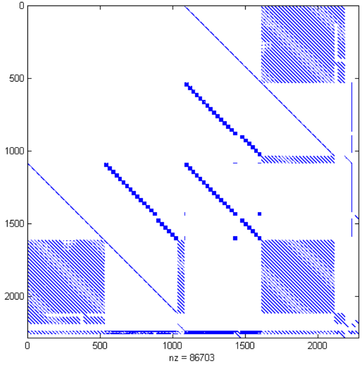
  vi H y

  dualvar λ defg
- EMP tool automatically creates an MCP

$$\nabla_x f(x,y) + \lambda^T \nabla g(x,y) = 0$$
$$0 \le -g(x,y) \perp \lambda \ge 0$$
$$H(x,y,\lambda) = 0$$

World Bank Project (Uruguay Round)

- 24 regions, 22 commodities
  - Nonlinear complementarity problem
  - Size: 2200 x 2200
- Short term gains $53 billion p.a.
  - Much smaller than previous literature
- Long term gains $188 billion p.a.
  - Number of less developed countries loose in short term
- Unpopular conclusions - forced concessions by World Bank
- Region/commodity structure not apparent to solver



Classic SPE Model (NLP + VI agents)

- One producer controlling all regions
- Price-taker in demand system
- Price-taker in transportation system

$$\max_{(D,S,T)\in\mathcal{F}} \sum_{l\in L} \overset{\pi_l}{\cancel{\theta_l(D_l)}} D_l - \sum_{l\in L} \Psi_l(S_l) - \sum_{i,j} \overset{p_{ij}}{\cancel{c_{ij}(T_{ij})}} T_{ij} \quad (1)$$

$$\text{s.t.} \quad S_l + \sum_{i,l} T_{il} = D_l + \sum_{l,j} T_{lj}, \quad \forall l \in L$$

$$p_{ij} = c_{ij}(T_{ij}) \quad (2)$$

$$\pi_l = \theta_l(D_l) \quad (3)$$

empinfo: vi tcDef tc
vi pricedef price

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EMP = MOPEC $\Longrightarrow$ MCP

Cournot-Nash equilibrium (multiple agents)

Assumes that each agent (producer):

- Treats other agent decisions as fixed
- Is a price-taker in transport and demand

EMP info file

```
equilibrium
max obj('one') vars('one') eqns('one')
max obj('two') vars('two') eqns('two')
max obj('three') vars('three') eqns('three')
vi tcDef tc
vi pricedef price
```

$\text{EMP} = \text{MOPEC} \implies \text{MCP}$

Nash Equilibria

- Nash Games: x^* is a Nash Equilibrium if

$$x_i^* \in \arg\min_{x_i \in X_i} \ell_i(x_i, x_{-i}^*, q), \forall i \in \mathcal{I}$$

  x_{-i} are the decisions of other players.
- Quantities q given exogenously, or via complementarity:

$$0 \leq H(x, q) \ \perp \ q \geq 0$$

- empinfo: equilibrium
  min loss(i) x(i) cons(i)
  vi H q
- Applications: Discrete-Time Finite-State Stochastic Games. Specifically, the Ericson & Pakes (1995) model of dynamic competition in an oligopolistic industry.

Key point: models generated correctly solve quickly

Here S is mesh spacing parameter

S	Var	rows	non-zero	dense(%)	Steps	RT (m:s)
20	2400	2568	31536	0.48	5	0 : 03
50	15000	15408	195816	0.08	5	0 : 19
100	60000	60808	781616	0.02	5	1 : 16
200	240000	241608	3123216	0.01	5	5 : 12

Convergence for $S = 200$ (with new basis extensions in PATH)

Iteration	Residual
0	1.56(+4)
1	1.06(+1)
2	1.34
3	2.04(−2)
4	1.74(−5)
5	2.97(−11)

Bimatrix Games: Golden Balls

- MOPEC can be used to formulate many standard problem instances corresponding to special choices of M and $\mathcal{C}$.
- Nash game: two players have I and J pure strategies.
- p and q (strategy probabilities) belong to unit simplex $\triangle_I$ and $\triangle_J$ respectively.
- Loss matrices $A \in R^{I \times J}$ and $B \in R^{I \times J}$, where $A_{i,j}$ is the loss incurred by the first player if strategy i is selected by the first player and j by the second, etc.
- The expected loss for the first and the second players are $p^T Aq$ and $p^T Bq$ respectively.
- A Nash equilibrium is reached by the pair of strategies (p^*, q^*) if and only if

$$p^* \in \arg \min_{p \in \triangle_I} p^T A q^* \quad \text{and} \quad q^* \in \arg \min_{q \in \triangle_J} (p^*)^T B q$$

Formulation using complementarity

The optimality conditions for the above problems are:

$$-Aq^* \in N_{\triangle_I}(p^*) \text{ and } -B^T p^* \in N_{\triangle_J}(q^*)$$

Therefore the corresponding VI is affine and can be written as:

$$0 \in \begin{bmatrix} 0 & A \\ B^T & 0 \end{bmatrix} \begin{bmatrix} p \\ q \end{bmatrix} + N_{\triangle_I \times \triangle_J}\left(\begin{bmatrix} p \\ q \end{bmatrix} \right). \tag{1}$$

General Equilibrium models

$$(C): \max_{x_k \in X_k} U_k(x_k) \text{ s.t. } p^T x_k \leq i_k(y,p)$$

$$(I): i_k(y,p) = p^T \omega_k + \sum_j \alpha_{kj} p^T g_j(y_j)$$

$$(P): \max_{y_j \in Y_j} p^T g_j(y_j)$$

$$(M): \max_{p \geq 0} p^T \left(\sum_k x_k - \sum_k \omega_k - \sum_j g_j(y_j) \right) \text{ s.t. } \sum_l p_l = 1$$

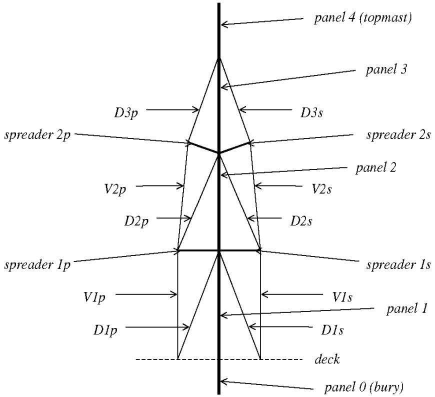
This is an example of a MOPEC

Optimal Yacht Rig Design

- Current mast design trends use a large primary spar that is supported laterally by a set of tension and compression members, generally termed the rig
- Reduction in either the weight of the rig or the height of the VCG will improve performance
- Design must work well under a variety of weather conditions

Complementarity feature

- Stays are tension only members (in practice) - Hookes Law
- When tensile load becomes zero, the stay goes slack (low material stiffness)
- $0 \geq s \perp s - k\delta \leq 0$
  - s axial load
  - k member spring constant
  - δ member extension
- Either $s_i = 0$ or $s_i = k\delta_i$



EMP: MPCC: complementarity constraints

$$\begin{aligned} \min_{x,y} \quad & f(x,y) \\ \text{s.t.} \quad & g(x,y) \leq 0, \\ & 0 \leq y \perp h(x,y) \geq 0 \end{aligned}$$

- g, h model "engineering" expertise: finite elements, etc
- $\perp$ models complementarity, disjunctions
- Complementarity "$\perp$" constraints available in AIMMS, AMPL and GAMS

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- NLPEC: use the convert tool to automatically reformulate as a parameteric sequence of NLP's
- Solution by repeated use of standard NLP software
  - Problems solvable, local solutions, hard
  - Southern Spars Company (NZ): improved from 5-0 to 5-2 in America's Cup!

MPCC approaches

- Implicit: $\min_x f(x, y(x))$
- Auxiliary variables: $s = h(x, y)$
- NCP functions: $\Phi(y, s) = 0$
- Smoothing: $\Phi_\mu(y, s) = 0$
- Penalization: $\min f(x, y) + \mu y^T s$
- Relaxation: $y^T s \leq \mu$

Different problem classes require different solution techniques

Parametric algorithm: NLPEC

- Reftype mult
- Aggregate none
- Constraint inequality
- Initmu $= 0.01$
- Numsolves $= 5$
- Updatefac $= 0.1$
- Finalmu $= 0$

A solution procedure whereby μ is successively reduced can be implemented as a simple option file to NLPEC

$$\begin{aligned} \min_{x \in \mathbf{R}^n, y \in \mathbf{R}^m, s \in \mathbf{R}^m} \quad & f(x,y) \\ \text{s.t.} \quad & g(x,y) \leq 0 \\ & s = h(x,y) \\ & y \geq 0, s \geq 0 \\ & y_i s_i \leq \mu, \quad i = 1, \ldots, m. \end{aligned}$$

Note that a series of approximate problems are produced, parameterized by $\mu > 0$; each of these approximate problems have stronger theoretical properties than the problem with $\mu = 0$

Bilevel Program (Stackelberg)

- Assumes one leader firm, the rest follow
- Leader firm optimizes subject to expected follower behavior
- Follower firms act in a Nash manner
- All firms are price-takers in transport and demand

EMP info file

bilevel obj('one') vars('one') eqns('one')
max obj('two') vars('two') eqns('two')
max obj('three') vars('three') eqns('three')
vi tcDef tc
vi pricedef price

EMP = bilevel $\Longrightarrow$ MPEC $\Longrightarrow$ (via NLPEC) NLP(μ)

Hierarchical models

- Bilevel programs:

$$\begin{array}{ll} \min_{x^*,y^*} & f(x^*,y^*) \\ \text{s.t.} & g(x^*,y^*) \leq 0, \\ & y^* \text{ solves } \min_y v(x^*,y) \text{ s.t. } h(x^*,y) \leq 0 \end{array}$$

- model bilev /deff,defg,defv,defh/;
  empinfo: bilevel min v y defv defh
- EMP tool automatically creates the MPCC

$$\begin{array}{lll} \min_{x^*,y^*,\lambda} & f(x^*,y^*) & \\ \text{s.t.} & g(x^*,y^*) \leq 0, & \\ & 0 \leq \nabla v(x^*,y^*) + \lambda^T \nabla h(x^*,y^*) & \perp y^* \geq 0 \\ & 0 \leq -h(x^*,y^*) & \perp \lambda \geq 0 \end{array}$$

Biological Pathway Models

Opt knock (a bilevel program)

max	bioengineering objective (through gene knockouts)		
s.t.	max cellular objective (over fluxes)		
	s.t.	fixed substrate uptake	
		network stoichiometry	
		blocked reactions (from outer problem)	
	number of knockouts $\leq$ limit		

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Also prediction models of the form:

$$\min \sum_{i,j} \|w_i - v_j\|$$
$$\text{s.t. } Sv = w$$
$$-\bar{v}_L \leq v \leq \bar{v}_U, \; w_j = \bar{w}_j$$

Can be modeled as an SOCP.

The overall scheme!

- Collection of algebraic equations
- Form a bilevel program via emp
- EMP tool automatically creates the MPCC (model transformation)
- NLPEC tool automatically creates (a series of) NLP models (model transformation)
- GAMS automatically rewrites NLP models for global solution via BARON (model transformation)
- Is this global? What's the hitch?

The overall scheme!

- Collection of algebraic equations
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- Is this global? What's the hitch?
- Note that heirarchical structure is available to solvers for analysis or utilization

Variational inequality (VI)

Given

a continuous function $F : \mathbf{R}^n \to \mathbf{R}^n$

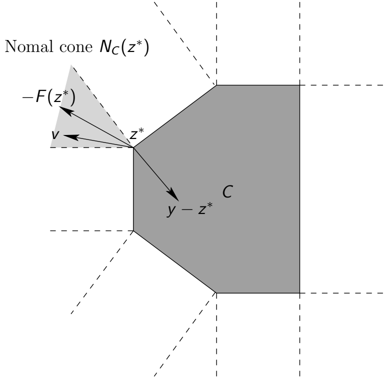
a closed convex set C

Find a $z^* \in C$ satisfying

$$\langle F(z^*), y - z^* \rangle \geq 0, \ \forall y \in C$$

$(\Longleftrightarrow) \ -F(z^*) \in N_C(z^*)$

$N_C(z^*) = \{v \mid \langle v, y - z^* \rangle \leq 0, \ \forall y \in C\}$



Solving a VI is equivalent to solving the generalized equation (GE)

$$0 \in F(z) + N_C(z) \qquad \text{(GE)}$$

Variational inequalities

- Find $z \in C$ such that

$$0 \in F(z) + \mathcal{N}_C(z)$$

- Many applications where F is not the derivative of some f
- model vi / F, g /;
  empinfo: vi F z g
- Convert problem into complementarity problem by introducing multipliers on representation of C
- Can now do MPEC (as opposed to MPCC)!
- Projection algorithms, robustness (evaluate F only at points in X)

What else can be modeled using complementarity

- $\min(F(x), G(x)) \leq y$
- $\min(F_1(x), F_2(x), \ldots, F_m(x)) = 0$
- kth largest of $\{F_1(x), F_2(x), \ldots, F_m(x)\} = 0$
- Switch off: $g(x)h(x) \leq 0$, $h(x) \geq 0$

Conclusions

- Modern optimization within applications requires multiple model formats, computational tools and sophisticated solvers
- EMP model type is clear and extensible, additional structure available to solver
- Extended Mathematical Programming available within the GAMS modeling system
- Able to pass additional (structure) information to solvers
- Embedded optimization models automatically reformulated for appropriate solution engine
- Exploit structure in solvers
- Extend application usage further