An Extended Mathematical Programming Framework

Michael C. Ferris

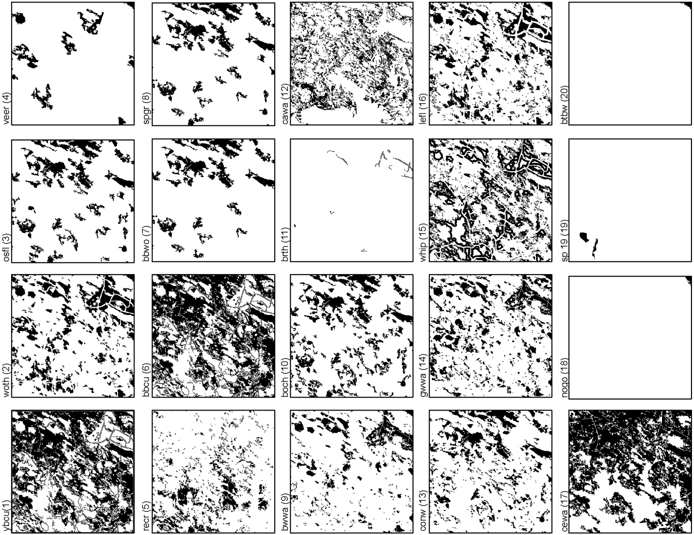
University of Wisconsin, Madison

SIAM National Meeting, Denver: July 6, 2009

Northern Wisconsin: Golden Winged Warbler

Golden-winged Warbler. Species maps are 14,309 columns by 11437 rows.

Northern Wisconsin: There's More



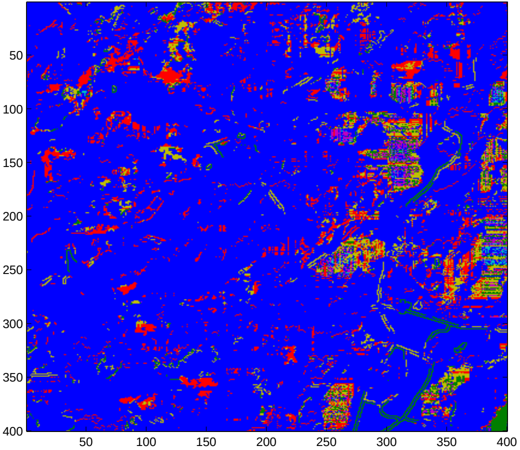
Some species require complementary habitats

The specs

- GIS data (77 million pixels with indicator that land type in 30 by 30 meter square can support species)
- Incompatibility matrix (cannot have certain species co-habiting)
- Threshold values (how much land required)
- Compact regions, limit total land conserved!

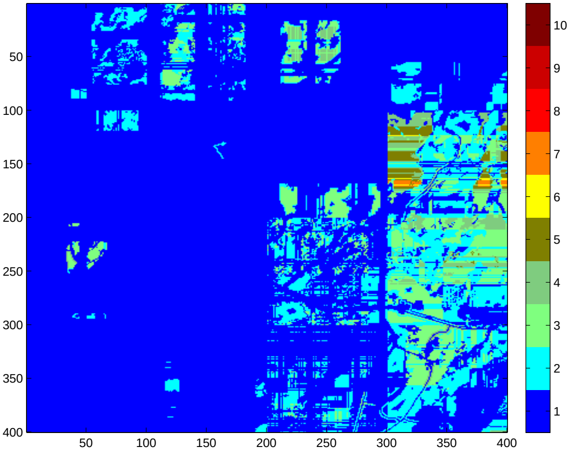
$$x_{s,i,j} = \begin{cases} 1 & \text{if } (i,j) \text{ conserved for species } s \\ 0 & \text{else} \end{cases}$$

A poor solution



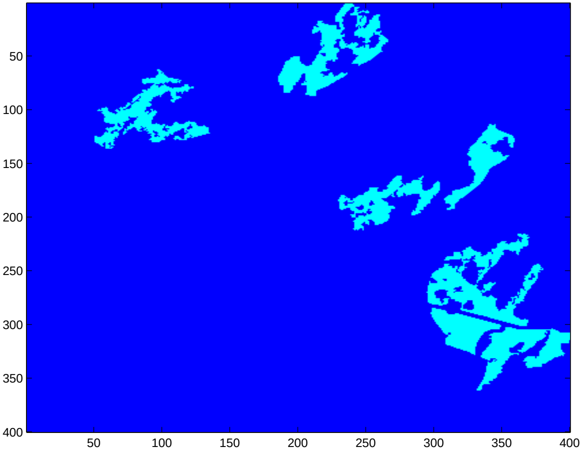
Mip solution needs enormous time, does not get compact boxes or multiple use [Use CPLEX with Matlab tool to visualize solution]

Partioning helps



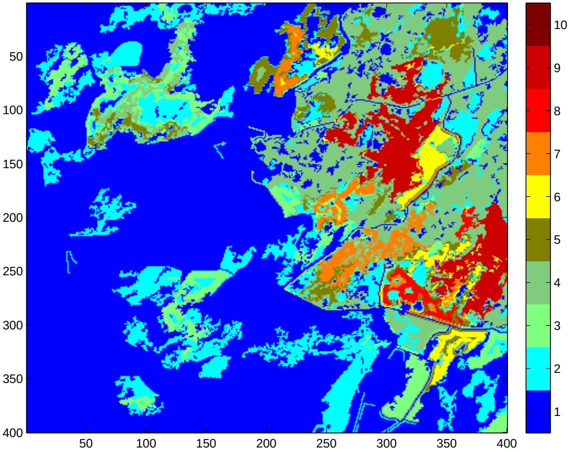
Split domain into multiple subsets. Solve in parallel (using Condor and GAMS/Grid).

Alternative approach



Data reduction (via largest connected components). Solve for these in parallel using network simplex.

Reassembling solution



Choose clusters for each species; ensure complementary habitat is satisfied; optimize multiple species overlap

Mathematical programming: modeling

- Optimization models improve understanding of underlying systems and facilitate operational/strategic improvements under resource constraints
- Application use requires multiple models, tools and solvers
- Modeling systems enable application interfacing, prototyping of optimization capability
- Problem format is old/traditional

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

  - Support for integer, sos, semicontinuous variables
  - Limited support for logical constructs
  - Support for complementarity constraints

Complementarity Problems in Economics (MCP)

- p represents prices, x represents activity levels
- System model: given prices, (agent) i determines activities x_i

$$G_i(x_i, x_{-i}, p) = 0$$

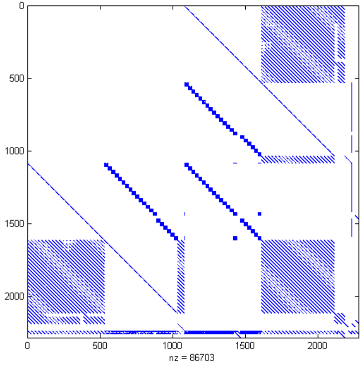
  x_{-i} are the decisions of other agents.
- Walras Law: market clearing

$$0 \leq S(x,p) - D(x,p) \perp p \geq 0$$

- Key difference: optimization assumes you control the complete system
- Complementarity solver (e.g. PATH) determines what activities run, and who produces what

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



EMP(i): Embedded models

- 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
  vifunc H y dualvar λ defg
- EMP tool automatically creates an MCP

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

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)
  vifunc 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)

General Equilibrium models

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

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

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

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

General Equilibrium models

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

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

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

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

Can reformulate as embedded problem (Ermoliev et al):

$$\max_{x \in X, y \in Y} \quad \sum_k \frac{t_k}{\beta_k} \log U_k(x_k)$$

$$\text{s.t. } \sum_k x_k \leq \sum_k \omega_k + \sum_j g_j(y_j)$$

$t_k = i_k(y, p)$ where p is multiplier on NLP constraint

Sequential Joint Maximization

$$\max_{x \in X, y \in Y} \quad \sum_k \frac{t_k}{\beta_k} \log U_k(x_k)$$

$$\text{s.t.} \quad \sum_k x_k \leq \sum_k \omega_k + \sum_j g_j(y_j)$$

$t_k = i_k(y, p)$ where p is multiplier on NLP constraint

- Embedded model often solves faster as an MCP than the original MCP from Nash game
- Can exploit structure to improve computational performance further

Sequential Joint Maximization

$$\max_{x \in X, y \in Y} \quad \sum_k \frac{t_k}{\beta_k} \log U_k(x_k)$$
$$\text{s.t.} \quad \sum_k x_k \leq \sum_k \omega_k + \sum_j g_j(y_j)$$

$t_k = i_k(y, p)$ where p is multiplier on NLP constraint

- Embedded model often solves faster as an MCP than the original MCP from Nash game
- Can exploit structure to improve computational performance further
- Can iterate (on m) $t_k^m = i_k(y^m, p^m)$, and solve sequence of NLP's

$$\max_{x \in X, y \in Y} \quad \sum_k \frac{t_k^m}{\beta_k} \log U_k(x_k)$$
$$\text{s.t.} \quad \sum_k x_k \leq \sum_k \omega_k + \sum_j g_j(y_j)$$

EMP(ii): Heirarchical models

- Bilevel programs:

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

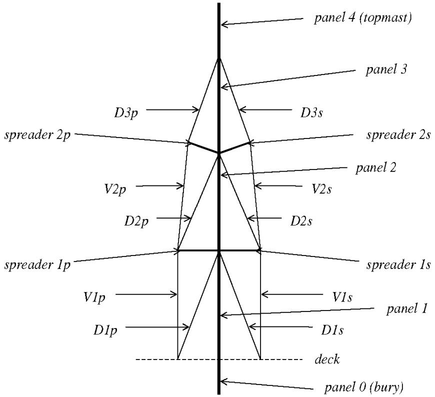
- model bilev /deff,defg,defv,defh/;
  empinfo: bilevel min v y defh
- EMP tool automatically creates the MPCC
- Note that heirarchical structure is available to solvers for decomposition approaches

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 $s_i = k\delta_i$



MPCC: complementarity constraints

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

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

MPCC: complementarity constraints

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

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

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	

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

Also prediction models of the form:

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

Can be modeled as an SOCP.

EMP(iii): Variational inequalities

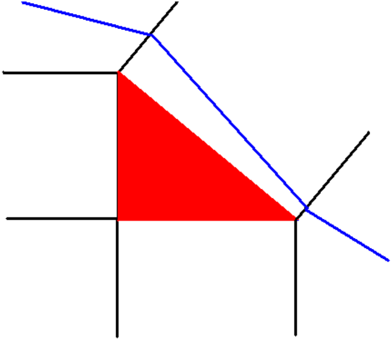
- Find $z \in C$ such that

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

- Many applications where F is not the derivative of some f
- model vi / F, g /;
  empinfo: vifunc F z
- 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 C)

The Path Idea

- Start in cell that has interior (face is an extreme point)
- Move towards a zero of affine map in cell
- Update direction when hit boundary (pivot)
- Solves or determines infeasible if M is copositive-plus on rec(C)
- Solves 2-person bimatrix games, 3-person games too, but these are nonlinear



But algorithm has exponential complexity (von Stengel et al)

Extensions and Computational Results

- Embed AVI solver in a Newton Method - each Newton step solves an AVI
- Compare performance of PathAVI with PATH on equivalent LCP
- PATH the most widely used code for solving MCP
- AVIs constructed to have solution with $M_{n \times n}$ symmetric indefinite

	PathAVI		*PATH*	
Size (m,n)	*Resid*	*Iter*	*Resid*	*Iter*
$(180, 60)$	3×10^{-14}	193	0.9	10176
$(360, 120)$	3×10^{-14}	1516	2.0	10594

- 2 - 10x speedup in Matlab using sparse LU instead of QR
- 2 - 10x speedup in C using sparse LU updates

EMP(iv): Other new types of constraints

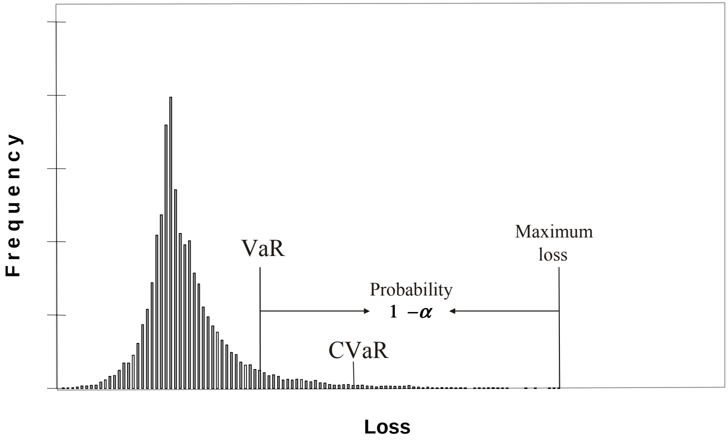
- range constraints $L \leq Ax - b \leq U$
- indicator constraints
- disjunctive programming
- soft constraints
- rewards and penalties
- robust programming (probability constraints, stochastics)

$$f(x, \xi) \leq 0, \forall \xi \in \mathcal{U}$$

- conic programming $a_i^T x - b_i \in K_i$

These constraints can be reformulated using EMP

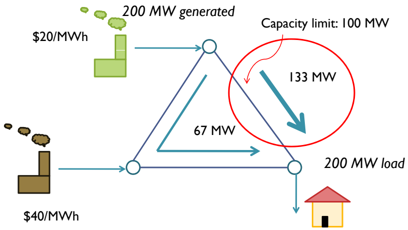
CVaR constraints: mean excess dose (radiotherapy)



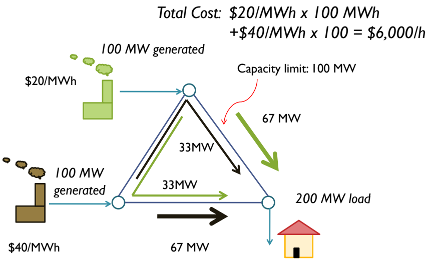
Move mean of tail to the left!

Transmission switching

Opening lines in a transmission network can reduce cost



(a) Infeasible due to line capacity



(b) Feasible dispatch

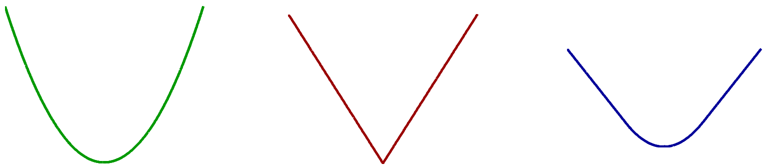
Need to use expensive generator due to power flow characteristics and capacity limit on transmission line

Use EMP to facilitate the disjunctive constraints (several equivalent formulations, including LPEC)

EMP(v): Extended nonlinear programs

$$\min_{x \in X} f_0(x) + \theta(f_1(x), \ldots, f_m(x))$$

Examples of different θ



least squares, absolute value, Huber function

Solution reformulations are very different

Huber function used in robust statistics.

Key point for our work (Rockafellar)

- For many interesting choices of θ, the conjugate θ^* is of the form $k(y^*) + I_{Y^*}(y^*)$, where k is nice (e.g., C^2) and Y^* is closed convex, as is X; often these have simple structure
- Then we can deal with this problem by solving first-order conditions for a saddle point problem over $X \times Y^*$ rather than as a nonsmooth minimization problem
- The new feature here is implementation and solution within the GAMS modeling language framework, which produces a tool usable without advanced knowledge in convex analysis and without cumbersome "hand tailoring" to accommodate different penalizations [Ferris, Dirkse, Jagla, and Meeraus 2008]
- This makes the theoretical benefits accessible to users from a wide variety of different fields

Solution Procedures

- Solution uses reformulation - one way: first order conditions

$$\text{VI}\left(\begin{bmatrix} \nabla_x \mathcal{L}(x,y) \\ -\nabla_y \mathcal{L}(x,y) \end{bmatrix}, X \times Y\right)$$

based on extended form of the Lagrangian:

$$\mathcal{L}(x,y) = f_0(x) + \sum_{i=1}^{m} y_i f_i(x) - k(y)$$

- EMP: allows "annotation" of constraints to facilitate library of different θ functions to be applied
- EMP tool automatically creates an MCP (or a smooth NLP)
- Available!
- To do: extend solvers to exploit X and Y beyond simple bound sets

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
- System can easily formulate and solve second order cone programs, risk measures, robust optimization, soft constraints via piecewise linear penalization (with strong supporting theory)
- Embedded optimization models automatically reformulated for appropriate solution engine
- Exploit structure in solvers
- Extend application usage further