Optimization, Wisconsin Institutes of Discovery, and SoccerManager.com: Is there a link?

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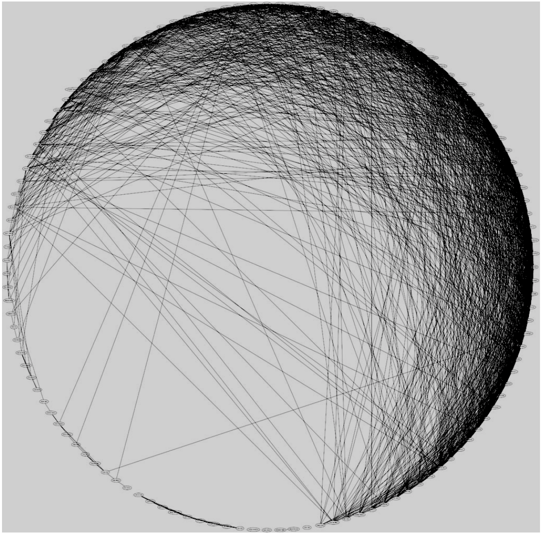
Innovations Seminar, Madison: March 10, 2010
Collaboration with Jeff Linderoth, Jim Luedtke, Ben Recht, Steve Wright and others.

Facebook: a friend wheel



- visual representation of relationships between the friends of any one person
- constructed by placing friends equidistant from each other on circumference of circle
- line segments are drawn between each point if those people are friends with each other
- Order to reduce amount of ink used

QAP (Koopmans and Beckman)

Given n facilities $\{f_1, \ldots, f_n\}$, n locations $\{l_1, \ldots, l_n\}$:
Determine to which location each facility must be assigned
$p : \{1, \ldots, n\} \mapsto \{1, \ldots, n\}$ is an assignment whose cost is

$$c(p) = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{i,j} d_{p(i),p(j)}$$

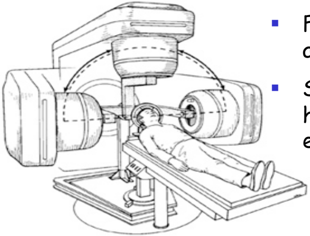
$$\text{QAP} : \min c(p) \text{ subject to } p \in \Pi_n$$

QAP is known to be strongly NP-hard

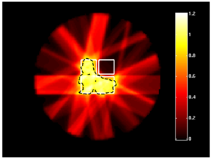
- n is the number of friends of a given individual
- $w_{i,j} = 1$ if i is a friend of j, and 0 otherwise
- $d_{r,s}$ is the distance from location r on the circle circumference to location s

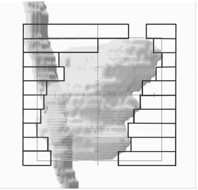
Cancer treatment

Conformal Radiotherapy

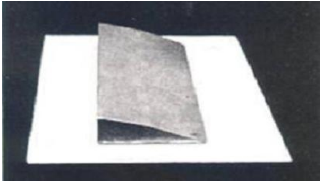


- Fire from multiple angles
- Superposition allows high dose in target, low elsewhere





- Beam shaping via collimator
- Gradient across beam via wedges



Extended Mathematical Programs

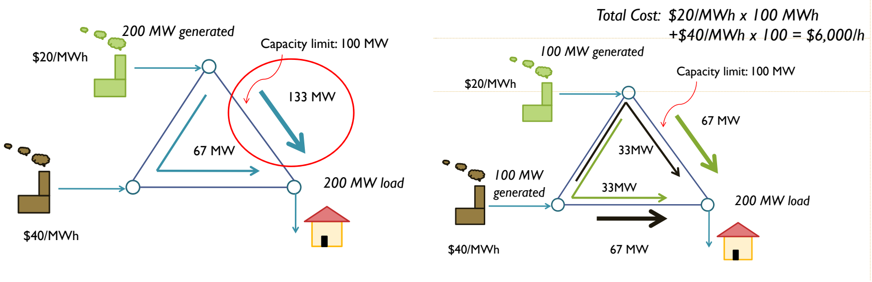
- Optimization models improve understanding of underlying systems and facilitate operational/strategic improvements under resource constraints
- Problem format is old/traditional

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

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

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

Determine which subset of lines to open at any given hour

The basic model

$$\begin{array}{lll} \min_{g,f,\theta} & c^T g & \text{generation cost} \\ \text{s.t.} & g - d = Af, f = BA^T\theta & A \text{ is node-arc incidence} \\ & \bar{\theta}_L \leq \theta \leq \bar{\theta}_U & \text{bus angle constraints} \\ & \bar{g}_L \leq g \leq \bar{g}_U & \text{generator capacities} \\ & \bar{f}_L \leq f \leq \bar{f}_U & \text{transmission capacities} \end{array}$$

with transmission switching (within a smart grid technology) we modify as:

$$\begin{array}{llll} \min_{g,f,\theta} & c^T g & & \\ \text{s.t.} & g - d = Af & & \\ & \bar{\theta}_L \leq \theta \leq \bar{\theta}_U & & \\ & \bar{g}_L \leq g \leq \bar{g}_U & & \\ \text{either} & f_i = (BA^T\theta)_i, \bar{f}_{L,i} \leq f_i \leq \bar{f}_{U,i} & \text{if } i \text{ closed} \\ \text{or} & f_i = 0 & \text{if } i \text{ open} \end{array}$$

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

Issues

- Models are critical to making hard business decisions
- Model needs enough detail so solutions are realistic
- Computation is hard - many possibilities!
- Need large scale solvers
- How to obtain data, get data into model, verify data integrity - more tools and models
- Interplay between model, data and decision maker is critical
- Visualization helps in motivating the answers

Nash equilibria: modeling competition

- 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:

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

- Can solve large instances of these problems
- Model competing agents, etc

EMP(ii): 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

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

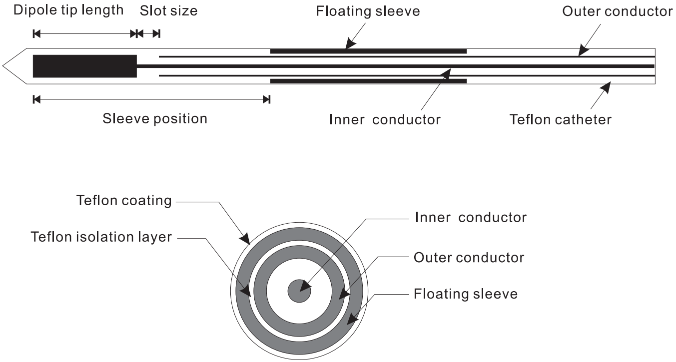
Issues

- New model paradigms available
- Models with continuous, discrete, categorical variables necessary
- Size matters
- Can solve realistic scale instances
- Data collection remains hard - new tools help
- Models are critical to making hard decisions

Simulation-based optimization problems

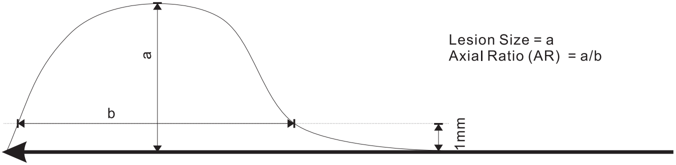
- Computer simulations are used as substitutes to evaluate complex real systems.
- Simulations are widely applied in epidemiology, engineering design, manufacturing, supply chain management, medical treatment and many other fields.
- The goal: Optimization finds the best values of the decision variables (design parameters or controls) that minimize some performance measure of the simulation.
- Other applications: calibration, design optimization, inverse optimization

Design a coaxial antenna for hepatic tumor ablation



Simulation of the electromagnetic radiation profile

Finite element models (COMSOL MultiPhysics v3.2) are used to generate the electromagnetic (EM) radiation fields in liver given a particular design



Metric	Measure of	Goal
Lesion radius	Size of lesion in radial direction	Maximize
Axial ratio	Proximity of lesion shape to a sphere	Fit to 0.5
S_{11}	Tail reflection of antenna	Minimize

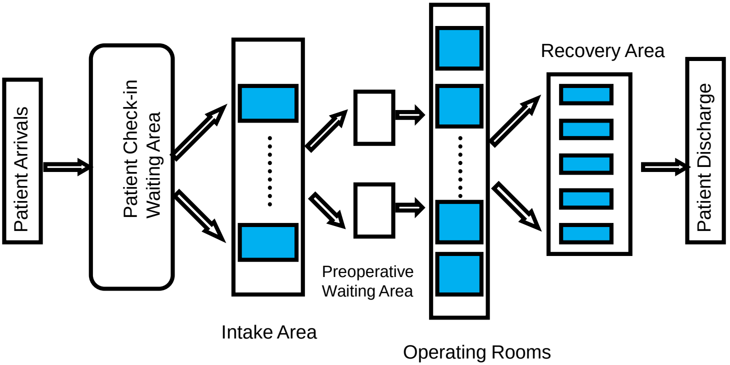
Issues

- Complex interactions of different types of models
- Large scale solution, in "real time"
- Models to aid in data collection/verification
- Uncertainties in data and model
- Moving effective models into practice - getting the checks done!

Scheduling surgeries: Denton and Miller

- Patient Intake: administrative activities, pre-surgery exam, gowning, site prep, anesthetic
- Surgery: incision, one or multiple procedures, pathology, closing
- Recovery: post-anesthesia care unit (PACU), ICU, hospital bed

Scheduling surgeries



Large scale interacting system: optimization can improve operation

Scheduling systems: a stochastic optimization problem

- Operating rooms (ORs): largest cost center and greatest source of revenue
- Uncertainty in surgery durations means scheduling of ORs can be very challenging
- Results in late starts, costs for overtime staffing
- Stochastic optimization model hedges against the uncertainty in surgery durations
- Simple sequencing rule based on surgery duration variance could be used to generate substantial reductions in total surgeon and OR team waiting, OR idling, and overtime cost

Stochastic Optimization Model

$$\min\{\underbrace{\sum_{i=1}^{n} c_i^w E_{\mathbf{Z}}[w_i]}_{\text{Cost of Waiting}} + \underbrace{\sum_{i=1}^{n} c^s E_{\mathbf{Z}}[s_i]}_{\text{Cost of Idling}} + \underbrace{c^L E_{\mathbf{Z}}[l]}_{\text{Cost of Overtime}}\}$$

$$w_i = \max(w_{i-1} + Z_{i-1} - x_{i-1}, 0),\ i = 1,..,n-1$$

$$s_i = \max(-w_{i-1} - Z_{i-1} + x_{i-1}, 0),\ i = 1,...,n-1$$

$$l = \max(w_n + Z_n + \sum_{i=1}^{n-1} x_i - d, 0)$$

Issues

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- Model needs enough detail so solutions are realistic
- Computation is hard - many possibilities!
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- Visualization helps in motivating the answers
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EMP(iii): Heirarchical models

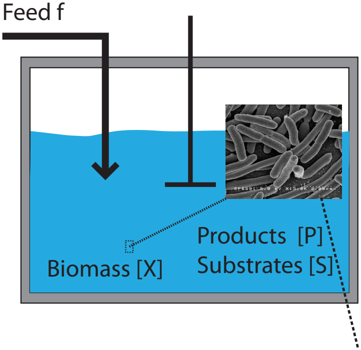
- Bilevel programs:

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

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

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

Large scale example: bioreactor



from: Rocky Mountain Laboratories, NIAID, NIH

- Challenge: Formulate an optimization problem that allows the estimation of the dynamic changes in intracellular fluxes based on measured external bioreactor concentrations
- Approach: Use existing constraint-based stoichiometric models of the cellular metabolism to formulate a bilevel dynamic optimization problem

  run time: **days**

  most industrial applications with biological processes, such as
  - fermentation
  - biochemical production
  - pharmaceutical protein production

Dynamic model of a bioreactor

Assumptions: well stirred, one phase!
Biomass:

$$\frac{d[X]}{dt} = (\mu - \frac{f}{V})[X]$$

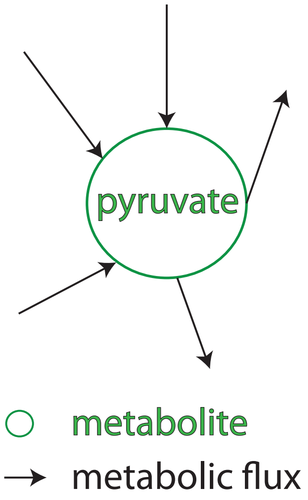
μ: growth rate
Product [P] or substrate [S] concentrations [C]:

$$\frac{d[C]}{dt} = q_{[C]}[X] + (f[C]^{\text{feed}} - \frac{f}{V}[C])$$

$q_{[C]}$: specific uptake or production rate of [C].
Volume V:

$$\frac{d[V]}{dt} = f$$

Stoichiometric constraints



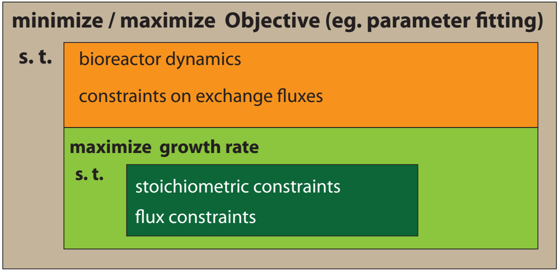
The stochiometry of the cellular metabolism is described by a stoichiometric matrix S.
S constrains steady-state flux distributions.

$$S \cdot v = 0$$

The above relation can be used in a linear programming problem, which maximizes for a cellular objective function
(**flux balance analysis).**

Dynamic optimization

Approach:
The different timescales of the metabolism (**fast**) and the reactor growth (**slow**), allows to assume steady-state for the metabolism.



Different mathematical programming techniques are used to transform the problem to a nonlinear program. The differential equations are transformed into nonlinear constraints using collocation methods.

Soccer Manager Analogy

- Optimize: selection of formation, who plays and tactics concurrently
- Equilibrium: competing agents, try to determine long term strategy
- Uncertainty: how to deal with uncertainty in function evaluations, underlying model parameters
- Heirarchical: how to get people to play (and sell adverts)
- Data mining: how to update your team via the transfer market (use of large amounts of ratings data, etc)

Conclusions

- Sparse Optimization/Data mining applications next week (Recht)
- Optimization models effective for large scale planning/operations
- Design optimization possible in conjunction with "expert" simulations
- Must treat uncertainties both in data and model
- New model paradigms (e.g. complementarity, conic programming, stochastic programming) effective for treating uncertainties and competition
- Engaged teams (including embedded optimizers) are most effective for timely, relevant solutions