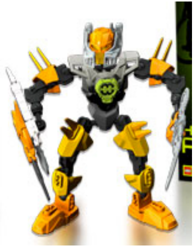

Why model?

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Math Bio III: Modeling
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Quote from Wikipedia: modeling

- A mathematical model is a description of a system using mathematical concepts and language.
- Mathematical models are used in:
  - the natural sciences (such as physics, biology, earth science, meteorology)
  - engineering disciplines (e.g. computer science, artificial intelligence)
  - in the social sciences (such as economics, psychology, sociology and political science)
- Physicists, engineers, statisticians, operations research analysts and economists use mathematical models extensively
- Lack of agreement between theoretical mathematical models and experimental measurements often leads to important advances as better theories are developed

Building mathematical models

- How to model: pencil and paper, excel, Matlab, R, python, ...

  - Linear vs nonlinear
  - Deterministic vs probabilistic
  - Static vs dynamic (differential or difference equations)
  - Discrete vs continuous
- Other issues: Large scale, stochasticity, data (rich and sparse)
- Must be able to model my problem easily/naturally
- Abstract/simplify:
  - Variables: input/output, state, decision, exogenous, random...
  - Exogenous = data/parameters
  - Objective/constraints
  - Black box/white box
  - Subjective information, complexity, training, evaluation
- Just solving a single problem isn't the real value of modeling: optimization finds "holes" in the model

Why model?

- to understand (descriptive process, validate principles and/or explore underlying mechanisms)
- to predict (and/or discover new system features)
- to combine (engaging groups in a decision, make decisions, operate/control a system of interacting parts)
- to design (strategic planning, investigate new designs, can they be economical given price of raw materials, production process, etc)

Understand: Sudoku Model

The aim of this puzzle is to enter a numerical digit from 1 through 9 in each cell of a 9x9 grid made up of 3x3 subgrids (called "regions"), starting with various digits given in some cells (the "givens"). Each row, column, and region must contain only one instance of each numeral.

- r, c, v, k (rows, cols, vals, regions) range from 1 to 9
- binary variables $x_{r,c,v}$

row entries unique: $$\sum_c x_{r,c,v} = 1, \quad \forall r, v$$

col entries unique: $$\sum_r x_{r,c,v} = 1, \quad \forall c, v$$

one val per cell: $$\sum_v x_{r,c,v} = 1, \quad \forall r, c$$

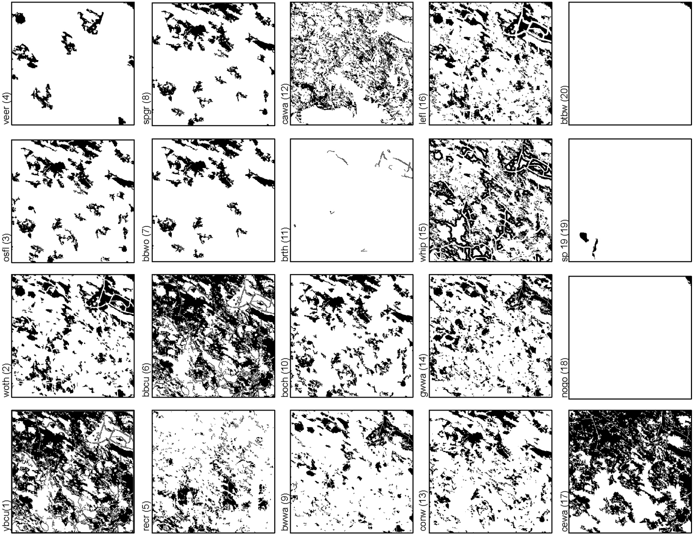
one val per region: $$\sum_{(r,c)\in\mathcal{R}_k} x_{r,c,v} = 1, \quad \forall k, v$$

Here $\mathcal{R}_k$ runs over all the k "regions"

Understand: Northern Wisconsin - Conservation

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

Northern Wisconsin: There's More



Some species require complementary habitats

Understand: abstraction

- 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!

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

- Example of an assignment model (e.g. Sudoku, etc)

$$x_{s,i,j} + x_{t,i,j} \leq 1, \text{ if } (s,t) \in \mathcal{I}$$

Many others...challenges and opportunities

- (Stochastic) differential equations
- Multiscale modeling and simulation
- Nonlinear optimization, including parameter estimation and inverse problems
- ...

Challenges:

- Abstraction/simplification/key drivers
- Size: (spatial/temporal/decision hierarchical) traditional approaches have proven inadequate, even with the largest supercomputers, due to range of scales and prohibitively large number of variables
- Nature of data: sparse, rich, uncertain

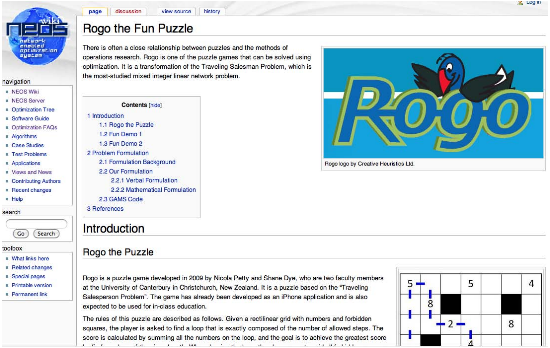
Opportunities: facilitates prediction, improved operation, strategic behavior and design

I: Show me on a problem like mine

- Repeated solutions of multiple (different) problems enables "understanding" of the solution space (or sensitivity)
- NEOS wiki (www.neos-guide.org) or try out NEOS solvers (www.neos-solvers.org) for extensive examples

Building a class of case studies:

- JAVA api to NEOS
- Web description of problem
- Solution on NEOS
- Ability to modify and resolve
- Comparison of results



Predict: tradeoff accuracy and simple structure

Many models from statistics: e.g. regression:

$$\min_x \|Ax - y\|^2$$

Additional structure: Compressed sensing: sparse signal to account for y

$$\min_x \|Ax - y\|_2^2 \text{ s.t. } \|x\|_0 \leq c$$

Regularized regression:

$$\min_x \|Ax - y\|_2^2 + \alpha \|x\|_1$$

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Machine learning: SVM for classification

$$\min_{w,\xi,\gamma} \sum_i \xi_i + \frac{\alpha}{2} \|w\|^2 \text{ s.t. } D(Aw - \gamma 1) \geq 1 - \xi$$

General model:

$$\min_{x \in X} E(x) + \alpha S(x)$$

X are constraints, E measures "error" and S penalizes bad structure

Image denoising (Wright)

Rudin-Osher-Fatemi (ROF) model (ℓ_2-TV). Given a domain $\Omega \subset \mathbb{R}^2$ and an observed image $f : \Omega \to \mathbb{R}$, seek a restored image $u : \Omega \to \mathbb{R}$ that preserves edges while removing noise. The regularized image u can typically be stored more economically. Seek to "minimize" both

- $\|u - f\|_2$ and
- the total-variation (TV) norm $\int_\Omega |\nabla u| \, dx$

Use constrained formulations, or a weighting of the two objectives:

$$\min_u P(u) := \|u - f\|_2^2 + \alpha \int_\Omega |\nabla u| \, dx$$

The minimizing u tends to have regions in which u is constant ($\nabla u = 0$). More "cartoon-like" when α is large.

Original, noisy, denoised (tol $= 10^{-2}, 10^{-4}$)

Many others...challenges and opportunities

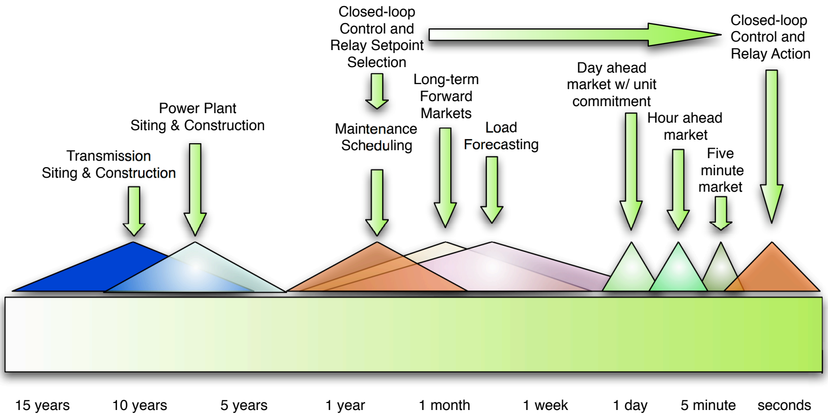
- Matrix completion (e.g. Netflix prize, covariance estimation)
- Machine learning: supervised, unsupervised, semi-supervised, reinforcement, and representation learning
- Probabilistic graphical modeling
- Stochastic processes, statistics, uncertainty quantification
- ...

Challenges:

- Terminology issues: active learning = optimal experimental design, reinforcement learning = approximate dynamic programming
- Incorporating domain knowledge into models
- Size and speed for realistic application settings (data sparse and rich environments)
- Online settings, stochastics

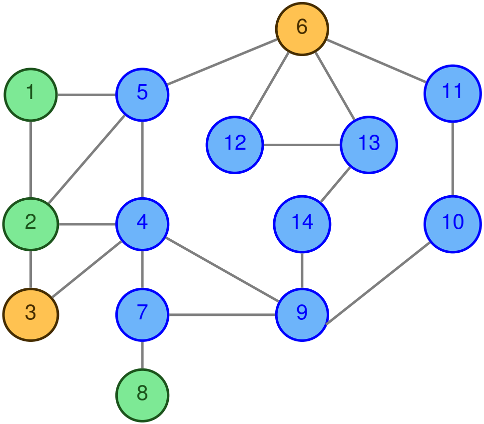
Opportunities: to exploit theory and structure to generate much more effective algorithms, generalizability, learning behavior

Combine: Representative decision-making timescales in electric power systems



Combine: Transmission Line Expansion Model

$$\min_{x \in X} \sum_{\omega} \pi_\omega \sum_{i \in N} d_i^\omega p_i^\omega(x)$$



- Nonlinear system to describe power flows over (large) network
- Multiple time scales
- Dynamics (bidding, failures, ramping, etc)
- Uncertainty (demand, weather, expansion, etc)
- $p_i^\omega(x)$: Price (LMP) at i in scenario ω as a function of x
- Use other models to construct approximation of $p_i^\omega(x)$

Stochastic competing agent models (with Wets)

- Competing agents (consumers, or generators in energy market)
- Each agent maximizes objective independently (utility)
- Market prices are function of all agents activities
- Additional twist: model must "hedge" against uncertainty
- Facilitated by allowing contracts bought now, for goods delivered later
- Conceptually allows to transfer goods from one period to another (provides wealth retention or pricing of ancillliary services in energy market)
- Can investigate new instruments to move to system optimal solutions from equilibrium (or market) solutions

Many others ... challenges and opportunities

Model predictive control, PDE constrained optimization,...

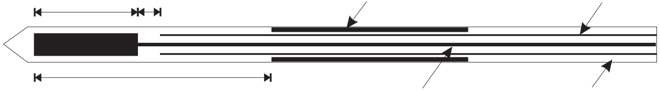
Challenges:

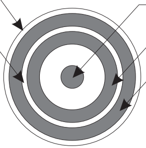
- Size: monster model unable to exploit underlying structure and provide solution quality guarantees
- Stochasticity: How to deal with noisy, sparse, incomplete or inconsistent data and models
- How to coupling collections of (sub)-models: design of interfaces

Opportunities:

- appropriate detail and consistency of sub-model formulation
- ability for individual subproblem solution verification and engagement of decision makers
- ability to treat uncertainty by stochastic and robust optimization at submodel level and with evolving resolution
- ability to solve submodels to global optimality

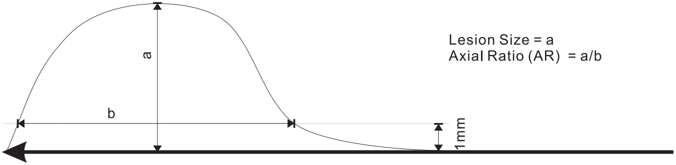
Design a coaxial antenna for hepatic tumor ablation





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



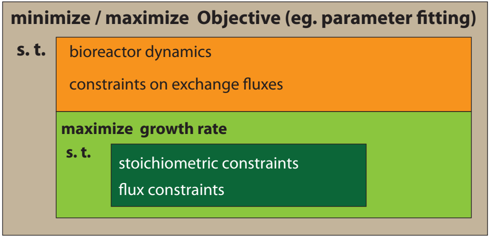
Metric	Measure of	Goal
Lesion radius	Size of lesion in radial direction	Maximize
Axial ratio	Proximity of lesion shape to a sphere	Fit to 0.5
S_{11}	Tail reflection of antenna	Minimize

Biological Hierarchical Models

I: 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

II: Bio-reactor dynamics:



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.

Challenges and opportunities

Challenges:

- Engaging the designer, collecting appropriate data
- Incorporating domain design tools into general (optimization) framework
- Modeling human behavior
- Determining appropriate model: Linear vs nonlinear, deterministic vs probabilistic, static vs dynamic, discrete vs continuous (smooth or nonsmooth)

Opportunities:

- Enormous: medical device design, drug design, radiation therapy machine and planning, bio-engineering
- economic instrument and policy design, smart grid, electric batteries, environmental remediation, offshore drilling and wind farms
- recommender systems, fabrication, election district gerrymandering