Computational Discovery of Scientific Models: Guiding Search with Knowledge and Data

Pat Langley

Department of Computer Science
University of Auckland
Private Bag 92019
Auckland 1142 NZ

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The Scientific Enterprise

Science is a unique collection of activities distinguished by some distinctive characteristics:

- Systematic collection and analysis of *observations*
- Formal statement of *theories*, *laws*, and *models*
- Use of the latter to *explain* and *predict* the former
- Use of observations to *evaluate* theorized structures

Moreover, science can apply these ideas to any area of enquiry, in principle even to *science itself*.

Philosophy of Science

One discipline – *philosophy of science* – has studied science itself since the 19th Century, including the:

- character of scientific observations and experiments
- structure of scientific theories, laws, and models
- nature of scientific explanations and predictions
- evaluation of scientific theories, models, and laws

However, philosophers of science have typically avoided one important topic: *scientific discovery*.

Mystical Views of Scientific Discovery

Philosophers largely ignored scientific discovery, believing it to be immune to logical analysis. Popper (1934) wrote:

> *The initial stage, the act of conceiving or inventing a theory, seems to me neither to call for logical analysis nor to be susceptible of it … My view may be expressed by saying that every discovery contains an 'irrational element', or 'a creative intuition'…*

He was not alone in this view. Hempel and many others believed discovery was inherently irrational and beyond understanding.

However, advances made by two fields – *cognitive psychology* and *artificial intelligence* – in the 1950s suggested otherwise.

Scientific Discovery as Problem Solving

Simon (1966) offered another view – that scientific discovery is a variety of *problem solving* that involves:

- *Search* through a space of connected *problem states*
- Generated from earlier states by mental *operators*
- Guided by *heuristics* that keep the search tractable

Heuristic search had been implicated in many cases of human problem solving, such as proving theorems and playing chess.

This idea offered a powerful new approach to understanding the rational character of scientific discovery.

But it also suggested ways to *automate* this mysterious process.

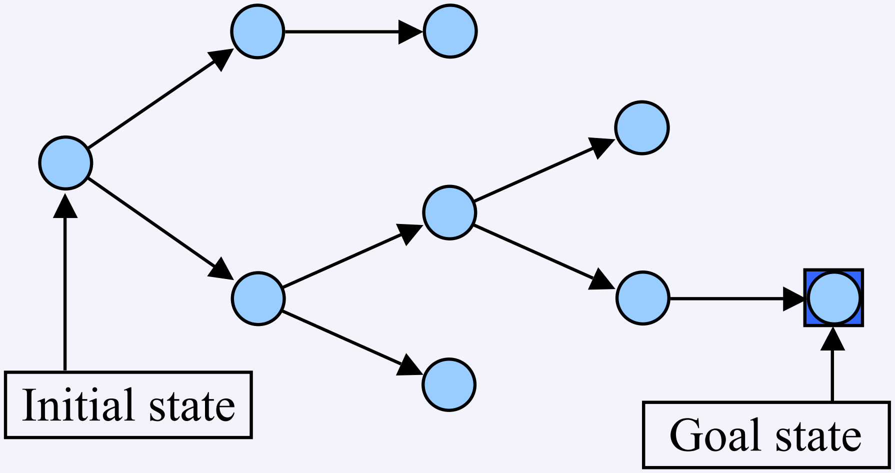
Heuristic Search in a Problem Space

Heuristic search is analogous to the traversal of a physical maze.

States in the problem space map onto locations in the maze.

Operators for producing new states map onto steps through the maze.

Solutions correspond to paths from the maze entrance to its exit (goal).



The initial state and the operators *implicitly* define a problem space.

Heuristics aid search by favoring likely choices and rejecting others to make solution finding tractable.

An Early Response

For my CMU dissertation research, I adapted Simon's ideas on scientific discovery, developing a computer program that:

- Carried out search in a problem space of theoretical terms;
- Using operators that combined old terms into new ones;
- Guided by heuristics that noted regularities in data; and
- Applied these recursively to formulate higher-level relations.

The result was *Bacon*, an early AI system that rediscovered laws from the history of physics and chemistry.

I named the system after Sir Francis Bacon because it adopted a data-driven approach to discovery.

Bacon on Kepler's Third Law

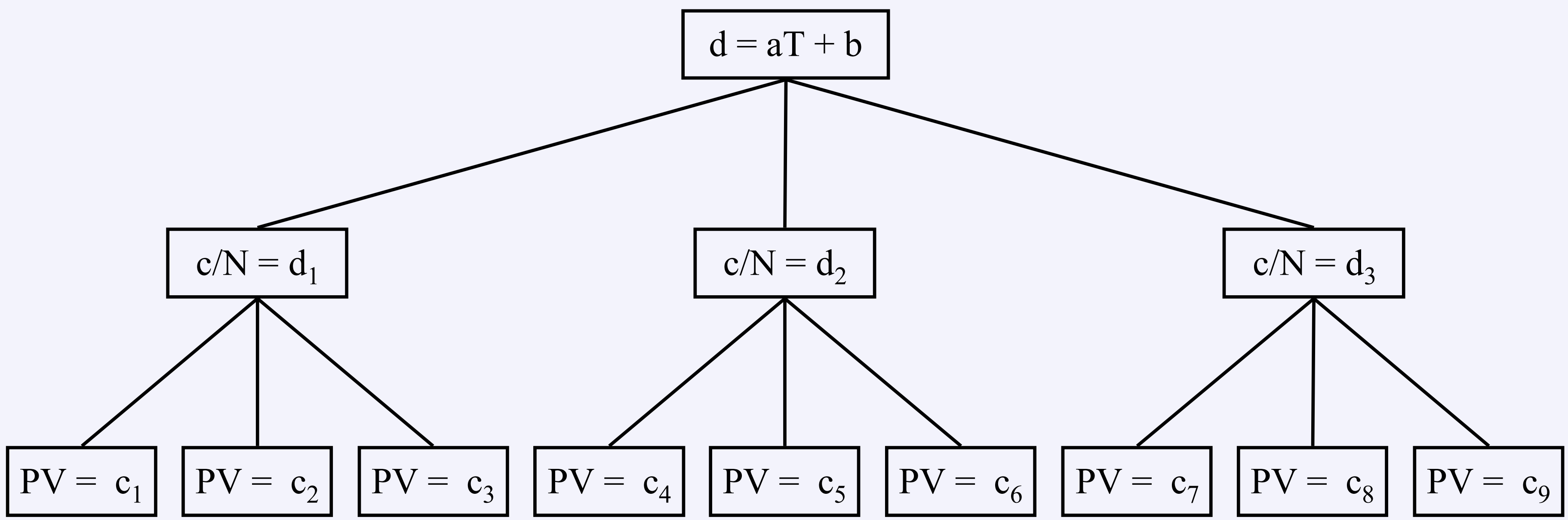
The Bacon system carried out heuristic search, through a space of numeric terms, looking for constants and linear relations.

moon	d	p	d/p	d^2/p	d^3/p^2
A	5.67	1.77	3.20	18.15	58.15
B	8.67	3.57	2.43	21.04	51.06
C	14.00	7.16	1.96	27.40	53.61
D	24.67	16.69	1.48	36.46	53.89

This table shows its progression from the distance and period of Jupiter's moons to a term with nearly constant value.

Bacon on the Ideal Gas Law

Bacon rediscovered the ideal gas law, $PV = aNT + bN$, in three stages, each at a different level of description.



Parameters for laws at one level became dependent variables in laws at the next level, enabling discovery of complex relations.

Some Laws Discovered by Bacon

Basic algebraic relations:

- Ideal gas law $PV = aNT + bN$
- Kepler's third law $D^3 = [(A - k) / t]^2 = j$
- Coulomb's law $FD^2 / Q_1Q_2 = c$
- Ohm's law $TD^2 / (LI - rI) = r$

Relations with *intrinsic properties*:

- Snell's law of refraction $\sin I / \sin R = n_1 / n_2$
- Archimedes' law $C = V + i$
- Momentum conservation $m_1V_1 = m_2V_2$
- Black's specific heat law $c_1m_1T_1 + c_2m_2T_2 = (c_1m_1 + c_2m_2)\,T_f$

Initial Responses to Bacon

Responses to the Bacon work were mixed, with some agreeing it clarified important aspects of scientific discovery.

But others claimed that *the real* key to discovery, which Bacon did not address, instead lay in:

- Deciding which variables to measure and relate
- Determining which problem space to search
- Selecting which scientific problem to address

Others held that Bacon only did what it was programmed to do, and thus did not really ‘discover’ anything.

We only claimed the system offered insights into the operation of scientific discovery, with much remaining to be done.

Ensuing Systems for Law Discovery

Indeed, Bacon inspired other AI systems for law discovery like:

- ABACUS (Falkenhainer, 1985) and ARC (Moulet, 1992)
- Fahrenheit (Zytkow, Zhu, & Hussam, 1990)
- COPER (Kokar, 1986) and E* (Schaffer, 1990)
- IDS (Nordhausen & Langley, 1990)
- Hume (Gordon & Sleeman, 1992)
- DST (Murata, Mizutani, & Shimura, 1994)
- SSF (Washio et al., 1997) and LaGramge (Todorovski et al., 2006)
- GP (Koza et al., 2001) and Eureqa (Schmidt & Lipson, 2009)

These relied on different methods but also searched for explicit mathematical laws that matched data.

Other Research on Discovery (from 1979 to 2000)

Interest in computational discovery spread to other aspects of science, including qualitative laws and explanatory models.

<table>
<tr><td>1979</td><td>1980</td><td>1981</td><td>1982</td><td>1983</td><td>1984</td><td>1985</td><td>1986</td><td>1987</td><td>1988</td><td>1989</td><td>1990</td><td>1991</td><td>1992</td><td>1993</td><td>1994</td><td>1995</td><td>1996</td><td>1997</td><td>1998</td><td>1999</td><td>2000</td></tr>
<tr><td colspan="6">Bacon.1–Bacon.5</td><td colspan="2">Abacus,
Coper</td><td colspan="4">Fahrehneit, E*,
Tetrad, IDS$_N$</td><td colspan="2">Hume,
ARC</td><td colspan="3">DST, GP$_N$
LaGrange</td><td colspan="2">SDS</td><td colspan="3">SSF, RF5,
LaGramge</td></tr>
<tr><td colspan="3">←AM</td><td></td><td colspan="3">Glauber</td><td colspan="2">NGlauber</td><td colspan="2"></td><td colspan="2">IDS$_Q$,
Live</td><td colspan="4"></td><td colspan="3">RL, Progol</td><td colspan="2">HR</td></tr>
<tr><td colspan="3">←Dendral</td><td></td><td colspan="3">Dalton,
Stahl</td><td colspan="3">Stahlp,
Revolver</td><td colspan="2">Gell-Mann</td><td colspan="2">BR-3,
Mendel</td><td colspan="2">Pauli</td><td colspan="2">BR-4</td><td colspan="4"></td></tr>
<tr><td colspan="6"></td><td colspan="2">IE</td><td></td><td colspan="3">Coast, Phineas,
AbE, Kekada</td><td colspan="2"></td><td colspan="6">Mechem, CDP</td><td colspan="2">Astra,
GP$_M$</td></tr>
</table>

Legend	Numeric laws	Qualitative laws	Structural models	Process models

Research in this tradition has continued to the present, in some cases producing new scientific results.

Successes of Computational Scientific Discovery

AI systems of this type have helped to discover new knowledge in many scientific fields:

- reaction pathways in catalytic chemistry (Valdes-Perez, 1994, 1997)
- qualitative chemical factors in mutagenesis (King et al., 1996)
- quantitative laws of metallic behavior (Sleeman et al., 1997)
- quantitative conjectures in graph theory (Fajtlowicz et al., 1988)
- qualitative conjectures in number theory (Colton et al., 2000)
- temporal laws of ecological behavior (Todorovski et al., 2000)
- models of gene-influenced metabolism in yeast (King et al., 2009)

Each of these has led to publications in the *refereed literature of the relevant scientific field*.

The Data Mining Movement

During the 1990s, a new paradigm known as *data mining and knowledge discovery* emerged that:

- Emphasized the availability of large amounts of data;
- Used computational methods to find regularities in the data;
- Adopted heuristic search through a space of hypotheses;
- Initially focused on commercial applications and data sets.

Most work used notations invented by computer scientists, unlike work on scientific discovery, which used *scientific formalisms*.

Data mining has been applied to scientific data, but the results seldom bear a resemblance to scientific *knowledge*.

Discovering Explanatory Models

The early stages of any science focus on *descriptive laws* that *summarize* empirical regularities.

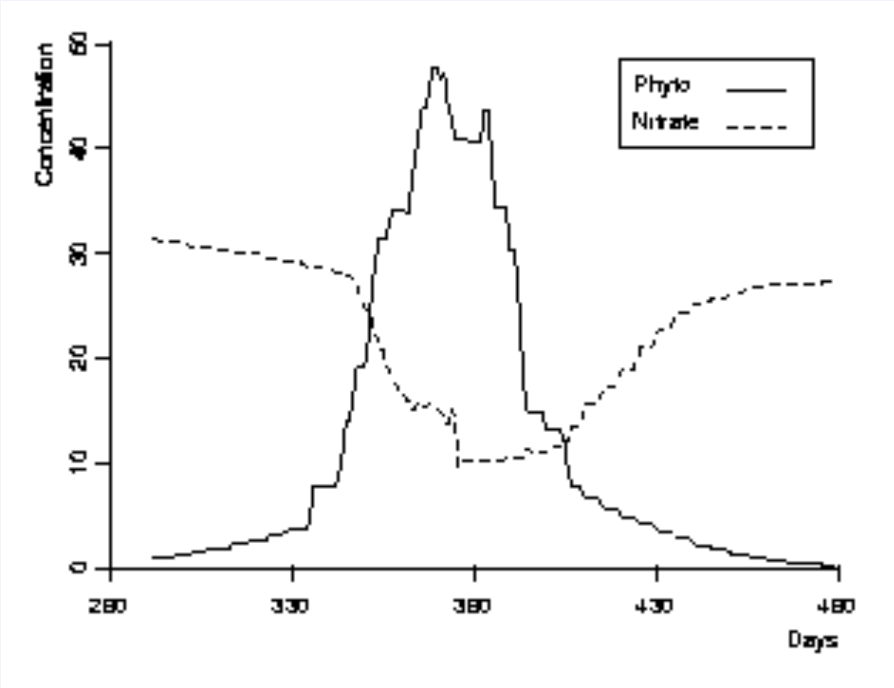
Mature sciences instead emphasize the creation of *models* that *explain* phenomena in terms of:

- Inferred *components* and *structures* of entities
- Hypothesized *processes* about entities’ interactions

Explanatory models move beyond description to provide deeper accounts linked to theoretical constructs.

Can we develop computational systems that address this more sophisticated side of scientific discovery?

An Example: The Ross Sea Ecosystem



Formal accounts of ecosystem dynamics are often cast as sets of differential equations.

Here four equations describe the concentrations of phytoplankton, zooplankton, nitrogen, and detritus in the Ross Sea over time.

Such models can match observed variables with some accuracy.

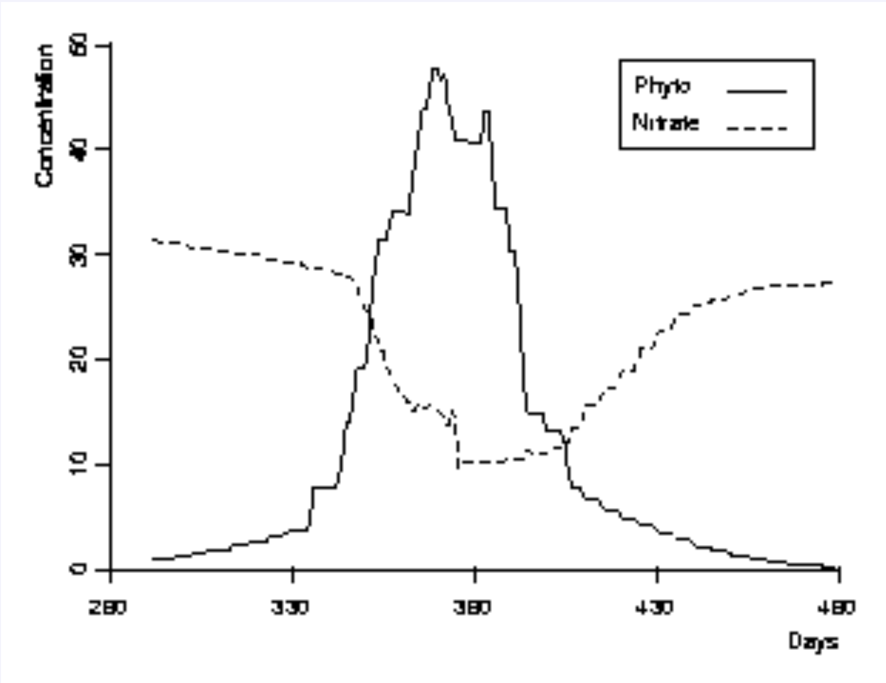
d[phyto,t,1] = – 0.307 × phyto – 0.495 × zoo + 0.411 × phyto

d[zoo,t,1] = – 0.251 × zoo + 0.615 × 0.495 × zoo

d[detritus,t,1] = 0.307 × phyto + 0.251 × zoo + 0.385 × 0.495 × zoo – 0.005 × detritus

d[nitro,t,1] = – 0.098 × 0.411 × phyto + 0.005 × detritus

A Deeper Account of Ross Sea Dynamics



As phytoplankton uptakes nitrogen, its concentration increases and the nitrogen decreases. This continues until the nitrogen is exhausted, which leads to a phytoplankton die off. This produces detritus, which gradually remineralizes to replenish nitrogen. Zooplankton grazes on phytoplankton, which slows the latter's increase and also produces detritus.

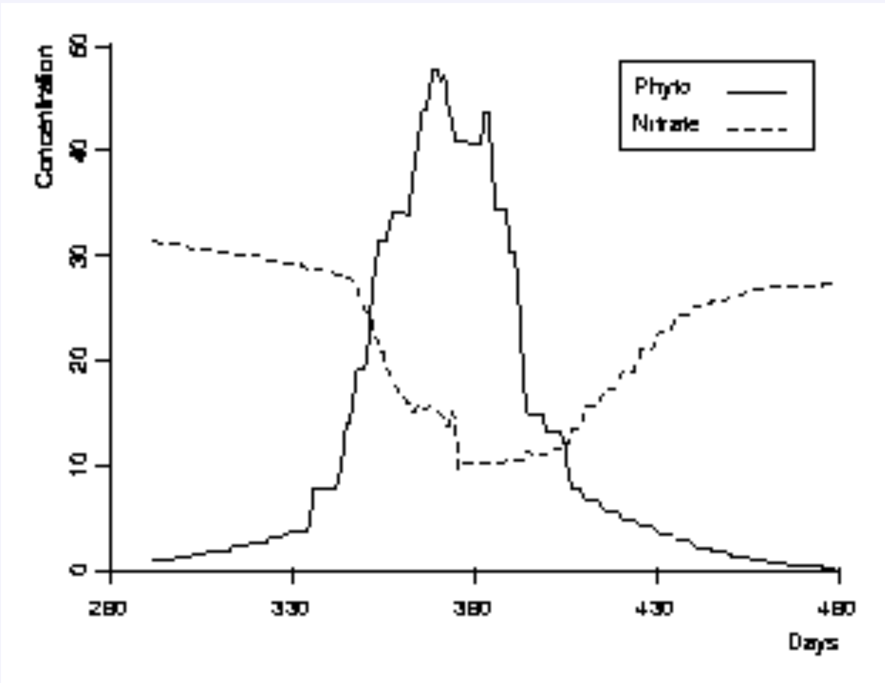
$$d[\text{phyto},t,1] = -\,0.307 \times \text{phyto} - 0.495 \times \text{zoo} + 0.411 \times \text{phyto}$$

$$d[\text{zoo},t,1] = -\,0.251 \times \text{zoo} + 0.615 \times 0.495 \times \text{zoo}$$

$$d[\text{detritus},t,1] = 0.307 \times \text{phyto} + 0.251 \times \text{zoo} + 0.385 \times 0.495 \times \text{zoo} - 0.005 \times \text{detritus}$$

$$d[\text{nitro},t,1] = -\,0.098 \times 0.411 \times \text{phyto} + 0.005 \times \text{detritus}$$

Processes in Ross Sea Dynamics



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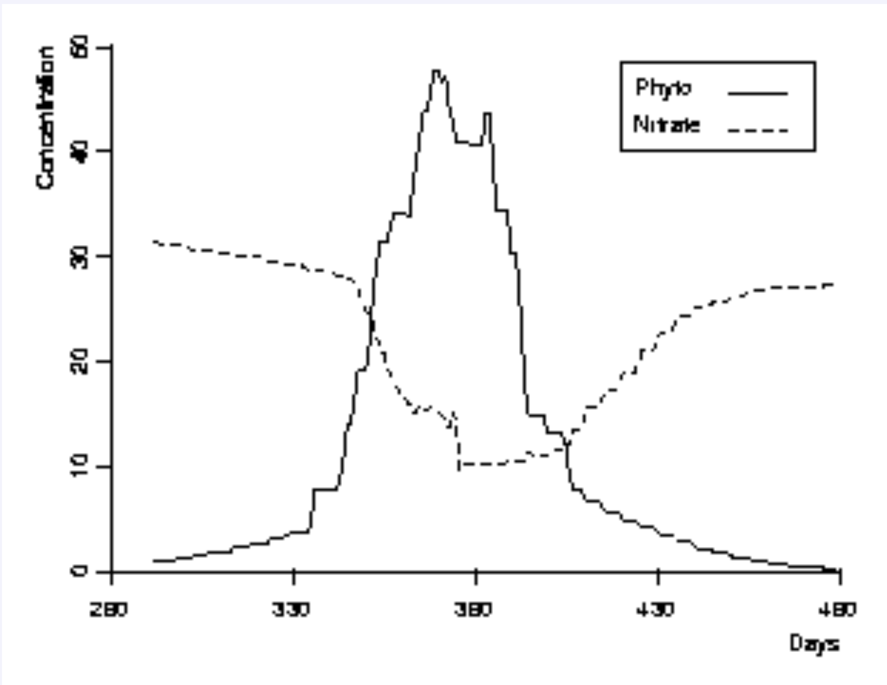
$$d[detritus,t,1] = 0.307 \times phyto + 0.251 \times zoo + 0.385 \times 0.495 \times zoo - 0.005 \times detritus$$

$$\boxed{d[nitro,t,1] = - 0.098 \times 0.411 \times phyto} + 0.005 \times detritus$$

Processes in Ross Sea Dynamics



As phytoplankton uptakes nitrogen, its concentration increases and the nitrogen decreases. This continues until the nitrogen is exhausted, which leads to a phytoplankton die off. This produces detritus, which gradually remineralizes to replenish nitrogen. *Zooplankton grazes on phytoplankton, which slows the latter's increase and also produces detritus.*

$$\boxed{d[phyto,t,1] =} - 0.307 \times phyto \boxed{- 0.495 \times zoo} + 0.411 \times phyto$$

$$\boxed{d[zoo,t,1] =} - 0.251 \times zoo + \boxed{0.615 \times 0.495 \times zoo}$$

$$\boxed{d[detritus,t,1] =} 0.307 \times phyto + 0.251 \times zoo + \boxed{0.385 \times 0.495 \times zoo} - 0.005 \times detritus$$

$$d[nitro,t,1] = - 0.098 \times 0.411 \times phyto + 0.005 \times detritus$$

A Process Model for the Ross Sea

```
model Ross_Sea_Ecosystem

entities: phyto, zoo, nitro, detritus
observables: phyto, nitro

process phyto_loss(phyto, detritus)
  equations:    d[phyto.conc,t,1] = –0.307 × phyto.conc
                d[detritus.conc,t,1] = 0.307 × phyto.conc

process zoo_loss(zoo, detritus)
  equations:    d[zoo.conc,t,1] = –0.251 × zoo.conc
                d[detritus.conc,t,1] = 0.251 × zoo.conc

process zoo_phyto_grazing(zoo, phyto, detritus)
  equations:    d[zoo.conc,t,1] = 0.615 × 0.495 × zoo.conc
                d[detritus.conc,t,1] = 0.385 × 0.495 × zoo.conc
                d[phyto.conc,t,1] = –0.495 × zoo.conc

process nitro_uptake(phyto, nitro)
  equations:    d[phyto.conc,t,1] = 0.411 × phyto.conc
                d[nitro.conc,t,1] = –0.098 × 0.411 × phyto.conc

process nitro_remineralization(nitro, detritus)
  equations:    d[nitro.conc,t,1] = 0.005 × detritus.conc
                d[detritus.conc,t,1 ] = –0.005 × detritus.conc
```

We can reformulate such an account by restating it as a *quantitative process model*.

Such a model is equivalent to a standard differential equation model, but it makes explicit assumptions about processes that are involved.

Each process indicates that certain terms in equations must stand or fall together.

A New Discovery Task

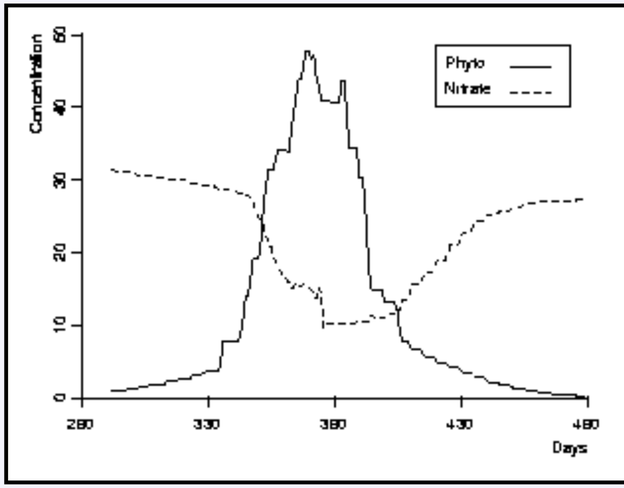
We can define the task of discovering such explanatory process models as:

- *Given:* A set of entities with associated variables
- *Given:* Times series for some of these variables
- *Given:* Knowledge about processes that might occur
- *Find:* Quantitative process models that explain the observed time series and predict new observations

We have referred to this class of computational discovery tasks as *inductive process modeling* (Bridewell et al., 2008).

Inductive Process Modeling

observations



Heuristic Search

generic processes

process exponential_growth
  variables: P {population}
  equations: d[P,t] = [0, 1,∞] × P

process logistic_growth
  variables: P {population}
  equations: d[P,t] = [0, 1, ∞] × P × (1 – P / [0, 1, ∞])

process constant_inflow
  variables: I {inorganic_nutrient}
  equations: d[I,t] = [0, 1, ∞]

process consumption
  variables: P1 {population}, P2 {population}, nutrient_P2
  equations: d[P1,t] = [0, 1, ∞] × P1 × nutrient_P2,
                  d[P2,t] = – [0, 1, ∞] × P1 × nutrient_P2

process no_saturation
  variables: P {number}, nutrient_P {number}
  equations: nutrient_P = P

process saturation
  variables: P {number}, nutrient_P {number}
  equations: nutrient_P = P / (P + [0, 1, ∞])

entities

phyto, nitro, zoo,
nutrient_nitro, nutrient_phyto

process model

model AquaticEcosystem

variables: nitro, phyto, zoo, nutrient_nitro, nutrient_phyto
observables: nitro, phyto, zoo

process phyto_exponential_growth
  equations: d[phyto,t] = 0.1 × phyto

process zoo_logistic_growth
  equations: d[zoo,t] = 0.1 × zoo / (1 – zoo / 1.5)

process phyto_nitro_consumption
  equations: d[nitro,t] = –1 × phyto × nutrient_nitro,
                  d[phyto,t] = 1 × phyto × nutrient_nitro

process phyto_nitro_no_saturation
  equations: nutrient_nitro = nitro

process zoo_phyto_consumption
  equations: d[phyto,t] = –1 × zoo × nutrient_phyto,
                  d[zoo,t] = 1 × zoo × nutrient_phyto

process zoo_phyto_saturation
  equations: nutrient_phyto = phyto / (phyto + 0.5)

Generic Processes for Aquatic Ecosystems

```
process exponential_loss(S, D)
  entities: S{species}, D{detritus}
  parameters: α [0, 1]
  equations:   d[S.conc,t,1] = −1 × α × S.conc
               d[D.conc,t,1] = α × S.conc

generic process grazing(S1, S2, D)
  entities: S1{species}, S2{species}, D{detritus}
  parameters: ρ [0, 1], γ [0, 1]
  equations:   d[S1.conc,t,1] = γ × ρ × S1.conc
               d[D.conc,t,1] = (1 − γ) × ρ × S1.conc
               d[S2.conc,t,1] = −1 × ρ × S1.conc

generic process nutrient_uptake(S, N)
  entities: S{species}, N{nutrient}
  parameters: τ [0, ∞], β [0, 1], μ [0, 1]
  conditions:  N.conc > τ
  equations:   d[S.conc,t,1] = μ × S.conc
               d[N.conc,t,1] = −1 × β × μ × S.conc

process remineralization(N, D)
  entities: N{nutrient}, D{detritus}
  parameters: π [0, 1]
  equations:
      d[N.conc, t,1] = π × D.conc
      d[D.conc, t,1] = −1 × π × D.conc

process constant_inflow(N)
  entities: N{nutrient}
  parameters: ν [0, 1]
  equations:   d[N.conc,t,1] = ν
```

Our aquatic ecosystem library contains about 25 generic processes, including ones with alternative functional forms for loss and grazing processes.

These form the *building blocks* from which to compose models.

Searching the Space of Model Structures

We have developed multiple 'IPM' systems that induce process models from generic components in four stages:

1. Instantiate known generic processes with specific entities, subject to type specifications;
2. Combine these instantiated processes into candidate model structures, rejecting disconnected structures;
3. For each model structure, carry out search through parameter space to find good coefficients;
4. Return the parameterized model with the best overall score (e.g., lowest squared error).

We have reported variants on this approach in numerous papers (Bridewell et al., *MLj*, 2008; Bridewell & Langley, *TopiCS*, 2010).

Searching the Space of Model Parameters

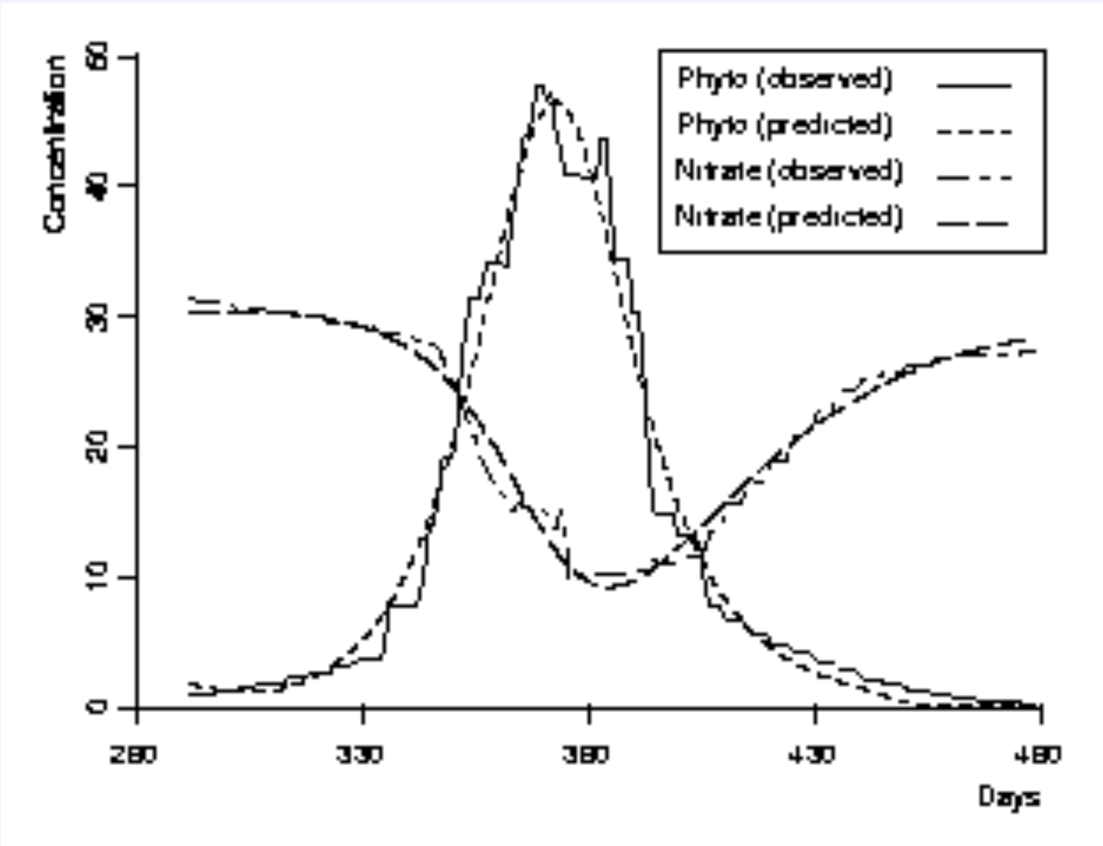
To estimate the parameters for each generic model structure, our induction algorithms:

1. Select random initial values that fall within ranges specified in the generic processes;
2. Improve these parameters using a conjugate gradient method (717) until it reaches a local optimum;
3. Repeat the process ten times and select the best-scoring set of parameter values.

This multi-level method gives reasonable fits to time-series data from a number of domains, but it is computationally intensive.

Each step in the gradient descent requires simulating the model's trajectory to calculate its error.

Results on Training Data from Ross Sea

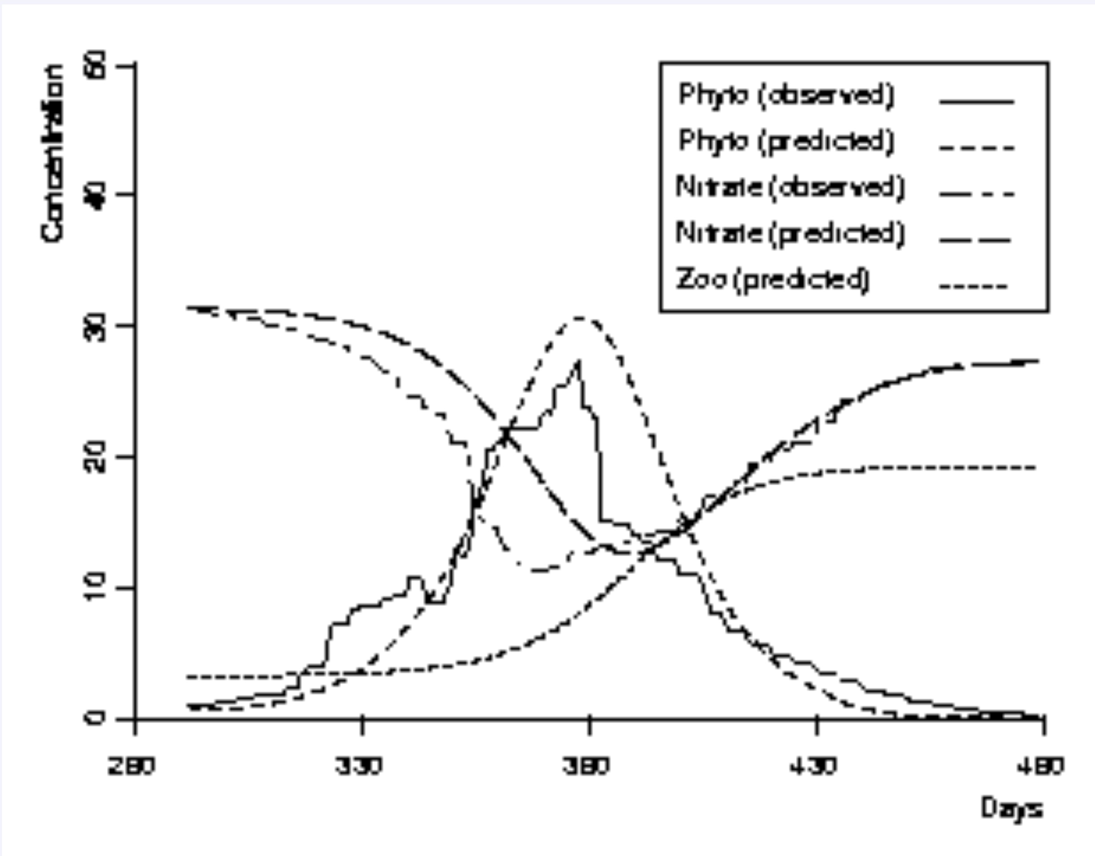


We provided IPM with 188 samples of phytoplankton, nitrate, and ice measures taken from the Ross Sea.

From 2035 distinct model structures, it found accurate models that limited phyto growth by the nitrate and the light available.

Some high-ranking models incorporated zooplankton, whereas others did not.

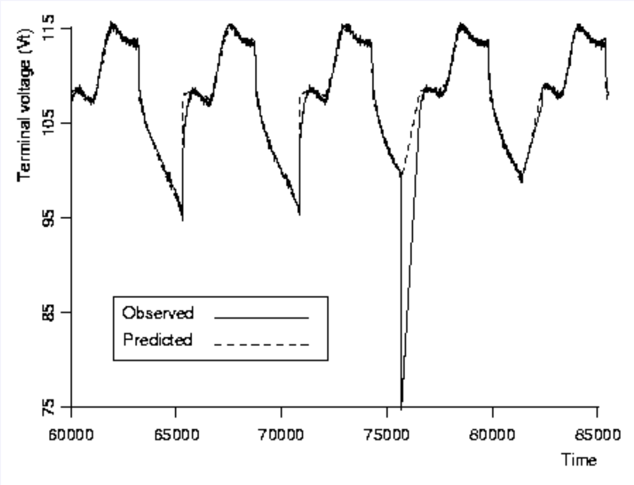
Results on Test Data from Ross Sea



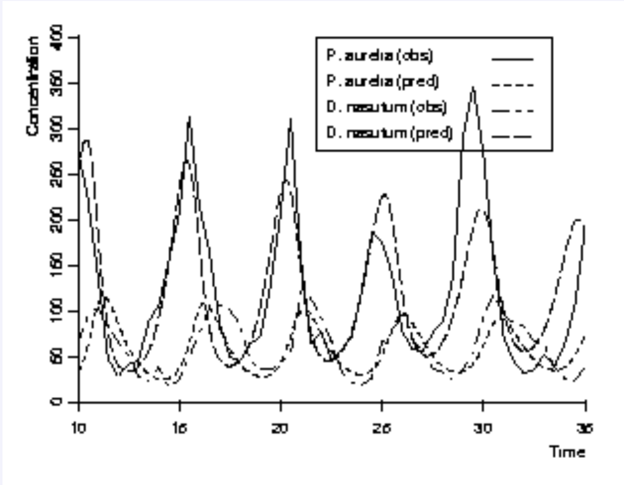
Generalization to a second year's data benefited from treating initial zooplankton concentration as a free model parameter.

Another good-fitting model suggested that the nitrogen to carbon ratio varies as a function of available light.

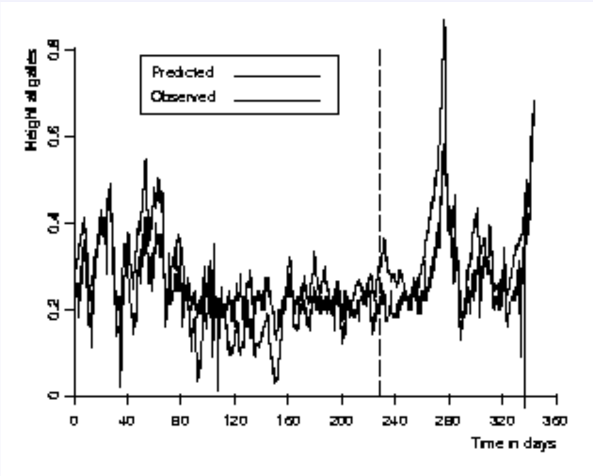
Other Results with Process Modeling



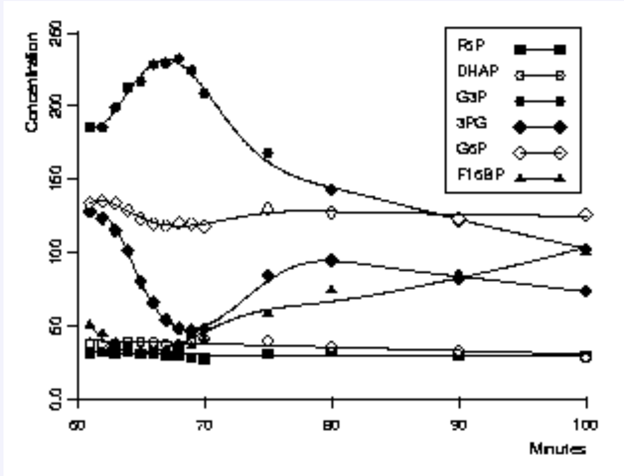
power systems



protist dynamics



hydrology



biochemical kinetics

Extensions to Inductive Process Modeling

In addition, we have extended the basic framework to support:

- Inductive revision of quantitative process models
  - Asgharbeygi et al. (*Ecological Modeling*, 2006)
- Hierarchical generic processes that constrain search
  - Todorovski, Bridewell, Shiran, and Langley (*AAAI-2005*)
- An ensemble-like method that mitigates overfitting effects
  - Bridewell, Bani Asadi, Langley, and Todorovski (*ICML-2005*)
- An EM-like method that estimates missing observations
  - Bridewell, Langley, Racunas, and Borrett (*ECML-2006*)

These extensions make the modeling framework more robust along a number of fronts.

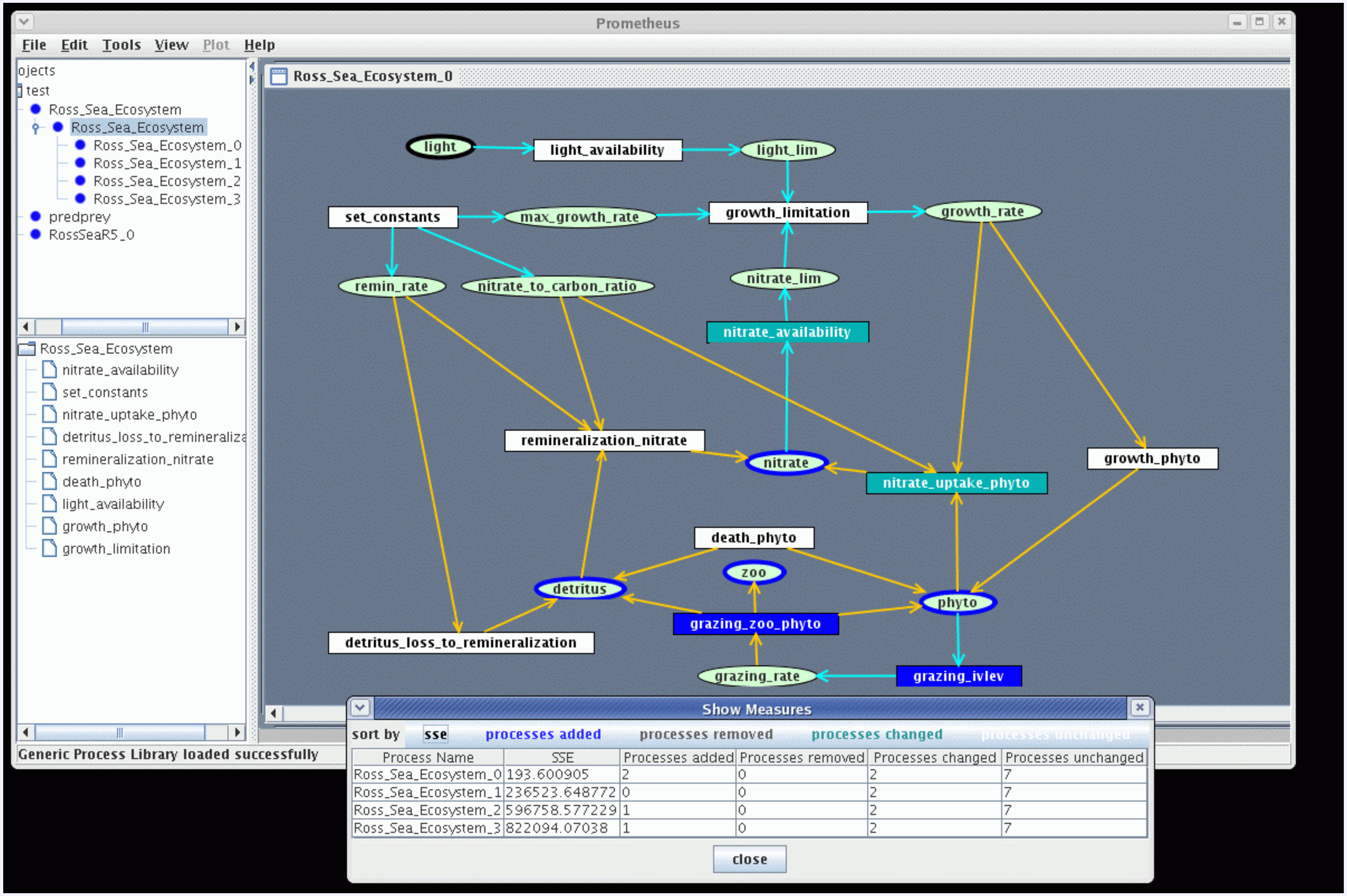
Interfacing with Scientists

Because few scientists want to be replaced, we also developed an interactive environment, PROMETHEUS, that lets users:

- specify a quantitative process model of the target system;
- display and edit the model's structure and details graphically;
- simulate the model's behavior over time and situations;
- compare the model's predicted behavior to observations;
- invoke a revision module in response to detected anomalies.

The environment offers computational assistance in forming and evaluating models but lets the user retain control.

The PROMETHEUS System



Details about PROMETHEUS are available in Bridewell et al. (*IJHCS*, 2007).

Knowledge and Search in Discovery

Traditional treatments of problem solving hold that knowledge reduces the amount of search.

- But adding generic processes leads to a combinatorial *increase* in the number of candidate structures.

Yet scientists are not overwhelmed by the size of model spaces and they reject many structures as unacceptable.

This suggests *two* forms of scientific background knowledge:

- *components* used to generate candidate model structures
- *constraints* on allowable combinations of such components

This distinction seldom occurs in the literature, but it appears key to understanding scientific explanation.

Constraints on Ecosystem Models

Our discussions with ecologists confirmed that constraints play an important role in model acceptability.

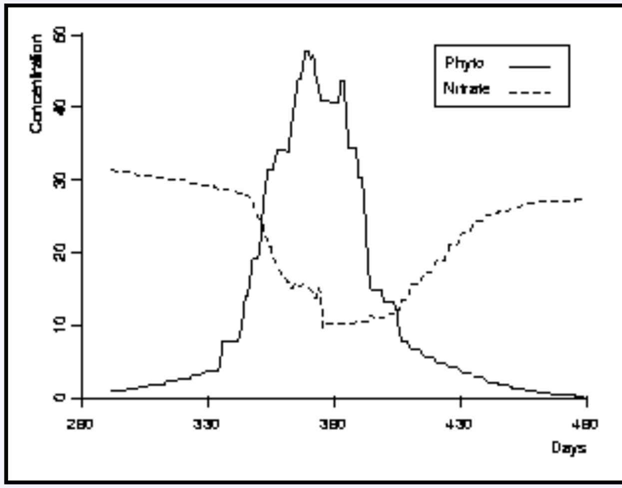
Some plausible constraints for models of ecosystems include:

- There must be at most one growth process for each species.
- A limited growth process cannot occur without a nutrient limitation process and vice versa.
- There must be no more than one predation process between any two species.

We have developed a formal notation that lets our systems use such constraints during inductive process modeling.

Inductive Process Modeling

observations



entities

phyto, nitro, zoo,
nutrient_nitro, nutrient_phyto

Reduction in search space

Heuristic Search

process model

model AquaticEcosystem

variables: nitro, phyto, zoo, nutrient_nitro, nutrient_phyto
observables: nitro, phyto, zoo

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  equations: d[phyto,t] = 0.1 × phyto

process zoo_logistic_growth
  equations: d[zoo,t] = 0.1 × zoo / (1 – zoo / 1.5)

process phyto_nitro_consumption
  equations: d[nitro,t] = –1 × phyto × nutrient_nitro,
             d[phyto,t] = 1 × phyto × nutrient_nitro

process phyto_nitro_no_saturation
  equations: nutrient_nitro = nitro

process zoo_phyto_consumption
  equations: d[phyto,t] = –1 × zoo × nutrient_phyto,
             d[zoo,t] = 1 × zoo × nutrient_phyto

process zoo_phyto_saturation
  equations: nutrient_phyto = phyto / (phyto + 0.5)

process exponential_growth
  variables: P {population}
  equations: d[P,t] = [0, 1,∞] × P

process logistic_growth
  variables: P {population}
  equations: d[P,t] = [0, 1, ∞] × P × (1 – P / [0, 1, ∞])

process constant_inflow
  variables: I {inorganic_nutrient}
  equations: d[I,t] = [0, 1, ∞]

process consumption
  variables: P1 {population}, P2 {population},
nutrient_P2
  equations: d[P1,t] = [0, 1, ∞] × P1 × nutrient_P2,
             d[P2,t] = – [0, 1, ∞] × P1 × nutrient_P2

process no_saturation
  variables: P {number}, nutrient_P {number}
  equations: nutrient_P = P

process saturation
  variables: P {number}, nutrient_P {number}
  equations: nutrient_P = P / (P + [0, 1, ∞])

generic processes

constraints

Always-together[growth(P), loss(P)]

Exactly-one[lotka-volterra(P, G), ivlev(P, G), watts(P, G)]

At-most-one[photoinhibition(P, E)]

Necessary[nutrient-mixing(N), remineralization(N, D)]

Inducing Process Models with Constraints

Our extended framework for the discovery of process models:

- Encodes modular constraints on process combinations
- Uses these constraints to eliminate unacceptable models
- Reduces search through the model space, which
  - Leads to far more efficient model construction
  - Produces little or no increase in generalization error
  - Improves the comprehensibility of generated models

The resulting systems are more robust in their ability to induce process models (Bridewell & Langley, *TopiCS*, 2010).

Discovering Constraints

In other recent work (Todorovski et al., AAAI-2012), we have developed a system that:

- Uses inductive process modeling to generate a set of models;
- Separates these into accurate and inaccurate model structures;
- Describes each model structure in terms of relational literals;
- Learns relational rules that can distinguish the two classes;
- Transforms the rules into constraints on model structures; and
- Uses these constraints to guide search on future modeling tasks.

Experiments suggests this produces a tenfold speedup on novel modeling tasks with little or no loss in accuracy.

Directions for Future Research

Despite the progress to date, we need further work in order to:

- apply approach to new data sets (oceanography, physiology)
- develop more efficient methods for fitting model parameters
- extend the framework to partial differential equation models
- design mechanisms for inducing new generic processes
- handle discovery of complex models with many variables
- embed these abilities in a PROMETHEUS-like environment

Together, these will make constraint-guided inductive process modeling a more robust approach to scientific explanation.

Summary Remarks

Inductive process modeling is a novel and promising approach to discovering scientific models that:

- Incorporates a formalism that is familiar to many scientists
- Utilizes two kinds of background knowledge about the domain
- Produces meaningful results from moderate amounts of data
- Generates models that explain, not just describe, observations
- Closes the loop between using and learning process constraints

Although work on this topic has focused on ecological modeling, the key ideas extend to other domains.

For more information, see *http://www.isle.org/process/* .

eScience and Discovery Informatics

The *escience* movement champions the use of computers to aid the scientific enterprise, emphasizing two themes:

- Creation and simulation of complex explanatory models
  - E.g., differential equation models for meteorology and biology
  - However, most such models are constructed *manually*
- Collection, storage, and mining of scientific data sets
  - E.g., learned classifiers in astronomy and planetology
  - But such analyses make no contact with scientific theory

Science is about the *relation between* theory and data, and work on computational scientific discovery offers a way to join them.

This idea is central to the emerging field of *discovery informatics*.

Big Data and Scientific Discovery

Digital collection and storage have led to rapid growth of data in many areas.

The *big data* movement seeks to capitalize on this content, but, in science at least, must address *three* distinct issues:

- Scaling to large and heterogeneous *data sets*
- Scaling to large and complex *scientific models*
- Scaling to large *spaces of candidate models*

Handling large data sets has been widely studied and poses the fewest challenges.

We need more work on the last two issues, for which the methods of computational scientific discovery are well suited.

Concluding Remarks

Scientific discovery does not involve any mystical or irrational elements; we can study and even partially automate it.

Our explanation of this fascinating set of processes relies on:

- Carrying out search through a space of laws or models;
- Utilizing operators for generating structures and parameters;
- Guiding search by data and by knowledge about the domain.

Work in this framework discovers laws and models stated in the formalisms and concepts familiar to scientists.

This paradigm has already started to aid the scientific enterprise, and its importance will only grow with time.

Publications on Computational Scientific Discovery

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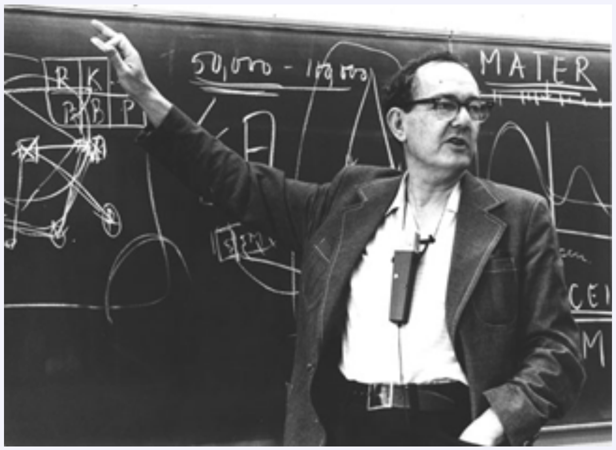
Todorovski, L., Bridewell, W., & Langley, P. (2012). Discovering constraints for inductive process modeling. *Proceedings of the Twenty-Sixth AAAI Conference on Artificial Intelligence*. Toronto: AAAI Press.

In Memoriam

In 2001, the field of computational scientific discovery lost two of its founding fathers.



Herbert A. Simon
(1916 – 2001)

Jan M. Zytkow
(1945 – 2001)

Both were interdisciplinary researchers who published in computer science, psychology, philosophy, and statistics.

Herb Simon and Jan Zytkow were excellent role models for us all.