AAAI Spring Symposium on

Computational Approaches to Scientific Discovery

Hyatt Regency / San Francisco Airport

March 27–29, 2023

Organizers:

Youngsoo Choi / Lawrence Livermore National Laboratory

Sašo Džeroski / Jozef Stefan Institute

J. Nathan Kutz / University of Washington

Pat Langley / Stanford University, CA

The Task of Scientific Discovery

We can state the discovery task in terms of the inputs provided and the outputs produced:

- Given: *Scientific data or phenomena to be described or explained*
- Given: *Knowledge and heuristics about the scientific domain*
- Given: *A space of candidate laws, hypotheses, or models*
- Find: *Laws or models that describe or explain the observations*

Ideally, the outputs should generalize well and be stated in an established *scientific formalism*.

Computational scientific discovery is the study of mechanisms for tackling this generic problem.

Einstein's Search Succeeds At Last

"*Now* that desk looks better. Everything's squared away, yessir, squaaaaaared away."

History of Computational Discovery

Computational scientific discovery is not a new field, with decades of work dating back to the 1970s.

- There was originally great resistance to the idea that computers might discovery scientific laws and models.
- Herbert Simon (1966) first proposed that we can view discovery as a form of heuristic search through a problem space.
- Philosophers of science, cognitive psychologists, and artificial intelligence researchers all played roles in the movement.

Research in this tradition continues, but the number of active groups has been modest until recently.

More History of Computational Discovery

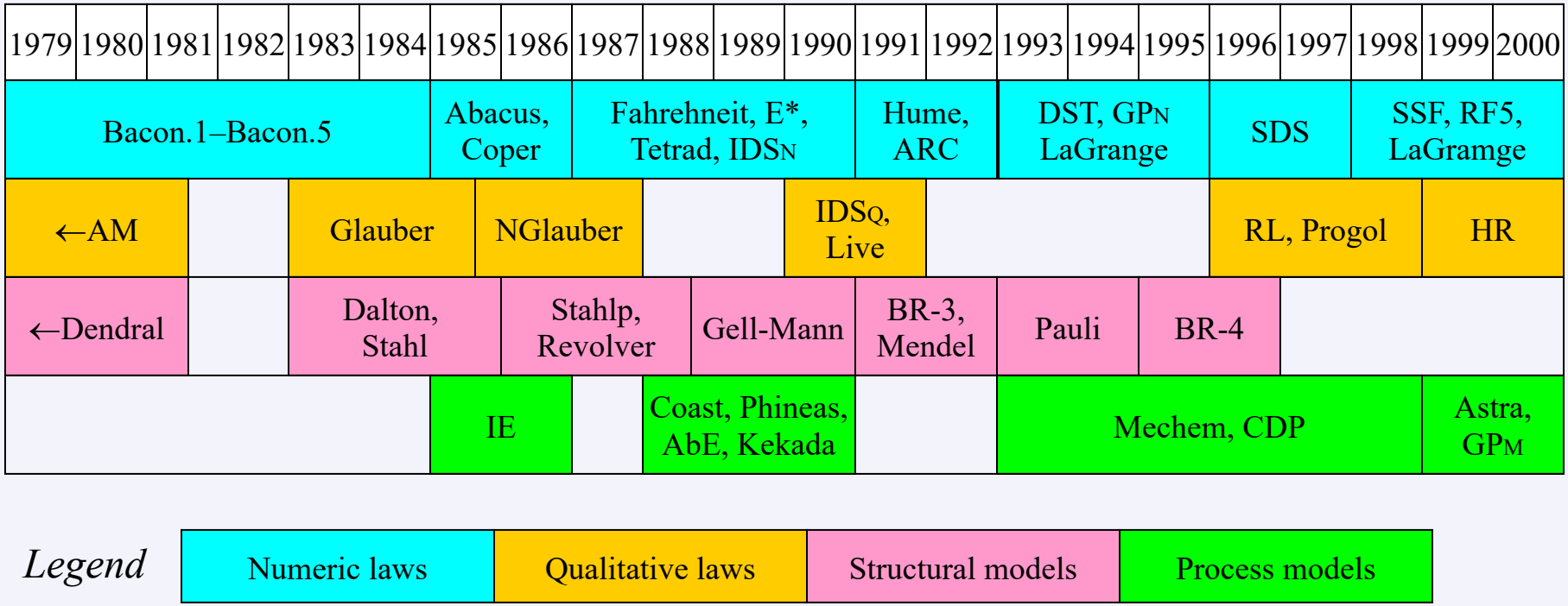
Early researchers aimed to find laws or models stated in terms of established scientific formalisms.

- Computers are *general symbol processors*, so they specified the search space in terms of *discrete symbolic expressions*.
- Researchers addressed a diverse set of discovery tasks, not all of them involving *induction from data*.
- These included constructing *qualitative models* that explained phenomena in terms of hidden structures or processes.

Replicating historical discoveries was a key step, but work soon produced novel scientific results (Langley, 2000).

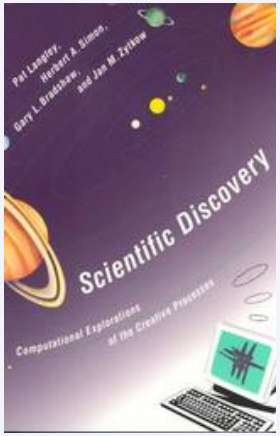
Early Decades of Scientific Discovery

Research on computational scientific discovery has addressed many different forms of laws and models.



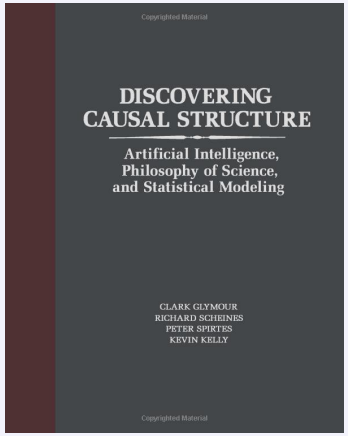
Books on Scientific Discovery

Research on computational discovery has led to multiple books.

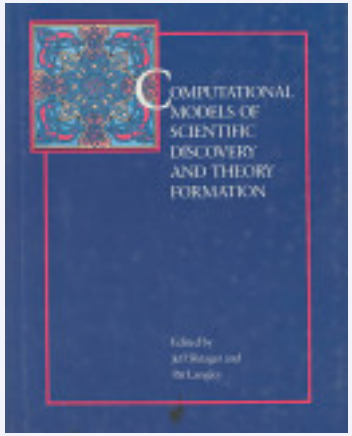


1987

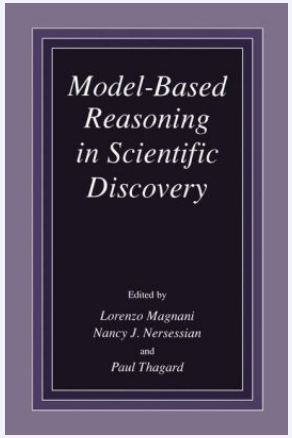
1987



1990



1999



2007

These demonstrate the field's diversity of problems and methods.

Meetings on Scientific Discovery

- Stanford University / January 1989
  Symposium on Computational Models of Scientific Discovery and Theory Formation
- Stanford University / March 1995
  AAAI Spring Symposium on Systematic Methods of Scientific Discovery
- Brighton, UK / August 1998
  ECAI-98 Workshop on Machine Discovery
- University of Pavia / December 1998
  Conference on Model-Based Reasoning in Scientific Discovery
- Stanford University / March 2001
  Symposium on Computational Discovery of Communicable Knowledge
- Stanford University / March 2008
  Symposium on Computational Approaches to Creativity in Science
- Arlington, VA / November 2012
  AAAI Fall Symposium on Discovery Informatics
- Carnegie Mellon Silicon Valley / June 2013
  Symposium on Cognitive Systems and Discovery Informatics

More Recent History

In the past decade, interest in computational discovery has spread to physics, applied mathematics, and other fields.

Research in this paradigm differs from earlier work in that it often:

- Assumes that computers are primarily *numeric processors*
- Focuses on models stated in *continuous mathematics*
- Carries out search through a *parameter space*
- Relies on *neural networks* and *continuous optimization*

Papers from this community use different terms and techniques, but they address many of the same challenges.

Aims of the Symposium

The main purpose of the symposium is to bridge the divide between the different discovery paradigms.

Thus, we have asked presenters to avoid discussing system details and instead to answer:

- What *original* discovery problem did they want to solve?
- How did they *formulate* the problem in computational terms?
- What *data* and *knowledge* did they provide as system *inputs*?
- What *types of models* did the system produce as *outputs*?
- What *criteria* did they use to *evaluate* candidate models?

These should help abstract away from computational details and suggest cross-paradigm insights.

Some General Questions

We hope that another outcome will be preliminary answers to five high-level questions:

- What are the major discovery tasks and how are they related?
- What challenges and responses cut across different paradigms?
- What computational abstractions are useful across disciplines?
- How can we evaluate discovery systems beyond accuracies?
- How can we move past informal accounts of interpretability?

Answers to these questions would help guide future research in this challenging arena.

Symposium Schedule

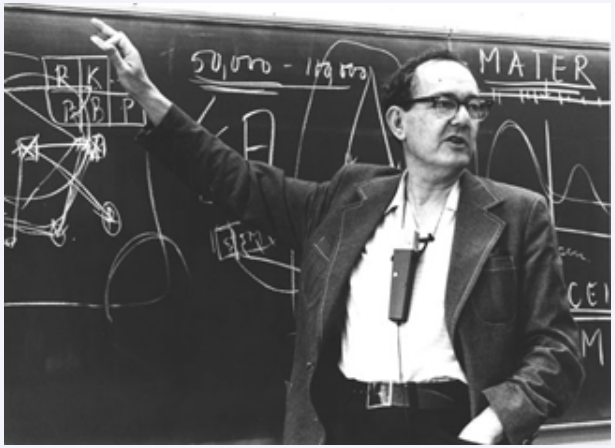
The symposium will run 2.5 days, from 9:00 am on Monday, March 27, to 1:00 pm on Wednesday, March 29.

- Each session will last 90 minutes and three talks
- Most talks will be 20 minutes with ten minutes for questions
- Time is limited, so please reserve questions to each talk's end
- AAAI will *not provide lunch*, so you are on your own
- We have one-hour poster sessions at 5 pm Monday and Tuesday
- There will be plenary events at 6 pm Monday and Tuesday
- We will end with a closing discussion about the community
- One topic of discussion is organizing a special issue

The schedule is at *http://cogsys.org/symposium/discovery-2023/* .

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.