Herbert A. Simon's Legacy

# Heuristics for Discovery in Cognitive Science

#### **Pat Langley**

Institute for the Study of Learning and Expertise 2164 Staunton Court, Palo Alto, California http://www.isle.org/~langley

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## **Heuristics and Scientific Discovery**

Herbert Simon was fascinated by many phenomena, but two that drew his attention repeatedly were:

- the heuristic nature of human problem solving
- the processes of scientific reasoning and discovery

Thus, it seems appropriate to examine Simon's career in terms of his personal heuristics for scientific research.

Moreover, it makes sense to illustrate these rules of thumb with examples from his own work on the discovery process.

#### **Mystical Views of Discovery**

Most philosophers have avoided scientific discovery, believing it 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'...

Hempel and many others also believed discovery was inherently irrational and beyond understanding.

## **Scientific Discovery as Problem Solving**

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

- *Search* through a space of *problem states*
- Generated by applying mental *operators*
- Guided by *heuristics* to make it tractable



Heuristic search had been implicated in many cases of human cognition, from proving theorems to playing chess.

This framework offered not only a path to understand discovery, but ways to automate this mysterious process.

## **Be Audacious**

Tackle challenging problems that others have been reluctant to face or even admit are solvable.

• Understand the cognitive and computational mechanisms that support the processes of scientific discovery.

In 1966, Herb Simon published "Scientific Discovery and the Psychology of Problem Solving".

This radical paper set the agenda for research on computational scientific discovery for the next 50 years.

## **Ignore Discipline Boundaries**

Become familiar with every field that is relevant to your research problem and incorporate good ideas from each one.

• To understand scientific discovery, borrow concepts not only from cognitive psychology and AI, but also from the history and philosophy of science.

Herb Simon applied his Renaissance scholarship to his discovery research, as he did to many other scientific problems.

Moreover, he made his results accessible to members of all these communities by publishing in many literatures.

## Use a Secret Weapon

Take advantage of metaphors and tools that you have mastered but that are not yet widely available.

• Cast the discovery task in terms of heuristic search through a problem space controlled by a production system.

Herb Simon repeatedly invoked the notion of heuristic search to model the discovery process, as to many other phenomena.

Ironically, he was also ready to share his secret weapons with any who were willing to learn them.

### **Balance Theory and Data**

Realize that scientific models must explain observations but also remain connected to existing knowledge.

- Examine discoveries from the history of science that require computational explanation.
- Constrain these historical models using established knowledge about human cognition.

Herb Simon's work on scientific discovery maintained a balance between theory and data, as did his other research efforts.

## Satisfice

Address challenging problems but idealize them enough to make them tractable.

- Focus on the discovery of descriptive laws from numeric data, giving BACON and its successors.
- Focus on discovery of simple structural models from qualitative data, giving STAHL and DALTON.
- Ignore issues of problem formulation, variable selection, and other aspects of scientific reasoning.

However, Herb Simon always acknowledged the limits of a given idealization and the need for additional research.

#### Persevere

Science is a gradual process. Build incrementally on previous results, extending them to cover ever more phenomena.

- *Herb Simon and his colleagues worked steadily, for over two decades, to model the process of scientific discovery.*
- Moreover, his research with Deepak Kulkarni on KEKADA itself modeled this central aspect of science.

This research programme changed the face of cognitive science and clarified the computational nature of discovery.

## **Evolution of Research on Computational Scientific Discovery**

1979	1980	1981	1982	1983	1984	1985	1986	1987	1988	1989	1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000
Bacon.1–Bacon.5				Aba Co	Abacus, Fa Coper T		Ihrenheit, E*, Tetrad, IDSN		Hu Al	ume, DS ARC La		ST, G aGran	GPN ange S		DS SS La		SF, RF5, Gramge				
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←Dendral Daltor Stahl			<b>1</b> ,	Stahlp, Revolve			Gell-Mann		BR-3, <b>Mendel</b>		Pa	uli	BR	<b>R-4</b>							
				Ι	IE		Coast, Phineas, AbE, <b>Kekada</b>					Mechem, CDP			Ast Gl	t <b>ra</b> , PM					

Legend	Numeric laws	Qualitative laws	Structural models	Process models
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## **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.

## A Long-Term Goal

The ultimate challenge in discovery research is to model the behavior of a scientist who:

- Formulates the notion of satisficing in human decision making
- Co-invents list processing and heuristic search on computers
- Co-develops theories of human memory and problem solving
- Uses his theories to model discovery and other key phenomena
- Fosters a new field that acknowledges no discipline boundaries

We know some of this scientist's heuristics, and we have detailed records of his accomplishments, but the task remains daunting.

## **A Closing Quotation**

We would like to imagine that the great discoverers, the scientists whose behavior we are trying to understand, would be pleased with this interpretation of their activity as normal (albeit highquality) human thinking . . .

But science is concerned with the way the world is, not with how we would like it to be. So we must continue to try new experiments, to be guided by new evidence, in a heuristic search that is never finished but always fascinating.

Herbert A. Simon, Envoi to Scientific Discovery, 1987.

## 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.

## End of Presentation