# Scientific Reasoning and Artificial Intelligence

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Science comprises some of the most challenging cognitive tasks in which humans engage, which makes it a natural target for AI research. Simon (1966) first proposed the idea that we might explain scientific discovery in computational terms and automate the processes involved on a computer. DENDRAL (Feigenbaum et al., 1971) demonstrated this by inferring the structures of organic molecules from mass spectra, a problem previously solved only by experienced chemists. Somewhat later, Lenat's (1977) AM and Langley's (1981) BACON rediscovered a number of conjectures and laws from the history of mathematics and science. Research continued during the 1980s, leading to multiple books on the topic (e.g., Shrager & Langley, 1990). Research in this period also focused on historical examples, but the 1990s saw repeated application of these ideas to discover new scientific knowledge, as Langley (2000) has recounted.

However, the past decade has seen a reduction of work on computational scientific reasoning and discovery, at least within the AI community. Undoubtedly, this has resulted partly from the allure of computational biology and bioinformatics, which has convinced many researchers to focus on domain-specific methods. Others have been attracted to the smaller movement in scientific data mining, which typically focuses on image analysis. Both developments have drawn people away from the computational study of science at a more general level, and many researchers in the new areas have little knowledge of well-established AI techniques that proved crucial to earlier efforts. Despite these trends, the original challenges remain, and we need more research on general principles for scientific reasoning and discovery that cut across domains.

One such challenge is to develop computational methods that cover the entire range of structures and processes that occur in science. These include taxonomies, laws, theories, models, explanations, anomalies, and the mechanisms that produce and operate over them. Another daunting task involves combining these mechanisms into integrated systems that cover the great variety of observed scientific behavior. Some researchers have taken preliminary steps along these lines (Kulkarni & Simon, 1988; Nordhausen & Langley, 1993), but we need more concerted efforts. A key subtask involves closing the loop between law/model construction and observation/experimentation, as Żytkow et al. (1990) did in their work on electrochemistry. We would also benefit from computational accounts of extended periods from the history of science, as this would force broader coverage and integration. Applications are also important, but we need not automate all facets of science to provide useful software; mixed-initiative systems are likely to find more ready adoption than fully automated ones. AI research on these topics would give us a much more complete understanding of science, one of the most intriguing activities of the human mind.



## References

Feigenbaum, E. A., Buchanan, B. G., & Lederberg, J. (1971). On generality and problem solving: A case study using the DENDRAL program. In B. Meltzer & D. Michie (Eds.), *Machine intelligence 6*. Edinburgh: Edinburgh University Press.

Kulkarni, D., & Simon, H. A. (1988). The processes of scientific discovery: The strategy of experimentation. *Cognitive Science*, *12*, 139–175.

Langley, P. (1981). Data-driven discovery of physical laws. *Cognitive Science*, *5*, 31–54.

Langley, P. (2000). The computational support of scientific discovery. *International Journal of Human–Computer Studies*, *53*, 393–410.

Lenat, D. B. (1977). The ubiquity of discovery. *Artificial Intelligence*, *9*, 257–285.

Nordhausen, B., & Langley, P. (1993). An integrated framework for empirical discovery. *Machine Learning*, *12*, 17–47.

Shrager, J., & Langley, P. (Eds.) (1990). *Computational models of scientific discovery and theory formation*. San Francisco: Morgan Kaufmann.

Simon, H. A. (1966). Scientific discovery and the psychology of human problem solving. In R. G. Colodny (Ed.), *Mind and cosmos: Essays in contemporary science and philosophy*. Pittsburgh: University of Pittsburgh Press.

Żytkow, J. M., Zhu, J., & Hussam, A. (1990). Automated discovery in a chemistry laboratory. *Proceedings of the Eighth National Conference on Artificial Intelligence* (pp. 889–894). Boston, MA: AAAI Press.