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Research in machine scientific discovery and the domain sciences: Invited response to "Computer science research in scientific discovery"

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In his thought-provoking paper, Valdes-Perez (1996, this volume) carefully describes the methodology and future directions for research in Machine Scientific Discovery (MSD), as viewed predominantly from the standpoint of computer science. Here, I shall offer some remarks from the angle of domain sciences (despite the fact that my basic area of expertise is actually general and computational linguistics).

MSD takes a meta-position in respect to the particular, or domain, sciences and thus can be viewed as "science of sciences". It is, therefore, similar to philosophy of science, but MSD offers, in addition, a computational treatment of science; hence its label "computational philosophy" (e.g. Thagard, 1988). Just like philosophy, then, the developments and results within MSD research will have significant impact on the developments and results within the diverse domain sciences (the influence in the opposite direction, from domain sciences to MSD, will also be relevant, recalling the contributions sciences have made to philosophical development, but I will generally ignore this question here).

Although MSD may be regarded as well-established within AI research, it is by no means so readily recognised by domain sciences (as traditional philosophy was, and still is). The attitude towards MSD, as far as could be judged by talks with scholars from diverse fields, is highly ambiguous, ranging from very strong skepticism, bordering on complete distrust, to unclouded optimism and unreserved belief. Generally, mathematicians and natural scientists (including such with considerable programming experience) would be on the negative side of the evaluation scale, while the humanitarians, who are (still) with understandably less computer skills, would be on the positive. This distribution invites the undesirable conclusion that the trust in the possibility of mechanical discovery is inversely proportional to someone's computer literacy.

There is a grain of truth in such an explanation, attributing, on the one hand, disbelief to people who are fully aware of the diverse and significant difficulties to be encountered in computer implementations, and on the other hand, uncritical trust to people hardly sensing those problems, and hence taking for granted the omnipotence of computers. My own explanation to this matter will be along different lines only insofar as non-humanitarians are concerned. It seems to me that the basic reason for the radical distrust on their part is not their computer competence, but is rather, partly, their general unfamiliarity with AI developments (and especially with work on MSD), and partly, the still predominant conception of "discovery", as connoting uniqueness, unprecedented grandeur, mysteriousness and similar things, all (or sufficiently many) of which are by definition irreplicable. As for humanitarians, the computer is often no less mysterious to them than a discovery itself, so that a mysterious thing, it could be trusted, could produce another of its own kind (surely, this is not intended as a rationalisation that humanitarians themselves would normally provide).

Researchers in MSD need to carefully evaluate such attitudes and take the necessary measures to promote the status of MSD within scientific communities. It seems that the best step to make to both convince disbelievers and support the trust in the faithful is merely to give good examples of

MSD research that could serve as models to be followed by philosophically-minded and computationally-trained scholars from domain sciences.

Some specification is necessary here due to the recent distinction in MSD research between "computational models" and "computational actors" (cf. Valdes-Perez (this volume); the distinction is also referred to as the "historical/cognitive" paradigm vs. the "expert-system" paradigm). This distinction is usually assumed to lie in the novelty of results achieved by a discovery system, and it has been argued that the old historical/cognitive paradigm, laying emphasis on historical reconstruction or plausible human problem solving, should be replaced by programs that are computational actors in the actual practice of science and would lead to really novel discoveries. My personal sympathies go equally with both camps, and I believe that all kinds of MSD research are actually needed for domain science research, and their merit needs to be judged by the convincingness of the cases made rather than proclaimed goal. Besides, I feel that the distinction somewhat unsurely rests on the idea of novelty, for both approaches may give (and have actually given) new results, only for different fields of study: for the psychology of scientific discovery or history of science (the historical/cognitive approach) and for concrete individual sciences (the expert system approach).

Besides good examples, it also seems essential that the exposition in MSD research should be in as accessible a form as possible, since it is not likely that domain scholars will have the AI competence of a computer scientist.

Retrospectively, a great deal has been done in MSD. Domain scientists would find early work like the Logic Theorist or the book by Langley et al. (1987) fundamental, and later research like the collections in Shrager and Langley (1990) and the recent *AAAI Spring Symposium* on discovery quite stimulating. A lot more remains to be done both as regards the understanding of discovery and as regards its computer simulation. The intregration of different facilities into one system, judging the novelty and importance of a discovery are still hard computational nuts to crack. Some aspects of science (e.g. its social structure) have remained, to my knowledge, outside the scope of computer implementations. A down-to-earth view would perhaps reveal that there are legion of problems awaiting machine discovery. Nevertheless, it will be clear that MSD research has provided the scientist with a more explicit theory of discovery, supplemented by methods and programs to be used in pursuing novel discoveries, which is a definite advancement over the previous (dignified) philosophical contributions and the highly penetrating discovery work by G. Polya.

On their part, domain scientists should show greater interest to MSD, and more generally to machine learning techniques, and a willingness (and the talent) to reconsider and recast their specific tasks in AI terms. This radically new perspective could hardly fail to be rewarding to the daring.

References

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