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Model-Based Scientific Discovery

A Study In Space Bioengineering

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Scientific discovery has been a focus of recent AI developments. Although not all researchers agree on the exact bounds of scientific discovery, theory formation is clearly at the core of the domain. Relevant AI research done in scientific discovery includes Kocabas (1992); Karp (1989); Prager, Belanger, and De Mori (1989); Kulkarni and Simon (1988); and Langley et al. (1987). My Ph.D. dissertation (Groleau 1992)[1] focuses on routine aspects of discovery. I consider model-based discovery to be a diagnosis and design problem. More precisely, model-based–theory refinement can be seen as a four-step process: (1) gather data, (2) compare the data to model-based predictions, (3) identify the sources of discrepancies between the predictions and the field data, and (4) fix these discrepancies by modifying the model. The first three steps are traditionally addressed by diagnosis systems, but the fourth step requires design techniques. In my dissertation, I present a system called MARIKA (model analysis and revision of implicit key assumptions) that performs model-based scientific discovery. It modifies the theory contained in a model of the human spatial-orientation system.

The Vestibular Domain

The *human orientation system* is a complex system in which the brain merges information from a variety of sensors to help maintain a coherent interpretation of body position and movement. These sensors include the semicircular canals and the otolith organs located in the inner ear as well as vision and somatosensory perception. I designed a model of this system based on the observer theory model (OTM), which was developed by Merfeld (1990) for the orientation system of the squirrel monkey. Under this scheme, the central nervous system has an internal representation of the sensor organs and tries to minimize the error between its estimate of the sensory afferent signals and the actual afferent signals.

As designed, MARIKA's goal is to classify the vestibular system of the subject as normal or abnormal and propose a corresponding model. It works iteratively until the results of the proposed experiment can be modeled. Additional experiments can be presented in succession to the same model.

I designed a model of the human orientation system based on the observer theory model

MARIKA comprises simulation, constraint-propagation, and model-revision modules (figure 1). The model is captured in a simulation environment that produces time-varying signals. The model parameters are represented as constrained range variables. The input, the output, and the intermediary signals are segmented in time. The signals are then approximated by linear combinations of a set of four simple shapes adequate for the vestibular domain. The model's linear[2] differential equations and boundary conditions are transformed into constraints on the curve-fit parameters and the model parameters. Clinical data are abstracted using the shapes predicted by the model. These data are then compared to simulation predictions by propagating the constraints relating the model and the curve-fit parameters. If the data and the predictions are compatible, the current model is returned, and another experiment can be considered. Otherwise, the system automatically extends the range of vestibular parameters or structurally modifies the model using a patch from a library of model patches. The modified vestibular model is used during the next iteration until a fit is achieved.

Model-Based Theory Formation as Diagnosis and Design

MARIKA starts from a theory expressed in a mathematical model of differential equations. Therefore, it doesn't consider the theory-generation problem for unorganized data. However, it is rare for a theory to survive without modification. I claim that the process of scrutinizing a theory to correct it can be viewed as a diagnosis and design problem. Hamscher and Davis (1987) make the following claim about the diagnosis process:

> A useful way to decompose this [diagnosis] task is to consider three separate tasks: (i) generating fault hypotheses, (ii) checking those hypotheses for consistency, and (iii) discriminating among the consistent hypotheses on the basis of further probes or tests.

MARIKA implements the first task by propagating constraints representing model parameters, equations, and signal shapes. Propagation failure directly indexes possible model modifications called *patches*. Structural patches include replacing defective versions of entire organs or nervous processing centers or suppressing nervous links between organs and processing centers. Nonstructural patches relax vestibular parameter constraints to account for subjects outside the normal distribution. Consistency of the patches is ensured

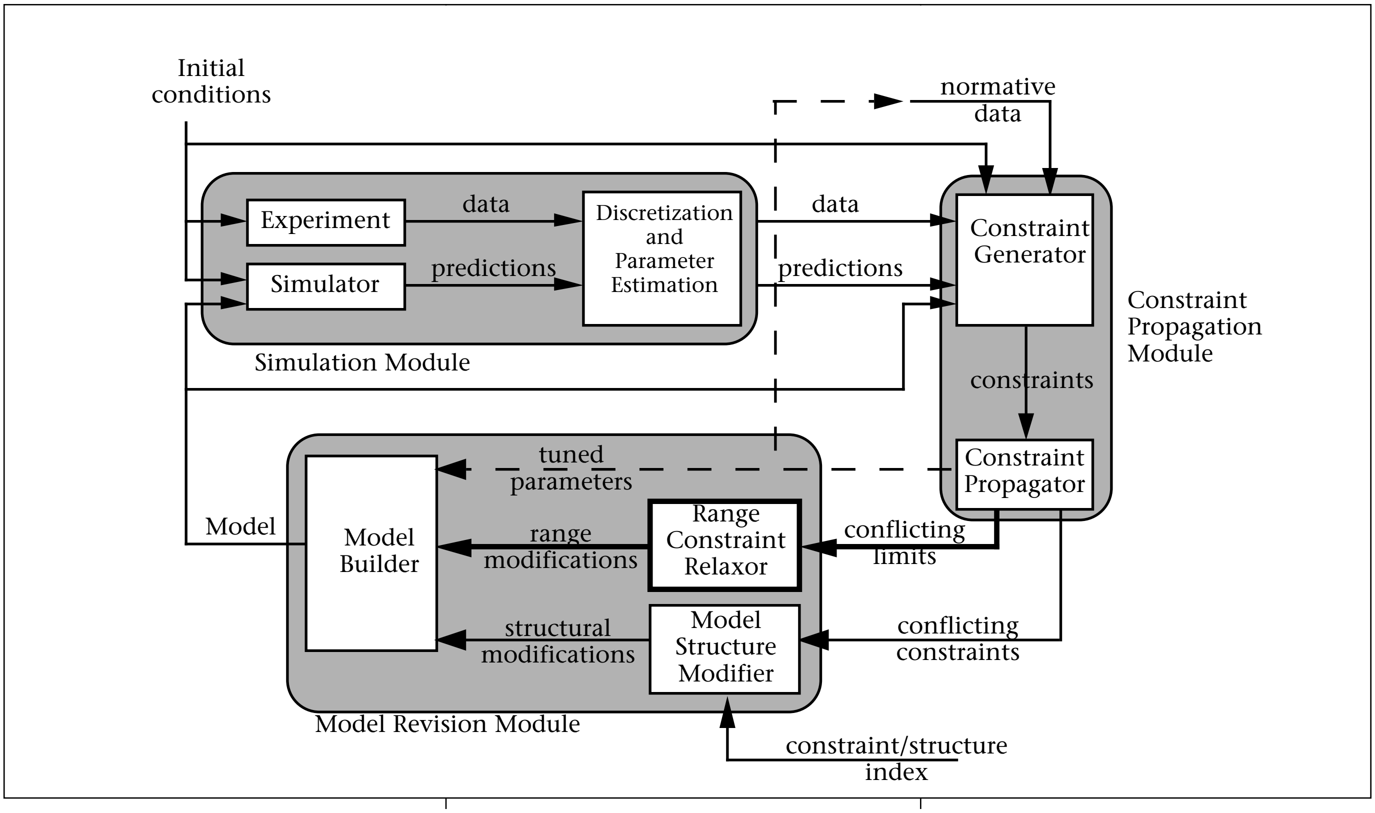

Figure 1. Overview of MARIKA's Structure.

by running the patched model through another constraint-propagation pass. Discrimination among competing patches requires further debugging and the application of parsimony considerations. I view model-based theory formation as a reverse form of diagnosis where the data are correct, but the model is wrong. To paraphrase Hamscher and Davis (1987), the goal of model-based scientific discovery can be described as follows: Given some valid experimental data, a description of the internal structure of the theoretical model, and descriptions of the behavior of its components, we wish to find which components of the model failed in such a way as to explain all discrepancies and suggest how to fix them.

The diagnosis approach to scientific discovery has to be complemented by a model-redesign step. The diagnosis process is concerned with locating the fault, assuming either that the component can be repaired or replaced according to established procedures. Scientific discovery must design a new model that leaves no unexplained data. MARIKA has a patch library that provides a small but interesting model space to search in. Thus, MARIKA correctly models normal vestibular data and several end-organ and nervous system–processing defects. The system was run on eight examples from two different experiments. Interestingly, MARIKA diagnosed a set of horizontal body-rotation data from the Massachusetts Eye and Ear Infirmary Vestibular Laboratory as abnormal, although the data were tagged as normal. Published results from other laboratories confirmed the finding.

Scientific Contributions

In the spirit of Widman and Loparo (1989), MARIKA provides a more intelligent simulation system because of its AI component and a more realistic reasoner because of its simulation component.

MARIKA contributes to the vestibular domain through the advanced modeling development it entails. It demonstrates the use of proven AI techniques adapted from diagnosis and design that help solve a problem often believed to require some level of intuition (see previous examples). It proves that the understanding of a mathematically modeled domain can be enhanced with the help of adapted AI techniques. It shows that an appropriate mix of qualitative and quantitative representations and methods can be used in synergy to provide adequate detail at reasonable computational cost. It uses a discrete representation of time to reason about time-varying signals in an efficient manner.

MARIKA demonstrates an automated discovery system in an actual scientific domain. Although the domain is clinical, not active, vestibular research, attention has been paid to understanding the domain thoroughly and crafting a representation that makes reasoning natural and efficient.

Limitations and Future Work

A knowledge-based patch suggester would also enhance the opportunistic nature of the system. Because of its simple model-patch indexing scheme, MARIKA explores a space of possible models that can be outlined when the library is designed. A system generating its own model patches would discover models in a more data-driven, exploratory, and dynamic fashion. Because it would be described implicitly, the model space explored could be an order of magnitude larger. MARIKA works well with models that can be represented as linear differential equations. The system handles four basic signal shapes at this stage but could easily be extended to others. However, no general mathematical mechanism is capable of recognizing or handling novel shapes. The segmentation of the signals is critical to proper approximation of the data. Other domains could require segmentation algorithms, as in the FLITE system by Prager, Belanger, and De Mori (1989).

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Notes

1. Copies of this dissertation are available from Beverly Linton, Man-Vehicle Laboratory, Room 37-215, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, 617/253-7805.

2. Some extensions are also provided to cover simple nonlinear cases and steady-state conditions.

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