

SELF-CALIBRATING MODELS FOR DYNAMIC MONITORING AND DIAGNOSIS

Benjamin Kuipers
Computer Science Department
University of Texas at Austin
Austin, Texas 78712 USA

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Abstract

The goal of our work in qualitative reasoning is to develop methods for automatically building qualitative and semi-quantitative models of dynamic systems, and to use them for monitoring and fault diagnosis. Our qualitative approach to modeling provides a guarantee of coverage while our semiquantitative methods support convergence toward a numerical model as observations are accumulated. In recent work, we and our collaborators have developed and applied methods for automatic creation of qualitative models; developed two methods for obtaining tractable results on problems that were previously intractable for qualitative simulation; and developed more powerful methods for learning semi-quantitative models from observations and deriving semi-quantitative predictions from them. With these advances, qualitative reasoning comes significantly closer to realizing its aims as a practical engineering method.

1 Introduction

The world is infinite, continuous, and continually changing over time. Human knowledge and human inference abilities are finite, apparently symbolic, and therefore incomplete. Nonetheless, people normally reason quite effectively about the physical world.

Models of particular systems or mechanisms play an important role in this capability. In service of a task such as diagnosis or design, simulation predicts the behaviors that follow from a particular model. In diagnosis or explanation, these predictions include testable consequences of a diagnostic hypothesis. In design, these predictions make explicit the consequences of a set of design choices.

A qualitative differential equation (QDE) model is a symbolic description expressing a state of incomplete knowledge of the continuous world, and is thus an abstraction of an infinite set of ordinary differential equations models. Qualitative simulation predicts the set of possible behaviors consistent with a QDE model and an initial state. Together, these methods support a meaningful and sound approach to "proof by simulation".

We have developed a substantial foundation of tools for model-based reasoning with incomplete knowledge: QSIM and its extensions for qualitative simulation; Q2, Q3 and their successors for semi-quantitative reasoning on a qualitative framework; and the CC and QPC model compilers for building QSIM QDE models starting from different ontological assumptions.

The QSIM representation for qualitative differential equations (QDEs) and qualitative behaviors was originally motivated by protocol analysis studies of expert explanations. A QDE represents a set of ODEs consistent with natural states of human incomplete knowledge of a physical mechanism. Qualitative simulation can be guaranteed to produce a set of qualitative behavior descriptions covering all possible behaviors of all ODEs covered by the QDE.

The subsequent evolution of QSIM has been dominated by the mathematical problems of retaining this guarantee while producing a tractable set of predictions. A variety of methods now exist for applying a deeper analysis, changing the level of description, or appealing to carefully chosen additional assumptions, to obtain tractable predictions from a wide range of useful models.

Quantitative information can be used to annotate qualitative behaviors, preserving the coverage guarantee while providing stronger predictions. Quantitative information may be expressed as bounds on landmarks and other symbolic elements of the qualitative description [Kuipers & Berleant, 1988], by adaptively inserting new time-points to improve the resolution of the description and converge to a numerical function [Berleant & Kuipers, 1992, 1993], and by deriving envelopes bounding the possible trajectories of the system [Kay & Kuipers, 1992, 1993]. Observations are interpreted by unifying quantitative measurements against the qualitative behavior prediction, yielding either a stronger prediction or a contradiction. As quantitative uncertainty in the QDE and initial state decrease to zero, the resulting behavioral description converges to the true quantitative behavior, though computational costs can still be high with current methods.

We have developed two model-compilers for QDE models: CC, which takes the component-connection view of a mechanism, and QPC, which implements an extended version of Qualitative Process Theory. Other model-compilers for QDEs, e.g. using bond graphs or compartmental models, have been developed elsewhere. These model-building tools will support deeper investigation into selection of views and modeling assumptions.

There are several inference schemes built on the set of all possible behaviors that are particularly well-suited to reliable model-based reasoning for diagnosis and design. For design, desirable and undesirable behaviors can be identified, and additional constraints inferred to guarantee or prevent those behaviors.

For monitoring and diagnosis, plausible hypotheses are unified against observations to strengthen or refute the predicted behaviors. In MIMIC [Dvorak & Kuipers, 1989, 1991], multiple hypothesized models of the system are tracked in parallel in order to reduce the "missing model" problem [Perrow, 1985]. Each model begins as a qualitative model, and is unified with *a priori* quantitative knowledge and with the stream of incoming observational data. When the model/data unification yields a contradiction, the model is refuted. When there is no contradiction, the predictions of the model are progressively strengthened, for use in procedure planning and differential diagnosis. Only under a qualitative level of description can a finite set of models guarantee the complete coverage necessary for this performance.

During the past year, we have made substantial progress in several areas: modeling of complex physical systems; semiquantitative reasoning and monitoring; and tractable qualitative simulation. We also constructed a QSIM model of the Space Shuttle Reaction Control System [Kay, 1992], which serves as a testbed for applying our methods. During the summer of 1992, our group hosted Prof. Lyle Ungar and three of his students from the Chemical Engineering Department at the University of Pennsylvania, who are applying our tools to problems in chemical engineering. The following sections present abstracts of publications summarizing many of our recent results.

2 Automated Model Building

2.1 QPC

Adam Farquhar has built the QPC model compiler into a substantial tool for building domain theories and qualitative models for complex physical systems. Farquhar's doctoral dissertation formalizes and proves the soundness of the QPC model-building algorithm, an essential step toward engineering-quality guarantees.

Automated Modeling of Physical Systems in the Presence of Incomplete Knowledge

Adam Farquhar

Department of Computer Sciences

University of Texas at Austin

This dissertation presents an approach to automated reasoning about physical systems in the presence of *incomplete knowledge* which supports formal analysis, proof of guarantees, has been fully implemented, and applied to substantial domain modeling problems. Predicting and reasoning about the behavior of physical systems is a difficult and important task that is essential to everyday commonsense reasoning and to complex engineering tasks such as design, monitoring, control, or diagnosis.

A capability for automated modeling and simulation requires

- expressiveness to represent incomplete knowledge,
- algorithms to draw useful inferences about non-trivial systems, and
- precise semantics to support meaningful guarantees of correctness.

In order to clarify the structure of the knowledge required for reasoning about the behavior of physical systems, we distinguish between the *model building* task which builds a model to describe the system, and the *simulation* task which uses the model to generate a description of the possible behaviors of the system.

This dissertation describes QPC, an implemented approach to reasoning about physical systems that builds on the expressiveness of Qualitative Process Theory [Forbus, 1984] and the mathematical rigor of the QSIM qualitative simulation algorithm [Kuipers, 1986].

The semantics of QPC's modeling language are grounded in the mathematics of ordinary differential equations and their solutions. This formalization enables the statement and proof of QPC's correctness. If the domain theory is adequate and the initial description of the system is correct, then the actual behavior of the system must be in the set of possible behaviors QPC predicts.

QPC has been successfully applied to problems in Botany and complex examples drawn from Chemical Engineering, as well as numerous smaller problems. Experience has shown that the modeling language is expressive enough to describe complex domains and that the inference mechanism is powerful enough to predict the behavior of substantial systems.

2.2 QPC Applied to Chemical Engineering

Catino [1993] constructed a large QPC domain theory within chemical engineering for the purpose of doing hazard and operability (HAZOP) studies of moderate-sized chemical process plants. The domain library consists of 50+ model-fragments, and has been used to construct models as large as 280 variables and 340 constraints, making it one of the largest qualitative models ever built. The

abstract of her doctoral dissertation, written under the supervision of Prof. Lyle Ungar, is quoted below.

**Automated Modeling of Chemical Plants
with Application to Hazard and Operability Studies**

Catherine A. Catino, Ph.D.
Department of Chemical Engineering
University of Pennsylvania

When quantitative knowledge is incomplete or unavailable (e.g. during design), qualitative models can be used to describe the behavior of chemical plants. Qualitative models were developed for several different process units with controllers and recycle, including a nitric acid plant reactor unit, and simulated using QSIM. In general, such systems produce an infinite number of qualitative states. Two new modeling assumptions were introduced, perfect controllers which respond ideally to a disturbance and ignore dynamics in controller variables, and pseudo steady state which ignores transients in all variables. Redundant constraints, reformulated equations, and quantitative information were also used to reduce ambiguity.

A library of general physical and chemical phenomena such as reaction and heat flow was developed in the Qualitative Process Compiler (QPC) representation and used to automatically build qualitative models of chemical plants. The phenomenon definitions in the library specify the conditions required for the phenomena to occur and the equations they contribute to the model. Given a physical description of the equipment and components present, their connectivity and operating conditions, the automatic model builder identifies the phenomena whose preconditions are satisfied and builds a mathematical model consisting of the equations contributed by these active phenomena. Focusing techniques were used to ignore irrelevant aspects of behavior. A dynamic condenser model was automatically generated illustrating QPC's ability to create a new model when a new phase exists.

Based on the ability to automatically build and simulate qualitative process models, a prototype hazard identification system, Qualitative Hazard Identifier (QHI), was developed which works by exhaustively positing possible faults, simulating them, and checking for hazards. A library of general faults such as leaks, broken filters, blocked pipes, and controller failures is matched against the physical description of the plant to determine all specific instances of faults that can occur in the plant. Faults may perturb variables in the original design model, or may require building a new model. Hazards including over-pressure, over-temperature, controller saturation, and explosion were identified in the reactor section of a nitric acid plant using QHI.

3 Tractable Qualitative Simulation

3.1 Qualitative Phase Portraits

The phase portrait is an important representational tool by which engineers capture the possible behaviors of a dynamical system. Wood Wai Lee has just completed a doctoral dissertation in which he shows that qualitative simulation can be used to construct qualitative phase portraits of non-trivial systems, inheriting the QSIM guarantees of complete coverage.

A qualitative method to construct phase portraits

Wood Wai Lee and Benjamin J. Kuipers

AAAI-93

We have developed and implemented a method based on qualitative simulation to construct phase portraits for a significant class of systems of two coupled first order autonomous differential equations, even in the presence of incomplete, qualitative knowledge.

Differential equation models are important for reasoning about physical systems. The field of nonlinear dynamics has introduced the phase portrait representation as a powerful tool for the global analysis of nonlinear differential equations.

QPORTRAIT uses qualitative simulation to generate the set of all possible qualitative behaviors of a system. Constraints on two-dimensional phase portraits from nonlinear dynamics make it possible to identify and classify the asymptotic limits of trajectories and constrain their possible combinations. By exhaustively forming all combinations of features, and filtering out inconsistent combinations, QPORTRAIT is guaranteed to generate all possible qualitative phase portraits.

We have applied QPORTRAIT to obtain tractable results for a number of nontrivial dynamical systems.

Guaranteed coverage of all possible behaviors of incompletely known systems complements the more detailed but approximation-based results of recently-developed methods for intelligently-guided numerical simulation [Nishida et al; Sacks; Yip; Zhao]. Together, these methods contribute to automated understanding of dynamical systems.

3.2 Behavior Abstraction

Daniel Clancy has developed a method for creating a lattice of abstractions of the tree of possible qualitative behaviors, providing a space of alternate descriptions with different degrees of tractability and discriminating power.

Behavior Abstraction for Tractable Simulation

Daniel J. Clancy and Benjamin Kuipers

QR-93

Most qualitative simulation techniques perform simulation at a single level of detail highlighting a fixed set of distinctions. This can lead to intractable branching within the behavioral description. The complexity of the simulation can be reduced by eliminating uninteresting distinctions. Behavior abstraction provides a hierarchy of behavioral descriptions allowing the modeler to select the appropriate level of description highlighting the relevant distinctions. Two abstraction techniques are presented. Behavior aggregation eliminates occurrence branching by providing a hybrid between a behavior tree representation and a history based description. Chatter box abstraction uses attainable envisionment to eliminate intractable branching due to chatter within a behavior tree simulation.

4 Semi-Quantitative Reasoning

Herbert Kay, collaborating with Kuipers and Ungar, has developed two major pieces of the puzzle of semiquantitative simulation. First, he has created, implemented, and proved the soundness of the dynamic envelope method for predicting improved bounds on behavior trajectories, given bounds on landmark values and envelopes around monotonic functions. Second, he and Ungar have developed a new method for learning envelopes around monotonic functions from a stream of observations.

4.1 Predicting Dynamic Bounds on Behaviors

Numerical Behavior Envelopes for Qualitative Models

Herbert Kay and Benjamin Kuipers

AAAI-93

Semiquantitative models combine both qualitative and quantitative knowledge within a single semiquantitative qualitative differential equation (SQDE) representation. With current simulation methods, the quantitative knowledge is not exploited as fully as possible. This paper describes *dynamic envelopes* – a method to exploit quantitative knowledge more fully by deriving and numerically simulating an *extremal system* whose solution is guaranteed to bound all solutions of the SQDE. It is shown that such systems can be determined automatically given the SQDE and an initial condition. As model precision increases, the dynamic envelope bounds become more precise than those derived by other semiquantitative inference methods. We demonstrate the utility of our method by showing how it improves the dynamic monitoring and diagnosis of a vacuum pumpdown system.

4.2 Learning Static Bounds on Functions

Deriving Monotonic Function Envelopes from Observations

Herbert Kay and Lyle H. Ungar

QR-93

Much work in qualitative physics involves constructing models of physical systems using functional descriptions such as “flow monotonically increases with pressure.” Semiquantitative methods improve model precision by adding numerical envelopes to these monotonic functions. Ad hoc methods are normally used to determine these envelopes. This paper describes a systematic method for computing a bounding envelope of a multivariate monotonic function given a stream of data. The derived envelope is computed by determining a simultaneous confidence band for a special neural network which is guaranteed to produce only monotonic functions. By composing these envelopes, more complex systems can be simulated using semiquantitative methods.

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Session A3: ARTIFICIAL INTELLIGENCE III

Session Chair: Dr. Peter Friedland

