Machine-Assisted Extraction of Formal Semantics from Domain Specific Semi-Formal Diagrams

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Abstract

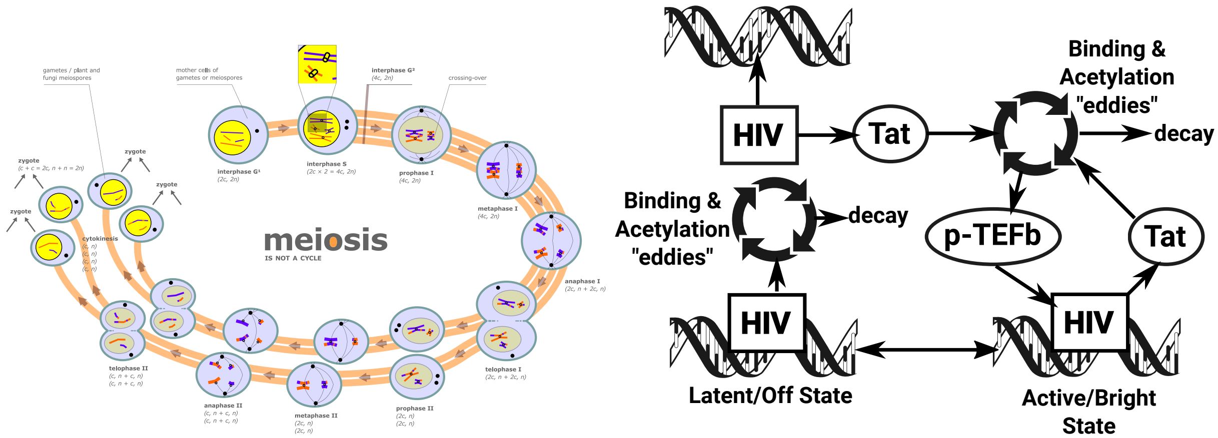
Analyzing complex systems is a challenging process which requires not only teams of domain experts but often also a multidisciplinary team of data scientists, mathematicians, statisticians, and software engineers in order to support the life cycle of model development, model-based inference, information extraction, and knowledge synthesis. The models that typically result from this process today are bespoke, lack generalizability, are not performable, lack reusability, and make the task of synthesizing actionable knowledge and policies from their raw outputs difficult. In this paper we describe AMIDOL: the Agile Metamodel Inference using Domain-specific Ontological Languages, a project that aims to reduce the overhead associated with the development, deployment, maintenance, and reuse of models of complex systems. Our technique utilizes a common intermediate representation which is designed to support a number of scientific, physical, social, and hybrid domains by allowing domain experts to define their models in a novel way: using domain specific ontological languages (VDSOLs). The intermediate representation provides formal, executable, meaning to the semi-formal diagrams domain experts normally create, and allows the inference engine to build prognostic queries on associated reward models. AMIDOL binds results from the inference engine to the original ontologies providing more explainability when compared to conventional methods.

1 Introduction

The construction of computational models is an important practice for scientists, engineers, policy makers, and other domain experts as it provides a way to make predictions of behavior, to test hypotheses, and to explain witnessed phenomena. The process of building suitable models, however, is a laborious one which requires diverse teams of experts, significant manual effort, and typical results in models with severe limitations, low performability, and little reusability or generalizability. Such models are not only costly to produce, both in time and effort, but are also prone to errors, difficult to verify, and do not utilize best practices in software development.

AMIDOL seeks to improve the problems inherent to modern machine-assisted inference with two high-level goals: 1) improving the ability of domain experts to build and maintain models and 2) improving the explainability and agility of the results of machine-inference. AMIDOL achieves these goals by utilizing a universal intermediate representation which provides executable representations to semantic concepts in a directed graph framework, and translates these representations to traditional machine learning and model solution techniques providing computational meaning to the semi-formal diagrams already being generated by domain experts.

Current modeling formalisms are often specified in formal languages which seem arcane and unnatural to domain experts, but have unambiguous formal mathematical meaning. By contrast domain experts have naturally developed visual semi-formal ways of describing the systems they study,



(a) Example of a semi-formal diagram of Meoisis. CC-BY-SA 3.0 Marek Kultys, July 2, 2008.

(b) Example of a semi-formal diagram of the molecular model of the Tat transactivation circuit.

Figure 1: Examples of semi-formal diagrams drawn by domain experts to represent operational semantics and complex system models.

such as those illustrated in Figure 1, but which are often ambiguous and lack formal mathematical meaning. In Luca Cardelli's paper on the abstract machines of systems biology [2] he notes that these semi-formal diagrams come close to capturing the operational semantics of process algebras, a concept he expanded on when deriving a formal calculus of membrane interactions [1]. While Cardelli was able to provide a calculus for a single sub-domain, the need for formal languages which describe biological, physical, or chemistry in an intuitive way was highlighted in Paul Nurse's 2008 paper [15]:

> "There should be a concerted programme . . . which will require both the development of the appropriate languages to describe information processing in biological systems and the generation of more effective methods to translate biochemical descriptions into the functioning of the logic circuits that underpin biological phenomena."
>
> (Paul Nurse (2008))

Significance AMIDOL seeks to provide a framework for the development of models which formally describe biological systems and complex systems from other domains using visual domain specific languages backed by a domain inspecific intermediate representation. This framework provides several significant advancements on the state of the art which seek to improve the usability, maintainability, reusability, and performability of scientific models. First, AMIDOL will provide translators from many Visual Domain Specific Ontological Languages (VDSOLs) to a single intermediate representation allowing VDSOLs to be specified for new domains and extended easily. Second, AMIDOL will provide transformations on models in its intermediate representation to optimize the execution of these models, compose models to build more powerful and complex representations, and to overlay reward structures on these models to specify metrics of interest and experiments to perform with AMIDOL's inference engine. Finally, AMIDOL provides translations from models in the intermediate representation into solver targets for the inference engine, checking constraints of composed reward structures and solving for measures of interest. AMIDOL allows these results to be communicated back to the user through the VDSOL, relating raw statistical and machine learning output to the original graph to improve explainability.

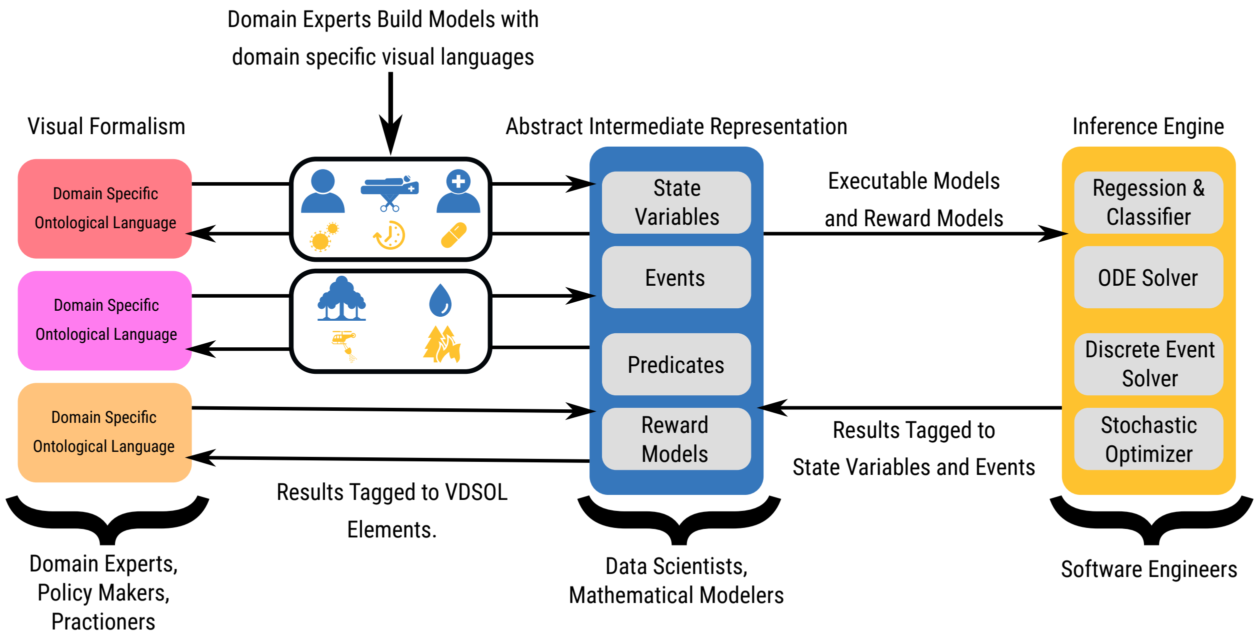


Figure 2: AMIDOL Architecture

2 AMIDOL

Figure 2 outlines AMIDOL's architecture and usage pattern. Users define models in one of a number of predefined VDSOLs using directed graphs connecting nouns and verbs. Each noun or verb has an underlying representation in the intermediate representation. These representations are then composed together with state sharing [18], and then composed with reward models which define metrics of interest. The resulting composed model can be further transformed in the intermediate representation for performability, efficiency, or other optimizations. AMIDOL then translates the model into a back end solver target, through code or script generation, and associates the results of executing a given solver with a set of nouns or verbs in the VDSOL to provide better explainability.

Visual Domain Specific Languages: AMIDOL is designed to support the definition of ontological languages which describe systems as directed graphs of nouns and verbs. Nouns and verbs for a given domain are organized into *palettes*. Nouns define elements which make up the state space of a system, and verbs define transitions in the state space. VDSOLs enable domain experts to build models of complex systems which are easier to maintain, validate, and verify, and avoid common pitfalls of monolithic and hand-coded implementations. To provide visual context for modelers AMIDOL supports the use of arbitrary scalable vector graphics (SVGs) to represent nouns and verbs, and features a canvas on which to draw nouns and verbs.

Composability of Atomic Models: AMIDOL is being designed to support the composition of individual models to enable model reuse, compositional methods for solution, to enhance backend support for performance optimizations such as symmetry detection, and to allow domain scientists to experiment by swapping out components of a model which may represent hypotheses about individual elements. Model composition in AMIDOL is being designed to support two primary mechanisms: *state-sharing* [17, 20] and *event-synchronization* [12].

Intermediate Representation: The Intermediate Representation (IR) for AMIDOL is designed to be a universal way to specify models, regardless of their domain, and provides a Turing-complete way to specify models performably, while avoiding domain specific considerations. The IR employed by AMIDOL has its roots in Markov models [11], Generalized Stochastic Petri-nets with inhibitor arcs [4] (which have been shown to be Turing complete), and stochastic activity networks [14, 19] (which are extensions of Petri-nets that allow more compact model specification). AMIDOL currently extends these concepts by creating ways to link to the original VDSOL, and by allowing embedded reward structures to be linked to a graph-based results database which stores the outcomes of experiments and can be used for the construction of arbitrary measures to support inference needs.

Formally, the IR is a 5-tuple, $(S, E, L, \Phi, \Lambda, \Delta)$ where:

- S is a finite set of state variables $\{s_0, s_1, \ldots, s_{n-1}\}$ that take on values in $\mathbb{N}$.
- E is a finite set of events $\{e_0, e_1, \ldots, e_{m-1}\}$ that may occur in the model.
- $L : S|E \to \mathbb{N}$ is the event and state variable labeling function that maps elements of S and E into the original ontology.
- $\Phi : E \times N_0 \times N_1 \times \ldots \times N_{n-1} \to \{0, 1\}$ is the event enabling predicate.
- $\Lambda : E \times N_0 \times N_1 \times \ldots \times N_{n-1} \to (0, \infty)$ is the transition rate specification.
- $\Delta : E \times N_0 \times N_1 \times \ldots \times N_{n-1} \to N_0 \times N_1 \times \ldots \times N_{n-1}$ is the state variable transition function specification.

Informally the IR is used to give formal definition to nouns, verbs, or entire models defined in a given VDSOL. **state-variables** and their current values make up the state of the model, and measure the configuration and capabilities of all modeled components. While state variables are defined as taking on values in $\mathbb{N}$, this does not restrict them from representing real numbers to arbitrary precision in modern computer hardware. In practice, they are implemented as integers, and floating point numbers by AMIDOL.

Events, when fired, change the state of a model by altering the value of state variables. Events in AMIDOL are associated with **input predicates** which define the enabling conditions of an event, **output predicates** which define the side effect of event firing, and a rate function which is used to calculate the inter-firing time of a given event.

An **input predicate** is associated with an event, and a set of state variables. Input predicates are functions of the value of their set of variables which map these sets and their values onto the set $\{0, 1\}$. When an input predicate evaluates to 1, the event is considered enabled and may fire. When the input predicate evaluates to 0, the event is considered disabled and cannot fire until subsequently enabled. An **output predicate** is associated with an event, and a set of state variables. Output predicates map a set of state variables, and their values, to new values for the same state variables defining the side effects of event firing on the state of the model.

3 Reward Variables, Reward Models, and Inference

The AMIDOL intermediate representation allows for the specification of reward variables or structures over a given model, and the composition of these structures with a model to produce new models which can be solved by the inference engine. We define two basic types of rewards structures, rewards over state variable values (rate rewards), and rewards over events (impulse rewards).

[16, 6, 5, 18] A rate reward is formally defined as a function $\mathcal{R} : P(S, \mathbb{N}) \to \mathbb{R}$ where $q \in P(S, \mathbb{N})$ is the reward accumulated when, for each $(s, n) \in q$, the value of the state variable s is n. Informally a rate reward variable x accumulates a defined reward whenever a subset of the state variables take on prescribed values. An impulse reward is formally defined as a function $\mathcal{I} : E \to \mathbb{R}$ where $e \in E, (I)_e$ is the reward for the completion of e. Informally an impulse reward variable x accumulates a defined reward whenever the event e fires.

Both rate and impulse reward variables measure the behavior of a model M with respect to time. As such, a reward variable θ is declared as either an instant-of-time variable, an interval-of-time variable, a time-averaged interval-of-time variable, or a steady state variable. An instant of time variable θ_t is defined as:

$$\theta_t = \sum_{\nu \in P(S,\mathbb{N})} \mathcal{R}(\nu) \cdot \mathcal{I}_t^{\nu} + \sum_{e \in E} \mathcal{I}(e) \cdot I_t^e$$

Intuitively a rate reward declared as an instant-of-time variable [10] can be used to measure the value of a state variable precisely at time t, and an impulse reward declared as an instant-of-time variable can be used to measure whether a given event fired at precisely time t. While the latter is not a particularly useful measure (as the probability of an event with a firing time drawn from a continuous distribution at time t is 0) it is defined for closure reasons, and for cases with discrete distributions and discrete time steps.

An interval-of-time variable intuitively accumulates reward over some fixed interval of time $[t, t+1]$. Given such a variable $\theta_{[t,t+1]}$ we formally define interval-of-time variables as:

$$\theta_{[t,t+1]} = \sum_{\nu \in P(S,\mathbb{N})} \mathcal{R}(\nu) \cdot \mathcal{J}_{[t,t+1]}^{\nu} + \sum_{e \in E} \mathcal{I}(e) N_{[t,t+1]}^{e}$$

where $J_{[t,t+1]}^{\nu}$ is a random variable which represents the total time the model spent in a state such that for each $(s, n) \in \nu$, the state variable s had a value of n during the period $[t, t + 1]$. Similarly $I_{t \to \infty}^{e}$ is a random variable which represents the number of times an event e fired during the period $[t, t + 1]$.

Time-averaged interval of time variables quantify accumulated reward averaged over some interval of time. Such a variable $\theta'_{[t,t+1]}$ is defined formally as $\theta'_{[t,t+1]} = \frac{\theta_{[t,t+1]}}{l}$.

Steady state reward variables are realized by testing for initial transients, and calculating an instant of time variable after a model has reached a stable steady state with high confidence.

4 Conclusions

We are currently testing AMIDOL using the SIS/SIR compartmental model of epidemiology. While simple, the SIS/SIR model utilizes real data from the CDC, and has a strong set of predictive capabilities. The primary objective of the SIS/SIR model is to identify the *basic reproduction number* associated with an infection, also known as R_0. The importance of estimating R_0 has been well established for many historical epidemics, including H1N1 [9] and Ebola [8]. This model also lends itself to testing AMIDOL's Design of Experiments module via public CDC Data on influenza infections by region and year [3], episodes which are well modeled by the SIR model.

Our initial tests with AMIDOL suggest that the framework can reduce the reliance of domain experts on bespoke and custom code. By providing an intermediate representation which is Turing complete, and expressive enough to allow the IR to be transformed to improve performance or tractability, such as when solving stiff systems of ODEs [7] we hope to enable domain experts to leverage the work of software engineers and mathematicians in a repeatable, and reusable way. By providing a common language for the expression of models and reward structures we hope to improve model maintainability, and to improve the ability of domain experts to share their results, and leverage models created by others in their domain, or even in adjacent domains. The end goal of AMIDOL is to create a community around this new framework similar to that of LLVM [13] with an open API for writing transformations for the IR, repositories of VDSOLs and models, and support for various back end solvers enabling more repeatable science utilizing machine-assisted inference.

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6 Resources, web sites, etc.

The current AMIDOL source code, including example models and documentation, is available at the AMIDOL Github site `https://github.com/GaloisInc/AMIDOL`.

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