Model-driven Design and Generation of Domain Simulators for Reinforcement Learning

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Abstract. Reinforcement learning (RL) is an important class of machine learning techniques, whereby intelligent agents optimize their behavior by observing and evaluating the outcomes of their interactions with their environment. Key for successful engineering of such agents is the availability of a large number of low-cost interactions with the target environment. This is often achieved through developing simulators of the latter, therewith different training strategies and parameters can be explored. However, specifying and implementing such simulators can be a complex endeavor requiring a systematic process for capturing and analyzing the associated goals, actions, and domain assumptions. We propose a model-driven goal-oriented framework for developing RL simulation environments. The framework utilizes a set of extensions to a standard goal modeling notation that allows automatic generation of a formal specification of the system to be simulated. The latter can be directly used by a specially constructed simulation engine to simulate the environment in question, such that off-the-shelf RL algorithms can use it as a training environment. We present the language extension, sketch its semantics, and show how models thereof can become executable.

Keywords: Goal Modeling Reinforcement Learning

1 Introduction

Over the past years, the demand for efficient Artificial Intelligence (AI) systems has been on the rise. Such systems perform tasks requiring human intelligence, such as driving vehicles, controlling devices, or making trading decisions. A specific kind of AI systems is based on Reinforcement Learning (RL), whereby intelligent software agents learn to optimize their behavior through continuously interacting with their environment [57]. RL has been studied in a variety of application domains including energy [4], traffic control [59], finance [52] and healthcare [27]. Intelligent RL agents can be seen as engaging in goal-oriented activity, whereby they perform actions to fulfill functional goals (e.g., administer a therapy, trade securities, control a heating device, etc.), while maximizing the satisfaction of higher level quality objectives (resp., health outcome, profit, occupant comfort) based on experience. Goal models [3, 16, 18, 25, 62] have been found to be suitable for model-driven analysis of the requirements for such agents [38], [37].

Key to successfully engineering an RL agent is the ability to subject it to a large number of opportunities for interaction with the target environment at a low cost. Using a *simulator* based on a model of the target environment allows RL agents to engage in a large number of training iterations that are unsafe or expensive to be performed in the real environment. When such model is accurate, the resulting policies are readily applicable to the target environment. When the model is provisional, approximate, or otherwise imprecise, simulator-based training is useful for exploring the performance of different learning algorithms under alternative problem formulations and parameter settings.

We propose a model-driven, goal-oriented framework for developing simulation environments for RL. The framework is based on developing goal models describing the required intentional structure of RL agents through representing how high-level agent goals are decomposed into low level actions, how the latter, upon their performance, give raise to stochastic outcomes, and how such outcomes, in turn, affect a variety of quality variables of interest, an aggregate of which is used to represent action/outcome rewards. The requirements model is then automatically translated into an action- and decision-theoretic formal specification which, through a set of proposed querying and simulation components, can be directly usable by RL agents as a training workbench. In this way, the training simulator is the result of a principled requirements-based approach that fully embraces modeling both for facilitating analysis and communication of the problem domain and for generating the actual simulator.

The paper is organized as follows. We describe the modeling language in Section 2 and the generation of simulators in Section 4. In Section 5 we discuss related work and we conclude in Section 6.

2 Modeling RL Domains

2.1 Motivating Example

Consider a large scale woodwork manufacturer who builds custom furniture and other wooden building structures in a make-to-order fashion. For every order they receive, they need to source the material and manufacture the requested product – among many other activities omitted here for simplicity. They have options as to how they perform these two steps. The material can be sourced from domestic or foreign sources. In the first case, the cost is higher, but in the latter case there are delay risks. Once the material is acquired, they can engage their in-house crafts-persons to build the product or subcontract to a more specialized group, who use precise manufacturing techniques but at a premium – plus they only work with domestic material. Importantly, a decision outcome of one step of the process, may affect what decision is best in a subsequent step. For example, a delay in sourcing may necessitate expedience in manufacturing to meet deadlines. In addition, choices have non-deterministic outcomes. For example, sourcing material from abroad may or may not delay, and the in-house crafts-persons may or may not produce a lower quality product.

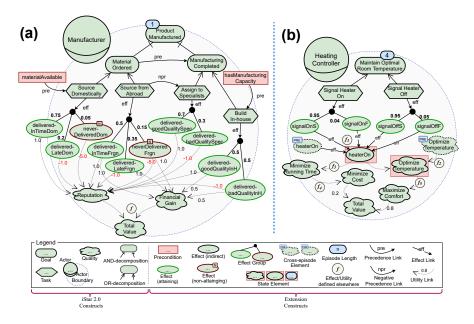


Fig. 1: An extended goal model.

The question for the manufacturer as they engage in this sequential decision making process for every incoming order is what decision they should be making at each step so that they are, on average, maximally satisfied in the end. Reinforcement learning (RL) refers to a set of techniques that have been proposed for addressing this problem via learning through experience [57]. Specifically, an RL agent actively engages with the environment by repeatedly performing actions which have the effect of (a) changing the state of the environment, typically in a non-deterministic way, and (b) offering to the agent a (positive or negative) reward reflecting the desirability of the action outcome or state change. They repeat until a goal state is reached and restart with a new effort to achieve the same goal. In the example case, an RL agent would, for each order, make a sourcing option, observe the outcome (delayed or not), proceed with a manufacturing option, observe that result (good quality or not) and move on to the next order. Various RL algorithms have been introduced for turning these repeated decision making sequences into a policy, which prescribes what action should be taken at each state, so that total reward is maximum on average.

As RL agents need to first process a potentially large number of cases before they can start making safe and good quality decisions, it is preferable that their training is not taking place in the actual environment but an executable model thereof, i.e., a simulator. Such a model should capture the decision points that are available to the RL agent, the corresponding alternative actions, the possible effects that these actions bring about, as well as the reward structure whereby the preferability of the effects is specified. The latter is particularly challenging in RL applications within socio-technical systems, such as the one of our example,

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where reward structures are abstract, subjective, and multi-dimensional. We next describe an extension to the standard goal modeling language that aims at developing such models.

2.2 Extending iStar for Reinforcement Learning: iStar-RL

The proposed language, which we will refer to as *iStar-RL*, extends iStar 2.0 [16], a language for goal-oriented modeling of socio-technical systems. Two examples of iStar 2.0 models can be viewed in Figure 1. Diagram (a) on the left shows the goals of the hypothetical woodwork manufacturer we discussed above.

As per the iStar 2.0 ontology, actors, such as Manufacturer, have goals, such as (Have) Material Ordered, which represent states of affairs that actors want to bring about and/or maintain. Through AND- and OR-decompositions, high-level goals are refined into lower-level ones, whereby satisfaction of all or, respectively, one subgoal(s) is necessary (resp. sufficient) for fulfilling the parent goal. At the leaf level, tasks signify concrete actions to be taken for fulfilling goals – e.g. Source Domestically. Quality goals (qualities) describe attributes for which actors desire some level of achievement, without the requirement that such level is precisely defined. Contribution links are used to signify that achievement of a goal/task affects a quality in a way that is described using an annotation on the link.

Models such as that of Figure 1(a) can encode a great number of subsets of leaf-level tasks and temporal orderings thereof that can fulfill top-level goals. Various ways of formalizing goal models for the purpose of identifying such task sequences have been introduced – e.g. [25, 30, 36, 46]. We adopt here a decision-theoretic extension to iStar for reasoning in the presence of probabilistic task effects [37,38] and further extend it with constructs that facilitate RL.

These extensions are showcased in Figure 1. A set of domain propositions are, firstly, introduced for describing the state of the environment at different points in time – for example, hasManufacturingCapacity and materialAvailable. Domain propositions are included in the model as the contents of precondition and effect elements. A precondition contains a boolean formula of domain predicates, whereas an effect contains one such predicate. Preconditions are connected to tasks through $precedence\ links \xrightarrow{pre}$ and, respectively, $negative\ precedence\ links \xrightarrow{npr}$ which denote that performance of the task is not possible unless (resp., if) the formula in the precondition is satisfied. Precedence (resp. negative precedence) links can also originate from goals meaning that the task cannot be performed unless (resp., if) the origin goal has been satisfied (resp., has been attempted, i.e. at least one of its descendant tasks has been successfully performed).

Further, tasks are connected with effects through the use of effect links $\stackrel{eff}{\longrightarrow}$, denoting that performance of the task from where the link originates can cause the effect which the link points at to occur, i.e., make the domain predicate contained in it true. As tasks may have several possible effects, they may be connected to effect groups which represent a collection of effects each carrying a distinct probability to occur once the task is performed. The probability is added as a label on the corresponding link on the diagram. Effects are marked

as task satisfying if their occurrence implies successful performance of the task, and non-satisfying otherwise. For example, an attempt to submit an order may be deemed successful (task satisfying) if it is finally delivered, despite delays, errors, etc., and non-satisfying if it is never delivered. Moreover, indirect effects, such as heaterOn in Figure 1(b), are effects whose truth status depends on other effects in a way that is defined outside the diagram – noted through an \bigcirc annotation. Effect links are used to connect regular effects with indirect effects.

Further, effects, including indirect, are connected to qualities through a specialization of iStar 2.0 contribution links which we call *utility links*. These are annotated either with a number representing the amount of satisfaction that the effect, if it occurs, adds to the quality or with the \bigcirc icon indicating that a more complex formula describes the relationship. Qualities, which can also be connected with each other using contribution links, form their own hierarchy with a top level goal o_{top} representing overall quality. In Figure 1, this goal is *Total Value*. Qualities in iStar-RL are considered to be continuous variables whose value represents level of satisfaction of the quality at a given state.

2.3 Task Histories, Goal Runs, and Episodes

Let us now focus tasks. Let task (performance) history be a sequence $tH^{|I} = [t_1, t_2, \ldots]^{|I|}$ of leaf-level tasks that (a) start from an initial state in which propositions and qualities have a value configuration I, and (b) is feasible with respect to the precondition and effect constraints, i.e., t_1 is feasible under I and each subsequent task is possible given the state that the previous task brought about. Attempt of each task results in the occurrence of an effect. Hence, a task history is mapped to a set of possible effect (occurrence) histories, $eH^{|I|} = [e_1, e_2, \ldots]^{|I|}$ we will henceforth omit the initial state superscript I unless needed. Further, let \mathcal{H} be the set of all goals and \mathcal{O} the set of all qualities in a model. The mappings $satG: \mathcal{H} \times \mathbf{eH} \mapsto \{true, false\}$ and $satQ: \mathcal{O} \times \mathbf{eH} \mapsto \mathbb{R}$, describe the satisfaction or not of a goal, and, respectively, the level of satisfaction of a quality, given an effect history eH from the set eH of all such. The former mapping reflects the AND/OR decomposition structure and the latter the structure of utility links; precisely how is discussed in a subsequent section.

Further, let \mathcal{G} be a goal model with root goal $r_{\mathcal{G}}$. A goal run for goal $r_{\mathcal{G}}$ is an effect history $eH = [e_1, e_2, \ldots]$ such that (a) $satG(r_{\mathcal{G}}, eH)$, i.e. the root goal is satisfied, (successful run) or (b) no other task can be performed at eH, due to precondition constraints, a situation we will call a deadlock.

Back in Figure 1(a), consider effect histories [deliveredInTimeDom, delivered-BadQualityInH] (materials sourced domestically and in-house production was of bad quality) and [neverDeliveredFrgn] (materials ordered from foreign sources and were never delivered). Both histories are goal runs: the former satisfies the root goal, whereas the latter cannot be continued due to the $\stackrel{pre}{\longrightarrow}$ link between Material Ordered and Manufacturing Completed. However neither [deliveredLate-Dom] nor [deliveredInTimeFrgn] are goal runs, as, in both cases, the root goal is not satisfied and there are actions that are still possible. The level of satisfaction satQ of quality Reputation for each of the aforementioned four histories is

+1.0 - 1.0 = 0, -5.0, -1.0, 1.0, respectively, calculated by simply adding up the annotations of utility links originating from effects included in the history.

We further define an episode to be a concatenation of n goal runs $eP^{|I} = [eH_1^{|I}, eH_2^{|I}, ..., eH_n^{|I}]$ such that for all $eH_i^{|I}$, i < n the root goal is satisfied. In other words, an episode describes a history of repeated goal runs all of which lead to the root goal being satisfied except for the last one, that may lead to a deadlock. For n > 1 the episode is a multi-run episode and for n = 1 a single-run episode. We can specify the maximum number of runs that comprise an episode $(episode\ length)$ as an annotation next to the root goal - see Figure 1. In multirun episodes, each run is, by default, assumed to start from the same initial configuration I. We may however wish to designate elements that carry their values across goal runs. We accomplish this through $cross-episode\ elements$.

To appreciate the rationale for multi-run episodes and the role of cross-episode elements in such episodes, consider the model of Figure 1(b). It describes the function of a heating device controller, contrived here to showcase additional features of the language. The controller periodically signals wirelessly to the device to turn on or off. This on or off signal can be lost with a probability. The overall quality accrued from a sequence of signaling tasks is a function of the distance of the temperature to an ideal one and the amount of time heating is on, which represents cost and environmental impact. To make meaningful optimal decisions one needs to look at the quality value accumulated over a sequence of events of attaining the top level goal, i.e., over several goal runs. According to the diagram this is set to four (4). Hence, if the controller makes a decision every, e.g., 5 minutes, which constitutes one goal run, an entire episode spans 20 minutes and overall quality is calculated for all 4 decisions made.

In Figure 1(b), cross-episode elements (dashed outline and with a "PRE" annotation) represent the (truth) value of the enclosed proposition or quality in the previous state. The previous state is the configuration of truth values before the latest action was performed within the episode, irrespective of goal run boundaries. Thus, the truth status of the proposition within indirect effect heaterOn (solid line effect), depends on its truth status at the end of the previous state (dashed line effect) and the current state of four regular effects in the second run, represented through the remaining four incoming effects. The symbol f denotes that the exact formula that translates the truth value of these five propositions into the new truth value for heaterOn is specified outside the diagram. Likewise, the current value of heaterOn. Again, a symbol f denotes that the formula for combining the two values is specified outside the diagram.

A final feature of the language is the designation of the exported state set, i.e., the set of propositions or qualities to be used for the calculation of policies. By default, we assume that the problem is modeled as discrete-state one, i.e., exported state set is the configuration of values of all propositions – the discrete state set. However, in some cases it is useful to designate the exported state to be a set of qualities of interest. In the heating controller example, whether the heater should turn on or off more obviously depends on the level to which

Reach Ideal Temperature has been achieved than the history of on and off. In the diagrams of Figure 1 we put a shaded rectangle at the background of an indirect effect or a quality, to mark its inclusion in the exported state. When the exported state contains at least one non-propositional element, we model the problem as a continuous-state one. In Figure 1(b) we designate variables heaterOn and Reach Ideal Temperature to exclusively comprise the exported state set – a continuous exported state set. Note that such designation does not affect the validity of task and effect histories which are based solely on the discrete state set; hence the "exported" qualification to prevent confusion.

2.4 iStar-RL and Reinforcement Learning

Let us now sketch how iStar-RL models can be used by an RL agent to allow for optimal decision making. Recall that RL-agents observe the state of the environment, perform an action from a set of available ones, and sense the state that results from the action along with the reward that the action yields. In our case, the state of the environment is, as we saw, the exported state, i.e., a combination of values of designated domain propositions and/or qualities. Upon sensing that state, the RL agent performs a task, which brings about the corresponding effect, which, in turn, augments the current episode eP with one more effect, and may also imply updated satG and satQ values. The RL agent will sense the new state and perceive the total value $satQ(o_{top}, eH_i)$ as the reward of the latest action. It will then repeatedly proceed with the next action until the episode is over, i.e., it reaches the maximum number of successful runs or a deadlock. During training, the RL agent will attempt a great number of such episodes, aimed at identifying a policy, i.e., a mapping from state to tasks that, when repeatedly followed, maximizes the average total value.

For the RL agent to accomplish such training using the domain model, the latter needs to be executable. In the next section, we describe how iStar-RL models can be formalized, aimed at both clarifying their semantics and paving the way for generating executable simulations of such models.

3 Semantics

3.1 DT-Golog

The semantics of iStar-RL are defined by means of its translation to DT-Golog, a high-level agent programming language [11,56] based on the situation calculus [53]. The basic constructs of DT-Golog are fluents, stochastic (or agent) actions, nature actions, and situations. Fluents play the role of state features and have different truth values in different situations. They are represented through predicates such as materialDelivered(s), with the situation s as one of the parameters. Stochastic actions a are first-order terms signifying specific activity initiated by agents and may have several alternative outcomes, each occurring with a different probability. These outcomes are modeled through a set of nature

actions $\hat{A} = \{\hat{a}_1, \hat{a}_2, ...\}$ associated with a through predicate $choice(a, \hat{A})$. The corresponding probabilities are represented using $prob(\hat{a}, v, s)$, where v is the probability of the occurrence of \hat{a} . Further, a situation s denotes a sequence of actions. Function $do(\hat{a}, s)$ denotes the situation which results from the performance of nature action \hat{a} in situation s. A special constant S_0 denotes the initial situation, where no action has been performed.

A DT-Golog specification contains axioms that prescribe what actions are possible in different situations and how the truth value of fluents is affected by the performance of actions. The former, *precondition axioms* are of the form:

$$\forall s.Poss(a,s) \leftrightarrow \Pi_a(s)$$

where $\Pi_a(s)$ is an arbitrary formula and special predicate Poss(a, s) states that action a is executable in situation s. Successor state axioms are of the form:

$$\forall \hat{a}, \mathbf{x}, s. f(\mathbf{x}, do(\hat{a}, s)) \leftrightarrow \Phi_f(\mathbf{x}, \hat{a}, s)$$

where \mathbf{x} signifies a list of arguments, f a fluent symbol and $\Phi_f(\mathbf{x}, \hat{a}, s)$ a formula whose truth value depends on the parameters, the current situation, and the nature action in question. Finally, by defining:

$$reward(v,s) \leftrightarrow \Psi_r(v,s)$$

where $\Psi_r(v,s)$ is a formula grounded on fluents, it is possible to assign a reward value v to any situation or action.

3.2 From iStar-RL to a DT-Golog specification

The DT-Golog-based semantics of iStar-RL is based on a treatment offered by Liaskos et al. [37], with the necessary additions for supporting RL. In what follows, let a goal model \mathcal{G} containing a set \mathcal{H} of goals, a set \mathcal{T} of tasks, a set \mathcal{E} of effects, a set \mathcal{Q} of domain predicates, and a set \mathcal{O} of qualities.

Primitives. Each element in the set is translated to a DT-Golog primitive as follows. For each domain proposition $q \in \mathcal{Q}$ introduce a fluent $\phi_q(s)$. For each task $t \in \mathcal{T}$ associated with an effect group $\mathcal{E}_t \subseteq \mathcal{E}$ introduce the following: a stochastic agent action a_t and a set of nature actions N_t each $\hat{a}_t \in N_t$ associated with an effect in \mathcal{E}_t . For each task $t \in \mathcal{T}$ and goal $h \in \mathcal{H}$, introduce fluents $\phi_t(s)$ and $\phi_h(s)$. For each quality $o \in \mathcal{O}$ introduce two fluents $\phi_o^{(r)}(v,s)$ and $\phi_o^{(m)}(v,s)$, respectively called *current satisfaction fluent* and *cumulative satisfaction fluent*; for both fluents, parameter $v \in \mathbb{R}$ represents satisfaction value of o.

Given the 1-1 correspondence between iStar-RL effects and situation calculus nature actions, effect histories $eH = [e_{t_1}, e_{t_2}, \ldots]$ also map 1-1 to situations $s = do(\ldots do(\hat{a}_{t_2}, do(\hat{a}_{t_1}, s_0)) \ldots)$, where \hat{a}_{t_i} is the nature action corresponding to effect e_{t_i} . For a goal h and quality o: satG(h, eH) iff $\phi_h(s)$ and satQ(o, eH) = v iff $\phi_o^{(r)}(v, s)$, where s is the situation corresponding to effect history eH.

Successor State Axioms. For each domain predicate q, collect all (if any) effects e_1, e_2, \ldots that mention it and consider the corresponding $\hat{a}_1, \hat{a}_2, \ldots$ nature actions. Introduce the following successor state axiom:

$$\phi_q(do(a,s)) \leftrightarrow (a = \hat{a}_1 \lor a = \hat{a}_2 \lor \ldots) \lor \phi_q(s).$$

Attempt and Attainment Formulae. Consider each task t connected with an effect group \mathcal{E}_t . Consider all the effects of \mathcal{E}_t , and the domain predicates

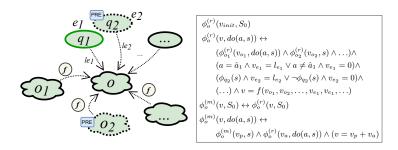


Fig. 2: Constructing quality formulae

 $q_1^{(t)}, q_2^{(t)}, \ldots$ contained in them. Generate the following task attempt formula for t: $\phi_t^{(att)}(s) \leftrightarrow \phi_{q_1^{(t)}}(s) \lor \phi_{q_2^{(t)}}(s) \lor \ldots$

A task attainment formula $\phi_t(s)$ is defined similarly with the only difference being that it excludes non-satisfying effects. Introduce also the a goal attainment formula for each goal h as follows:

$$\phi_h(s) \leftrightarrow f_{\text{AND/OR}}(\phi_{t_1}(s), \phi_{t_2}(s), \ldots)$$

where t_1, t_2, \ldots are the tasks that are descendants of h in the goal hierarchy, $\phi_{t_1}(s), \phi_{t_2}(s), \ldots$ their corresponding task attainment formulae, and $f_{\text{AND/OR}}$ an AND/OR formula reflecting the corresponding goal decomposition structure. A goal attempt formula for h, $\phi_h^{(att)}(s)$, is similarly defined but grounded on task attempt, rather than attainment, formulae.

Quality Formulae. Consider each quality or domain variable $o \in \mathcal{O}$, all the contribution links toward it coming from effects e_1, e_2, \ldots labeled with values l_{e_1}, l_{e_2}, \ldots , and all contribution links coming from other qualities o_1, o_2, \ldots see Figure 2 left side. Recalling that o is associated with fluents $\phi_o^{(r)}$ and $\phi_o^{(m)}$, the value of each is defined by the formulae at the right side of Figure 2. In the formulae, \hat{a}_i are the nature actions associated with effects e_i . Intuitively, the value v of quality o is a function f of the corresponding current or previous (depending on cross-episode status) values of the other qualities and/or the labels of utility links coming from effects that are(/were) currently(/previously) true.

Action Precondition Axioms. For each task t which receives precedence links from a precondition element, a set of tasks $\{t_1, t_2, \ldots\}$, a set of goals $\{h_1, h_2, \ldots\}$ and a set of effects containing predicates $\{q_1, q_2, \ldots\}$ introduce:

$$poss(a_t,s) \leftrightarrow \phi_{q_1}(s) \land \phi_{q_2}(s) \land \ldots \land \phi_{t_1}(s) \land \phi_{t_2}(s) \land \ldots \land \phi_{h_1}(s) \land \phi_{h_2}(s) \land \ldots \land g_{prec}(s) \land \neg \phi_t^{(att)}(s)$$
 where $g_{prec}(s)$ is the formula inside the precondition element, grounded on

where $g_{prec}(s)$ is the formula inside the precondition element, grounded on fluents of type $\phi_q(s)$, and $\phi_t^{(att)}(s)$ is the attempt formula for the task in question itself. As will become apparent below, the latter addition prevents the RL learning agent from selecting the same task more than once in a given episode. The above formula can be extended to include $\stackrel{npr}{\longrightarrow}$ incoming links, omitted here for simplicity; however it must be noted that for these links specifically, we utilize task and goal attempt formulae rather than attainment ones. **Reward.** The

total reward calculated for each situation is simply the *current* quality value of what has been designated as o_{top} as per the quality formula:

$$reward(v,s) \leftrightarrow \phi_{o_{top}}^{(r)}(v,s)$$

Probabilities. For each link that connects an effect e with its effect group, introduce $prob(\hat{a}, p, \cdot)$, where \hat{a} is the nature action associated with e, and p is the probability label of the link – independent of situation, hence \cdot instead of s. **OR-decomposition exclusivity.** We finally demand that all children of OR-decompositions are connected in pairs with $\stackrel{npr}{\longrightarrow}$ links. More formally, let g_1, g_2, \ldots be children (goals or tasks) of an OR-decomposition. Then, assume $g_i \stackrel{npr}{\longrightarrow} g_j$ for all $i \neq j$. The additions appear in action precondition axioms for the involved goals, following from the semantics of $\stackrel{npr}{\longrightarrow}$.

4 Making Models Executable

4.1 The Function of RL Simulation Components

So far we have discussed the iStar-RL modeling language and how it can be formalized into a DT-Golog specification. We now describe how the latter specification can serve as a domain simulator usable by software agents implementing arbitrary RL algorithms. We adopt a widely used interface specification for RL simulators, Open AI's Gym framework [1], called *gym.Env*, which offers a small collection of functions that satisfy the RL observe-decide-act interaction pattern. Specifically, the most important of *gym.Env*'s functions is:

observation, reward, terminated, info \leftarrow step(action)

The function requests the simulator to perform *action*, identified as an integer within a range, and return: (a) the state which results from the performance of *action*, which is encoded in variable *observation* as a state-identifying integer for discrete-space problems or as an array of real values for continuous-space problems, (b) the *reward* obtained for performing the action, and (c) whether the current episode is *terminated*, and (d) other miscellaneous *info*. Our goal is, hence, to use the formalized iStar-RL model to implement *step* (along with other auxiliary functions), so that the latter is compliant with the goal model, allowing thereby accurate simulation of the high-level iStar-RL model.

To achieve this we introduce two software components. The $Query\ Engine\ (QE)$ offers a number of functions that answer queries about the domain relative to a given a history of actions, such as what fluents are true and what actions are possible. These services are used by a GMEnv component which implements the gym.Env standard. GMEnv maintains information about the current state of execution of a simulated episode, and executes actions or relays information as per the requests of the client environment. The latter is an arbitrary RL agent, implementing some RL learning algorithm (e.g, A2C [41], Deep Q Network (DQN) [42], etc.) and requiring the gym.Env interface for its training. We examine the development of the QE and the GMEnv components in sequence.

The Query Engine (QE) 4.2

QE offers a set of functions whereby the iStar-RL model can be queried with respect to an effect history eH. The supported functions are listed in Table 1 and are implemented as logic programs in Prolog and in accordance to DT-Golog semantics also seen in the table. Below we present these semantics in more detail.

Extracting State Information. Consider the set $Q = q_1, q_2, \ldots$ of domain predicates in the goal model and an effect history $eH = [e_1, e_2, \ldots]$. Define also list $L_{\mathcal{Q}} = [ql_1, ql_2, \ldots]$ where $ql_i = 1$ if the predicate q_i is satisfied after effect history eH has been observed, and $ql_i = 0$ otherwise. For discrete-state problems, $L_{\mathcal{O}}$ offers a representation of discrete exported state and it is easily translatable to an integer identifier. For continuous-state problems, list $L_{\mathcal{O}} = [ol_1, ol_2, \ldots]$, where $ol_i = satQ(o_i, eH)$, represents continuous exported state for the goal model after eH for continuous exported state set $\{o_1, o_2, \ldots\} \subseteq \mathcal{O}$.

The semantics of $L_{\mathcal{Q}}$ and $L_{\mathcal{O}}$ in DT-Golog terms are understood as follows. Recall that there is a 1-1 correspondence between domain predicates Q = $\{q_1,q_2,\ldots\}$ and DT-Golog fluents $\Phi_{\mathcal{Q}}=\{\phi_{q_1},\phi_{q_2},\ldots\}$, as well as between an effect history eH and a DT-Golog situation s. The following rule then defines $L_{\mathcal{O}}$ in terms of situation s:

$$\begin{split} getState(s,L_{\mathcal{Q}}) \leftrightarrow (\phi_{q_1}(s) \wedge (ql_1=1) \vee \neg \phi_{q_1}(s) \wedge (ql_1=0)) \wedge \\ (\phi_{q_2}(s) \wedge (ql_2=1) \vee \neg \phi_{q_2}(s) \wedge (ql_2=0)) \wedge \dots \end{split}$$

Thus, $getState(s, L_Q)$ holds when binary list L_Q captures the truth value of every fluent in situation s. The predicate is the semantics of QE function getState(eH): bit[] seen in entry 5 of Table 1. For continuous exported states, recall that qualities $o \in \mathcal{O}$ in the goal model are associated with fluents of the form $\phi_o^{(r)}(v,s)$ in which v is a real value representing o's satisfaction satQ(o,eH). Hence, for continuous exported state set $\{o_1, o_2, \ldots\} \subseteq \mathcal{O}$: $getContState(s, L_{\mathcal{O}}) \leftrightarrow \phi_{o_1}^{(r)}(v_1, s) \land (ol_1 = v_1) \land \phi_{o_2}^{(r)}(v_2, s) \land (ol_2 = v_2) \land \ldots$

$$getContState(s, L_{\mathcal{O}}) \leftrightarrow \phi_{o_1}^{(r)}(v_1, s) \land (ol_1 = v_1) \land \phi_{o_2}^{(r)}(v_2, s) \land (ol_2 = v_2) \land ...$$

The predicate effectively maps a situation s with the value of fluents representing the qualities included in the exported state set, and constitutes the semantics of QE function getContState(eH):float[] - entry 6 of Table 1.

Episodes and Goal Runs. We now express the semantics of goal runs and episodes in terms of DT-Golog constructs. Recall that a task history is a goal run iff the root goal is satisfied or it leads to a deadlock. Recall also that for goal h, satG(h, eH) iff $\phi_h(s)$, where s is the situation corresponding to history eH. Thus, root goal $r_{\mathcal{G}}$ is satisfied iff $\phi_{r_{\mathcal{G}}}(s)$. Secondly, to decide if a situation s is a deadlock we examine if any of the action precondition axioms allow the performance of any task at s. Let $\mathcal{N}_{\mathcal{G}}$ to be the set of all nature actions \hat{a} (each corresponding to an effect $e \in \mathcal{E}_{\mathcal{G}}$), a situation s is a deadlock according to the following definition:

$$deadlock(s) \equiv \forall \hat{a} \in \mathcal{N}_{\mathcal{G}}. \neg poss(\hat{a}, s)$$

where $poss(\hat{a}, s)$ are, as we saw, the left-hand sides of action precondition axioms. Given the above, we can now define predicate done(s) (entry 7 of Table 1) that holds when a situation s is a complete run with respect to root goal r_G :

$$done(s) \equiv \phi_{r_{\mathcal{G}}}(s) \vee deadlock(s)$$

Cross-episode Elements. Recall from Figure 2 that in the initial situation S_0 , qualities are assigned an initial value v_{init} , while all other predi-

	QE Function	Semantics		QE Function	Semantics
1	<pre>possibleAt(t,eH): bool</pre>	$poss(a_t, s)$	7	done(eH):bool	$done(s) \equiv \\ \phi_{r_{\mathcal{G}}}^{att} \vee deadlock(s)$
2	<pre>getOutcomes(t): integer[]</pre>	$choice(a_t, \{\hat{a}_t^{(1)}, \hat{a}_t^{(2)},\})$	8	deadlock(eH):	$\forall \hat{a} \in \mathcal{N}_{\mathcal{G}}. \neg poss(\hat{a}, s)$
3		(, , , , , , , , , , , , , , , , , , ,			
	<pre>getProbs(t,eH):</pre>	$getProbs(a_t,$	9	<pre>getCrState(eH):</pre>	crossState(L, s)
	float[]	$\{p_t^{(1)}, p_t^{(2)}, \ldots\}, s\}$		float/bool[]	, , ,
4	reward(eH): float	reward(s,r)	10	setCrState(X)	(V)
				(X: initializations)	assert(X)
5	getState(eH):bit[]	$getState(s, L_{\mathcal{Q}})$	11	rootAchieved(eH):	4 (2)
				bool	$\phi_{r_{\mathcal{G}}}(s)$
6	<pre>getContState(eH):</pre>	getConState			
	float[]	$(s, L_{\mathcal{O}})$			

Table 1: Query Engine (QE) functions and their semantics. The functions assume a mapping of nature and stochastic actions to integers, hence t and eH are respectively an integer and an array thereof.

cates/fluents are assumed to be false. QE allows the client environment to both assert these initial values and to read the values at a given situation s. This is useful for implementing cross-episode elements within multi-run episodes. Let $L = \{ol_1, ol_2, \ldots, ql_1, ql_2, \ldots\}$ represent the values of all cross-episode qualities o_1, o_2, \ldots and propositions q_1, q_2, \ldots , where $ol_i = v$ iff $\phi_{o_i}(v, s)$ and $ql_i = 1$ iff $\phi_q(s)$, 0 otherwise. Predicate crossState(s, L) (the semantics of QE's getCrState – see entry 9 of Table 1) allows extraction of cross-state information given situation s corresponding to effect history eH:

 $crossState(s, L) \leftrightarrow \phi_{o_1}^{(m)}(v_1, s) \land (ol_1 = v_1) \land \phi_{o_2}^{(m)}(v_2, s) \land (ol_2 = v_2) \land \dots \\ [\phi_{q_1}(s) \land (ql_1 = 1) \lor \neg \phi_{q_1}(s) \land (ql_1 = 0)] \land [\phi_{q_2}(s) \land (ql_2 = 1) \lor \neg \phi_{q_2}(s) \land (ql_2 = 0)] \land \dots$

Dynamically defining initial states is a matter of asserting in the specification, using setCrState the list of initializations $\{\phi_{o_1}(v_1',s_0),\,\phi_{o_2}(v_2',s_0),\ldots,\varPhi_q^T(s_0)\}$, where v_i' are the desired initial values, $\varPhi_q^T(s_0)$ the subset of fluents representing propositions that are true in s_0 – see entry 10 of Table 1. Thanks to the above two functions, GMEnv can implement multi-run episodes by reading the values of cross-episode elements $o_1,o_2,\ldots,q_1,q_2,\ldots$ at the end of a run using getCrState and setting these as the initial values of the next episode using setCrState.

Other predicates. The query engine offers additional functions, which can be viewed on Table 1, along with their DT-Golog semantics. One of them: $getProbs(a_t, \{p_1, p_2, ...\}, s) \leftrightarrow choice(a_t, \{\hat{a}_t^{(1)}, \hat{a}_t^{(2)}, ...\}) \wedge$

 $prob(\hat{a}_t^{(1)}, p_1, s) \wedge prob(\hat{a}_t^{(2)}, p_2, s) \wedge \dots$

uses $choice(a_t, \hat{A})$ to collect probabilities $\{p_1, p_2, \ldots\}$ for all nature actions $\hat{A} = \{\hat{a}_t^{(1)}, \hat{a}_t^{(2)}, \ldots\}$ associated with task t's stochastic action a_t .

4.3 The GMEnv component

GMEnv implements gym.Env through utilizing the QE's services. While QE is stateless, GMEnv maintains episode information including the history of tasks that have been attempted from the beginning of an episode, the history of effects that has occurred upon such performance, the run count since the episode's beginning, as well as the state after the performance of the latest action.

Algorithm 1 Implementation of the Step function of GMEnv.

```
1: GLOBAL: eH,tH = []
                                                   ▷ run-wide effect and task history
            eH_Ep,tH_Ep =[]
                                               ▷ episode-wide effect and task history
2:
3:
            curRun = 0
                                           ▶ the goal run under current consideration
            penaltyReward

▷ default penalty for infeasible actions

 4:
                                            ▷ reference to a QE implementing object
5:
            qe
 6: function STEP(t)
7:
       if qe.possibleAt(t,eH) then
                                                                  \triangleright E_t: list of effects
8:
          E_t = qe.getOutcomes(t)
9:
          P_t = qe.getProbs(t,eH)
                                                       \triangleright P_t: list of effect probabilities
10:
          e_t = pickRndAction(E_t, P_t)
                                                               ▷ randomly pick effect
11:
           eH = append(eH,et)
                                                           ▶ append effect to history
12:
          tH = append(tH,t)
                                                            ▶ append task to history
13:
          reward = qe.reward(eH)
                                                                    ▷ retrieve reward
14:
                                                         > retrieve new discrete state
          state = qe.getState(eH)
15:
          c_state = qe.getConState(eH)
                                                                  ▷ optional: retrieve
                                                                new continuous state
16:
                                                                    ⊳ bit array to int
          n_state = bitToInt(State)
17:
       else
                                                          ▷ penalize infeasible action
18:
          reward = penatlyReward
19:
       end if
       if qe.rootAchieved(eH) then
20:
21:
          X = constructInitClauses(qe.getCrState(eH))
22:
          qe.setCrState(X)
23:
          eH_Ep.append(eH),tH_Ep.append(tH)
24:
          eH,tH = []
25:
          curRun = curRun + 1
26:
       end if
       return n_state, reward, DONE, [c_state]
27:
28: end function
29.
30: function DONE
31:
       return ((curRun == N) or qe.deadlock(eH))
32: end function
```

Of the gym.Env functions that GMEnv implements, the most important is, as we saw, step(task): state, reward, terminate, info. Algorithm 1 sketches the implementation of the function. The function is iteratively called by the RL agent, with parameter a task t of its choosing. Upon its call, step checks first if the task is feasible given the current history of effect occurrences, stored in eH, through the use of QE's possibleAt(t,eH). If yes, through getOutcomes(t) it retrieves a list of possible effects E_t that t may have and through getProbs(t,eH) their probabilities P_t . A random choice on the basis of the probabilities is made and both task t and the chosen effect e_t are appended to the corresponding lists, tH and eH respectively. The state resulting from the performance of t is calculated through getState(eH), which translates a history of effect occurrences to an array of bits representing the truth values of domain

	Model Characteristics			Learning Tests										
	Model Size	Size			Learning Reward A2C DON PPO		Training Steps A2C DQN PPO		Training Time (s)			Rnd.*		
			#	Space	AZC	DQN	PPU	AZC	DQN	PPU	AZC	DQN	PPO	
Discrete	Material	1.12	1	2^{6}	0.924	0.924	0.924	10K	10K	10K	6.813	5.000	24.00	0.771
	Ordered 1,12	2	2^{12}	1.711	1.712	1.715	10K	10K	10K	106.2	4.469	113.9	1.465	
	Product	2.20	1	2^{10}	0.477	0.480	0.465	10K	150K	20K	81.97	848	147.8	-78.42
	Manuf.	2	2^{20}	0.946	0.705	0.710	10K	80K	20K	8,123	23.49K	20.32K	-90.95	
	Organize Travel	3,29	1	2^{14}	0.789	0.694	0.788	20K	150K	10K	400.3	1,957	436.7	-94.46
	HVAC Control	1,13	4	2^{16}	-1.36	-1.37	-1.36	10K	70K	10K	585	702.4	724.2	-5.000
Conts.	Product	1ct 2,20	1	\mathbb{R}^2	0.456	0.472	0.048	50K	80K	50K	778.4	972.9	181.3	-78.42
	Manuf. 2,20	2	\mathbb{R}^2	0.286	0.667	0.325	70K	4.5M	70K	62.59	30,379	343.5	-90.95	
	HVAC Control	1,13	4	\mathbb{R}^2	-1.36	-1.36	-1.37	10K	110K	10K	709.5	390.1	769.8	-5.000

Table 2: Training with off-the-shelf RL agents. Times in CPU seconds. \mathbf{Rnd}^* excludes deadlock penalty. Model size n, m: n is total # of OR-nodes, m total # of elements.

propositions. An integer representation of the bit array, n_state, is, in turn, returned to the calling environment as per the *gym.Env* requirements. Likewise, getConState(eH) is called to retrieve any continuous exported state set.

If task t is not feasible at eH, step does not proceed with any changes to history lists and state, but may, based on user configuration, result in a negative reward to bias the learning procedure against performance of the task in the specific state. On the other hand, if the goal is achieved, the current run has concluded at eH. Consequently (a) the cross-run elements at eH are retrieved and reasserted as initial state for the next run, (b) the action and effect lists are added to the episode-wide record and (c) reset, and (d) the run counter increases by one. As we saw above, the episode is done if the root of the Nth goal run has been achieved or a deadlock has been detected.

Finally, the second important gym.Env function to be implemented by GMEnv reset(), simply empties the history lists and resets state to its initial values.

4.4 In Action

The proposed components QE and GMEnv along with any appropriately formalized iStar-RL model can be used by off-the-shelf algorithms for learning optimal policies. We performed tests with three such implementations, namely, Advantage Actor Critic (A2C) [41], Deep Q Network (DQN) [42] and Proximal Policy Optimization (PPO) [55], as implemented for the Stable-Baselines3 RL package [51]. For the experiments, we used discrete and continuous versions of models such as those of Figure 1. As a benchmark, for discrete-space problems, we also calculated optimal policies and their expected rewards using the DT-Golog interpreter. A modest Intel(R) Core(TM) i7-8650U CPU @ 1.90GHz, 4 Core(s), 16Gb RAM computer was used. In all cases, using default hyperparameters, the RL agents converged close to the optimal reward and away from the reward of the random policy. Further, the three algorithms performed differently both in terms of optimization outcome and in terms of numbers of

steps and time required, showing how the toolset can be useful for assessing the feasibility of various training techniques. A more extensive presentation of the experimental study along with a reproducibility package can be found at [?].

Note, that, while the formalized iStar-RL models can be used by DT-Golog for exact, search-based identification of optimal policies (vs. learning-based that RL agents do), this option is restricted to discrete-state problems, may not scale for larger models, and requires accurate probabilities. In the absence of accurate probabilities, where neither exact nor learning-based methods can calculate the true optimal, the generated simulators can still be useful for exploring the behavior of different RL algorithms using provisional probabilities.

5 Related Work

Substantial interest has developed over the past few years in studying the intersection of conceptual modeling (CM) with artificial intelligence (AI), a space referred to as CMAI [9,10]. The latter describes both the application of AI to support CM tasks (AI4CM), and reversely, the application of CM to systematize, streamline, and support various qualities AI-intensive systems (CM4AI). In the AI4CM context, machine learning has been used in tasks such as supporting extraction of models or schemas from data (e.g., [54,63–65]), supporting model transformation [13, 23], classification of models or repositories thereof [40, 47], model auto-completion [21], or assessment of realism of generated models [39]. In the CM4AI space, where our work finds a natural fit, the idea of using models organize, systematize, and support the ML development pipeline (from input collection and preparation, to training and inference) has been underlined [17]. Here, models have been proposed for quality assuring the AI/ML process [33], detecting bias [61], supporting meta-learning [29], chatbots generation [50] or generation of neural architectures [35].

The problem of systematically devising AI solutions has also been studied from the RE point of view. Major theme in that context is the quality of the end-result [28], with an emphasis on explainability [12,14,15], how such systems can be specified [8,58], and how the RE process can be organized [49]. In search for a solution to the RE4AI [2] problem, Nalchigar et al. [44,45] propose a goal-oriented conceptual framework for expressing machine learning requirements and designs organized around three main modeling views (business, analytics design, and data preparation). Ahmad et al. [2] review, among other things, modeling approaches for conducting RE for AI, to find that Goal Oriented RE languages, along with UML/SySML, are the most popular for modeling in that space.

Goal models have indeed been known to be effective vehicles for allowing formal reasoning about requirements and designs in various ways [19, 20, 25, 30, 36]. This capability of goal models has been utilized also in the area of adaptive systems [5, 7, 24] and multi-agent systems [26]. The modeling approach proposed here, iStar-RL, is heavily based on an iStar dialect proposed for modeling decision-theoretic domains and, through formalization, perform search-based reasoning thereof [37, 38]. The strength of the modeling approach we adopt,

compared to common approaches for modeling probabilistic transition systems (e.g., [32]) lies in the combined ability of goal models both to concisely encode high-variability processes and behaviors, stemming from overarching stakeholder goals, and to compare variants vis-à-vis intricate, multi-dimensional quality requirements structures [43]. Hence, efforts such as on probabilistic logic shields [60] using ProbLog [34], or on using DT-Golog for Q-learning [6], indicate promising destinations of iStar-RL transformations. Probabilistic reasoning using conceptual models other than goal models, such as BPMN [48], has also been proposed [22,31], with not clear connection to RL however.

6 Concluding Remarks and Future Work

We presented a framework for goal-oriented modeling and generation of RL simulators. Through an extension to a standard goal modeling language, designers can systematically identify the action, effect, and state spaces of the environments to be simulated through analysis of agent goals, while utilizing quality contribution structures for designing reward functions. Models constructed using the proposed language are subsequently translated to a formal specification, which is used by a set of interpreting components to allow step-wise execution of the model. Such step-wise execution lies at the heart of the RL process, hence the result is directly usable by a variety of RL algorithms. The framework is aimed at supporting investigations of the feasibility and performance of different training techniques against different action, reward, and probability models, and, when these models are deemed accurate, identifying a directly usable optimal or nearoptimal policy when dealing with continuous state spaces or, potentially, with problems that are too large for model-based techniques to solve. The approach is, hence, promising for systematically developing adaptive high-variability systems, such as adaptive business processes or behaviorally customizable software, while following well-studied goal oriented requirements engineering processes.

Future research effort can be dedicated towards exploring how the goal model representations can assist the learning process. Of particular interest is the exploration of novel RL algorithms that are allowed partial access to the domain specification (e.g., the precondition and contribution structures, or some presumed probability intervals) to be used for informing the training process. Further, potential may exist in applying some version of our proposal to the problems of AI safety and explainability. Firstly, the framework ensures that AI agent training is based on interaction data stemming from well-studied and well-behaved models, arguably confining the learned behavior to what is permitted by the model that trained it, or, conversely using the model as the source of safety standards (e.g., non violation of temporal constraints) for the trained agent. Secondly, by being faithful to i^* 's fundamental principle of centering the analysis around action and decision rationale, the iStar-RL model can serve as a suitable explanatory device for the respective actions and decisions performed by the acting RL agent that was trained against the model. Applications and case studies in various problem domains can be helpful in assessing the utility of the approach in these areas.

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