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# Schema Networks: Zero-shot Transfer with a Generative Causal Model of Intuitive Physics

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### Abstract

The recent adaptation of deep neural networkbased methods to reinforcement learning and planning domains has yielded remarkable progress on individual tasks. Nonetheless, progress on task-to-task transfer remains limited. In pursuit of efficient and robust generalization, we introduce the Schema Network, an objectoriented generative physics simulator capable of disentangling multiple causes of events and reasoning backward through causes to achieve goals. The richly structured architecture of the Schema Network can learn the dynamics of an environment directly from data. We compare Schema Networks with Asynchronous Advantage Actor-Critic and Progressive Networks on a suite of Breakout variations, reporting results on training efficiency and zero-shot generalization, consistently demonstrating faster, more robust learning and better transfer. We argue that generalizing from limited data and learning causal relationships are essential abilities on the path toward generally intelligent systems.

# 1. Introduction

A longstanding ambition of research in artificial intelligence is to efficiently generalize experience in one scenario to other similar scenarios. Such generalization is essential for an embodied agent working to accomplish a variety of goals in a changing world. Despite remarkable progress on individual tasks like Atari 2600 games (Mnih et al., 2015; Van Hasselt et al., 2016; Mnih et al., 2016) and Go (Silver et al., 2016), the ability of state-of-the-art models to *transfer* learning from one environment to the next remains limited. For instance, consider the variations of Breakout illustrated in Fig. 1. In these environments the positions of ob-



*Figure 1.* Variations of Breakout. From top left: standard version, middle wall, half negative bricks, offset paddle, random target, and juggling. After training on the standard version, Schema Networks are able to generalize to the other variations without any additional training.

jects are perturbed, but the object movements and sources of reward remain the same. While humans have no trouble generalizing experience on the basic Breakout to its variations, deep neural network-based models are easily fooled (Taylor & Stone, 2009; Rusu et al., 2016).

The model-free approach of deep reinforcement learning (Deep RL) such as the Deep-Q Network and its descendants is inherently hindered by the same feature that makes it desirable for single-scenario tasks: it makes no assumptions about the structure of the domain. Recent work has suggested how to overcome this deficiency by utilizing *object-based representations* (Diuk et al., 2008; Usunier et al., 2016). Such a representation is motivated by the well-acknowledged Gestalt principle, which states that the ability to perceive objects as a bounded figure in front of an unbounded background is fundamental to all perception

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(Weiten, 2012). Battaglia et al. (2016) and Chang et al.
(2016) go further, defining hardcoded *relations* between
objects as part of the input.

113 While object-based and relational representations have 114 shown great promise alone, they stop short of modeling 115 causality – the ability to reason about previous observations 116 and explain away alternative causes. A causal model is es-117 sential for regression planning, in which an agent works 118 backward from a desired future state to produce a plan 119 (Anderson, 1990). Reasoning backward and allowing for 120 multiple causation requires a framework like Probabilis-121 tic Graphical Models (PGMs), which natively supports ex-122 plaining away (Koller & Friedman, 2009). 123

124 Here, we introduce Schema Networks - a generative model 125 for object-oriented reinforcement learning and planning. 126 Schema networks incorporate key desiderata for the flexible and compositional transfer of learned prior knowl-128 edge to new settings<sup>1</sup>. 1) Knowledge is represented using 129 "schemas" - causal graphical model fragments involving 130 entities, their attributes, and learnable interactions among 131 entities; 2) In a new setting, the appropriate knowledge 132 fragments are automatically instantiated to guide action se-133 lection; and 3) The representation deals with uncertainty, 134 multiple-causation and explaining away, and stochastic-135 ity in a principled way. We describe the representational 136 framework and learning algorithms and demonstrate how 137 action policies can be generated by treating planning as 138 inference. We evaluate the end-to-end system on Break-139 out variations and compare against Asynchronous Advan-140 tage Actor-Critic (A3C) (Mnih et al., 2016) and Progressive 141 Networks (PNs) (Rusu et al., 2016), the latter of which ex-142 tends A3C explicitly to handle transfer. We show that the 143 rich structure of the Schema Network enables efficient and 144 robust generalization beyond the Deep RL models. 145

# 2. Related Work

148 The field of reinforcement learning has witnessed signifi-149 cant progress with the recent adaptation of deep learning 150 methods to traditional frameworks like O-learning. Since 151 the introduction of the Deep Q-network (DQN) (Mnih 152 et al., 2015), which uses experience replay to achieve 153 human-level performance on a set of Atari 2600 games, 154 several innovations have enabled faster convergence and 155 better performance with less memory. The asynchronous 156 methods introduced by Mnih et al. (2016) exploit multi-157 ple agents acting in copies of the same environment, com-158 bining their experiences into one model. As the Asyn-159 chronous Advantage Actor-Critic (A3C) is the best among 160 these methods, we use it as our primary point of compari-

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son.

Model-free deep RL models like A3C are unable to substantially generalize beyond their training experience (Jaderberg et al., 2016; Rusu et al., 2016). To address this limitation, recent work has attempted to introduce more structure into the neural network-based models. The Interaction Network (Battaglia et al., 2016) and the Neural Physics Engine (Chang et al., 2016) use object-level and pairwise relational representations to learn models of intuitive physics. The primary advantage of these models is their amenability to gradient-based methods, though such techniques might be applied to Schema Networks as well. Schema Networks offer two key advantages: latent physical properties and relations (schemas) need not be hardcoded; and planning can make use of backward search, since the model can distinguish different causes.

Schema Networks build upon the ideas of the Object-Oriented Markov Decision Process (OO-MDP) introduced by Diuk et al. (2008) (see also (Scholz et al., 2014)). Related frameworks include relational and first-order logical MDPs (Guestrin et al., 2003a). These various formalisms, which harken back to classical AI's roots in symbolic reasoning, are designed to enable robust generalization. Recent work by Garnelo et al. (2016) on "deep symbolic reinforcement learning" makes this connection explicit, marrying first-order logic with deep RL. This effort is similar in spirit to our work with Schema Networks, but like Interaction Networks and Neural Physic Engines, it remains limited without a mechanism for backward planning (also referred to as regression planning).

Generalization is the ability to transfer experience from one scenario to other similar scenarios, or, ideally, dissimilar scenarios that exhibit repeatable structure and sub-structure (Taylor & Stone, 2009). Schema networks achieve this by building an inductive model of the world after observing a limited and biased sample of it. It is also possible to attempt task-to-task transfer by directly using the learned model from one task to begin learning another, without attempting to generalize. This strategy is taken by Rusu et al. (2016) in their work on Progressive Networks (PNs). A PN is constructed by successively training copies of A3C on each task of interest. With each new task, the existing network is frozen, another copy of A3C is added, and lateral connections between the frozen network and the new copy are established to facilitate transfer of features learned during previous tasks. The obvious limitation of PNs is that the number of network parameters must grow quadratically with the number of tasks. However, even if this growth rate was improved, the PN would still be unable to generalize in the manner of Schema Networks to create one coherent model of all experiences.

Schema Networks are built on the technical foundations

 <sup>&</sup>lt;sup>161</sup>
 <sup>1</sup>We borrow the term "schema" from Drescher (1991), whose schema mechanism inspired the early development of our model.

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Figure 2. Construction and architecture of a Schema Network. A schema is a template for a factor that predicts future reward (A) or the value of an entity-attribute (B) based on entity states and actions taken in the present. Self-transitions (C) predict the value of entity-attributes in the absence of other factors. Selftransitions allow continuous or categorical variables to be represented by a set of binary variables (depicted as smaller nodes). The grounded schema factors and self-transitions are combined to create a Schema Network (D), which gives a generative model of the MDP transition and reward distributions.

of probabilistic graphical models (PGMs), which provide not only an expressive and powerful modeling language, but also a rich toolbox of inference techniques, including the ability to learn the structure of models. More importantly, reasoning with uncertainty and explaining away are naturally supported by PGMs. We direct the readers to (Koller & Friedman, 2009) and (Jordan, 1998) for a thorough overview of PGMs. In particular, early work on factored MDPs established how PGMs can be applied in RL and planning settings (Guestrin et al., 2003b).

## 3. Schema Networks

### 3.1. MDPs and Notation

The traditional formalism for the Reinforcement Learning problem is the Markov Decision Process (MDP). An MDP M is a five-tuple  $(S, A, T, R, \gamma)$ , where S is a set of states, A is a set of actions,  $T(s^{(t+1)}|s^{(t)}, a^{(t)})$  is the probability of transitioning from state  $s^{(t)} \in S$  to  $s^{(t+1)} \in S$  after action  $a^{(t)} \in A$ ,  $R(r^{(t+1)}|s^{(t)}, a^{(t)})$  is the probability of receiving reward  $r^{(t+1)} \in \mathbb{R}$  after executing action  $a^{(t)}$ while in state  $s^{(t)}$ , and  $\gamma \in [0, 1]$  is the rate at which future rewards are exponentially discounted.

#### 3.2. Model Definition

A Schema Network is a structured generative model of an MDP. We first describe the architecture of the model informally. An image input is parsed into a list of *entities*, which may be thought of as instances of objects in the sense of OO-MDPs (Diuk et al., 2008). All entities share the same collection of *attributes*. We refer to a specific attribute of a specific entity as an *entity-attribute*, which is represented as a binary variable to indicate the presence of that attribute for an entity. An *entity state* is an assignment of states to all attributes of the entity, and the complete model state is the set of all entity states.

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A grounded schema is a binary variable associated with a particular entity-attribute in the next timestep, conditioned on the present values of other entity-attributes. Each entityattribute that conditions the distribution is associated with 0 or 1, and the event that the entity-attribute assumes this value is called a *precondition* of the grounded schema. When the preconditions of a grounded schema are satisfied, we say that the schema is active, and it predicts the activation of its associated entity-attribute. Grounded schemas may also predict *rewards* and may be conditioned on *ac*tions, both of which are represented as binary variables. For instance, a grounded schema might define a distribution over Entity 1's "position" attribute at time 5, conditioned on Entity 2's "position" attribute at time 4 and the action "UP" at time 4. Grounded schemas are instantiated from *ungrounded schemas*, which behave like templates for grounded schemas to be instantiated at different times and in different combinations of entities. For example, an ungrounded schema could predict the "position" attribute of Entity x at time t+1 conditioned on the "position" of Entity y at time t and the action "UP" at time t; this ungrounded schema could be instantiated at time t = 4 with x = 1 and y = 2 to create the grounded schema described above. In the case of attributes like "position" that are inherently continuous or categorical, several binary variables may be used to discretely approximate the distribution (see the smaller nodes in Figure 2). A Schema Network is a factor graph that corresponds to the instantiation of a set of ungrounded schemas for a particular set of entities over some window of time. See Figure 2 for a high-level illustration of the Schema Network architecture.

We now formalize the Schema Network factor graph. For simplicity, suppose the number of entities and the number of attributes are fixed at N and M respectively. Let  $E_i$  refer to the  $i^{th}$  entity and let  $\alpha_{i,j}^{(t)}$  refer to the  $j^{th}$  attribute of the  $i^{th}$  entity at time t. We use the notation  $E_i^{(t)} = (\alpha_{i,1}^{(t)}, ..., \alpha_{i,M}^{(t)})$  to refer to the state of the  $i^{th}$  entity at time t. The complete state of the MDP modeled by the network at time t is then  $s^{(t)} = (E_1^{(t)}, ..., E_N^{(t)})$ . Actions and rewards are also represented with sets of binary

variables, denoted  $a^{(t)}$  and  $r^{(t+1)}$  respectively. A Schema 330 Network for time t will contain the variables in  $s^{(t)}$ ,  $a^{(t)}$ , 331  $s^{(t+1)}$ , and  $r^{(t+1)}$ . 332

333 Let  $\phi^k$  denote the variable for grounded schema k.  $\phi^k$ 334 is bound to a specific entity-attribute  $\alpha_{i,j}$ , and acti-335 vates it when the schema is active. Multiple grounded 336 schemas can try to predict the same attribute, and those 337 are combined through an OR gate. For binary vari-338 ables  $v_1, ..., v_n$ , let AND $(v_1, ..., v_n) = \prod_{i=1}^n P(v_i)$ 339 1), and  $OR(v_1, ..., v_n) = 1 - \prod_{i=1}^n (1 - P(v_i) =$ 340 1)). A grounded schema is connected to its precondi-341 tion entity-attributes with an AND factor, written as  $\phi^k =$ 342 AND $(\alpha_{i_1,j_1},...,\alpha_{i_H,j_H},a)$  for H entity-attribute precondi-343 tions and an optional action a. There is no restriction on 344 how many entities or attributes from a single entity can be 345 preconditions of a grounded schema. 346

347 An ungrounded schema (or template) is represented 348 as  $\Phi_l(E_{x_1},...,E_{x_H}) = \text{AND}(\alpha_{x_1,y_1},\alpha_{x_1,y_2}...,\alpha_{x_H,y_H}),$ 349 where  $x_h$  determines the relative entity index of the *h*-th 350 precondition and  $y_h$  determines which attribute variable is 351 the precondition. The ungrounded schema is a template 352 that can be bound to multiple specific entities and locations, 353 thus generating grounded schemas.

354 A subset of attributes corresponds to discrete positions. 355 These attributes are treated differently from all others, 356 whose semantic meanings are unknown to the model. 357 When a schema predicts a movement to a new position, 358 we must inform the previously active position attribute to 359 be inactive unless there is another schema that predicts it 360 to remain active. We introduce a self-transition variable to 361 represent the probability that a position attribute will re-362 main active in the next time step when no schema predicts 363 a change from that position. We compute the self-transition 364 variable as  $\Lambda_{i,j} = \text{AND}(\neg \phi^1, ..., \neg \phi^k, s_{i,j})$  for entity i 365 and position attribute j, where the set  $\phi^1 \dots \phi^k$  includes all 366 schemas that predict the future position of the same entity 367 *i* and include  $s_{i,j}$  as a precondition. 368

369 With these terms defined, we may now compute the transition function, which can be factorized as  $T(s^{(t+1)}|s^{(t)}, a^{(t)}) = \prod_{i=1}^{N} \prod_{j=1}^{M} T_{i,j}(s_{i,j}^{(t+1)}|s^{(t)}, a^{(t)}).$ 370 An entity-attribute is active at the next time step if either 372 373 a schema predicts it to be active or if its self-transition vari-374 able is active: 375

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$$T_{i,j}(s_{i,j}^{(t+1)}|s^{(t)}) = OR(\phi^{k_1}, ..., \phi^{k_Q}, \Lambda_{i,j})$$
(1)

Where  $k_1...k_Q$  are the indices of all grounded schemas that predict  $s_{i,j}$ .

### 3.3. Construction of Entities and Attributes

In practice we assume that a vision system is responsible for detecting and tracking entities in an image. It is therefore largely up to the vision system to determine what constitutes an entity. Essentially any trackable image feature could be an entity, which most typically includes objects, their boundaries, and their surfaces. Recent work has demonstrated one possible method for unsupervised entity construction using autoencoders (Garnelo et al., 2016). Depending on the task, Schema Networks could learn to reason flexibly at different levels of representation. For example, using entities from surfaces might be most relevant for predicting collisions, while using one entity per object might be most relevant for predicting whether it can be controlled by an action. The experiments in this paper utilize surface entities, described further in Section 5.

Similarly, entity attributes can be provided by the vision system, and these attributes typically include: color/appearance, surface/edge orientation, object category, or part-of an object category (e.g. front-left tire). For simplicity we here restrict the entities to have fully observable attributes, but in general they could have latent attributes such as "bounciness" or "magnetism".

### **3.4.** Connections to Existing Models

Schema Networks are closely related to Object-Oriented MDPs (OO-MDPs) (Diuk et al., 2008) and Relational MDPs (R-MDPs) (Guestrin et al., 2003a). However, neither OO-MDPs nor R-MDPs define a transition function with an explicit OR of possible causes, and traditionally transition functions have not been learned in these models. In contrast, Schema Networks provide an explicit OR to reason about multiple causation, which enables regression planning. Additionally, the structure of Schema Networks is amenable to efficient learning.

Schema Networks are also related to the recently proposed Interaction Network (IN) (Battaglia et al., 2016) and Neural Physics Engine (NPE) (Chang et al., 2016). At a high level, INs, NPEs, and Schema Networks are much alike - objects are to entities as relations are to schemas. However, neither INs nor NPEs are generative and hence do not support regression planning from a goal through causal chains. Because Schema Networks are generative models, they support more flexible inference and search strategies for planning. Additionally, the learned structures in Schema Networks are amenable to human interpretation, explicitly factorizing different causes, making prediction errors easier to relate to the learned model parameters.

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# 4. Learning and Planning in Schema Networks

In this section we describe how to train Schema Networks
(i.e., learn its structure) from interactions with an environment, as well as how they can be used to perform planning.
Planning is needed not only at test time to maximize reward, but also to improve exploration during the training
procedure.

### 4.1. Training Procedure

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451 Given a series of actions, rewards and images, we repre-452 sent each possible action and reward with a binary variable, 453 and we convert each image into a set of entity states S. 454 The number of entities is allowed to vary between adjacent 455 frames, accounting for objects appearing or moving out of 456 view. For each entity we record the attributes of the entities 457 at each position within a local neighborhood. Empty posi-458 tions in the neighborhood are represented by setting all its 459 attributes (other than position) to zero. This collection of 460 attributes can then be converted into a fixed-length binary 461 feature vector for a given neighborhood radius. This data 462 is aggregated across all frames and provided to the schema 463 learning algorithm described in Section 4.2. 464

465 While gathering data, actions are chosen by planning using 466 the schemas that have been learned so far. This planning 467 algorithm is described in Section 4.3. We use an  $\varepsilon$ -greedy 468 approach to encourage exploration, taking a random ac-469 tion at each timestep with small probability. We found no 470 need to perform any additional policy learning, and after 471 convergence predictions were accurate enough to allow for 472 successful planning. As shown in Section 5, since learning only involves understanding the dynamics of the game, 473 474 transfer learning is simplified and there is no need for pol-475 icy adaptation.

### 4.2. Schema learning

478 Structure learning in graphical models is a well studied 479 topic in machine learning (Koller & Friedman, 2009; Jor-480 dan, 1998). To learn the structure of the Schema Network, 481 we cast the problem as a supervised learning problem over 482 a discrete space of parameterizations (the schemas), and 483 then apply a greedy algorithm that solves a sequence of LP 484 relaxations. See Jaakkola et al. (2010) for further work on 485 applying LP relaxations to structure learning. 486

487 Let us arrange the observed inputs to the Schema Network 488 as a binary matrix  $X \in \{0, 1\}^{N \times D}$ , with one observation 489 per row. Similarly, let binary vector  $y \in \{0, 1\}^N$  represent 490 the observed binary outputs corresponding to the previous 491 inputs. Both X and y are collected during the environment 492 exploration. The output of the Schema Network is an esti-493

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mation of y and can be expressed as

$$\hat{y} = f_W(X) = \overline{\overline{X}W}\vec{1}$$

where all the involved variables are binary and operations follow Boolean logic: addition corresponds to ORing, and overlining to negation.  $W \in \{0, 1\}^{D \times M}$  is a binary matrix, with each column representing one (ungrounded) schema. The variables set to 1 in each schema represent an existing connection between that schema and an input condition (see Fig. 2). The outputs of each individual schema are ORed to produce the final prediction.

We would like to minimize the prediction error of Schema Networks while keeping them as simple as possible. A suitable objective function is

$$\min_{W \in \{0,1\}^{D \times M}} \frac{1}{N} |y - f_W(X)|_1 + C|W|_1, \qquad (2)$$

where the first term computes the prediction error, the second term estimates the complexity and parameter C controls the trade-off between both. This is an NP-hard problem for which we cannot hope to find an exact solution, except for very small environments.

We consider a greedy solution in which linear programming (LP) relaxations are used to find each new schema. Starting from the empty set, we greedily add schemas (columns to W) that have perfect precision and increase recall for the prediction of y (See Algorithm 1 in the Supplementary). In each successive iteration, only the input-output pairs for which the current schema network is predicting an output of zero are passed. This procedure monotonically decreases the prediction error of the overall schema network, while increasing its complexity. The process stops when we hit some predefined complexity limit. In our implementation, the greedy schema selection produces very sparse schemas, and we simply set a limit to the number of schemas to add. For this algorithm to work, no contradictions can exist in the input data (such as the same input appearing twice with different labels). Such contradictions might appear in stochastic environments, and would not be artifacts in real environments, so we preprocess the input data to remove them.

### 4.3. Planning as Probabilistic Inference

The full Schema Network graph (Fig. 2) provides a probabilistic model for the set of rewards that will be achieved by a sequence of actions. Finding the sequence of actions that will result in a given set of rewards becomes then a MAP inference problem. This problem can be addressed approximately using max-product belief propagation (MPBP) (Attias, 2003). Another option is variational inference. Cheng et al. (2013) use variational inference for planning, but also 495 496 497

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550 end up resorting to MPBP to optimize the variational free 551 energy functional. We will follow the first approach.

552 Without lack of generality, we will consider the present 553 time step to be t = 0. The state, action and reward variables 554 for  $t \leq 0$  are observed, and we will consider inference over 555 the unobserved variables in a look-ahead window of size<sup>2</sup> 556  $T, \{s^{(t)}, a^{(t)}, r^{(t)}\}_{t=0}^{T-1}$ . Since the Schema Network is built 557 exclusively of compatibility factors that can take values 0 558 or 1, any variable assignment is either impossible or equally 559 probable under the joint distribution of the graph. Thus, if 560 we want to know if there exists any global assignment that 561 activates a binary variable (say, variable  $r_{(+)}^{(t)}$  signaling pos-itive reward at some future time t > 0), we should look at the max-marginal  $\tilde{p}(r_{(+)}^{(t)} = 1)$ . It will be 0 if no global 562 563 564 assignment compatible with both the SN and existing ob-565 servations can lead to activate the reward, or 1 if it is fea-566 sible. Similarly, we will be interested in the max-marginal 567  $\tilde{p}(r_{(-)}^{(t)} = 0)$ , i.e., whether it is feasible to find a configuration that avoids a negative reward. 568 569

570 At a high-level, planning proceeds as follows: Identify feasible desirable states (activating positive rewards and de-572 activating negative rewards), clamp their value to our de-573 sires by adding a unary potential to the factor graph, and 574 then find the MAP configuration of the resulting graph. 575 The MAP configuration contains the values of the action 576 variables that are required to reach our goal of activating/deactivating a variable. We can also look at S to see how the model "imagines" the evolution of the entities un-579 til they reach their goal state. Then we perform the actions 580 found by the planner and repeat. We now explain each of these stages in more detail.

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Potential feasibility analysis First we run a feasibility analysis. To this end, a forward pass MPBP from time 0 to time T is performed. This provides a (coarse) approximation to the desired max-marginals for every variable. Because the SN graph is loopy, MPBP is not exact and the forward pass can be too optimistic, announcing the feasibility of states that are unfeasible<sup>3</sup>. Actual feasibility will be verified later, at the backtracking stage.

Choosing a positive reward goal state We will choose the potentially feasible positive reward that happens sooner within our explored window, clamp its state to 1 and backtrack (see below) to find the set of actions that lead to it. If backtracking fails, we will repeat for the remaining potentially feasible positive rewards.

Avoiding negative rewards Keeping the selected positive reward variable clamped to 1 (if it was found in the previous step), we now repeat the same procedure on the negative rewards. Among the negative rewards that have been found as potentially feasible to turn off, we clamp to zero as many negative rewards as we can find a jointly satisfying backtrack. If no positive reward was feasible, we backtrack from the earliest predicted negative reward.

**Backtracking** This step is akin to Viterbi backtracking, a message passing backward pass that finds a satisfying configuration. Unlike the HMM for which the Viterbi algorithm was designed, our model is loopy, so a standard backward pass is not enough to find a satisfying configuration (although can help to find good candidates). We combine the standard backward pass with a depth-first search algorithm to find a satisfying configuration.

# **5.** Experiments

We compared the performance of Schema Networks, A3C, and PNs (Progressive Networks) on several variations of the game Breakout. The chosen variations all share similar dynamics, but the layouts change, requiring different policies to achieve high scores. A diverse set of concepts must be learned to correctly predict object movements and rewards. For example, when predicting why rewards occur, the model must disentangle possible causes to discover that reward depends on the color of a brick but is independent of the ball's velocity and position where it was hit. While these causal relationships are straightforward for humans to recover, we have yet to see any existing approach for learning a generative model that can recover all of these dynamics without supervision or curriculum and transfer them effectively.

Because Schema Networks rely on an input of entity states instead of raw images, we attempted to provide the same information to A3C and PNs by augmenting the three color channels of the image with 34 additional channels. Four of these channels indicated the shape to which each pixel belongs, including shapes for bricks, balls, walls, and obstacles. Another 30 channels indicated the positions of parts of the paddle, where each part consisted of a single pixel. To reduce training time, we did not provide A3C and PN with part channels for objects other than the paddle, since these are not required to learn the dynamics or predict scores. However, Schema Networks were provided separate entities for each part (pixel) of each object, and each entity contained 78 attributes corresponding to the available part labels (21 for bricks, 30 for the paddle, 25 for obsta-

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<sup>&</sup>lt;sup>2</sup>In contrast with MDPs, the reward is discounted with a rolling square window instead of an exponentially weighted one.

<sup>&</sup>lt;sup>3</sup>To illustrate the problem, consider the case in which it is feasible for an entity to move at time t to position A or position B(but obviously not both) and then some reward is conditioned on that type of entity being in both positions: A single forward pass will not handle the entanglement properly and will incorrectly report that such reward is also feasible.



*Figure 3.* Comparison of learning rates. (a) Schema Networks and A3C were trained for 100k frames in Mini Breakout. (b) PNs and Schema Networks were pretrained on 100K frames of Standard Breakout, and then training continued on 45K additional frames of the Middle Wall variation. We show performance as a function of training frames for both models. Note that Schema Networks are ignoring all the additional training data, since all the required schemas were learned during pretraining. For Schema Networks, zero-shot transfer learning is happening.

	Standard Breakout	Offset Paddle	Middle Wall	Random Target	Juggling
A3C Image Only	N/A	$0.60\pm20.05$	$9.55 \pm 17.44$	$6.83 \pm 5.02$	$-39.35 \pm 14.57$
A3C Image + Entities	N/A	$11.10 \pm 17.44$	$8.00 \pm 14.61$	$6.88 \pm 6.19$	$-17.52 \pm 17.39$
Schema Networks	$36.33 \pm 6.17$	$41.42\pm6.29$	$35.22 \pm 12.23$	$21.38 \pm 5.02$	$-0.11\pm0.34$

Table 1. Zero-Shot Average Score per Episode Average of the 2 best out of 5 training attempts for A3C, and average of 5 training attempts for Schema Networks. A3C was trained on 200k frames of Standard Breakout (hence its zero-shot scores for Standard Breakout are unknown) while Schema Networks were trained on 100k frames of Mini Breakout. Episodes were limited to 2500 frames for all variations. In every case the average Schema Network scores are better than the best A3C scores by more than one standard deviation.

cles, 1 for walls, and 1 for the ball). Only one of these part attributes was active per entity. In this way, Schema Networks did not treat any object differently, and they were forced to learn that some part attributes, like bricks or obstacles, were irrelevant for predicting the ball's movement. We intentionally provided A3C and PN only with the relevant part information (for the paddle) while ignoring irrelevant information (for other other objects), to give them a strict advantage over the input to the Schema Networks.

## 5.1. Transfer Learning

This experiment examines how effectively Schema Networks and PNs are able to learn a new Breakout variation after pretraining, which examines how well the two models can transfer existing knowledge to a new task. Fig. 3a shows the learning rates during 100k frames of training on Mini Breakout. In a second experiment, we pretrained on Large Breakout for 100k frames and continued training on the Middle Wall variation, shown in Fig. 1b. Fig. 3b shows that PNs require significant time to learn in this new environment, while Schema Networks do not learn anything new because the dynamics are the same. 72.2

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### 5.2. Zero-Shot Generalization

While the moving obstacles variation required additional training to adapt to the new dynamics, many Breakout variations can be constructed that all involve the same dynamics. If a model correctly learns the dynamics from one variation, in theory the others could be played perfectly by planning using the learned model. Rather than comparing transfer with additional training using PNs, in these variations we can compare zero-shot generalization by training A3C only on Standard Breakout and Schema Networks only on Mini Breakout. Fig. 1b-e shows some of these variations.

	Half Negative Bricks
A3C Image Only	$5.95 \pm 5.53$
A3C Image + Entities	$-1.75\pm6.93$
Schema Networks	$6.34 \pm 4.53$

Table 2. Average Score per Episode on Half Negative Bricks A3C was trained on 200k frames of Random Negative Bricks, and Schema Networks were trained on 100k frames of Mini Random Negative Bricks, both to convergence. Testing episodes were limited to 1000 frames.

ations. Here are brief descriptions:

- Offset Paddle (Fig. 1d): The paddle is shifted upward by a few pixels.
- **Middle Wall** (Fig. 1b): A wall is placed in the middle of the screen, requiring the agent to aim around it to hit the bricks.
- **Random Target** (Fig. 1e): A group of bricks is destoyed when the ball hits any of them and then reappears in a new random position, requiring the agent to delibarately aim at the group.
- **Juggling** (Fig. 1f, enlarged from actual environment to see the balls): Without any bricks, three balls are launched in such a way that a perfect policy could juggle them without dropping any.

Table 1 shows the average scores per episode in each Breakout variation. These results show that A3C has failed to recognize the common dynamics and adapt its policy accordingly. This comes as no surprise, as the policy it has learned for Standard Breakout is no longer applicable in these variations. Simply adding an offset to the paddle is sufficient to confuse A3C, which has not learned the causal nature of controlling the paddle with actions and controlling the ball with the paddle. The Middle Wall and Random Target variations illustrate that Schema Networks are aiming to deliberately cause positive rewards from ball-brick collisions, while A3C struggles to adapt its policy accordingly. The Juggling variation is particularly challenging, since it is not clear which ball to respond to unless the model understands that the lowest downward-moving ball is the most imminent cause of a negative reward. By transferring the correct causal dynamics from Mini Breakout, Schema Networks outperform A3C in all variations.

### 5.3. Testing for Learned Causes

To better evaluate whether these models are truly learning the causes of rewards, we designed one more zero-shot generalization experiment. We trained both Schema Networks

825 and A3C on a Mini Breakout variation in which the color of a brick determines whether a positive or negative reward 826 is received when it is destroyed. Six colors of bricks pro-827 828 vide +1 reward, and two colors provide -1 reward. Negative bricks occurred in random positions 33% of the time dur-829 830 ing training. Then during testing, the bricks were arranged into two halves, with all positive colored bricks on one half 831 and negative colored bricks on the other. If the causes of re-832 wards have been correctly learned, the agent should prefer 833 834 to aim for the positive half whenever possible. As Table 1 shows, Schema Networks have correctly learned from ran-835 836 dom arrangements which brick colors cause which rewards, preferring to aim for the positive half during testing, while 837 A3C demonstrates no preference for one half or the other, 838 achieving an average score near zero. 839

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# 6. Discussion and Conclusion

In this work, we have demonstrated the promise of Schema Networks with strong performance on a suite of Breakout variations. Instead of learning policies to maximize rewards, the learning object for Schema Networks is designed to *understand causality* within these environments. The fact that Schema Networks are able to achieve rewards more efficiently than state-of-the-art model-free methods like A3C is all the more notable, since high scores are a byproduct of learning an accurate model of the game.

The success of Schema Networks is derived in part from the entity-based representation of state. Our results suggest that providing Deep RL models like A3C with such a representation as input can improve both training efficiency and generalization. This finding corroborates recent attempts (Usunier et al., 2016; Garnelo et al., 2016; Chang et al., 2016; Battaglia et al., 2016) to incorporate object and relational structure into neural network-based models.

The environments considered in this work are conceptually diverse but also simplified in a number of ways with respect to the real world: states, actions, and rewards are all discretized as binary random variables; the dynamics of the environments are deterministic; and there is no uncertainty in the observed entity states. In future work we plan to address each of these limitations, adapting Schema Networks to continuous, stochastic domains.

Schema Networks have shown promise toward multi-task transfer where Deep RL struggles. This transfer is enabled by the causal understanding embedded in the networks, which in turn allows for planning in novel tasks. As progress in RL and planning continues, robust generalization from limited experience will be vital for future intelligent systems.

# 880 **References**

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- Anderson, John R. Cognitive psychology and its implications. WH Freeman/Times Books/Henry Holt & Co, 1990.
  - Attias, Hagai. Planning by probabilistic inference. In *AIS*-*TATS*, 2003.
- Battaglia, Peter, Pascanu, Razvan, Lai, Matthew, Rezende,
  Danilo Jimenez, et al. Interaction networks for learning about objects, relations and physics. In *Advances in Neural Information Processing Systems*, pp. 4502–4510,
  2016.
- Chang, Michael B, Ullman, Tomer, Torralba, Antonio, and Tenenbaum, Joshua B. A compositional object-based approach to learning physical dynamics. *arXiv preprint arXiv:1612.00341*, 2016.
- Cheng, Qiang, Liu, Qiang, Chen, Feng, and Ihler, Alexander T. Variational planning for graph-based mdps. In *Advances in Neural Information Processing Systems*, pp. 2976–2984, 2013.
- Diuk, Carlos, Cohen, Andre, and Littman, Michael L.
  An object-oriented representation for efficient reinforcement learning. In *Proceedings of the 25th international conference on Machine learning*, pp. 240–247. ACM, 2008.
  - Drescher, Gary L. Made-up minds: a constructivist approach to artificial intelligence. MIT press, 1991.
  - Garnelo, Marta, Arulkumaran, Kai, and Shanahan, Murray. Towards deep symbolic reinforcement learning. *arXiv preprint arXiv:1609.05518*, 2016.
  - Guestrin, Carlos, Koller, Daphne, Gearhart, Chris, and Kanodia, Neal. Generalizing plans to new environments in relational mdps. In *Proceedings of the 18th international joint conference on Artificial intelligence*, pp. 1003–1010. Morgan Kaufmann Publishers Inc., 2003a.
- Guestrin, Carlos, Koller, Daphne, Parr, Ronald, and
  Venkataraman, Shobha. Efficient solution algorithms
  for factored mdps. *Journal of Artificial Intelligence Research*, 19:399–468, 2003b.
- Jaakkola, Tommi S, Sontag, David, Globerson, Amir,
  Meila, Marina, et al. Learning bayesian network structure using lp relaxations. In *AISTATS*, pp. 358–365,
  2010.
- Jaderberg, Max, Mnih, Volodymyr, Czarnecki, Wojciech Marian, Schaul, Tom, Leibo, Joel Z, Silver, David, and Kavukcuoglu, Koray. Reinforcement learning with unsupervised auxiliary tasks. *arXiv preprint arXiv:1611.05397*, 2016.

- Jordan, Michael Irwin. *Learning in graphical models*, volume 89. Springer Science & Business Media, 1998.
- Koller, Daphne and Friedman, Nir. *Probabilistic graphical models: principles and techniques*. MIT press, 2009.
- Mnih, Volodymyr, Kavukcuoglu, Koray, Silver, David, Rusu, Andrei A, Veness, Joel, Bellemare, Marc G, Graves, Alex, Riedmiller, Martin, Fidjeland, Andreas K, Ostrovski, Georg, et al. Human-level control through deep reinforcement learning. *Nature*, 518(7540):529– 533, 2015.
- Mnih, Volodymyr, Badia, Adria Puigdomenech, Mirza, Mehdi, Graves, Alex, Lillicrap, Timothy, Harley, Tim, Silver, David, and Kavukcuoglu, Koray. Asynchronous methods for deep reinforcement learning. In *Proceedings of The 33rd International Conference on Machine Learning*, pp. 1928–1937, 2016.
- Rusu, Andrei A, Rabinowitz, Neil C, Desjardins, Guillaume, Soyer, Hubert, Kirkpatrick, James, Kavukcuoglu, Koray, Pascanu, Razvan, and Hadsell, Raia. Progressive neural networks. *arXiv preprint arXiv:1606.04671*, 2016.
- Scholz, Jonathan, Levihn, Martin, Isbell, Charles, and Wingate, David. A physics-based model prior for objectoriented mdps. In *Proceedings of the 31st International Conference on Machine Learning (ICML-14)*, pp. 1089– 1097, 2014.
- Silver, David, Huang, Aja, Maddison, Chris J, Guez, Arthur, Sifre, Laurent, Van Den Driessche, George, Schrittwieser, Julian, Antonoglou, Ioannis, Panneershelvam, Veda, Lanctot, Marc, et al. Mastering the game of go with deep neural networks and tree search. *Nature*, 529(7587):484–489, 2016.
- Taylor, Matthew E and Stone, Peter. Transfer learning for reinforcement learning domains: A survey. *Journal of Machine Learning Research*, 10(Jul):1633–1685, 2009.
- Usunier, Nicolas, Synnaeve, Gabriel, Lin, Zeming, and Chintala, Soumith. Episodic exploration for deep deterministic policies: An application to starcraft micromanagement tasks. *arXiv preprint arXiv:1609.02993*, 2016.
- Van Hasselt, Hado, Guez, Arthur, and Silver, David. Deep reinforcement learning with double q-learning. In *AAAI*, pp. 2094–2100, 2016.
- Weiten, W. *Psychology: Themes and Variations.* PSY 113 General Psychology Series. Cengage Learning, 2012. ISBN 9781111354749. URL https://books. google.com/books?id=a4tznfeTxV8C.