

# Enhanced Equivalence Projective Simulation: a Framework for Modeling Formation of Stimulus Equivalence Classes

**Asieh Abolpour Mofrad**<sup>1</sup>

**Anis Yazidi**<sup>1</sup>

**Samaneh Abolpour Mofrad**<sup>2, 3</sup>

**Hugo L. Hammer**<sup>1, 4</sup>

**Erik Arntzen**<sup>5</sup>

<sup>1</sup>Dept. of Computer Science, OsloMet - Oslo Metropolitan University, Oslo, Norway

<sup>2</sup> Dept. Computer Science, Electrical Engineering, and Mathematical Sciences, Western Norway University of Applied Sciences, Bergen, Norway

<sup>3</sup> Mohn Medical Imaging and Visualization Center, Haukeland University Hospital, Bergen, Norway

<sup>4</sup>Simula Metropolitan Center, Oslo, Norway

<sup>5</sup>Dept. of Behavioral Science, OsloMet - Oslo Metropolitan University, Oslo, Norway

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## Abstract

Formation of Stimulus Equivalence classes has been recently modeled through Equivalence Projective Simulation (EPS), which is a modified version of Projective Simulation (PS) learning agent. PS, is endowed with an episodic memory which resembles the internal representation in the brain and the concept of cognitive map. PS flexibility and interpretability enables EPS model, and consequently the current model, to simulate a broad range of behaviors in matching-to-sample experiments. The episodic memory, which is the basis for agent decision-making, is formed during training phase. Derived relations in EPS model, that are not trained directly but can be established via the network's connections, are computed on demand during the test phase trials by likelihood reasoning. In this article, we investigate the formation of derived relations in the EPS model using an iterative diffusion process called Network Enhancement (NE) which yields an offline approach to the agent decision-making at the testing phase. NE process is applied after the training phase to denoise the memory network so that derived

relations are formed in the memory network and retrieved during testing phase. During the NE phase, indirect relations get enhanced and the structure of episodic memory changes. This approach can also be interpreted as agent’s replay after training phase which is in line with recent findings in behavioral and neuroscience studies. In comparison with EPS, the current model is able to model the formation of derived relations and other features such as the nodal effect in a more intrinsic manner. Decision-making in the test phase is not an ad-hoc computational method, but rather a retrieval and update process of the cached relations from memory network based on the test trial. In order to study the role of parameters on the agent performance, the proposed model is simulated and the results are discussed through various experimental settings.

## 1 Introduction

Stimulus Equivalence (SE) phenomenon was identified and explored by Sidman (1971) and refers to the condition that members of an equivalence class evoke the same response in human and animal subjects. The introduced SE methodology uses matching-to-sample (MTS) procedure to train arbitrary relations between unfamiliar stimuli, and test derived relations through mathematical relations in equivalence sets i.e. reflexivity, symmetry, and transitivity. SE framework, as an efficient learning method, has been vastly studied by employing humans or animals as experimental participants (see Sidman et al., 1974, 1982; Sidman & Tailby, 1982; Sidman et al., 1986; Devany et al., 1986; Hayes, 1989; Fields et al., 1990; Spencer & Chase, 1996; Groskreutz et al., 2010; Steingrimsdottir & Arntzen, 2011; Arntzen & Mensah, 2020, to mention a few). Computational models constitute another alternative to understand SE and study variables that are challenging to examine on humans or animals due to time constraints or ethical issues (see, e.g., Barnes & Hampson, 1993; Cullinan et al., 1994; Lyddy et al., 2001; Lew & Zanutto, 2011; Tovar & Westermann, 2017; Ninness et al., 2018, for some computational models of the learning of equivalence relations).

Equivalence Projective Simulation (EPS) is a computational model that has been proposed to SE in our previous article (Mofrad et al., 2020). In brief, EPS has modeled formation of SE classes through a MTS procedure. Projective Simulation (PS) framework (Briegel & De las Cuevas, 2012) was the basis of the model and we have proposed several methods to address the test phase and derived relations, including max-product, memory sharpness, and random walk on the memory network with absorbing action sets. The EPS model, similar to the original PS model, has an internal episodic memory which is updated during training phase which is used to cope with new, derived relations in the testing phase. The PS model, and therefore EPS model, is pretty flexible and easy to interpret which allows modeling a broad range of behaviors in MTS experiments including typical participants or participants with some disabilities. Many parameters of the model can be controlled such as learning rate, forgetting rate, and nodal effect.

The EPS model relies on the assumption that the derived relations are derived upon request, i.e. when they appear in a MTS trial, during the testing phase while updated during the training phase. We slightly change this assumption and form those relations in the end of the training phase, thus the output network from training phase of EPS assumed to be a noisy version of the agent’s memory network that is supposed to contain

all trained and derived relations. Using a denoising approach, we could produce a new less noisy clip network that contains information regarding the equivalence class formation. The trained relations in the training phase are mapped into a transition matrix whose values describe the strength of the trained relations. By resorting to Network Enhancement (Wang et al., 2018), we address the formation of SE classes using an iterative update of the transition matrix. Interestingly, the update process permits to naturally denoise the transition matrix and enhance indirect relations<sup>1</sup> while preserving the initial direct relations learned during the training phase. The denoised network can be assimilated to an updated clip network, later used in the test phase. Furthermore, it can also be used to assess the overall agent performance on eventual equivalence tests. In summary, the contribution of this paper is as follows:

- (a) Instead of using reasoning, i.e. computing the likelihood of the different alternatives during testing by following some indirect paths over the clip network, we update memory and retrieve the updated memory at the test phase.
- (b) As in the EPS model, we still control symmetry relations with a multiplicative parameter. We are able to control the ability to derive transitivity relations using parameter  $\alpha$ . This turns out to be of great importance when modeling subjects with learning disabilities.
- (c) We further enhance the NE and propose DNE in which we can control the agent ability to derive symmetry and also control its ability to derive transitivity.
- (d) A comparison between PS, EPS and E-EPS together with supporting studies from neuroscience literature is provided that justify the proposed model.
- (e) From computational point of view, the new updating rule has less parameters to fine tune in comparison with the EPS. The approach to derive relations in EPS model can be seen as routing in the clip network, with action sets as destination points. In E-EPS model, a diffusion model explores the clip network by simultaneous propagation of flow without a specific target.
- (f) The updated clip network can be considered as a cognitive map of the stimuli which can be used in analysing the results of different settings.
- (g) The testing phase in the E-EPS model, involves less computation at the decision time in comparison with EPS. E-EPS uses the updated network during the testing phase, rather than processing the trained relations to compute derived relation links at each test trial.
- (h) Using simulation of several configurations, we study the parameters in detail.
- (i) We compare three training procedures linear series (LS), many-to-one (MTO), and one-to-many (OTM) in the final experiment. In line with the main stream literature in behavior analysis (see, e.g. Arntzen et al., 2010; Arntzen & Hansen,

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<sup>1</sup> According to the theory of SE, indirect relations are derived through reflexivity, symmetry, transitivity, and equivalence.

2011; Arntzen, 2012), the model yields better performance in OTM and MTO cases in comparison with LS which is a qualitative property of our model confirming that it is a realistic model.

- (j) We provide theoretical analysis of the model and a convergence guarantee see Appendix A.

In the rest of paper, we begin by a brief overview of SE, EPS, and Network Enhancement in section 2. The architecture of the Enhanced Equivalence Projective Simulation (E-EPS) model is provided in section 3, where we also compare the new proposed approach to the original PS model and recent EPS model. We consider seven experimental scenarios to study the parameters of the model in section 4. Finally, section 5 is a summary of the paper, discussion and concluding remarks.

## 2 Background and Related Works

First in section 2.1, the concept of SE from behavior analysis perspective is reviewed. In section 2.2, the EPS model is shortly explained and we provide a brief section about Network Enhancement (Wang et al., 2018) in section 2.3. It is noteworthy that the updating rule which we have considered as the main approach, is introduced and discussed in section 3.

### 2.1 Stimulus Equivalence (SE)

SE is a research method on complex human behavior, including memory and problem solving (Sidman, 1990). In the MTS or conditional discrimination procedure, which is used in SE, a given stimulus, say  $A_1$ , must be paired with  $B_1$  among a given comparison stimuli set, say  $B_1$ ,  $B_2$ , and  $B_3$ . The discrimination happens through programmed consequences.

The MTS procedure has two phases, the training phase where the participant learns some relations and the testing phase where the participant is tested with derived relations. Trial types in the test phase includes baseline, symmetry, transitivity, and equivalence. It is noteworthy that equivalence relations are sometimes referred to as combined transitivity and symmetry.

The evaluation of participant learning is usually through a threshold or mastery criterion ratio (e.g.,  $0.95 - 1$ ). Only if the participant is able to pass the criterion the derived relations will be tested. In the test phase, there is no programmed consequences and usually the criterion ratio in the test phase is lower than training phase (e.g.,  $0.9 - 1$ ). Whenever the evidence (passing the criterion for testing) shows the emergence of all relations, the equivalence class is considered to be formed (Sidman & Tailby, 1982).

In equivalence literature, three training structures have been used in establishing conditional discrimination with MTS procedure: linear series (LS), many-to-one (MTO), and one-to-many (OTM) (see Arntzen, 2012, for more details about MTS training and testing procedures and parameters in SE formation). Generally, a class with  $n$  stimuli, requires training of only  $(n - 1)$  stimulus-stimulus relations. The condition is that each

component of these relations needs to be present in at least one trained relation, and further none of the trained relations can have the same two stimuli as components. Even with these constraints, many possible ways for structuring training relations remain, some of them might be more efficient than the others (see Fields et al., 1990; O’Mara, 1991; Arntzen & Holth, 1997; Hove, 2003; Lyddy & Barnes-Holmes, 2007; Arntzen et al., 2010; Arntzen & Hansen, 2011; Fienup et al., 2015, for instance). Appendix B formally analyzes the size of the training design space which is shown to be exhaustive even for a small number of categories and number of classes. Therefore, it is complex to design and run experiments involving human subjects that explore different training and testing scenarios. Computational models, on the other hand, could be used for exploring new ideas through simulation. For instance, one could try several configurations and find the optimum scenario according to some design criterion in the computational model before running a real experiment. Moreover, components of the computational model can be easily manipulated, disrupted, impaired, and removed to see the effect of those components on the results. Having more control over the experimental variables including a controllable environment is a considerable advantage of these models over real experiments (Barnes & Hampson, 1993; McClelland, 2009; Ninness et al., 2018).

## 2.2 Equivalence Projective Simulation (EPS)

EPS is based on PS, which can be seen as an reinforcement learning (RL) model that can be embodied in an environment, perceive stimuli, execute actions, and learn through trial and error (see, e.g., Briegel & De las Cuevas, 2012; Melnikov et al., 2017, for details of PS model).

PS agent, and therefore EPS agent, has an episodic memory which is literally a directed, weighted network of clips, where each clip represents a remembered percept or action (stimulus in EPS). Memory can be described as a probabilistic network of clips so called “clip network”<sup>2</sup>. The learning in PS is realized by updating weights and structure through adding new clips and new transition links.

Simulation of MTS procedure via EPS has two phases, the training phase where the memory network will be formed through trials and guided feedback, and the test phase in which no new memory clips are created. Even though there is no guided feedback in the testing phase connection weights might be updated. The test phase is the main part of the model and in (Mofrad et al., 2020) three different approaches dealing with the derived relations are discussed, i.e. max-product, memory sharpness, and absorbing action sets.

At the beginning of a MTS training phase, the agent memory space which is shown by  $\mathcal{C} = \{c_1, \dots, c_p\}$  is empty. Based on trial settings, a memorized clip could either play the role of percept clip or action clip. At each time step, the environment (experimenter in the real experiments) shows a sample stimulus and some comparison alternatives which are referred as percept and actions. The percept and actions belong to the percept set  $\mathcal{S}$  and action set  $\mathcal{A}$  respectively. The sample stimulus (percept,  $s \in \mathcal{S}$ ) and the comparison stimuli (actions  $a \in \mathcal{A}_t$ ) belong to different categories (say category  $A$ , or  $B$ , etc.), where  $\mathcal{A}_t$  denotes the action space at time  $t$  and consists of set of

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<sup>2</sup>The terms episode and clip are used interchangeably.

comparison at the given trial. The training phase will be as follows:

- Agent perceives stimulus  $s \in \mathcal{S}$  from environment. Clip  $c_s \in \mathcal{C}$  is either created (the first time) or activated.
- Perceiving action set  $\mathcal{A}_t$  from environment, agent establishes and initializes connections between sample and comparison stimuli the first time with  $h$ -values equal to  $h_0$ . If there exist connections from previous trials there is no need for initialization.
- Agent computes  $p^{(t)}(c_a|c_s), a \in \mathcal{A}_t$  based on the  $h$ -values using the “softmax” distribution function:

$$p^{(t)}(c_j|c_i) = \frac{e^{\beta h^{(t)}(c_i, c_j)}}{\sum_k e^{\beta h^{(t)}(c_i, c_k)}}, \quad (1)$$

where at this stage clip  $c_i = c_s$  and clip  $c_j \in \mathcal{A}_t$ . A larger value of  $\beta \geq 0$  creates a probability distribution that is more biased to the choice of the largest  $h$ -value, and therefore parameter  $\beta$  can be used for tuning the learning rate as well.

- Agent selects one of the actions based on the computed probability distribution and receives a positive or negative reward from environment, say  $\lambda^{(t)} \in \Lambda = \{-1, 1\}$ .<sup>3</sup>
- Connection weights,  $h$ -values, will be updated as a result of the environment feedback as follows:

$$h^{(t+1)}(c_s, c_a) = h^{(t)}(c_s, c_a) - \gamma(h^{(t)}(c_s, c_a) - 1) + \lambda^{(t)}, \quad (2)$$

Moreover, the opposite link,  $(c_a, c_s)$  will be updated in a similar way, but with parameter  $0 < K \leq 1$ :

$$h^{(t+1)}(c_a, c_s) = h^{(t)}(c_a, c_s) - \gamma(h^{(t)}(c_a, c_s) - 1) + K\lambda^{(t)}. \quad (3)$$

- Environment provides new trials until all training relations meet the mastery criterion.

It is noteworthy that parameter  $K$  was used in the learning rule of original PS model (Briegel & De las Cuevas, 2012) to determine the growth rate of “associative” or “compositional” connections relative to the direct connections. This parameter, for instance, enables the PS agent to learn faster by recognizing similarity between the existing clips in memory and new perceptual input (see Figure 11 and Figure 12 in Briegel & De las Cuevas, 2012, for more detail on associative learning in PS agent). The parameter  $K$

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<sup>3</sup>It is noteworthy that  $\Lambda$  could have any positive or negative values including asymmetric rewards. For instance, negative feedback might have greater impact (see Baumeister et al., 2001, as an example of positive-negative asymmetry effect).

in the EPS model, however, quantifies the relative growth of symmetric relations compared to the direct, or baseline, relations<sup>4</sup>. This parameter is different from the original PS in the sense that the stimuli in EPS (and E-EPS) are arbitrary, i.e. have no physical similarity, and therefore the parameter  $K$  does not capture similarity. The notion of associative memory, however, can be added to the EPS model by introducing compound stimuli which is not addressed in the current paper.

After that agent passes the training phase, the test phase will be started consequently in which the formation of derived relations are tested. At this stage, no feedback is provided from the environment.

- Agent perceives  $s \in \mathcal{S}$ , activates the memory clip  $c_s \in \mathcal{C}$  and tries to chooses the best action among the given action set  $\mathcal{A}_t$  based on its memory as follows.
- If connections between the sample and comparisons exist, the agent computes the  $p^{(t)}(c_a|c_s)$ ,  $a \in \mathcal{A}_t$  based on the  $h$ -values using a probabilistic distribution achieved either by softmax or a normalized vector of  $h$ -values (called “standard” in PS and EPS). If such connections do not exist, in the transitivity or equivalence relation cases, agent computes the transition probabilities using max-product scenario, or absorbing states scenario and selects one of the possible actions.
  1. In the max-product case, agent finds the most probable paths between  $c_s$  and each action  $c_a, a \in \mathcal{A}_t$ . Please note that there are many possible paths that might link  $c_s$  to a particular action  $c_a$  and thus the procedure might be computationally exhaustive.
  2. The absorbing state scenario can be considered as a random walk in clip network, starting from  $c_s$  and ending with a clip in  $\mathcal{A}_t$ . So, unlike the max-product method, the probability of reaching each action from  $c_s$  is important but not the path itself. These probabilities, can be computed when actions  $c_a \in \mathcal{A}_t$  are set to be absorbing states of the underlying Markov chain, at time  $t$ .
- Memory sharpness,  $0 \leq \theta \leq 1$ , functions as a mechanism to control the formation of transitivity relations, and also consequently controls equivalence relations and the effect of the nodal number (see, e.g., Sidman, 1994, for nodal number ), in line with the baseline relations training. In (Mofrad et al., 2020), this is discussed as a separate method. However, it can be used in combination with either max-product or the concept of absorbing states.

It is noteworthy that for the sake of brevity we just review the parts of EPS model that are necessary for understanding the new perspective on derived relations. Moreover, an overview of some other behavior-analytic computational approaches to formation of SE classes is provided in the EPS article (see Mofrad et al., 2020, for the detailed version of EPS model).

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<sup>4</sup>Please note that in (Mofrad et al., 2020) we use  $K_1, K_2, K_3$ , and  $K_4$  which play the same role as  $K$  in this paper but with a higher level of control.

## 2.3 Network Enhancement (NE)

NE (Wang et al., 2018) is a computational approach that has been proposed for denoising biological networks. NE converts a noisy, undirected, weighted network into a new network possessing the same nodes but with different connections and weights. NE assumes that nodes which are connected through paths with high weight edges, have a high chance to be directly connected with a high-weight edge. The diffusion process of NE uses random walks of length three or less and a regularized information flow in order to produce new edge weights.

For formal description of NE, let  $W$  be the matrix of edge weights and  $\mathcal{N}_i$  be the  $K$ -nearest neighbors of the  $i$ -th node, including node  $i$  itself. The localized network  $\mathcal{T}$  is constructed from  $W$  as follows:

$$P_{i,j} \leftarrow \frac{W_{i,j}}{\sum_{k \in \mathcal{N}_i} W_{i,k}} \mathbb{I}_{\{j \in \mathcal{N}_i\}}, \quad \mathcal{T}_{i,j} \leftarrow \sum_{k=1}^n \frac{P_{i,k} P_{j,k}}{\sum_{v=1}^n P_{v,k}} \quad (4)$$

where  $\mathbb{I}_{\{\cdot\}}$  is the indicator function. Then the diffusion process is defined as an iterative relation:

$$W_{t+1} = \alpha \mathcal{T} \times W_t \times \mathcal{T} + (1 - \alpha) \mathcal{T} \quad (5)$$

where  $\alpha$  is a regularization parameter,  $t$  shows iteration step and  $W_0$  can be initialized with the input matrix  $W$ . The update rule in equation 5 for each entry is:

$$(W_{t+1})_{i,j} = \alpha \sum_{k \in \mathcal{N}_i} \sum_{l \in \mathcal{N}_j} \mathcal{T}_{i,k} (W_t)_{k,l} \mathcal{T}_{l,j} + (1 - \alpha) \mathcal{T}_{i,j}. \quad (6)$$

There are many theoretical properties for this diffusion process which are discussed in (Wang et al., 2018). It is shown that  $W_t$  remains a symmetric, doubly stochastic matrix (DSM) for each iteration  $t$  and  $W_t$  converges to a non-trivial equilibrium network. Moreover, NE does not change eigenvectors of the initial DSM  $\mathcal{T}$ , but the spectrum of the eigenvalues is changed non-linearly so that the eigengap is increased. This effect of NE process on the eigenspectrum improves the network to achieve more accurate detection of clusters. Although this method produces promising results in our model, as we will explain in the results section 4, it is not the main approach for formation of equivalence classes in the EPS model, but NE and discussions in (Wang et al., 2018) is the main motivation for the update rule. The method we use does not have all the properties that NE has and we refer to the theoretical aspect of the diffusion process we used in Appendix A. In the rest of this paper we refer to NE method due to (Wang et al., 2018) as Symmetric Network Enhancement (SNE).

## 3 Enhanced Equivalence Projective Simulation (E-EPS)

The training phase of the proposed E-EPS model is generally the same as the original PS and the EPS in the sense that the clip network is formed by adding new clips and updating the  $h$ -values based on the environment feedback. However, since in the current paper the probability distribution over the action set is modeled using the softmax function, we let the network have negative  $h$ -values and simplify the training by



removing some parameters associated to positive  $h$ -values. However, the approach to formation of SE classes and the testing phase is quite different compared to the EPS model (Mofrad et al., 2020). As explained in section 2.2, after training phase, we have a network of  $h$ -values for baseline relations and the symmetry relations. To add reflexivity to the clip network, we can either consider an updating method during training phase<sup>5</sup> or after training phase. In order to keep the model simpler, we add a self-loop to each clip after training phase and assign it an  $h$ -value equal to the maximum  $h$ -value of input or output connections. The argument is in the case that the agent can identify the members of a class (say  $A_1, B_1, C_1$ ), it must be able to differentiate members of each category (say  $A_1$  from  $A_2$  and  $A_3$ ). We refer to the adjacency matrix of this network of  $h$ -values as  $W_h$ .

In this work we are proposing a new NE model called Directed Network Enhancement (DNE) which can be used for the testing phase, including baseline, reflexivity, symmetry, transitivity, and equivalence relations. Suppose the following rule as the update rule (or diffusion process):

$$W_{t+1} = \alpha P \times W_t \times P + (1 - \alpha)P, \quad (7)$$

where  $W_0$  is a right stochastic matrix achieved from  $W_h$ . We put  $W_0 = P$  where  $P$  is the transition probability matrix of  $W_h$  applying softmax function on non-zero values at each row using  $\beta_h$  parameter.  $P$  is not symmetric and  $P\mathbf{1} = \mathbf{1}$ , where  $\mathbf{1}$  represents the all-one eigenvector of  $P$  associated with eigenvalue one. In other term,  $P$  is a right stochastic matrix so can be used as initial matrix in DNE process. In the theoretical analysis of SNE process provided by Wang et al. (2018), and the supplementary note 3, the converged network is proved to be:

$$W_{t \rightarrow \infty} = (1 - \alpha)\mathcal{T}(\mathcal{I} - \alpha\mathcal{T}^2)^{-1}. \quad (8)$$

As it is discussed in appendix A, the convergence in DNE process remains valid for a network where we substitute  $\mathcal{T}$  with  $P$  in equation 8

$$W_{t \rightarrow \infty} = (1 - \alpha)P(\mathcal{I} - \alpha P^2)^{-1}. \quad (9)$$

This post-processing phase transforms the  $h$ -value network obtained by training, into a new network which can represent the agent predictive representations in cognitive map (or successor representation similar to Momennejad et al., 2017b).

$W_{t \rightarrow \infty}$  matrix can be seen as the memory representation where we ignore the effect of context (or actions) and assume all the transitions in the network is based on the random walk on the graph (or diffusion). For instance, we can interpret the  $(i, j)$  entry of  $W_{t \rightarrow \infty}$  matrix as the transition probability from clip  $i$  to clip  $j$  when there is no external control.

When it comes to the testing phase, the softmax function with  $\beta_t$  is applied to calculate the probability distribution for each test trial. In order to accommodate the controlling effect of the test trials, the input values to the softmax function are set to be

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<sup>5</sup>For instance, this can simply achieved by adding a self loop edge initialized with  $h_0$  to each clip the first time which is perceived by the agent and update it whenever get involved in a trial.

conditional probabilities given the trial which can be calculated using Bayes' rule. As an example, if the test trial consists of  $A_1$  as sample stimulus and  $F = \{F_1, F_2, F_3\}$  as the comparison stimuli, input values for the softmax function are  $P(A_1F_1|A_1F)$ ,  $P(A_1F_2|A_1F)$  and  $P(A_1F_3|A_1F)$  where event  $A_1F$  is either  $A_1F_1$ ,  $A_1F_2$  or  $A_1F_3$ . These conditional values can be calculated due to the Bayes' rule; for instance

$$\begin{aligned} P(A_1F_1|A_1F) &= \frac{P(A_1F_1)P(A_1F|A_1F_1)}{P(A_1F_1)P(A_1F|A_1F_1) + P(A_1F_2)P(A_1F|A_1F_2) + P(A_1F_3)P(A_1F|A_1F_3)} \\ &= \frac{P(A_1F_1)}{P(A_1F_1) + P(A_1F_2) + P(A_1F_3)} \end{aligned}$$

which can be seen as a normalization. Note that all the conditional probabilities in the right hand side are equal to one and therefore are removed. Parameter  $\beta_t$  in the softmax function can characterize the agent's memory and ability to link an internal representation to the real action. When a test trial is given to the agent, the memory is conditioned based on the test trials (sample and comparison stimuli), and the Bayes' rule is used to characterize the environment effect.

Another way to formalize the behavior of agent in the test phase is to use a trial-based  $\beta_t$  for softmax function, which is defined as  $\beta_t$  divided by the summation over weights for comparison stimuli. In the above example,  $A_1$  as sample stimulus and  $F = \{F_1, F_2, F_3\}$  as comparison stimuli, uses  $\frac{\beta_t}{P(A_1F_1) + P(A_1F_2) + P(A_1F_3)}$  as the  $\beta$  in softmax function. As clear from the example, in this formalization, the results will remain exactly the same, but opens up room to interpret the agent behavior differently. Using Bayes's rule and fixed  $\beta_t$  approach, emphasizes the effect of environment and the agent characteristics separately, but variable  $\beta_t$  approach avoids the interpretation that the agent probabilities are calculated twice.

Before comparing the E-EPS with the original PS and the EPS model, and relating it to other studies, we summarize the parameters of the agent model as follows:

- (a) Parameter  $0 < K \leq 1$  controls the formation of symmetry relations.  $K = 1$  means that the relations are bidirectional and the  $h$ -value network is symmetric (see Experiment 2).
- (b) Parameter  $0 \leq \gamma < 1$  represents the forgetting rate during training phase. The training structure (order of relations to be trained) is more important when forgetting rate is high (see Experiment 4).
- (c) Parameter  $\beta_h > 0$  converts  $h$ -values to probabilities during training trials and generates the input matrix  $W_0$  for the NE process (see Experiment 1 and 3).
- (d) Parameter  $0 \leq \alpha < 1$  controls to what extent the NE affects the initially trained network, when there is no test trial in place.  $\alpha$  could characterize the amount of abstract mental process or replay that the agent performs. Even a small value of  $\alpha$  could form derived relations that are weak in comparison with direct relations, but the ratio or conditional probabilities (which is used as an input to the softmax function) is strong. A value close to one for  $\alpha$  means too much diffusion which

can erase the trained relations. One might find the appropriate diffusion based on the expected agent abilities and the training criterion (see Experiment 5 and appendix A for more details)

- (e) Parameter  $\beta_t > 0$  controls agent’s performance in a test trial (see Experiment 6).

### 3.1 PS, EPS, and E-EPS: Discussion and Comparison

As mentioned by Briegel & De las Cuevas (2012), the idea of clip network in PS, is similar to the idea of cognitive maps of Tolman (1948) which refers to a rich internal model of the world that represents relationships between events and simulates the consequences of actions. Although cognitive maps are mostly used for modeling spatial behavior (O’keefe & Nadel, 1978), they are more general and cover organization of knowledge in other types of behaviors including flexible behavior. Cognitive maps can be constructed from abstract representations to describe relational knowledge and new cognitive problems can then be considered as inference in this relational basis (Behrens et al., 2018).

Brain studies suggest multiple solutions to predicting long-term reward in RL problem (Daw et al., 2005). Learning a model of environment, or cognitive map of environment, and using it to simulate future states step-by-step to predict long-term reward is one solution, which can be referred to as a model-based RL (Daw et al., 2005, 2011; Sutton & Barto, 2018). Forming simple world models in human hippocampus for relational knowledge sorting and value spreading across associated stimulus representations, is shown to directly influence behaviour in novel decision-making situations (Wimmer & Shohamy, 2012). Repeating patterns during both awake experiential states and non-engaged states and reshaping of neural circuits has been studied in both hippocampus and in the neocortex (see, Liu & Watson, 2020, for a review). Functional magnetic resonance imaging (fMRI) similarity measures in hippocampus and entorhinal cortex (Stachenfeld et al., 2017; Garvert et al., 2017) suggest the existence of statistical transitions of discrete state-spaces. The usage of precompiled transition distances, rather than simulating all possible transitions online, is studied by Momennejad et al. (2017b), where these precompiled distances depend on offline activity, or replay, in hippocampus and ventral frontal cortex (Momennejad et al., 2017a). Caching of multi-step predictive representations is also referred to as “predictive map” (Stachenfeld et al., 2017). These predictive representations link model-based RL to model-free mechanisms through an offline replay mechanisms (Russek et al., 2017) resembling Dyna-style planning (Sutton et al., 2008).

PS is much more primitive than Dyna-style planning. PS only changes the weights of the clip transition and performs a random walk on the clip network (for detailed comparison, see Briegel & De las Cuevas, 2012). The multiple reflection in PS model, is different from “experiment replay” (Lin, 1992) in the sense that PS uses short-term memory, or emotional tags, to evaluate the result of a simulation and repeat the random walk if the remembered reward for the chosen action in previous round was negative. So repeatedly presenting its past experiences to its learning algorithm is not performed just for the sake of memory consolidation. (see also, Momennejad, 2020, for a review on role of replay on how the brain learns and generalizes relational structures with a

focus on RL approach)

In the EPS model (Mofrad et al., 2020), two scenarios called “standard” and “softmax” were used for training phase and various ways for deriving relations in the test phase were studied and discussed due to the aim to define EPS as a general and flexible model. The EPS (and E-EPS) training phase is similar to the PS model with extra links and update rule for symmetry relations. In this article, we just survey the training method that uses softmax function in order to calculate probability distributions over the action sets. Although, the training phase in this article could be similar to EPS, for simplicity we just consider the softmax scenario where negative  $h$ -values are allowed, so we can formalize the learning with just one parameter,  $K$ , to control the growth ratio of symmetry relations in comparison with the direct relations.

The main difference with PS, which is the most important part of the EPS (E-EPS) model, is the testing phase where there is no feedback. In the EPS model, the derived relations were calculated on demand at the decision time, whenever they appear in a test trial. The probabilities are either calculated based on the probabilities of the paths with maximum values, using max-product algorithm, or the probability of reaching each of the action points having a random walk on the episodic memory started at sample stimulus. The symmetry relations, as mentioned earlier, are controlled via a multiplicative parameter and the transitivity could be controlled with a parameter called memory sharpness.

In EPS test phase, the only change to the clip network  $h$ -values is related to the parameter  $\gamma$ , the forgetting factor, and all the computations for the test trials are performed at the decision time which can be seen as an ad-hoc computational tool rather than an intrinsic feature of the model. The perspective to the derived relation in E-EPS, is quite different where NE, an iterative diffusion process, is used after the training phase. This alternative approach updates the structure of clip network by adding new connections between the clips and updating connection weights. In other words, the approach to derive relations in EPS model can be seen as routing in the clip network, where the action sets play the role of destination, while in E-EPS model, in the absence of test trials, the approach involves a diffusion model to explore the clip network by simultaneous propagation of flow without an specific target. The NE process is in line with the random walk based decision-making in the PS approach. It is noteworthy that diffusion models have been successfully used in various cognitive tasks involving decision-making (see, e.g., Shrager et al., 1987; Ratcliff et al., 2016). Stella et al. (2019) show that hippocampal circuits can reactivate random trajectories of varying lengths and timescales which resembling Brownian diffusion. NE process, can also be interpreted as a kind of replay similar to the offline replay that contributes to generalization via multi-step predictive representations of upcoming clips (or the successor representation) (Momennejad et al., 2017b,a; Russek et al., 2017). It is different from the online replay, or multiple reflection, in the PS model and closer to the offline replay that accommodates planning based on inferential piecing data together and multi-step dependencies. REMERGE (recurrency and episodic memory results in generalization) model of memory trace activation (Kumaran & McClelland, 2012) also uses replay, and iterative update of episodic memory, for modeling rapid generalization in, for example, transitive inference task.

The final abilities of the E-EPS agent to master derived relations strongly depends on two parameters,  $\alpha$ , which controls how much the NE affects the initially trained net-

work, and  $\beta_t$  which generates the probability distribution over the comparison stimuli. The post-processed network,  $W_{t \rightarrow \infty}$ , can be seen as an unconditioned network which will be biased in present of a test trial. To account for the environment effect, we use a Bayesian approach and then apply the softmax function (see, McClelland, 2013, for different models of contextual effects on perception). It is noteworthy that, the PS model uses Bayesian updating and therefore this update is in harmony with the PS agent (see, Schwöbel et al., 2018; Parr et al., 2019, for modeling goal-directed behavior as an inference process).

The approach to the testing phase in the E-EPS model, needs less computation at the decision time since it uses the cached updated network, rather than processing the trained relations to compute derived relation links at each test trial.

In the rest of the paper, we will discuss and conduct experiments on both models SNE and DNE, but the emphasis will be on the DNE which as we will show is more adequate for E-EPS model than the SNE.

## 4 Simulation Results

In this section, we study the model parameters in order to present insight on how parameters can be tuned to simulate various behaviors including typical people behavior or behavior of people with some disabilities. To study the model in more details, we consider a similar training setting as in the experiment by Spencer & Chase (1996) which is addressed in EPS paper (Mofrad et al., 2020) as well.

Spencer & Chase (1996) study addresses the relatedness or nodal number using three 7-member stimulus classes. Stimuli are nonsense figures and the training order is  $A \rightarrow B \rightarrow C \rightarrow D \rightarrow E \rightarrow F \rightarrow G$ . The training consists of seven stages as summarized in Table 1<sup>6</sup>. The first training block contains 48 trials of  $AB$  relations. Since the number of classes are three, this means the block for training  $AB$ , contains 16 trials with correct match  $A_1B_1$ , 16 trials with correct match  $A_2B_2$ , and 16 trials with correct match  $A_3B_3$ . The order of presented trials is random in the block and the order of comparison stimuli, in this case  $B_1, B_2, B_3$ , is also randomly changed. If we consider the training of  $EF$  relation, for instance, the training block contains six  $AB$  relations (which means each trial with  $A_1B_1, A_2B_2$ , and  $A_3B_3$  as the correct pair appears twice), six  $BC$  relations (i.e. each trial with  $B_1C_1, B_2C_2$ , and  $B_3C_3$  as the correct pair appears twice), six  $CD$  relations and six  $DE$  relations, and finally the new relation  $EF$  with 24 relations (i.e. each trial with  $E_1F_1, E_2F_2$ , and  $E_3F_3$  as the correct pair appears eight times). In the baseline maintenance stage no new relation is provided and each correct relation appears only once. The mastery criterion is set to 0.9 and if agent passes the mastery criterion for all stages and the final baseline maintenance, then we can test the agent for formation of derived relations.

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<sup>6</sup>It is noteworthy that in (Spencer & Chase, 1996) each stage of training has 48 trials per stage, due to simulation ease the fourth stage for  $DE$  training is changed, so we consider 9 trials for  $AB, BC$ , and  $CD$  relations instead of 8 trials. Therefore, this stage has 51 trials in the simulation instead of original 48.

Table 1: The training stages in (Spencer & Chase, 1996) study; number and type of training trials.

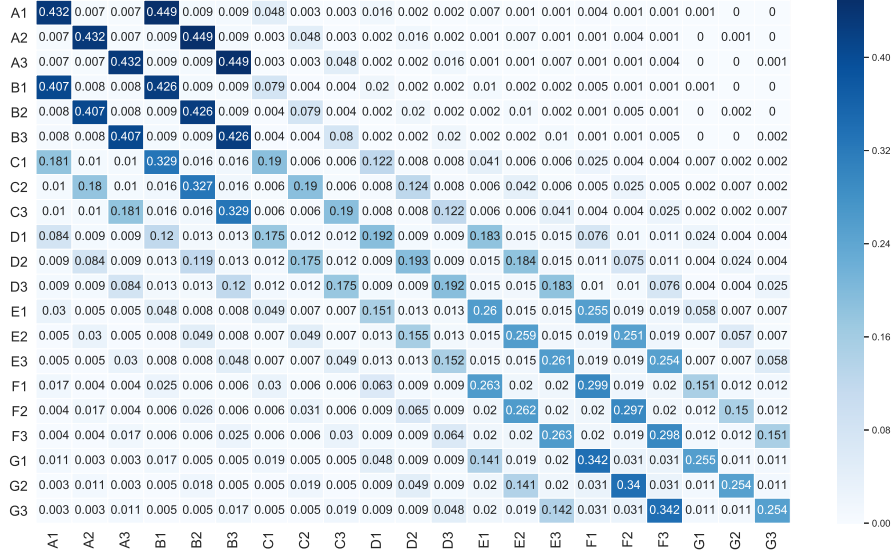
Training	Number of trials per relation					
	<i>AB</i>	<i>BC</i>	<i>CD</i>	<i>DE</i>	<i>EF</i>	<i>FG</i>
<i>AB</i>	48					
<i>BC</i>	24	24				
<i>CD</i>	12	12	24			
<i>DE</i>	9	9	9	24		
<i>EF</i>	6	6	6	6	24	
<i>FG</i>	3	3	3	6	9	24
Bsl Maint	3	3	3	3	3	3

The reported simulation results are the average over 1000 simulations.

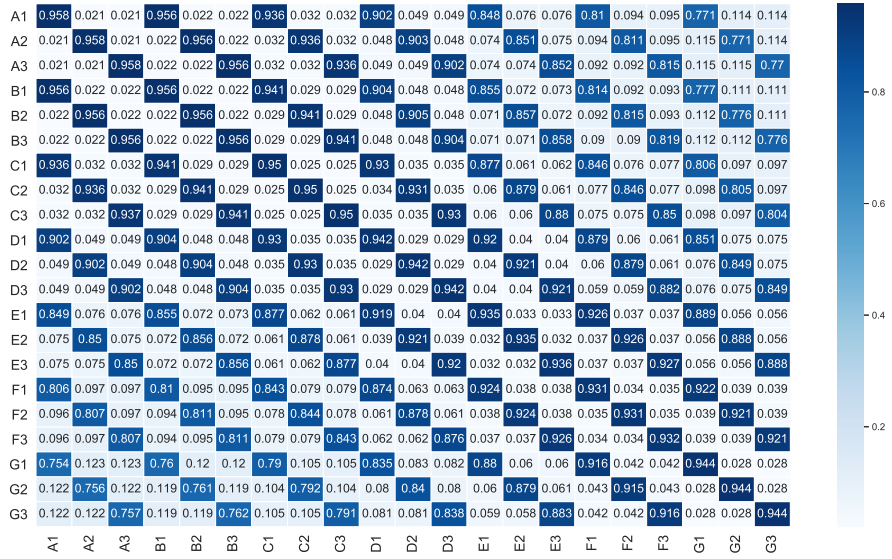
### Experiment 1: Step by Step Process

In this experiment, we illustrate the different computation steps. In Figure 1a, the network  $h$ -values after training phase (based on Table 1) is depicted where the parameters are set to  $\gamma = 0.001$ ,  $K = 1$ ,  $\beta_h = 0.1$ ,  $\beta_t = 4$ , and  $\alpha = 0.7$ . Note that the symmetry and reflexivity connections in addition to the baseline connections appeared in Figure 1a. The reflexivity  $h$ -values are the maximum  $h$ -value at each row (input-output connections). Moreover, since  $K = 1$ , the  $W_h$  matrix is symmetric, for instance  $A_1B_1 = B_1A_1 = 51.82$ . To compute the transition probability matrix, softmax function with parameter  $\beta_h = 0.1$  is used. Note that the transition probability matrix is just row-normalized and not symmetric. All the reported values are rounded either by two or three decimal places.





(a) Converged network  $W_{t \rightarrow \infty}$  using  $\alpha = 0.7$ .



(b) Category-based probability distributions for the test phase using  $\beta_t = 4$ .

Figure 2: The new network adjacency matrix when the regularization parameter is  $\alpha = 0.7$  with the input matrix  $W_0 = P$  which is given in Figure 1b. The test phase probabilities in Figure 2b, are calculated by normalizing the weights for the specific category and then using softmax function with parameter  $\beta_t = 4$ .

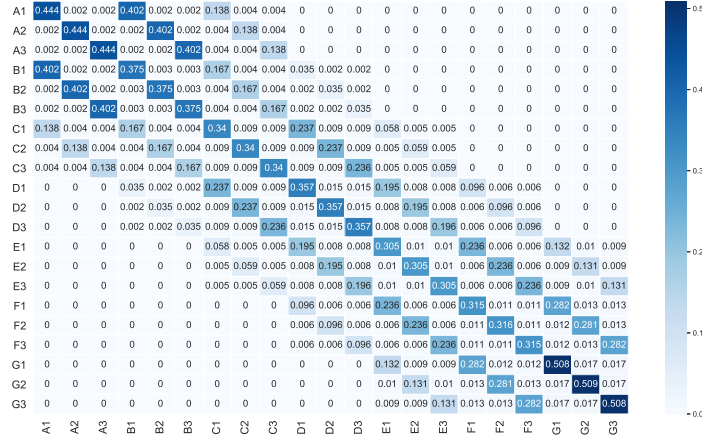
Figure 2a shows the general internal map of the network clip before the testing phase. One can interpret these values as how the stimuli are prioritized in the agent memory when there is no external trial that measures the accuracy of answers in MTS trials. Figure 2b shows the performance of agent when it comes to the testing phase. For instance, if the sample stimulus be  $A_3$  and the comparison stimuli be  $F_1, F_2$  and  $F_3$ ,



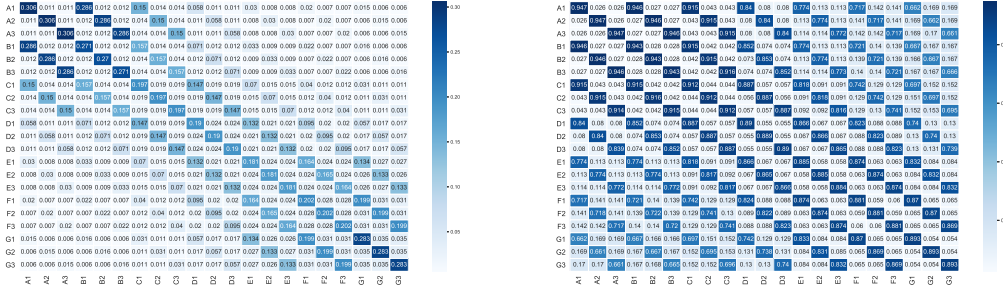
then the agent chooses  $F_1$  and  $F_2$  with probability 0.092 and selects  $F_3$  with probability 0.815.

To calculate these category-based probability distributions, first the conditional probability for any specific category is calculated based on Bayes' rule and then softmax function transfers these vectors to the desired probabilities based on the chosen parameter  $\beta_t$ . The conditional input aims to show the context, or environment state, effect and therefore we can apply the same  $\beta_t$ , as a characteristic of agent, for all the categories.

If we use SNE, first we have to compute  $\mathcal{T}$ , which is reported in Figure 3a, and then update the network using  $\alpha = 0.7$  parameter. The localized network  $\mathcal{T}$  add weights to the one-node relations and we have two more diagonals in  $\mathcal{T}$  in comparison with  $P$ .



(a) The localized network  $\mathcal{T}$ .



(b) Converged network  $W_{t \rightarrow \infty}$  using  $\alpha = 0.7$ . (c) Category-based probability distributions for the test phase using  $\beta_t = 4$ .

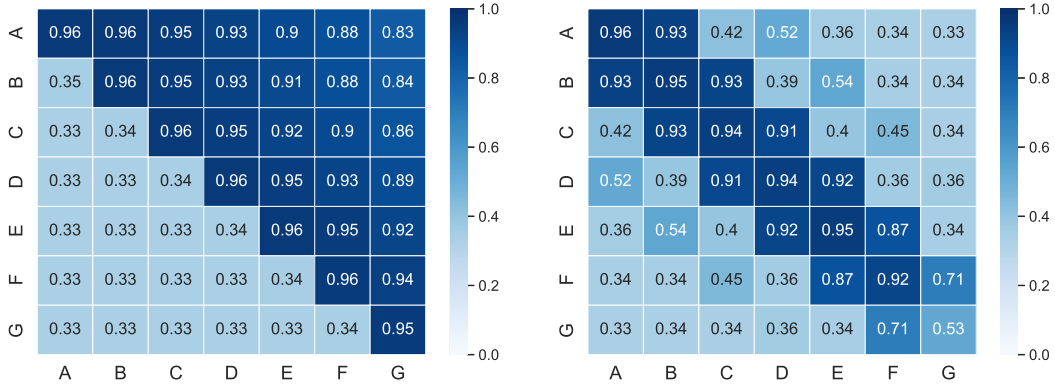
Figure 3: The new network adjacency matrix using SNE update when the regularization parameter is  $\alpha = 0.7$  and the input matrix  $W_0 = P$  which is given in Figure 1b. The test phase probabilities in Figure 3c, are calculated by normalizing the weights for the specific category and then using softmax function with parameter  $\beta_t = 4$ .

This experiment is supposed to illustrate how both DNE and SNE are working. In Experiment 2, we compare the two updating methods for symmetry and transitivity relations and discuss why DNE could be a more appropriate option for enhancing EPS model.

## Experiment 2: Isolating Symmetry and Transitivity

Two main differences between DNE and SNE is shown in this experiment. In this regard, we consider two extreme cases to isolate the symmetry and transitivity effects.

First, we isolate the effect of symmetry relations; in other words, we suppose that agent is able to answer the transitive relations, but unable to derive symmetry relations. For this, we set the parameters to  $\gamma = 0.001$ ,  $K = 0.01$ ,  $\beta_h = 0.1$ ,  $\beta_t = 4$ , and  $\alpha = 0.05$ .

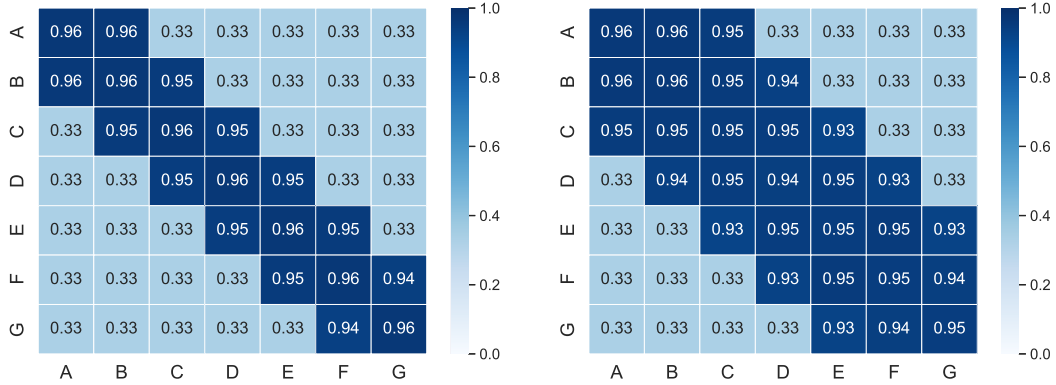


(a) Final category-based results applying DNE (b) Final category-based results applying SNE

Figure 4: Probability of choosing correct pairs between categories when  $\gamma = 0.001$ ,  $K = 0.01$ ,  $\beta_h = 0.1$ ,  $\beta_t = 4$ , and  $\alpha = 0.05$ . The reported values are calculated by taking average over all relations in each category.

As illustrated in Figure 4a, the symmetry relations and therefore equivalence relations can be altered by parameter  $K$ . However, in Figure 4b, due to the symmetric behaviour of updates, symmetry relations are exactly the same as baseline relations and transitive and equivalence relations are altered by setting  $K = 0.01$ . We can conclude that a DNE type agent can handle non-symmetric relations, but SNE agent is unable to control symmetry relations independently.

Next, we simulate a scenario that agent learns the baseline relations, but no transitive relation is derived. Suppose the symmetry relations are derived perfectly, so that we only isolate the transitive relations. Let the parameters of such an agent be  $\gamma = 0.001$ ,  $K = 1$ ,  $\beta_h = 0.1$ ,  $\beta_t = 4$ , and  $\alpha = 0$ .



(a) Final category-based results applying DNE (b) Final category-based results applying SNE

Figure 5: Probability of choosing correct pairs between categories when  $\gamma = 0.001$ ,  $K = 1$ ,  $\beta_h = 0.1$ ,  $\beta_t = 4$ , and  $\alpha = 0$ .

In Figure 5a, using DNE method, the transitive and therefore equivalence relations are not formed, while the symmetry relations are strong. In Figure 5b we see that the one-node relations such as  $AC$  and  $BD$  are derived in SNE. This is expected due to the definition of  $\mathcal{T}$ . In the EPS model though, we are seeking to control all the transitive and equivalence relations.

Therefore, since SNE is not an appropriate method for controlling symmetry and transitivity completely, we consider DNE as the main approach in this paper to cover more general cases, such as cases with weak symmetry relations or weak transitivity relations. In the rest of simulations we just report the results for DNE method.

### Experiment 3: Effect of $\beta_h$ Parameter

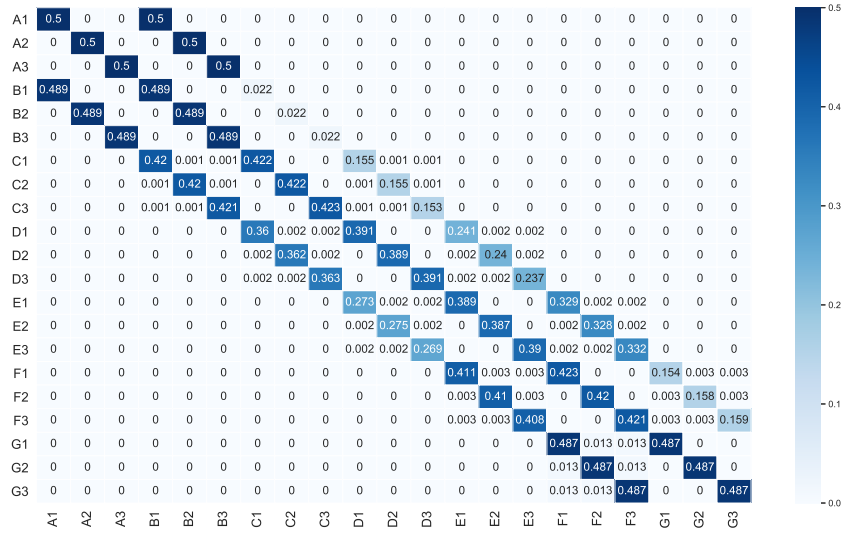
The softmax function parameter  $\beta_h$ , is used in the training phase for checking the mastery criterion as well as computing the transition matrix from  $W_h$ . As reported in Table 2, a higher value of  $\beta_h$  causes that the agent be able to pass the training phase faster, while for smaller values of  $\beta_h$ , it takes much more iterations to pass the training phase and learning baseline relations. See Table 2 for the learning speed for three values of  $\beta_h = 0.2$ ,  $0.1$  and  $0.05$  when  $\gamma = 0.001$ ,  $K = 1$ ,  $\beta_t = 4$ , and  $\alpha = 0.05$ .

Table 2: The average of required repetition of training blocks until reaching mastery criterion ratio 0.9 when  $\gamma = 0.001$ ,  $K = 1$ ,  $\beta_t = 4$ , and  $\alpha = 0.05$  for three values of  $\beta_h = 0.2, 0.1$  and  $0.05$

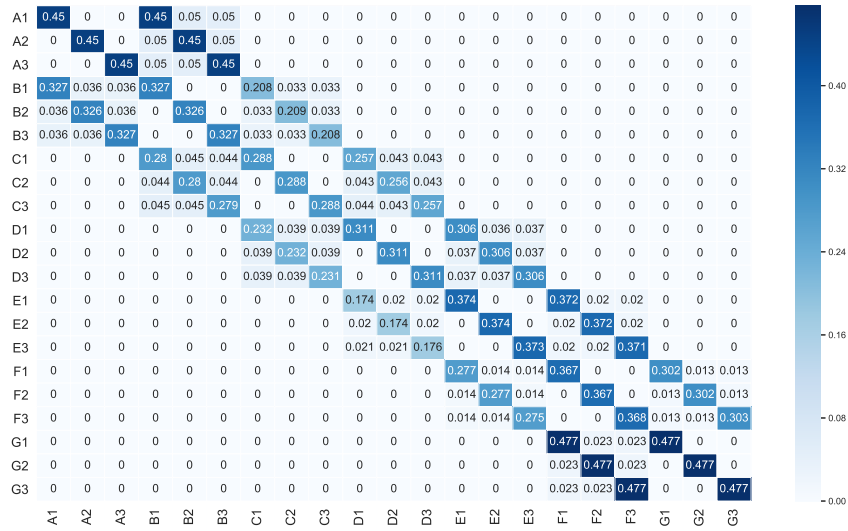
Training	Number of trials per relation						Time		
	<i>AB</i>	<i>BC</i>	<i>CD</i>	<i>DE</i>	<i>EF</i>	<i>FG</i>	$\beta_h = 0.2$	$\beta_h = 0.1$	$\beta_h = 0.05$
<i>AB</i>	48						2.133	3.423	5.907
<i>BC</i>	24	24					2.885	4.757	8.751
<i>CD</i>	12	12	24				2.959	4.977	9.641
<i>DE</i>	9	9	9	24			2.791	4.661	9.469
<i>EF</i>	6	6	6	6	24		2.992	5.208	11.736
<i>FG</i>	3	3	3	6	9	24	3.008	5.339	12.978
Bsl Maint	3	3	3	3	3	3	1.038	1.407	7.561

Table 2 shows that parameter  $\beta_h$  can be used to control the learning speed. For instance, an agent with  $\beta_h = 0.2$  learns *AB* relations with repeating the training blocks 2.1 times in average. This value will be 3.4 for  $\beta_h = 0.1$  and 5.9 for  $\beta_h = 0.05$ .

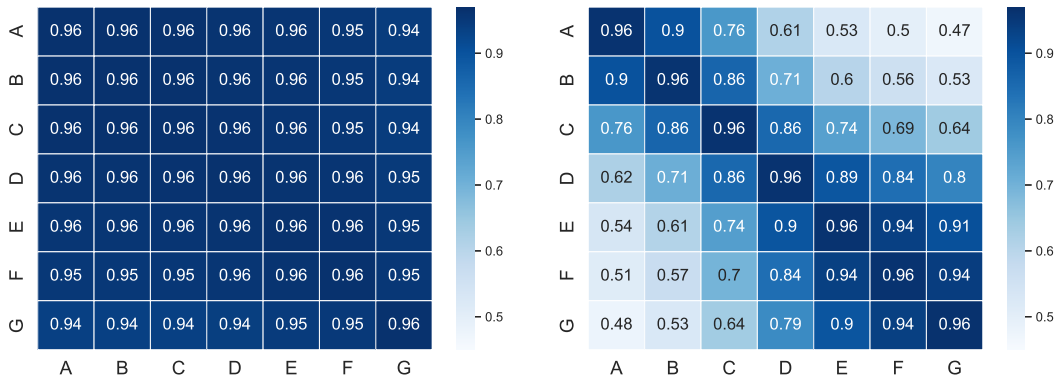
Another effect of  $\beta_h$  appears in computation of probability matrix and consequently the final network shape. In Figure 6, we report the  $P$  matrix and the computed nodal effect in the test phase for two choices of  $\beta_h = 0.2$  and  $\beta_h = 0.05$  when we keep all parameters similar;  $\gamma = 0.001$ ,  $K = 1$ ,  $\beta_t = 4$ , and  $\alpha = 0.05$ .



(a) The transition probability matrix  $P$  using  $\beta_h = 0.2$



(b) The transition probability matrix  $P$  using  $\beta_h = 0.05$



(c) Final category-based probability of correct choice in the test phase when  $\beta_h = 0.2$

(d) Final category-based probability of correct choice in the test phase when  $\beta_h = 0.05$

Figure 6: Comparison of probability matrix out of training and final category-based probability of correct choice in the test phase for two choices of  $\beta_h = 0.2$  and  $\beta_h = 0.05$ , when  $\gamma = 0.001$ ,  $K = 1$ ,  $\beta_t = 4$ , and  $\alpha = 0.05$ .

By comparing Figure 6a and Figure 6b, we notice that probability of direct relations are weaker when  $\beta_h = 0.05$ . Since this matrix is considered as  $W_0$ , the input matrix to the NE iterative method, the final results will be altered. In Figure 6c, the nodal effect is negligible and all the transitive and equivalence relations are formed equally well as baseline relations. Figure 6d, however, shows the nodal effect and agent’s weak performance in relations with higher nodal number. We conclude that  $\beta_h$  can be used both for controlling the speed of learning and the nodal effect. In other words, if we fix all other parameters than  $\beta_h$ , the smaller value of  $\beta_h$  results slower learning and lower chance to form transitive and equivalence relations with higher nodal number. It is noteworthy that the effect of  $\beta_h$  and  $\gamma$  are somehow intertwined. As we see in Experiment 4,  $\gamma$  also controls the learning speed and nodal effect. Indeed, if the agent does not forget at all, i.e.  $\gamma = 0$ , then  $\beta_h$  just controls the speed of learning. However,  $\gamma = 0$  is not a plausible choice for replication of human behavior.

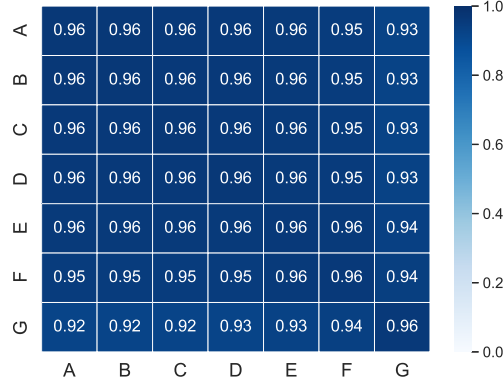
#### Experiment 4: Effect of $\gamma$ Parameter

In (Mofrad et al., 2020), the effect of  $\gamma$  in the training phase of EPS agents has been studied, where learning speed can be adjusted via  $\gamma$ . In Table 3, average number of repeating times at each stage is provided for three choices of  $\gamma = 0, 0.001$  and  $0.005$ . There is a general trend that increasing the forgetting factor will increase the repetition times in all stages. But the rate of increase for later stages and the baseline maintenance are different. The explanation is that forgetting factor affects the initial learned relations more since at the final blocks we have less of them. In other words, in the final blocks, we have fewer trials of them, and thus the forgetting factor will cause a stronger adverse impact. This is why we need around 7 iterations of maintenance phase when  $\gamma = 0.002$  while we need just one iteration by removing forgetting factor, i.e.  $\gamma = 0$ .

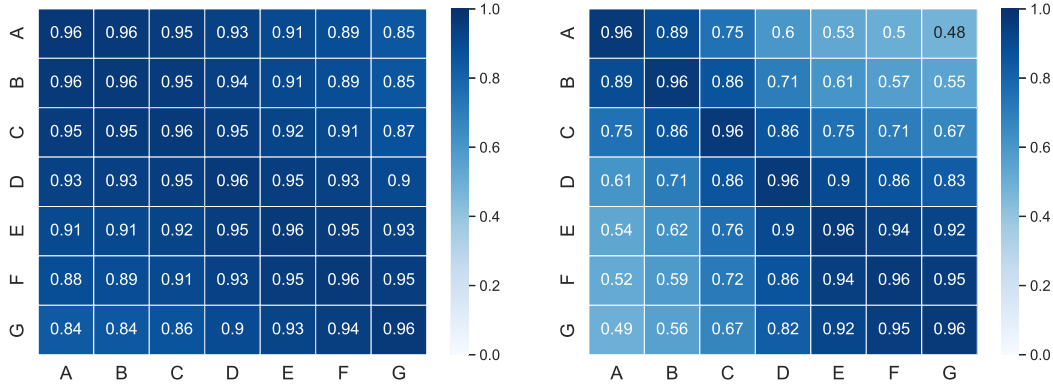
Table 3: The average of required repetition of training blocks until reaching mastery criterion ratio 0.9 when  $K = 1, \beta_h = 0.1, \beta_t = 4$ , and  $\alpha = 0.05$  for three values of  $\gamma = 0, 0.001$  and  $0.005$ .

Training	Number of trials per relation						Time		
	<i>AB</i>	<i>BC</i>	<i>CD</i>	<i>DE</i>	<i>EF</i>	<i>FG</i>	$\gamma = 0.0$	$\gamma = 0.001$	$\gamma = 0.002$
<i>AB</i>	48						3.318	3.452	3.580
<i>BC</i>	24	24					4.391	4.703	5.088
<i>CD</i>	12	12	24				4.570	4.951	5.584
<i>DE</i>	9	9	9	24			4.200	4.654	5.514
<i>EF</i>	6	6	6	6	24		4.649	5.190	6.951
<i>FG</i>	3	3	3	6	9	24	4.637	5.324	7.884
Bsl Maint	3	3	3	3	3	3	1.089	1.414	7.281

The forgetting factor will affect the final shape of  $h$ -values network  $W_h$ , and therefore for similar parameters we have different probability matrices and therefore final outcomes in the test phase. In Figure 7, final results of testing phase for three different values of forgetting factor is provided;  $\gamma = 0, 0.001, 0.002$ .



(a) Final category-based results when  $\gamma = 0$ .



(b) Final category-based results when  $\gamma = 0.001$

(c) Final category-based results when  $\gamma = 0.002$

Figure 7: Probability of choosing correct pairs between categories when  $K = 1$ ,  $\beta_h = 0.1$ ,  $\beta_t = 4$ , and  $\alpha = 0.05$  for three forgetting factors values  $\gamma = 0, 0.001$  and  $0.002$ .

When  $\gamma = 0$  (Figure 7a), there is no forgetting and therefore the training order does not matter and all the relations are considered equally the same. In Figure 7b, still all the relations are formed but we can easily notice the nodal effect. For instance, if we test  $AB$  relation the probability of correct choice by agent is 0.96 while it is about 0.85 for  $AG$  with five nodes in between. Figure 7c shows that a higher forgetting factor can be used to model impaired equivalence class formation. If we test the agent with  $AB$  relation, the probability of correct choice would be 0.89 while it is about 0.48 for  $AG$ . Comparing correct choice probabilities for  $AB$  and  $FG$  (0.89 for  $AB$  vs. 0.95 for  $FG$ ), shows the importance of training order in this setting. The agent forgets the initial stage relations and these relations need to be repeated. If the training trial blocks are totally separate, like Experiment 1 in (Mofrad et al., 2020), the initial trained relations drop dramatically in the case with high forgetting factor.

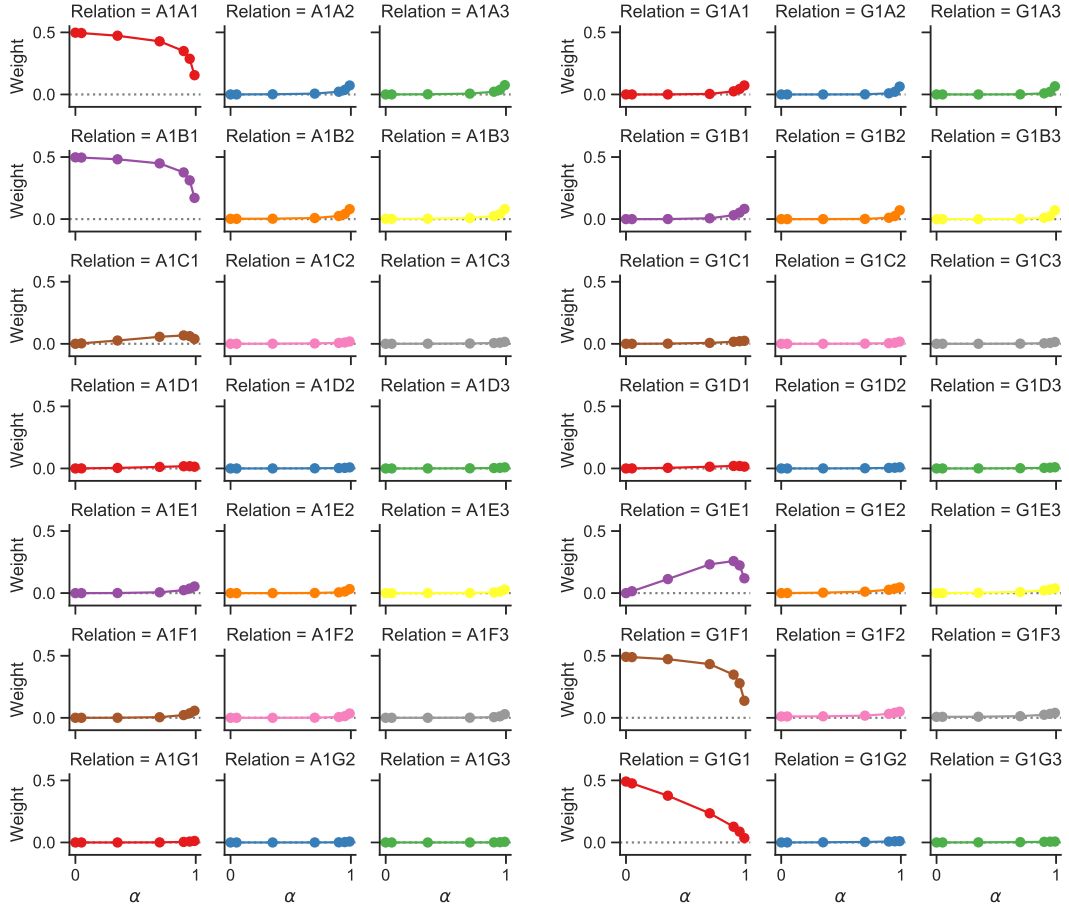
It is noteworthy that in the EPS model, to show the importance of testing order in the model, similar to the SE literature, we simulate the test phase with different test orders so the trials that appear late in the test phase, have weaker results when forgetting factor is high. Here, for simplicity, we calculate the probability distribution for different test trials and evaluate the agent behavior based on them. This means the forgetting factor is

not effective on the test results in the current simulations. However, the forgetting factor can be used by defining  $\beta_t$  as a function of time and  $\gamma$  to model the forgetting in the test phase of E-EPS. Another argument is that the forgetting might affect the network, in this case the network weights must be updated in a way to keep each row summing to one. Therefore, it is not as straightforward as the EPS where matrix with  $h$ -values is the basis for test phase.

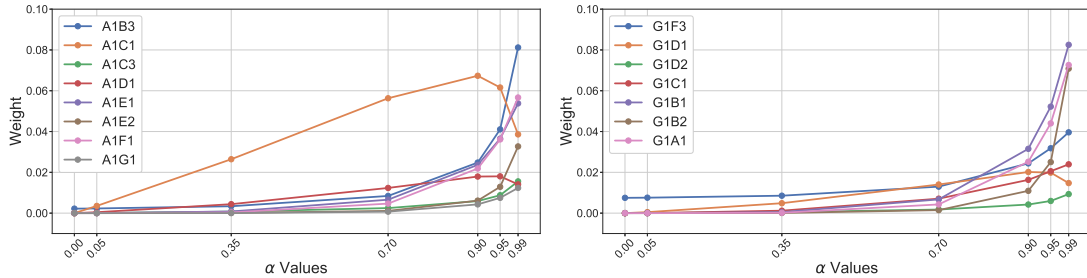
### **Experiment 5: Effect of $\alpha$ Parameter**

This parameter shapes the final representation of the clip network (see appendix A for a theoretical discussion). A smaller value of  $\alpha$  biases the converged matrix  $W_{t \rightarrow \infty}$  to keep the connections from  $W_0$  stronger, while a bigger value of  $\alpha$  enhances transitive relations. In the case of  $\alpha = 0$ , as represented in Figure 5a, there is no enhancement in the network using DNE. Figure 8a and Figure 8b respectively represent the connection values from  $A_1$  and  $G_1$  to other stimuli in the converged network for  $\alpha = 0, 0.05, 0.35, 0.7, 0.9, 0.95, \text{ and } 0.99$ , when  $\gamma = 0.001, K = 1$ , and  $\beta_h = 0.1$ .





(a) The connection weights in the converged matrix between  $A_1$  and other stimuli in  $W_{t \rightarrow \infty}$ . (b) The connection weights in the converged matrix between  $G_1$  and other stimuli in  $W_{t \rightarrow \infty}$ .



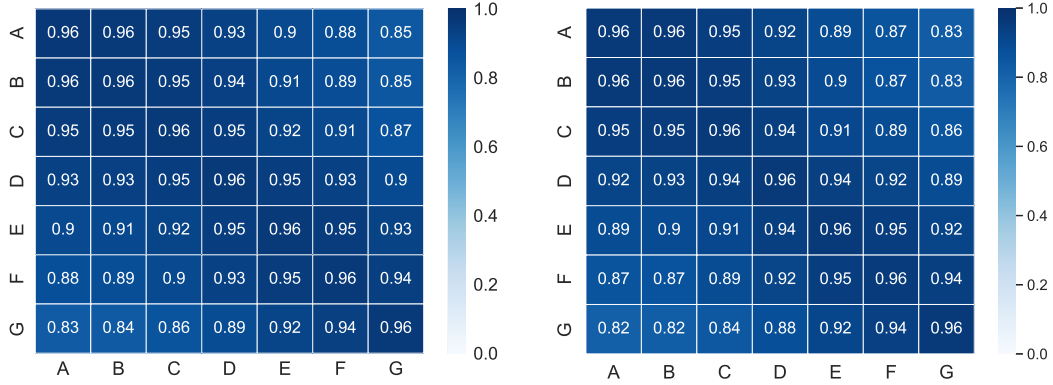
(c) A comparison between behavior of some desired and undesired relations between  $A_1$  and other stimuli based on different  $\alpha$  values. (d) A comparison between behavior of some desired and undesired relations between  $G_1$  and other stimuli based on different  $\alpha$  values.

Figure 8: The connection weights in the converged matrix  $W_{t \rightarrow \infty}$  for  $A_1$  and  $G_1$  for  $\alpha = 0, 0.05, 0.35, 0.7, 0.9, 0.95, 0.99$ , when  $\gamma = 0.001$ ,  $K = 1$ , and  $\beta_h = 0.1$ .

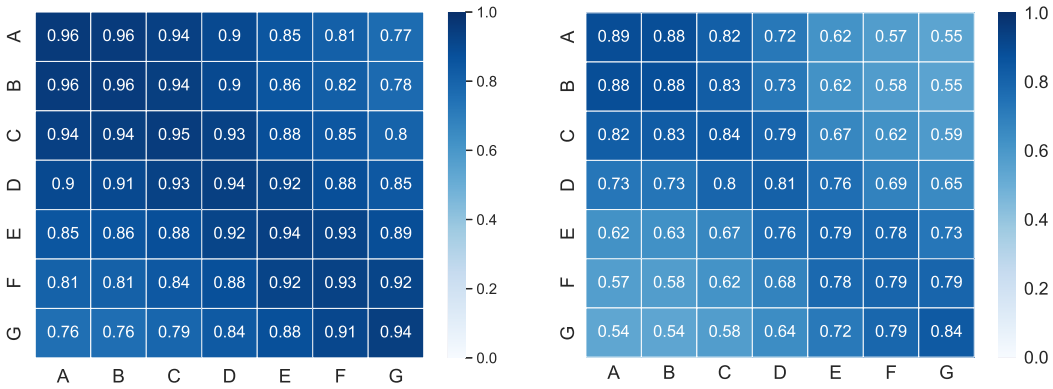
As depicted in Figure 8, smaller values of  $\alpha$  keep the relations in the input network, i.e. trained relations together with symmetry and reflexivity, stronger. On the other hand, a higher  $\alpha$  value, reinforces the transitive and equivalence relations. For each  $\alpha$  value, the connection weights for all relations must sum to one, for instance the values for  $\alpha = 0.9$  in all sub-plots of Figure 8a sum to one as they show the transition proba-

bility from  $A_1$  to all other points when using  $\alpha = 0.9$ . As a result, increasing the values for transitive relations means decrease in initial relations, see the decrease in  $A_1A_1$ ,  $A_1B_1$  relation weights and the increase in other values, say  $A_1C_1$  and  $A_1G_1$ . Along with construction and enhancing the desired relations (first columns in Figure 8a and Figure 8b), the undesired relations are also constructed and enhanced to some extent. This can be explained by the fact that the values for undesired relations such as  $A_1B_2$ ,  $A_1B_3$ ,  $G_1F_2$ , and  $G_1F_3$  are not zero in the initial matrix; since the training criterion was set to 0.9. These values could enhance undesired relations especially when  $\alpha$  is higher. For instance, as depicted in Figure 8c, the connection weight for  $A_1C_1$  relation, which is a desired relation, decreases for  $\alpha$  values higher than 0.9. Similarly, the connection weight for  $A_1D_1$  relation decreases at  $\alpha = 0.99$  in comparison with  $\alpha = 0.9, 0.95$ . The connection weight for  $A_1B_3$  relation, which has a very small weight in the beginning (i.e. when  $\alpha = 0$ ) increases with  $\alpha$  with acceleration in the rate of change for  $\alpha$  values greater than 0.7.  $A_1C_3$  and  $A_1E_2$  are two sample relations that are undesired and get enhanced during the diffusion process as a function of  $\alpha$  value. The same kind of behavior can be observed for relations from  $G_1$ . In Figure 8d, relation  $G_1D_1$  increases as desired, but when  $\alpha$  is too high, i.e.  $\alpha = 0.95, 0.99$ , starts to decrease. Undesired relations such as  $G_1F_3$  and  $G_1D_2$  are enhanced with a higher rate when  $\alpha$  approaches to one. Therefore, inappropriate choice of  $\alpha$  could play a destructive role; in this example higher values of  $\alpha = 0.9$  sounds inappropriate.

Different  $\alpha$  values and therefore different configurations of  $W_{t \rightarrow \infty}$  matrix results into different testing performance. In Figure 9, we report the testing results for four values of  $\alpha = 0.05, 0.35, 0.7, 0.95$  when  $\gamma = 0.001$ ,  $K = 1$ ,  $\beta_h = 0.1$ , and  $\beta_t = 4$ .



(a) Final category-based results when  $\alpha = 0.05$ . Average number of iterations is 4.0. (b) Final category-based results when  $\alpha = 0.35$ . Average number of iterations is 9.0.



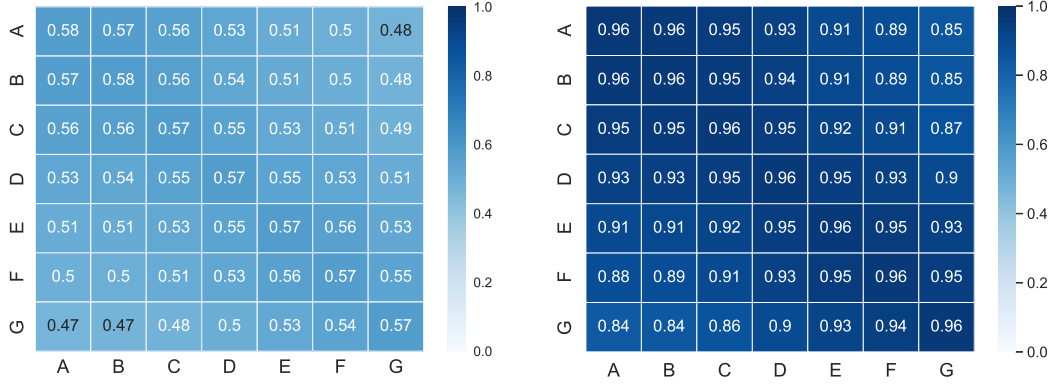
(c) Final category-based results when  $\alpha = 0.7$ . Average number of iterations is 23.96. (d) Final category-based results when  $\alpha = 0.95$ . Average number of iterations is 102.0.

Figure 9: Probability of choosing correct pairs between categories when  $\gamma = 0.001$ ,  $K = 1$ ,  $\beta_h = 0.1$ , and  $\beta_t = 4$  for four choices of  $\alpha = 0.05, 0.35, 0.7$ , and  $0.95$ .

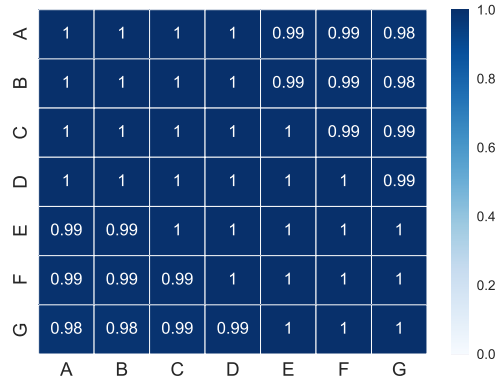
We observe that probability of choosing correct relations in Figure 9c and 9d respectively for  $\alpha = 0.05$  and  $\alpha = 0.35$ , are almost the same. In Figure 9a when  $\alpha = 0.7$  the transitive and equivalence relations are affected negatively. In Figure 9d, we see from the converged transition matrix that values for all the relations are decreased. Moreover, for smaller values of  $\alpha$  the convergence of the network needs less iterations, compare 4, 9, 23, and 102 for respectively  $\alpha = 0.05, 0.35, 0.7$  and  $0.95$ . For more details in  $\alpha$  parameter effect, see Table 4 where connection weights of  $AB$  and  $AG$  in  $W_{t \rightarrow \infty}$  for different  $\alpha$  choices, along with the calculated probabilities based on three choices of  $\beta_t = 1, 4, 8$  is reported.

### Experiment 6: Effect of $\beta_t$ Parameter

To study the effect of  $\beta_t$ , first we keep other parameters fixed  $\gamma = 0.001$ ,  $K = 1$ ,  $\beta_h = 0.1$ ,  $\alpha = 0.05$ , and simulate the agent behavior for three values of  $\beta_t = 1, 4, 8$  (see Figure 10).



(a) Final category-based results when  $\beta_t = 1$ . (b) Final category-based results when  $\beta_t = 4$ .



(c) Final category-based results when  $\beta_t = 8$ .

Figure 10: Probability of choosing correct relations between categories when  $\gamma = 0.001$ ,  $K = 1$ ,  $\beta_h = 0.1$ , and  $\alpha = 0.05$  for three values of  $\beta_t = 1, 4, 8$ .

We see a decrease in all types of relations by decreasing the value of  $\beta_t$ . In Figure 10a, when  $\beta_t = 1$  all relations including baseline relations become weaker. When  $\beta_t = 4$  in Figure 10b we see that the relations are well formed across all nodal numbers. Figure 10c shows that with a higher value of  $\beta_t = 8$ , all the relations are almost completely formed. This experiment illustrates that by changing  $\beta_t$  one can control the agent performance in the testing phase and even impair the baseline relations. In Table 4, we have a closer look to the simultaneous effect of  $\alpha$  and  $\beta_t$  when  $\gamma = 0.001$ ,  $K = 1$ ,  $\beta_h = 0.1$ .

Table 4: The simultaneous effect of  $\alpha$  and  $\beta_t$  values on the test results for  $AB$  and  $AG$  relations.  $W_{t \rightarrow \infty}$  row reports the weights in the converged network.  $W_{t \rightarrow \infty C}$  refers to the input weights conditioned based on the category which softmax function uses to generate the probability distribution. The  $C$  in the index of  $W_{t \rightarrow \infty C}$  refers to the conditional weights for the category calculated with Bayes rule.

$(\alpha, \beta_t)$		Baseline relation $AB$			Derived relation $AG$		
		$A_1B_1$	$A_1B_2$	$A_1B_3$	$A_1G_1$	$A_1G_2$	$A_1G_3$
$\alpha = 0$	$W_{t \rightarrow \infty}$	0.49837	0.00163	0.00163	0	0	0
	$W_{t \rightarrow \infty C}$	0.99350	0.00325	0.00325	0	0	0
	$\beta_t = 1$	0.57134	0.21419	0.21447	0.33333	0.33333	0.33333
	$\beta_t = 4$	0.9619	0.01904	0.01906	0.33333	0.33333	0.33333
	$\beta_t = 8$	0.99925	0.00037	0.00037	0.33333	0.33333	0.33333
$\alpha = 0.05$	$W_{t \rightarrow \infty}$	0.49686	0.0017	0.0017	$4.1276e^{-08}$	$5.6875e^{-09}$	$8.6627e^{-09}$
	$W_{t \rightarrow \infty C}$	0.9932	0.0034	0.0034	0.74202	0.10225	0.15573
	$\beta_t = 1$	0.57115	0.21429	0.21456	0.48349	0.25909	0.25743
	$\beta_t = 4$	0.96178	0.01909	0.01912	0.83865	0.08146	0.07989
	$\beta_t = 8$	0.99925	0.00037	0.00037	0.99049	0.00509	0.00442
$\alpha = 0.9$	$W_{t \rightarrow \infty}$	0.39782	0.02119	0.0223	0.003	0.00092	0.00112
	$W_{t \rightarrow \infty C}$	0.90145	0.04802	0.05053	0.59524	0.18254	0.22222
	$\beta_t = 1$	0.51983	0.24069	0.23948	0.4146	0.29794	0.28746
	$\beta_t = 4$	0.91757	0.04108	0.04135	0.69558	0.17058	0.13384
	$\beta_t = 8$	0.99726	0.00137	0.00136	0.96297	0.02154	0.01549
$\alpha = 0.95$	$W_{t \rightarrow \infty}$	0.34433	0.03844	0.04031	0.00464	0.00185	0.00212
	$W_{t \rightarrow \infty C}$	0.81387	0.090858	0.095278	0.53891	0.21487	0.24623
	$\beta_h = 1$	0.47784	0.2627	0.25945	0.39334	0.31058	0.29608
	$\beta_h = 4$	0.85289	0.0733	0.0738	0.61673	0.22268	0.16059
	$\beta_h = 8$	0.99183	0.0041	0.00407	0.92776	0.04397	0.02827

In Table 4, baseline relation  $AB$  and transitive relation  $AG$  with nodal number five are addressed. We use the conditioned weights (row  $W_{t \rightarrow \infty C}$  in Table 4) as the input vector to the softmax function to generate the probability distribution for the test phase. When  $\alpha = 0$ , there is no NE and any choice of  $\beta_t$  results to equal probability of all relations in  $AG$ . However,  $\beta_t$  could effect  $AB$  relation so that agent performs very poor (chooses  $A_1B_1$  with probability 0.57134 for  $\beta_t = 1$ ) or very strong (chooses  $A_1B_1$  with probability 0.99925 for  $\beta_t = 8$ ). When  $\alpha = 0.05$ , after about just four iterations,  $W_{t \rightarrow \infty}$  is achieved. We observe an insignificant reduction in  $A_1B_1$  weight in  $W_{t \rightarrow \infty}$  (from 0.49837 to 0.49686) and an insignificant increase in the  $A_1B_2$ ,  $A_1B_3$ ,  $A_1G_1$ ,  $A_1G_2$  and  $A_1G_3$ . Interestingly, since we use conditioned weights and apply softmax function, very tiny values for  $AG$  in  $W_{t \rightarrow \infty}$  transfers into noticeable values when condi-

tioned which could show the formation of derived relations. For instance, with  $\beta_t = 4$ ,  $(A_1G_1, A_1G_2, A_1G_3)_{W_{t \rightarrow \infty}} = (4.1276e^{-08}, 5.6875e^{-09}, 8.6627e^{-09})$  is transformed to  $(0.74202, 0.10225, 0.15573)$  that using softmax is converted into  $(0.83865, 0.08146, 0.07989)$ ; i.e.  $A_1G_1$  relation is formed for the agent. This means a small value of  $\alpha$  and consequently a few steps of NE could produce the desired network with an appropriate choice of  $\beta_t$ . If we consider higher values of  $\alpha$ , we see that the weight of baseline relation  $A_1B_1$  in  $W_{t \rightarrow \infty}$  is reduced, but all other relations are enhanced.

It is also noteworthy that increasing the value of  $A_1G_1$  which happens with higher choice of  $\alpha$  is not equivalent to a better performance in the test phase as it is reported in Table 4.

The reason is that NE changes the proportion of weights in  $W_{t \rightarrow \infty}$  which affects the conditioned vector in favor of undesired options (see  $W_{t \rightarrow \infty_C}$  values), and finally the probability of correct choice computed through softmax function is reduced. For instance when  $\alpha = 0.05$  the  $A_1G_1$  weight is  $4.1276e^{-08}$  but its proportion in the conditioned vector is 0.74202. For  $\alpha = 0.95$  the  $A_1G_1$  weight is 0.00464 which is much higher than  $\alpha = 0.05$ , but its proportion in the conditioned vector is 0.53891 which is less than the case with  $\alpha = 0.05$ . So, different configurations of  $\alpha$  and  $\beta_t$  could produce different behaviors upon request.

### Experiment 7: Study the Training Order; Comparing LS MTO, and OTM

There are many studies on the differences between LS OTM, and MTO training structures (see, e.g., Arntzen et al., 2010; Arntzen & Hansen, 2011; Arntzen, 2012). In this experiment we re-arrange the training blocks from LS in Table 1 to similar training stages for OTM and MTO training structures, represented in Table 5 and Table 6 respectively. For OTM training structure, the training relations in order are  $AB, AC, AD, AE, AF$ , and  $AG$ . For MTO training structure the training relations in order are  $AG, BG, CG, DG, EG$ , and  $FG$ .

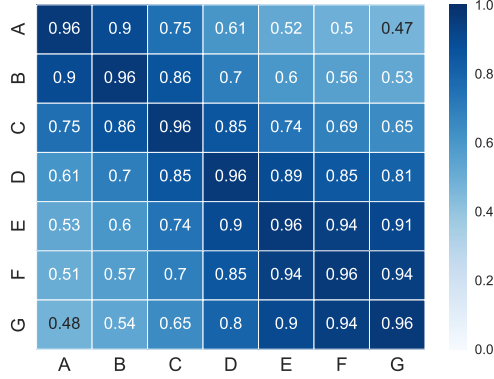
Table 5: The training order for OTM training structure

Training	Number of trials per relation					
	$AB$	$AC$	$AD$	$AE$	$AF$	$AG$
$AB$	48					
$AC$	24	24				
$AD$	12	12	24			
$AE$	9	9	9	24		
$AF$	6	6	6	6	24	
$AG$	3	3	3	6	9	24
Bsl Maint	3	3	3	3	3	3

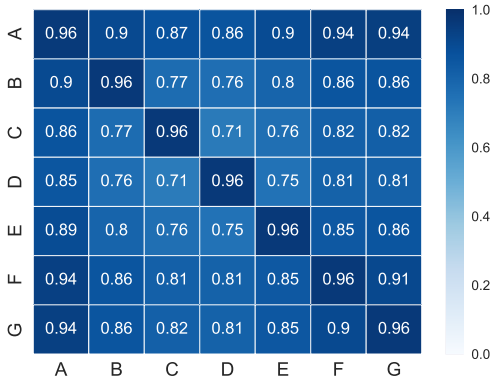
Table 6: The training order for MTO.

<b>Training</b>	<b>Number of trials per relation</b>					
	<i>AG</i>	<i>BG</i>	<i>CG</i>	<i>DG</i>	<i>EG</i>	<i>FG</i>
<i>AG</i>	48					
<i>BG</i>	24	24				
<i>CG</i>	12	12	24			
<i>DG</i>	9	9	9	24		
<i>EG</i>	6	6	6	6	24	
<i>FG</i>	3	3	3	6	9	24
<b>Bsl Maint</b>	3	3	3	3	3	3

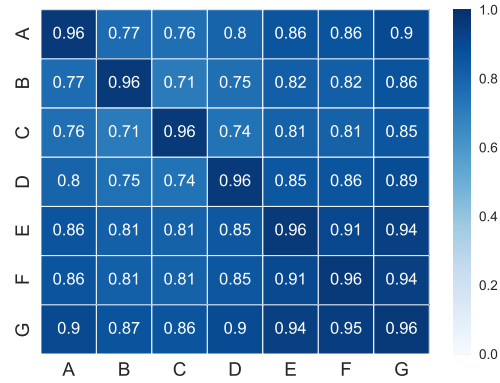
The three training structures, LS OTM, and MTO can be studied in various levels and with several parameter assemblies. But the aim of this experiment is to show the potential of proposed E-EPS model in reflecting the differences between LS OTM, and MTO training structures reported in the literature. In Figure 11, the results of the final test phase of the three cases for an agent with parameters  $\gamma = 0.001$ ,  $K = 1$ ,  $\beta_h = 0.05$ ,  $\alpha = 0.05$ , and  $\beta_t = 4$  is reported.



(a) Final category-based results for LS.



(b) Final category-based results for OTM.



(c) Final category-based results for MTO.

Figure 11: Probability of choosing correct relations between categories when  $\gamma = 0.001$ ,  $K = 1$ ,  $\beta_h = 0.05$ ,  $\alpha = 0.05$ , and  $\beta_t = 4$  for three training structures LS, MTO, and OTM.

According to Figure 11a, the agent performance when the LS is used is not satisfactory for higher nodal numbers. The weakest value belongs to  $AG$  which is 0.47. The equivalence classes are not formed in this case. Figure 11b, shows a better performance where the weakest connections are for  $CD$  and  $DC$  and equals to 0.71. This minimum value is also found in Figure 11c but for relations  $BC$  and  $CB$ . So in this experiment, the overall results in terms of formation of equivalence classes are the same for MTO and OTM, but due to the order of training, the agent might exhibit different performance for specific relations in MTO and OTM training structures. For instance, calculated probability for  $FA$  relation in OTM is 0.94 and in MTO is 0.86. On the other hand, calculated probability for  $DE$  relation in OTM is 0.75 while in MTO is 0.85.

It is noteworthy that the training time, i.e. number of repetition of each block before mastery in all three cases for all training procedures are similar. This can be explained by the independence of designing baseline relations. The reported results in Figure 11 confirms that our model shows better performance in the OTM and MTO cases in comparison with LS (see, e.g. Arntzen et al., 2010; Arntzen & Hansen, 2011; Arntzen, 2012).



## 5 Conclusion

In summary, the main contribution of this article is to propose a new perspective in formation of SE classes in recently introduced model, called EPS. EPS is a modified version of PS model (Briegel & De las Cuevas, 2012), that can be seen as an RL agent which has a directed, weighted network of clips. Each clip represents a remembered stimulus that is added to the clip network during the training phase.

To replicate the test phase of SE, i.e. examining the agent ability to encounter with new relations that can be derived from baseline relations, EPS model relies on some type of likelihood reasoning whenever tested via a MTS trial. In other words, in the EPS model, derived relations were calculated on demand in the test phase trials, but the new alternative approach to the testing phase is an offline approach and relies rather on memory retrieval during test phase than on complex logical processing. Derived relations in the new model, called E-EPS, are achieved by applying an iterative diffusion process so called Network Enhancement (NE) (Wang et al., 2018). During the network enhancement phase, the structure of clip network changes where indirect relations get enhanced. The NE is a denoising method and one way to interpret the model is to consider a typical memory as a less noisy memory, whilst a disabled memory is a noisy memory which can not form equivalence relations. Since in the NE connections are bidirectional, it is called Symmetric Network Enhancement (SNE) in this paper. We further modify the SNE and propose Directed Network Enhancement (DNE) in which the connections are directed and we can control the agent’s ability to derive transitivity and also control its ability to derive symmetry. One might use SNE in study SE formation with the assumption that all the relations are bidirectional and transitive and equivalence relations are formed. DNE is a better option to replicate real experiments with the possibility of non-formation of classes and non-symmetric relations.

In the simulation part, we study the role of parameters on the agent performance and show that the model is able to replicate either a typical memory or a disabled memory with different learning and forgetting rates, and accomplishing the trial tasks in the test phase. We also compare the main training structures; LS MTO, OTM, and notice better outcome of MTO and OTM training structures than LS which is consistent with evidences from behavioral analysis literature. Many other configurations can be considered in simulations. For instance, we consider  $K = 1$  to reduce the variety of results, or to study each parameter, we fixed all the other parameters.

Another alternative is to execute the NE phase during training and not merely at the end of the training. The argument would be that brain does not wait until the end of training to start process of formation of these relations. Although this might sound a plausible argument and can be easily added to the model, we avoid NE during training. The most obvious reason is to keep the model simple with less computations. As we are studying the agent behavior, the timing of events inside the brain is not the main priority. Moreover, baseline relations are independent and not derived from each other. So there is no need to update them earlier when the formation of relations are tested in the test phase. On the other hand, as discussed in section 3.1, these updates could be analogous to the replay in brain which generates a predictive map in an offline process.

The probability distribution over comparison stimuli in the test trial is calculated based on the direct links in the updated clip network. It is similar to the EPS in the sense

that whenever there are links between the sample stimulus and comparison stimuli, the probabilities are calculated based on the  $h$ -values either by averaging or using softmax function. In E-EPS, however, there are links through the whole network updated by NE process, and therefore no extra calculation is made. Although, one might still consider the random walk on the network similar to PS model, the cyclic nature of the network in E-EPS model might generate problems and extra conditions (such as gating) might be necessary. We avoid this scenario, since the calculated weights are based on the random walk and diffusion and we consider these cached links at the decision time. The EPS and E-EPS could further be developed to model more complex tasks with more sophisticated structures that PS model offers. For instance, we might use compound stimuli and benefit from PS model with associative learning (Briegel & De las Cuevas, 2012), or a multi-layer memory clip where agent is able to generate and add additional clips to the memory, called wildcard clips (Melnikov et al., 2017). Such multi-layer PS agent has been further developed to address abstract compositional concepts which is closer to the concept of SE (Ried et al., 2019).

The mathematical understanding of the properties of the converged network that guarantees the converged solution is an advantage of NE over other network denoising methods. DNE maintains many properties of SNE with the advantage of controlling formation of symmetry and transitivity in the E-EPS model. Finally, it is worth to mention that we choose NE, as the source of inspiration for updating the network clip, since in the updates, there is no requirement for supervision or prior knowledge. After training phase, we have a clip network without further feedback or supervision. Hence, NE provides a proper solution with the emphasis on the indirect paths, which is what we have in derived relations.

## Abbreviations

**DNE** Directed Network Enhancement. 3, 9, 13, 15, 17–19, 33, 34, 39–42

**DSM** doubly stochastic matrix. 8

**E-EPS** Enhanced Equivalence Projective Simulation. 3, 4, 7, 8, 10–13, 24, 31, 33, 34, 43, 47

**EPS** Equivalence Projective Simulation. 1–5, 7–13, 17, 19, 22–24, 33, 34, 43, 47

**fMRI** Functional magnetic resonance imaging. 11

**LS** linear series. 3, 4, 30–33, 44

**MTO** many-to-one. 3, 4, 30–33, 44–46

**MTS** matching-to-sample. 1, 2, 4, 5, 16, 33, 43, 47

**NE** Network Enhancement. 1–4, 8–10, 12, 15, 22, 29, 30, 33, 34

**OTM** one-to-many. 3, 4, 30–33, 44–46

**PS** Projective Simulation. 1–8, 10–13, 33, 34

**RL** reinforcement learning. 5, 11, 12, 33

**SE** Stimulus Equivalence. 1–4, 7, 9, 23, 33, 34

**SNE** Symmetric Network Enhancement. 8, 9, 13, 17–19, 33, 34

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## A Theoretical Analysis of Directed Network Enhancement (DNE)

Here we explain why the proposed diffusion process in equation 7 improves the results and can be used to form equivalence classes. As mentioned in the main part of paper, the theoretical analysis in this part is mostly based on the supplementary note 3, of (Wang et al., 2018). However, since  $W_t$  in the DNE, is not a symmetric doubly stochastic matrix, the proofs and discussions need to be revised for DNE. It is noteworthy that the largest eigenvalue of each right stochastic matrix, such as  $P$ , is 1, associated with eigenvector  $\mathbf{1}$ . In the following first we prove that  $W_t$  remains right stochastic in each iteration of DNE and converges to a non-trivial equilibrium matrix. Then, we show that DNE preserves the eigenvectors of the stochastic matrix  $W_0$ , but increases the gap between large eigenvalues and reduces the gap between small eigenvalues (see Figure 13). Larger eigengap in the final converged matrix  $W_{t \rightarrow \infty}$ , is associated with better equivalence class formation.

### The convergence of DNE process

We show that  $W_t$  remains stochastic during the updates. By definition  $W_0 \mathbf{1} = \mathbf{1}$ , for all-one eigenvector  $\mathbf{1}$  associated with eigenvalue one. We assume that  $W_{t-1} \mathbf{1} = \mathbf{1}$ , and show that the rows of  $W_t$  remain normalized, i.e.

$$\begin{aligned}
W_t \mathbf{1} &= \alpha P W_{t-1} P \mathbf{1} + (1 - \alpha) P \mathbf{1} \\
&= \alpha P W_{t-1} \mathbf{1} + (1 - \alpha) P \mathbf{1} \\
&= \alpha P \mathbf{1} + (1 - \alpha) P \mathbf{1} \\
&= P \mathbf{1} \\
&= \mathbf{1}.
\end{aligned} \tag{10}$$

Now, we show that  $W_t$  converges to a non-trivial equilibrium graph. A closed form solution for the final, converged network can be achieved through induction. Consider the following expression for the network at iteration  $t$

$$W_t = \alpha^t P^t W_0 P^t + (1 - \alpha) P \sum_{k=0}^{t-1} (\alpha P^2)^k. \tag{11}$$

This formula is similar to equation 6 of the supplementary note 3 by Wang et al. (2018) where  $\mathcal{T}$  is replaced by  $P$ , and can be guessed by iterating the process for the first few steps.

- Define  $W_0 = W_{t=0}$ . For  $t = 1$ , equation 11 holds true:

$$W_{t=1} = \alpha P W_0 P + (1 - \alpha) P$$

- We assume equation 11 holds true for iteration  $t$ , then:

$$\begin{aligned}
W_{t+1} &= \alpha P W_t P + (1 - \alpha) P \\
&= \alpha P \left( \alpha^t P^t W_0 P^t + (1 - \alpha) P \sum_{k=0}^{t-1} (\alpha P^2)^k \right) P + (1 - \alpha) P \\
&= \alpha^{t+1} P^{t+1} W_0 P^{t+1} + (1 - \alpha) P \sum_{k=0}^{t-1} (\alpha P^2)^{k+1} + (1 - \alpha) P \\
&= \alpha^{t+1} P^{t+1} W_0 P^{t+1} + (1 - \alpha) P \sum_{k=0}^t (\alpha P^2)^k,
\end{aligned}$$

which satisfies equation 11. Using geometric series when  $t \rightarrow \infty$ , we have this non-trivial equilibrium matrix:

$$W_{t \rightarrow \infty} = (1 - \alpha) P (\mathcal{I} - \alpha P^2)^{-1}. \tag{12}$$

## Spectral Analysis of DNE

We show that DNE process does not change eigenvectors of the input matrix  $W_0 = P$  but mapping eigenvalues through a non-linear function.

Suppose  $(\lambda, v)$  be the eigen-pair of  $P$ . We know that the absolute value of eigenvalues of any stochastic matrix satisfy  $|\lambda| \leq 1$  relation. Let the eigendecomposition of  $P$  be  $V D V^{-1}$  where  $D$  is a diagonal matrix formed from eigenvalues of  $P$  and the columns of  $V$  are the corresponding eigenvectors of  $P$ . We have



$$\begin{aligned}
W_{t \rightarrow \infty} &= (1 - \alpha)P(\mathcal{I} - \alpha P^2)^{-1} \\
&= (1 - \alpha)VDV^{-1}(\mathcal{I} - \alpha VDV^{-1}VDV^{-1})^{-1} \\
&= (1 - \alpha)VDV^{-1}(VV^{-1} - \alpha VDV^{-1}VDV^{-1})^{-1} \\
&= (1 - \alpha)VDV^{-1}(V(\mathcal{I} - \alpha D^2)V^{-1})^{-1} \\
&= (1 - \alpha)VDV^{-1}(V(\mathcal{I} - \alpha D^2)^{-1}V^{-1}) \\
&= (1 - \alpha)V(D(\mathcal{I} - \alpha D^2)^{-1})V^{-1} \\
&= V((1 - \alpha)(D(\mathcal{I} - \alpha D^2)^{-1})V^{-1}) \\
&= VD'V^{-1}.
\end{aligned}$$

This testifies that DNE process keeps the eigenvectors unchanged, but the eigenvalues become  $D'_{ii} = \frac{(1 - \alpha)\lambda_i}{1 - \alpha\lambda_i^2}$ . Therefore, DNE process functions non-linearly on the eigenvalues of the input matrix, i.e. the final converged matrix,  $W_{t \rightarrow \infty}$ , transforms  $(\lambda, v)$  to  $(f_\alpha(\lambda), v)$  where  $f_\alpha(\lambda) = \frac{(1 - \alpha)\lambda}{1 - \alpha\lambda^2}$ . It is trivial that  $f_\alpha(\lambda)(0) = 0$ ,  $f_\alpha(\lambda)(1) = 1$ . The below relations show that the DNE always decreases the absolute value of eigenvalues

$$\begin{aligned}
1 &\geq |\lambda| \\
1 &\geq \lambda^2 \\
\alpha &\geq \alpha\lambda^2 \\
1 - \alpha &\leq 1 - \alpha\lambda^2 \\
|\lambda|(1 - \alpha) &\leq |\lambda|(1 - \alpha\lambda^2) \\
\frac{|\lambda|(1 - \alpha)}{1 - \alpha\lambda^2} &\leq |\lambda|,
\end{aligned}$$

where the rate of this decrease is higher for eigenvalues with greater absolute values. Figure 12 depicts the behavior of  $f_\alpha$  and how does this non-linear function can be regularized with  $\alpha$  parameter. Increasing the eigengaps between large eigenvalues, enhances the robustness of the converged network which in our case means better formation of classes (see, e.g. Joseph et al., 2016; Wang et al., 2018; Mavroeidis & Bingham, 2010, for more details in spectral eigengap).

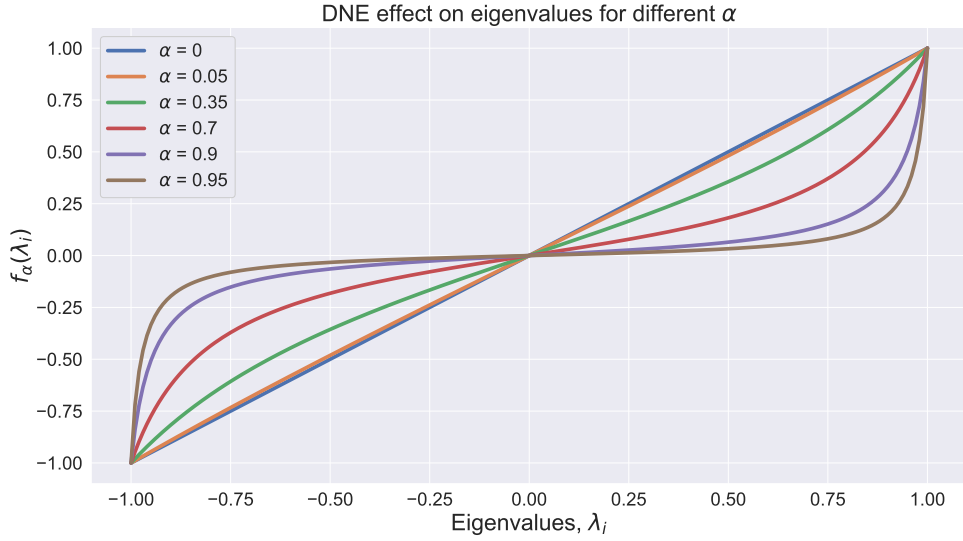


Figure 12: Role of  $\alpha$  on the non-linear transformation of eigenvalues using  $f_\alpha(\lambda)$  in DNE process.

Figure 12 shows that by increasing the regularization parameter, higher eigengaps are achieved. In Figure 13, the associated eigenvalues of a sample network clip<sup>7</sup> and the new eigenvalues of the converged network with different  $\alpha$  values is represented.

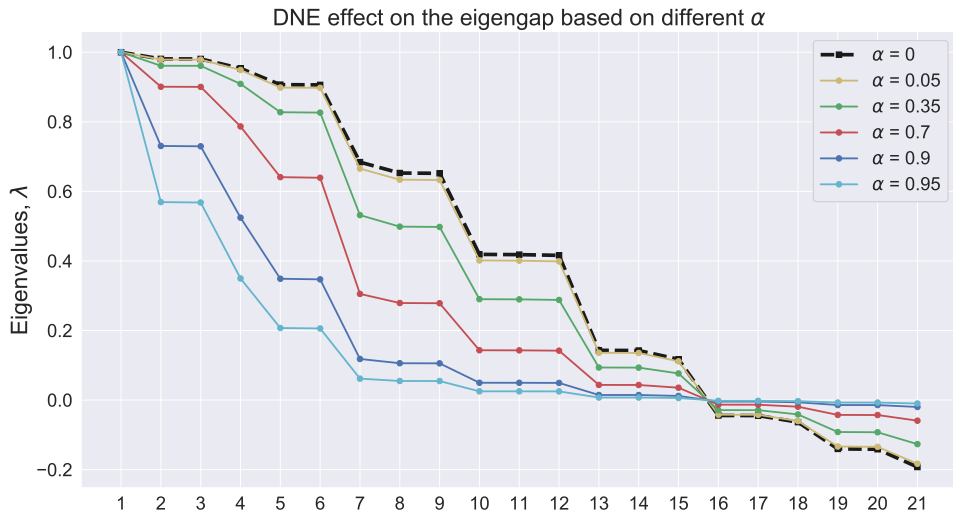


Figure 13: The effect of  $\alpha$  on the eigenvalues of the transition matrix of a clip network obtained from Experiment 1 in the results section 4 (see Table 1 for training structure).

<sup>7</sup>The training order represented in Table 1, we will explain the experiments in section 4.

## B Training Structure Design Complexity

Here we provide some mathematical calculations to show that how complex the design of different training structures could be both in real experiments and in artificial EPS or E-EPS agents.

Let the set of all classes be  $\mathbf{C}$ , where each class has  $m$  members. Each member of the classes belongs to a separate category; usually labeled by letters  $A, B, C$ , etc. As a result, there are  $m$  categories each with  $n = |\mathbf{C}|$  members, so the total number of stimuli equals  $m|\mathbf{C}| = mn$ . In an arbitrary MTS procedure, experimenter usually decides how to label categories (among  $m!$  possibilities) and which stimuli sets form classes (among  $mn!$  possibilities). In real-life experiments, changing the order of two categories (or label) or how the members of the same class are assembled across different categories, might have impact on the learning and testing outcome.

However, in the computational model, all the categories and stimuli are abstract symbols and literally the same. We just use the category labels and class indices to differentiate the stimuli. By differentiation between categories, as real-life experiment, the total number of baseline relation configurations, defined as  $\mathbf{T}$ , would be:

$$\begin{aligned} \mathbf{T} &= \binom{m}{1} \binom{m-1}{1} \left( 2 \binom{2}{1} \binom{m-2}{1} \right) \left( 2 \binom{3}{1} \binom{m-3}{1} \right) \cdots \left( 2 \binom{m-1}{1} \binom{1}{1} \right) \\ &= 2^{m-2} m! (m-1)! \end{aligned} \quad (13)$$

In the EPS model, we can remove the repetitions by assuming the category label describes the order of adding a category. For instance, the first relation for training would be  $AB$ , the next training could be one of  $AC, BC, CA$  or  $CB$ , etc. The number of different training configurations for the agent in this case is:

$$\mathbf{T} = 1 \times \left( 2 \binom{2}{1} \right) \times \left( 2 \binom{3}{1} \right) \cdots \left( 2 \binom{m-1}{1} \right) = 2^{m-2} (m-1)! \quad (14)$$

To make these calculations more intuitive, consider the case with seven categories, i.e.  $m = 7$ , with labels  $A, B, C, D, E, F$ , and  $G$  each with three members  $n = 3$ . In Figure 14,  $C_1$  to  $C_7$  refers to the seven categories where at each time step, one relation to a new category will be added. The first training stage, contains  $C_1$  to  $C_2$  relation, which is shown via a directed connection.  $C_1$  could be any of seven categories, and  $C_2$  could be one of the remained six categories. The next stage, represented with  $t = 2$  is to add  $C_3$  which is one of the remained five categories. There are four options to train:  $C_1C_3, C_3C_1, C_2C_3$ , and  $C_3C_2$ , which are shown with undirected connections. Similarly, we see that for  $t = 3$ , there are four choices for categories and  $2 \times 3$  ways to choose the relation that connects  $C_4$  to previous categories. Therefore, we can easily investigate that the number of possible maps of categories to  $C_1$  to  $C_7$  is  $7!$  and the possibilities to connect them with six relations is  $2^5(6!)$ . In total, if we distinguish between categories and therefore their order, the number of possible training procedures based on equation 13 and above explanation equals  $2^5(7!)(6!) = 32 \times 5040 \times 720 = 116, 121, 600$ .

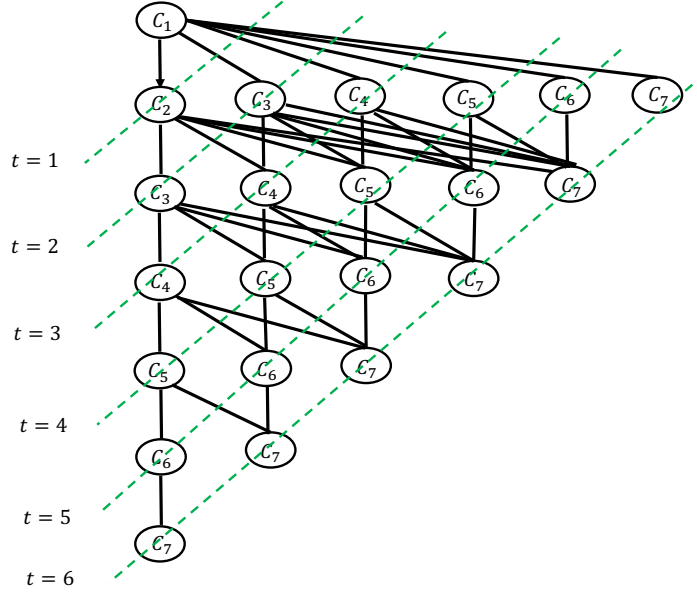


Figure 14:  $C_1$  to  $C_7$  refers to the seven categories and the number of possible maps from categories to  $C_i$ s,  $i = 1, \dots, 7$  is  $7!$ . Each time step, which is shown by green dashed lines, a category is added to the previously trained relations. At time  $t = 1$ ,  $C_1$  to  $C_2$  relation, which is shown via a directed connection, is trained as the first relation. This can be any relation. Then at each time step a new category is connected to the previously trained relations.

If we consider that the order of categories to be the same and map  $C_1 \rightarrow A$ ,  $C_2 \rightarrow B$ ,  $C_3 \rightarrow C$ ,  $C_4 \rightarrow D$ ,  $C_5 \rightarrow E$ ,  $C_6 \rightarrow F$ , and  $C_7 \rightarrow G$ , different configurations will be reduced to  $2^5(6!) = 32 \times 720 = 23,040$ , according to equation 14. This one-to-one mapping is shown in Figure 15 along with a sample training order in directed red connections which is not LS, OTM, or MTO; see Table 7 for the summary of training.

Table 7: The Training Order for Training Structure Depicted in Figure 15. A training block can be formed by only new relation at each stage or a combination of new relation and previously trained relations.

Time step	New relation	Possible previous relations
$t = 1$	$AB$	
$t = 2$	$CB$	$AB$
$t = 3$	$AD$	$CB$ $AB$
$t = 4$	$EA$	$AD$ $CB$ $AB$
$t = 5$	$DF$	$EA$ $AD$ $CB$ $AB$
$t = 6$	$GE$	$DF$ $EA$ $AD$ $CB$ $AB$

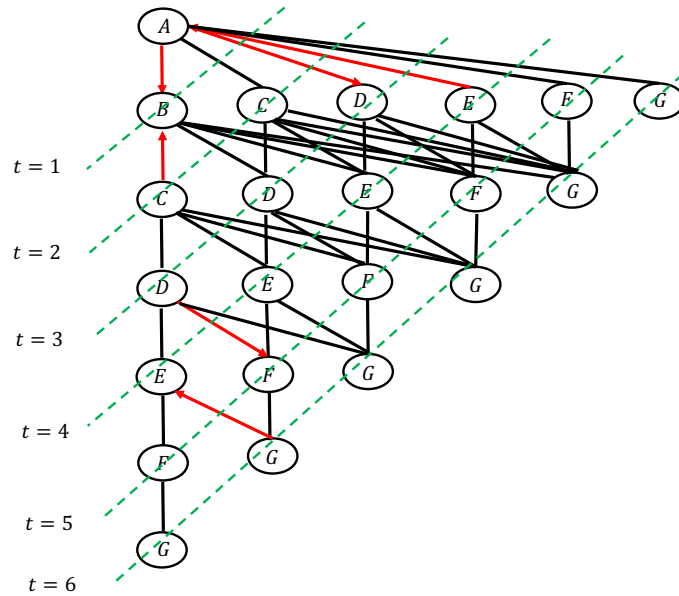
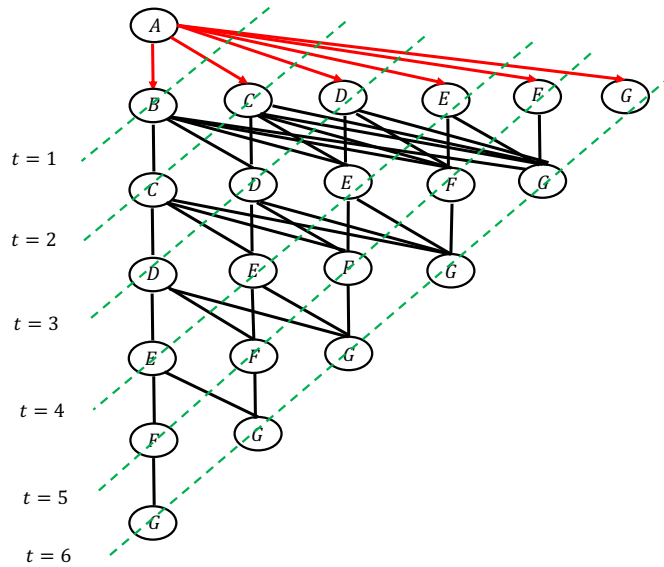
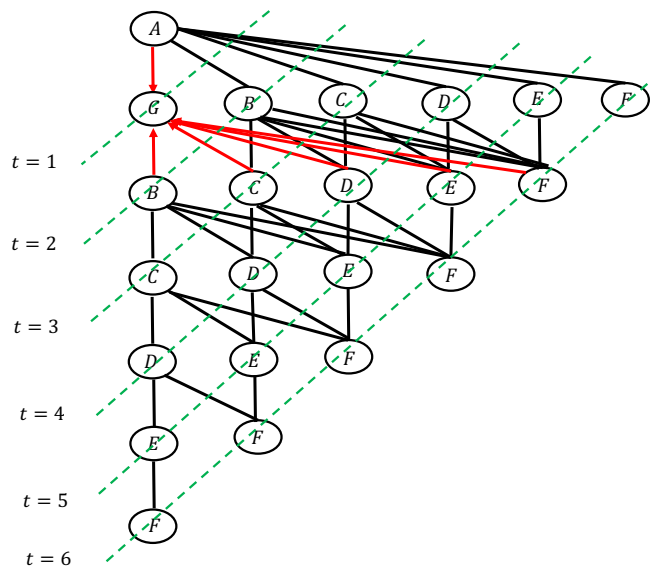


Figure 15: A possible training structure shown in red:  $AB, CB, AD, EA, DF, GE$  when the order of categories in the training structure is not important.

In Figure 16a and Figure 16b, respectively the order of adding new relations to the training blocks for OTM and MTO are depicted. Both training structures are addressed in Experiment 1 and reported in Table 5, and Table 6.



(a) The order of adding new relations in OTM training structure:  $AB$ ,  $AC$ ,  $AD$ ,  $AE$ ,  $AF$ , and  $AG$ .



(b) The order of adding new relations in MTO training structure:  $AG$ ,  $BG$ ,  $CG$ ,  $DG$ ,  $EG$ , and  $FG$ .

Figure 16: Graphical representation of training order for OTM and MTO, shown in red.

Although the above argument and equations 13-14 show the complexity of studying the effect of training structure in MTS procedure on the participant/agent performance, it is noticeable that the training structure and training block design is much more complex. We just address the order of adding new training relation to the previously trained relations. There are many other parameters that can be included in the analysis, such as: the number of trials in each block, the combination of previously trained relations together with the new relation, testing derived relations during training or not, testing order, number of classes (members of each category), and so on. Moreover, the possibility to train a mixture of relations between two categories, say  $A_1B_1, B_2A_1, A_3B_3$  will increase this amount. An example of such training is simulated in our previous work (Mofrad et al., 2020). Therefore, finding some optimal training structure either theoretically or via simulation with EPS or E-EPS is an interesting problem in its own right, but it is out of the scope of this paper.