Model-free reinforcement learning operates over information stored in working-memory to drive human choices

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1 Abstract

Model-free learning creates stimulus-response associations, but are there limits to the types of stimuli it can operate over? Most experiments on reward-learning have used discrete sensory stimuli, but there is no algorithmic reason to restrict model-free learning to external stimuli, and theories suggest that model-free processes may operate over highly abstract concepts and goals. Our study aimed to determine whether model-free learning can operate over environmental states defined by information held in working memory. We compared the data from human participants in two conditions that presented learning cues either simultaneously or as a temporal sequence that required working memory. There was a significant influence of model-free learning in the working memory condition. Moreover, both groups showed greater model-free effects than simulated model-based agents. Thus, we show that model-free learning processes operate not just in parallel, but also in cooperation with canonical executive functions such as working memory to support behavior.

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1 Introduction

Reinforcement learning theory and the computational algorithms associated with it have been extremely influential in the behavioral, biological, and computer sciences. Reinforcement learning theory describes how an agent learns by interacting with its environment [1]. In a typical reinforcement learning paradigm, the agent selects an action and the environment responds by presenting rewards and taking the agent to the next situation, or state. A reinforcement learning algorithm 19 determines how the agent changes its action selection strategy as a result of experience, with the goal of maximizing future rewards. Depending on how algorithms accomplish this goal, they are classified as model-free or model-based [1]. Model-based algorithms acquire beliefs about how the 22 environment generates outcomes in response to their actions and select actions according to their 23 predicted consequences. By contrast, model-free algorithms generate a propensity to perform, in each state of the world, actions that were more rewarding in previous visits to that environmental state. Model-free reinforcement learning algorithms are of considerable interest to behavioral and biological scientists, in part because they offer a compelling account of the phasic activity of dopamine neurons, but also more generally can explain many observed patterns of behavior in human and non-human animals [2, 3, 4, 5, 6, 7]. A key concept in reinforcement learning theory is the environmental state. Typically, empiri-30 cal tests of reinforcement learning algorithms use discrete sensory stimuli to define environmental 31 states. However, there is no theoretical or algorithmic constraint to define the states of the en-32 vironment exclusively by sensory stimuli. State definitions may also include the agent's internal stimuli, such as its memory of past events, thirst or hunger level, or even subjective characteristics such as happiness or sadness [1]. Thus, model-free reinforcement learning might operate over a wide variety of both external and internal factors. Indeed, recent work suggests that model-free learning algorithms can support a large set of cognitive processes and behaviors beyond the formation of habitual response associations with discrete sensory stimuli [8, 9, 10]. For instance, it has been proposed that the model-free system can perform the action of selecting a goal for goal-directed planning [11] or conversely that a modelbased decision can trigger a habitual action sequence [12, 13, 14, 15]. Model-free algorithms have 41 also been suggested to gate working memory [16]. However, many of these important theoretical proposals about model-free algorithms have not been directly tested empirically. Here, we determine the ability of model-free reinforcement learning algorithms to operate over states defined by information held in working memory, an internal state. Specifically, we use an experimental paradigm and computational modeling framework designed to dissociate model-

free from model-based influences on behavior [17] to test if temporally separated sequences of individually uninformative cues can drive model-free learning and behavior. If an agent can store the elements of a temporal sequence in its memory to form a unique and predictive cue and use the memorized information as the state definition, then, theoretically, it can use model-free algorithms to learn the associations between a specific sequence of individually uninformative cues and action outcomes [18]. Our approach has several important facets. First, we use an experimental paradigm that allows us to determine not only if our participants learn from information in working memory, but also whether that learning is supported by model-based or model-free algorithms. Second, the cues in our temporal sequences are individually uninformative; in other words, any single cue in isolation provides no information about which response is correct. It is well-known that modelfree algorithms can shift response associations to the earliest occurring predictor of the correct response in a temporal sequence of informative cues and can integrate predictive information across individual cues. Neither of these mechanisms is possible in our paradigm because the individual cues themselves contain no information about the previous or subsequent cues or which response is best. Temporal pattern learning is a fundamental and early developing human cognitive ability. It allows people to form predictions about what will happen from what has happened and select their actions accordingly. Humans can learn patterns both explicitly and implicitly in the absence of specific instructions or conscious awareness [19]. Moreover, they can do so as early as two months of age [20]. In fact, people identify patterns even when, in reality, no pattern exists [21]. These empirical results together with the theoretical potential for model-free learning to operate over internal stimuli suggest that temporal pattern learning could be supported by model-free processes. However, to date, studies of reinforcement learning and decision making have focused 70 primarily on tasks in which the relevant stimuli are presented simultaneously just prior to or at the time of decision-making, or on implicit motor sequence learning, wherein participants learn a sequence of movements automatically, without full awareness (for instance, 22, 23, 24, 25, 26). Thus, the degree to which model-free processes do in fact operate over temporal sequences or any other information stored in working memory has not yet been directly tested and compared with model-free learning from traditionally employed external, static environmental cues. Here, we directly test whether model-free processes can access and learn from information stored in working memory. We adapted a decision-making paradigm originally developed by Daw et al. [17] that can behaviorally dissociate the influence of model-free and model-based learning on choice. The task was performed by two groups of human participants either in a simultaneous

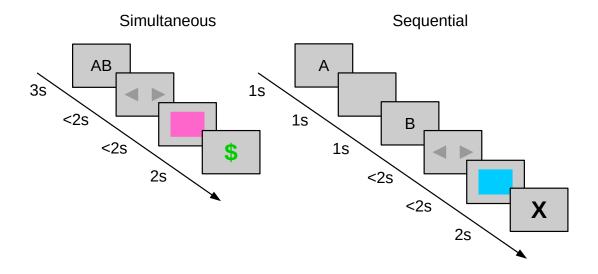


Figure 1: Timelines of events in a trial. The two symbols that represent the initial state are presented simultaneously in the simultaneous condition (left) and separately as a temporal sequence in the sequential condition (right). In this example, AB is the initial state. The simultaneous condition participant goes to the pink final state and receives a reward (signaled by the green \$ symbol). The sequential condition participant goes to the blue final state and does not receive a reward (signaled by the black X symbol).

condition (i.e. static and external), wherein visual stimuli were presented simultaneously, or in a sequential condition, wherein the same visual stimuli were presented as a temporal sequence that required working memory processing. We also simulated a series of experiments in which artificial model-based agents whose behavioral processes we determined were compared to the human participants. Our analysis indicates that our temporal sequences, and consequently information stored in working memory, can trigger model-free learning. Moreover, we found no evidence that the degree to which model-free learning influenced behavior differed between conditions in which environmental states were defined by external sensory stimuli compared to those defined by internal representations stored in working memory. Our findings support the theoretical proposition that model-free learning can act on stimuli internally represented in working memory as well as on external ones.

92 Results

2.1 Determining model-free and model-based influences on choice be havior

- Forty-one young human participants completed a behavioral task adapted from Daw et al. [17].
- ⁹⁶ In our task, participants began each trial in a randomly selected initial state represented by one

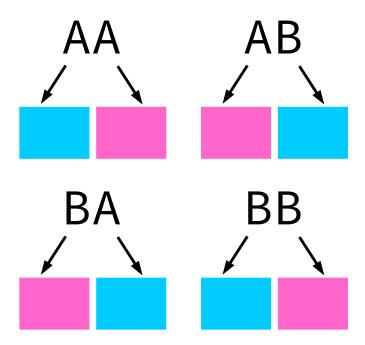


Figure 2: Common state transitions in the behavioral task's model. These graphics highlight the uninformative nature of each single element (i.e. A or B symbols) in the simultaneous or sequential cues. Knowledge of only the first or final element of the combined cue provides no indication of how likely the right and left responses are to lead to a specific state.

of four possible sequences of two symbols: AA, AB, BA, or BB (Figure 1). At this initial state, participants chose one of two possible actions: going left or going right. They were then taken to one of two possible final states, the blue state or the pink state. If they had gone left, they were taken with 0.8 probability to the final state given by the rule $AA \to blue$, $AB \to pink$, $BA \to pink$, 100 $BB \rightarrow blue \text{ or with } 0.2 \text{ probability to the other final state. If they had gone right, they were taken$ 101 with 0.8 probability to the final state not given by the previous rule or with 0.2 probability to the 102 other final state. The common (most probable) transitions between the initial and final states are 103 shown in Figure 2. To predict the final state accurately, participants had to know both elements of the sequence. If they knew only one, the final state might have been either blue or pink with 0.5 probability and they would not be able to perform above chance. This feature is key and separates our work from others in which each element of a sequence is predictive on its own. One of the final states delivered a monetary reward with 0.7 probability and the other with 108 0.3 probability. The optimal strategy was to always select the action that led with 0.8 probability 109

0.3 probability. The optimal strategy was to always select the action that led with 0.8 probability to the final state with 0.7 reward probability. Initially, participants were instructed to learn the common transitions between the initial and final states in the absence of rewards. They were told that each final state might be rewarded with different probabilities, but not what the probabilities were nor that they were fixed. The task comprised 250 trials and participants received the total reward they obtained at the end.

Twenty-one participants were randomly allocated to a simultaneous condition and twenty to a 115 sequential condition (Figure 1). In the simultaneous condition, both symbols that represented the 116 initial state were displayed simultaneously on the screen. In the sequential condition, each symbol 117 was displayed consecutively by itself, as a temporal sequence. The specific objective of this study 118 was to determine if participants in the sequential condition could use states represented in working 119 memory to learn the task in a model-free way or if their learning was necessarily model-based. The 120 simultaneous condition is already known to support model-free learning as well as model-based learning [17, 27, 28, 29, 30]. We thus sought to determine the difference between the standard simultaneous and working-memory dependent sequential conditions. 123

The two-stage task we used can differentiate between model-free and model-based learning because algorithms that implement them make different predictions about how a reward received 125 in a trial impacts a participant's choices in subsequent trials. The SARSA ($\lambda = 1$) model-free 126 algorithm learns this task by strengthening or weakening associations between initial states and 127 initial-state actions depending on whether the action is followed by a reward or not [1]. Therefore, 128 it simply predicts that an initial-state action that resulted in a reward is more likely to be repeated 129 in the next trial with the same initial state [17]. On the other hand, the model-based algorithm considered in this study uses an internal model of the task's structure to determine the initialstate choice that will most likely result in a reward [17]. To this end, it considers which final state, pink or blue, was most frequently rewarded in recent trials and selects the initial-state action, left or right, that will most likely lead there. Therefore, the model-free algorithm predicts that the 134 participant will choose the mostly frequently rewarded action in past trials with the same initial 135 state, while the model-based algorithm predicts that the participant will choose the action with the 136 highest probability of leading to the mostly frequently rewarded *final state* in past trials, regardless 137 of their initial states. 138

The model-free and model-based algorithms thus generate different predictions about the *stay*probability, which is the probability that in the next trial with the same initial state the participant will stay with their previous choice and take the same initial-state action. For instance, if in a given trial whose initial state was AA the participant chose left, and in the next trial with AA as the initial state the participant also chose left, this was considered a stay. The model-free prediction is that the stay probability will increase if the previous trial with the same initial state was rewarded and decrease if it was not. The model-based prediction, on the other hand, depends on the transition structure of the task and how the estimated reward probabilities of the two final states have changed since the previous trial with the same initial state (see Methods for a detailed description of how model-based predictions were calculated).

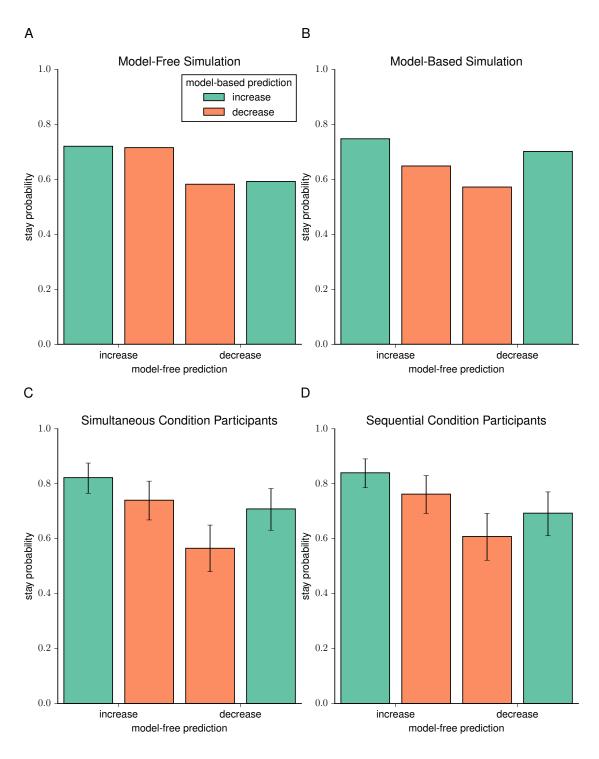


Figure 3: Stay probabilities for simulated agents and human participants as a function of mode-free and model-based predictions. The bar graphs show the choice probabilities derived from the logistic regressions as a function of model-free (separated along the x-axis) and model-based predictions (indicated by the color of the bars). The four panels demonstrate the behavior of $\bf A$) model-free simulations (N=10,000), $\bf B$) model-based simulations (N=10,000), $\bf C$) human participants in the simultaneous condition (N=21) and $\bf D$) human participants in the sequential condition (N=20). Error bars on the data from human participants represent the 95% highest density interval.

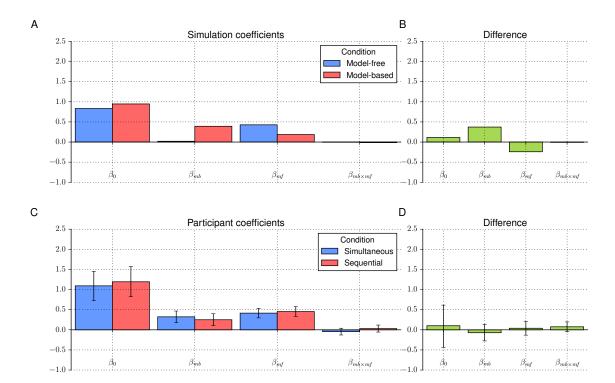


Figure 4: The relative effects of model-free and model-based learning on choice behavior. A) The regression coefficients from a logistic regression on stay vs switch choices for the model-free (blue; N=10,000) and the model-based simulations (purple; N=10,000). B) The difference between model-based and model-free simulation coefficients (i.e. red minus blue from panel A). C) Logistic regression coefficients from the same model used for panel A, but here estimated on choices from the simultaneous (blue; N=21) and sequential condition (purple; N=20) participants. D) The difference between sequential and simultaneous condition participants' coefficients (i.e. red minus blue from panel C). In all panels, β_0 is the logistic regression's intercept, β_{mb} is the model-based coefficient, β_{mf} is the model-free coefficient, and $\beta_{mb \times mf}$ is the coefficient of the interaction between the model-based and model-free effects. Error bars on the data from human participants represent the 95% highest density interval.

We simulated model-free and model-based agents performing this task for comparison with the 149 behavior of human participants in each condition. In all cases, we analyzed the data using Bayesian 150 hierarchical logistic regression analyses. The correspondence between theoretical predictions of the 151 model-free and model-based algorithms and choices of the simulated agents are shown in the top row of Figure 3. The correspondence between theoretical predictions of the model-free and modelbased algorithms and choices of the human participants in each experimental condition are shown in the bottom row of Figure 3. 155 In addition to examining the stay choice probabilities, we directly tested the degree to which the 156 human participants' and simulated agents' choices were influenced by model-based and model-free 157 signals. The coefficients of these logistic regression analyses are shown in Figure 4. The positive 158 value of the intercept β_0 indicates that the stay probabilities tended to be above 0.5, i.e., simulated 159 agents and human participants were more likely to repeat their previous choice than switch to the

other choice in the next trial with the same initial state. This is also visible in the stay probabilities 161 shown in Figure 3. The coefficients for the regressions on the simulated agents' choices show the 162 expected pattern with the model-free and model-based coefficients primarily determining behavior 163 for the model-free and model-based agents, respectively (Figure 4A) and differing substantially 164 between agent types (Figure 4C). 165 In the human participants, behavior was influenced by both model-based and model-free processes regardless of whether the states were defined by external sensory cues or internal workingmemory representations. The model-based and model-free coefficients, β_{mb} and β_{mf} , were positive for both the simultaneous and sequential conditions with 0.999 posterior probability (Figure 4B). 169 The model-based coefficient was 0.32 (95\% highest density interval [0.18, 0.47]) for the simultaneous condition and 0.25 (95% HDI [0.10, 0.40]) for the sequential condition, and the model-free coefficient 171 was 0.41 (95% HDI [0.30, 0.54]) for the simultaneous condition and 0.45 (95% HDI [0.33, 0.58]) for 172 the sequential condition. The differences between the sequential and simultaneous conditions were 173 -0.07 (95% HDI [-0.28, 0.14]) for the model-based coefficient and 0.04 (95% HDI [-0.13, 0.21]) 174 for the model-free coefficient. The posterior probability that the model-free coefficient is smaller in 175 the sequential group than in the simultaneous group is 0.32, and the posterior probability that the model-based coefficient is greater in the sequential group than in the simultaneous group is 0.24 (Figure 4D). Thus, we find no evidence that sequentially presented, working-memory-dependent state cues shift the balance of model-based and model-free effects on choice behavior compared to traditional, static, external cues. 180 The model-based predictions in our two-stage decision task differ from those reported in pre-181 vious work using similar tasks. In the version of the two-stage task used by Daw et al. [17], the 182 model-based prediction is that the heights of the two orange bars should be (nearly) equal to one 183 another and that the heights of the two green bars should be (nearly) equal as well (note, that the 184 precise prediction depends on the exact parameterization of the model). However, in our task the model-based prediction includes a reward effect. Consequently, we find that the stay probabilities in the model-based agent simulations are influenced by the outcome of the most recent trial with the same initial state as can be seen in the differences in magnitude between the two inner, orange bars as well as the two outer, green bars in Figure 3B. Specifically, if the previous matching-state trial was rewarded, then the stay probabilities are greater than if it was not rewarded. This reward 190 effect in the model-based choices is similar to a model-free effect, but not identical because the 191 model-based value updating procedure incorporates the transition probabilities while the model-192 free algorithm does not. However, the reward-effect does lead to model-free-like choice patterns 193

in the data that result in a small, but significant model-free coefficient in the logistic regressions

on model-based agents' choices (Figure 4A). Therefore, small model-free-like patterns in the stay
probabilities do not necessarily indicate the influence of model-free learning, because we know the
model-based agents do not use this learning algorithm. We directly address the potential for spurious effects mimicking the influence of a model-free algorithm in our human participants in the
working-memory-dependent sequential condition in the following paragraphs.

2.2 Direct comparisons between human participants and simulated modelbased agents

Our goal was to test the hypothesis that working-memory-dependent, temporal patterns can be learned through a model-free process in humans. Given that our model-based simulations showed a reward effect that shared some properties with a model-free learning process, we sought to determine if the same results obtained by the human participants in the sequential condition, including the estimated model-free effect, could have been generated through the use of a model-based algorithm alone. Despite the fact that we find no evidence for differences in behavior between participants in the sequential and simultaneous conditions, this additional test is important because as Figures 3 and 4 show, the model-based simulated agents exhibited behavior that mimicked a model-free effect even though they operated solely on the basis of a model-based algorithm by design.

This raises the question, could purely model-based agents exhibit a model-free effect as large as the participants in the sequential condition? To this end, we fitted the model-based algorithm to the sequential condition results using a Bayesian hierarchical model. We then simulated 10,000 experiments in which we first created behavior for 20 simulated model-based agents (replacing the 20 sequential condition human participants) and then combined those data with that from the 21 human participants in the simultaneous condition and estimated the same hierarchical logistic regression on stay/switch choices described above and summarized in Figure 4. These 10,000 regressions give us a measure of what the coefficients in the sequential condition participants would be if they were purely model-based.

We found that while the simulated purely-model-based (PMB) agents showed a level of model-based influence comparable to participants in the sequential condition, the degree of model-free influence in PMB agents was substantially lower. The mean value of the model-based coefficient, β_{mb} , was 0.23 (95% HDI [0.05, 0.49]), which, as expected, is very close to the mean value of 0.25 from the sequential participants' behavior. Likewise, the mean difference across simulations between the PMB agents and the participants in the simultaneous condition for β_{mb} was -0.09

(95% HDI [-0.28, 0.15]), similar to the -0.07 value for the difference between the sequential and simultaneous conditions in humans. In contrast, the mean value of the model-free coefficient, β_{mf} , 228 in the simulated agents was 0.15 (95% HDI [0.07, 0.23]), and it was smaller than 0.45, the mean value obtained for the sequential condition, in more than 99.9% (in fact all 10,000) of the simulated 230 experiments. Furthermore, the mean difference between the PMB agents and the participants in 231 the simultaneous condition for β_{mf} (i.e. the difference corresponding to Figure 4D) was -0.26 (95%) 232 $\mathrm{HDI}\ [-0.34, -0.18]),\ \mathrm{and}\ \mathrm{more\ than}\ 99.9\%\ (\mathrm{in\ fact\ all}\ 10,000)\ \mathrm{of\ simulated}\ \mathrm{experiments\ yielded}$ a difference for β_{mf} smaller than 0.04, the observed difference between human participants in the sequential and simultaneous conditions. In summary, the model-free coefficient observed in the 235 sequential condition is three times the size one would expect to see from a purely model-based agent, which strongly suggests that the observed effect is due to a true model-free influence and 237 not mimicked by the reward-effect. 238

3 Discussion

In this study, we empirically tested the hypothesis that human participants can develop model-free associations between temporal sequences of stimuli stored in working memory and a motor response. To that end, we developed a behavioral task based on a previous decision-making paradigm that can determine the model-free and model-based influences on choice [17]. The participants in the simultaneous condition performed this task with the two visual symbols presented together simul-244 taneously and those in the sequential condition performed it with the same two visual symbols presented as a temporal sequence that had to be held in working memory. The model-free effect estimated for the sequential condition was similar to the one estimated for the simultaneous condition and higher than that predicted by a purely model-based algorithm. Our results suggest that both model-based and model-free learning influenced the participants' choices whether they saw the entire set of stimuli at once or saw each stimulus by itself at separate times. Our study thus provides experimental support to proposed model-free algorithms of temporal pattern learning [18] and the view that model-free learning and habituation can be triggered by external or internal stimuli [8, 9, 10] 253 A key element of our experimental paradigm is that the individual symbols within each temporal 254 sequence convey no information about the best response in isolation. This fact rules out the 255 possibility that the sequential condition's model-free effect is due to an association between a single symbol in the sequence and a response rather than one between the entire sequence and a response. Each sequence element is completely uninformative by itself: it cannot predict reward delivery above chance. Therefore, the task cannot be learned by simple stimulus-response associations with individual symbols in the temporal sequence.

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Model-free learning processes support habit formation, and thus our results suggest that stim-261 uli stored in working memory can trigger habitual responses. To the best of our knowledge, no 262 study has yet tested for habituation to temporal sequences directly, using procedures such as con-263 tingency degradation or outcome devaluation. Although two-stage choice tasks similar to the one we use here have been reported to share construct validity with outcome devaluation measures of habitual responding [31], direct tests of outcome devaluation and contingency degradation following temporal sequence learning are still needed. If such additional tests show positive evidence for habituation, this would indicate that habits can be triggered by internally generated stimuli as well as by external ones. Conversely, if no evidence is found for habituation to temporal sequences, this 269 would indicate that model-free learning processes can use internal stimuli, but do not necessarily 270 produce habits. Experimental evidence already suggests that habits are not exclusively learned in 271 a model-free way [32]; it may also be true that habituation involves additional mechanisms beyond 272 the model-free caching of state-action-reward contingencies. Our study also raises the question 273 of which neural systems are commonly versus distinctly recruited in order to learn from stimuli represented in working memory (e.g. temporal sequences) compared to purely external stimuli in a reinforcement learning task. While numerous studies have investigated the neural systems mediating reinforcement learning over externally presented stimuli (see 33 for a review), to date, only a single study has investigated brain activity involved in temporal pattern learning using fMRI [21]. However, the sequence of events in that study was random, and any pattern that occurred was 279 spurious. Moreover, participants were required to respond to the stimuli instead of predicting 280 them, and might thus be implicitly learning a motor sequence. It remains to be determined what 281 brain regions support explicit learning from temporal sequences, or other stimuli held in working 282 memory, and to what degree these systems overlap with those shown to underlie learning from external environmental cues. In conclusion, we have presented experimental evidence that temporal pattern learning, and consequently learning from internal stimuli held in working memory, can be model-free. Our study has helped delineate the contexts that support model-free learning—a subject of current debate. Temporal pattern learning is a fundamental aspect of human cognition and model-free

Our study has helped delineate the contexts that support model-free learning—a subject of current debate. Temporal pattern learning is a fundamental aspect of human cognition and model-free
learning and habit formation are subjects of immediate relevance for research on typical learning
as well as for the study of neuropsychiatric disorders ranging from addiction, obsessive-compulsive
disorder, and Tourette syndrome to anxiety disorders and major depression [34]. It is thus important to continue investigating temporal pattern learning, including whether the model-free learning

of temporal sequences produces outcome-insensitive, habitual responses and how such learning is implemented in the brain.

Methods $\mathbf{4}$

Participants 4.1

Forty-one healthy young adults participated in the experiment, 21 (13 female) randomly assigned 297 by a random number generator to the simultaneous condition and 20 (13 female) to the sequential condition. The inclusion criterion was speaking English and no participants were excluded from the analysis. The sample size was chosen by the precision for research planning method [35, 36], by comparing the estimated differences between participant groups in the logistic regression analysis with those between model-free and model-based simulated agents. The experiment was conducted in accordance with the Zurich Cantonal Ethics Commission's 303 norms for conducting research with human participants, and all participants gave written informed consent.

4.2Task

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The task's state transition model defines four possible initial states, which were randomly selected with uniform distribution in each trial and represented by four different stimuli, each composed of two symbols: AA, AB, BA, or BB. At the initial state, two actions were available to the participant: pressing the left or the right arrow keys. By pressing one of the keys, the participant was taken 310 to a final state, which might be either the blue state or the pink state. If the left arrow key was 311 pressed, the participant was taken to the final state given by the rule $AA \rightarrow blue$, $AB \rightarrow pink$, 312 $BA \rightarrow pink$, $BB \rightarrow blue$ with 0.8 probability or to the other state with 0.2 probability; if the right arrow key was pressed, the participant was taken to the final state not given by the previous rule with 0.8 probability or to the other state with 0.2 probability. There was no choice of action at the final state, but participants were required to make a button press to potentially earn the reward. Each final state was rewarded according to an associated probability, which was 0.7 for one state and 0.3 for the other. The highest reward probability was associated with the blue state for half 318 of the participants and to the pink state for the other half. Participants were told that each final 319 state might be rewarded with different probabilities, but not what the probabilities were nor that 320 they were fixed. 321

In contrast with our task design, in which the final states' reward probabilities were fixed, in

the original task design proposed by Daw et al. [17] the reward probabilities slowly drifted over time, because those authors were interested in the trade-off between model-based and model-free mechanisms, which is assumed to happen on the basis of their relative uncertainties. In this study we were interested instead in testing if model-free learning of temporal patterns is possible and keeping the task environment stable helps making the model-free associations stronger and more likely to influence choice [37, 38].

Participants were initially instructed to learn the common transitions between the initial and the final states in the absence of reward. Participants then performed the task defined by the model above in the simultaneous or sequential condition. Half of the participants were randomly allocated 331 to the simultaneous condition and the other half to the sequential condition (Figure 1). In the simultaneous condition, both symbols that define the initial state were displayed simultaneously 333 on the screen for 3 seconds. In the sequential condition, each symbol is an element of a sequence 334 and each element was presented for 1 second, but never conjointly, and with a 1-second delay 335 (blank screen) in between. Two triangles pointing left and right then appeared and the participant 336 was given 2 seconds to make a decision about whether to press the left or the right arrow keys; 337 if they did not press any keys, the word SLOW was displayed for 1 second, and the trial was aborted and omitted from analysis. A blue or pink rectangle appeared immediately afterward, indicating the final state. The participant then pressed the up-arrow key and, if the final state was rewarded, a green dollar sign appeared on the screen for 2 seconds; otherwise, a black X appeared for 2 seconds. The task comprised 250 trials, with a break every 50 trials, and participants received the total reward they obtained by the end of the task (0.18 CHF per reward).

4.3 Model-free algorithm

The SARSA model-free algorithm with replacing eligibility traces [1, 17] was used to simulate model-free learning agents. For each action a and state s, it estimated the value Q(s,a) of performing that action in that state. The task's initial states s_i were AA, AB, BA, and BB, and the actions a_i available at the initial states were left and right. The final states were pink and blue, and the only action a_f available at those states was up. The initial value of Q(s,a) for every state and action was 0.5. In each trial t, the simulated agent at the initial state s_i chose left as its initial-state action with probability p_{left} and right with probability $1 - p_{left}$, according to the following equation:

$$p_{left} = \frac{1}{1 + e^{-\beta[Q(s_i, left) - Q(s_i, right)]}},\tag{1}$$

where $\beta > 0$ is an inverse temperature parameter that determines the algorithm's propensity to choose the option with the highest estimated value. After the final state s_f was observed and a reward $r \in \{0,1\}$ was received, state-action values were updated according to the following equations:

$$Q(s_i, a_i) = (1 - \alpha_1)Q(s_i, a_i) + \alpha_1 Q(s_f, up) + \alpha_1 \lambda [r - Q(s_f, up)], \tag{2}$$

$$Q(s_f, up) = (1 - \alpha_2)Q(s_f, up) + \alpha_2 r, \tag{3}$$

where $0 \le \alpha_1, \alpha_2, \lambda \le 1$ are parameters: α_1 is the initial learning rate, α_2 is the final learning rate, and λ is the eligibility trace [1, 17].

In the special case where $\lambda = 1$, the update of initial state-action values becomes

$$Q(s_i, a_i) = (1 - \alpha_1)Q(s_i, a_i) + \alpha_1 r,$$
(4)

that is, the estimated values of choosing *left* and *right* in each initial state are updated independently of the final state's estimated value. Thus, SARSA ($\lambda = 1$) ignores the identity of the final state when making initial-state decisions, and an initial-state action that resulted in a reward will necessarily lead to a higher stay probability when the respective initial state recurs. This is true even if the action will probably lead to the final state with the lowest value.

365 4.4 Model-based algorithm

In simulations of model-based agents [17], values were assigned to initial-state actions and to final states. The value V of a final state $s \in \{pink, blue\}$ in the first trial t = 1 was V(s, 1) = 0.5. An initial-state choice $c \in \{left, right\}$ in trial t had a value V given by

$$V(c,t) = \Pr(c \to pink)V(pink,t) + \Pr(c \to blue)V(blue,t), \tag{5}$$

where $Pr(c \to s)$ is the probability that choosing c will lead to the final state s, which might be 0.8 or 0.2 according to the task's transition model. The value of an initial-state choice can thus be understood as the expected value of the final state the agent will go to after making that choice.

If V(left,t) > V(right,t), the agent was more likely to choose left and vice-versa.

In each trial t, the agent's initial state action was left with probability p_{left} and right with

probability $1 - p_{left}$, given by

$$p_{left} = \frac{1}{1 + e^{-\beta[V(left,t) - V(right,t)]}},$$
(6)

where β is an inverse temperature parameter. After the agent made its initial-state choice and went to a final state s, that final state's value was updated according to the following equation:

$$V(s,t+1) = (1-\alpha)V(s,t) + \alpha r(t), \tag{7}$$

where $r(t) \in \{0,1\}$ indicates if the agent received a reward and $0 \le \alpha \le 1$ is a learning-rate parameter of the model. The value of a final state is thus the moving average of the rewards received in that state.

• 4.4.1 Model-based predictions

Our method of determining model-based predictions for the stay probability was different from
the method used by Daw et al. [17]. In that study, there was only one initial state and the modelbased and model-free algorithms predicted how the stay probability would change from one trial
to the next. The present study's task, on the other hand, had four initial states and the model-free
algorithm made predictions about how rewards would affect the participant's choices from one trial
to the next trial with the same initial state, which is not necessarily the next trial. We therefore
had to devise an alternative method of calculating the model-based predictions.

Our method relies directly on how the model-based algorithm estimates the reward probabilities of the initial-state choices, which either increase or decrease from one trial to the next with the same initial state depending on what happened, and was therefore learned about reward probabilities, in the intervening trials. If the participant's initial-state choice in a trial t_1 was left, for instance, the model-based prediction was that in a future trial t_2 with the same initial state the stay probability 392 should increase if $V(left, t_2) - V(right, t_2) > V(left, t_1) - V(right, t_1)$ and decrease otherwise. The 393 model-based predictions depended on the parameter α . The data analysis results were obtained by 394 setting $\alpha = 0.4$, as this was the mean value that Daw et al. [17] found in their experiment by fitting 395 to their experimental data an expanded reinforcement learning model that combines model-based 396 and model-free learning. For comparison, we tried other values for α , but the analysis results did not vary significantly.

Data analysis by logistic regression 4.5

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For each human participant or simulated agent, we calculated the stay probability as a function of model-free and model-based predictions. In each trial, if the human participant or simulated agent chose an action that was the same as that chosen in the previous trial with the same initial state, this was considered a stay. The four initial-state choices following the first occurrence of an initial state were not analyzed. The remaining initial-state choices were coded as the random variable yand classified as a stay (y = 1) or not a stay (y = 0). 405 We then analyzed the resulting data using a hierarchical logistic regression model whose parameters were estimated through Bayesian computational methods. The dependent variable was 407 p_{stay} , the stay probability for a given trial, and the independent variables were x_{mf} , which indi-408 cated what the model-free algorithm predicted about p_{stay} (+1 if it predicted an increase, -1 if it 409 predicted a decrease), x_{mb} , which indicated what the model-based algorithm predicted about p_{stay} 410 (+1) if it predicted an increase, -1 if it predicted a decrease), and the interaction between the two. Thus, for each participant, we determined a four-dimensional vector $\vec{\beta}$ whose components were the β coefficients of the following equation:

$$p_{\text{stay}} = \frac{1}{1 + \exp[-(\beta_0 + \beta_{mb}x_{mb} + \beta_{mf}x_{mf} + \beta_{mb \times mf}x_{mf}x_{mb})]}.$$
 (8)

The distribution of y was Bernoulli (p_{stay}) . The distribution of the $\vec{\beta}$ vectors was $\mathcal{N}(\vec{\mu_c}, \vec{\sigma^2})$ if the participant was in the simultaneous condition and $\mathcal{N}(\vec{\mu_e}, \vec{\sigma^2})$ if the participant was in the 415 sequential condition; in other words, the group means for each $\vec{\beta}$ were allowed to vary independently. The parameters of the $\vec{\beta}$ distribution were given vague prior distributions based on preliminary 417 analyses—the $\vec{\mu}$ vectors' components were given a $\mathcal{N}(\mu=0,\sigma^2=25)$ prior, and the $\vec{\sigma^2}$ vector's 418 components were given a Half-normal(0,25) prior. Other vague prior distributions for the model 419 parameters were tested and the results did not change significantly. To obtain parameter estimates from the model's posterior distribution, we coded the model 421 into the Stan modeling language version 2.14.0 [39, 40] and used the PyStan Python package [41] 422 to obtain 100,000 samples of the joint posterior distribution from four chains of length 50,000 (warmup 25,000). Convergence of the chains was indicated by $\hat{R} \approx 1.0$ for all parameters. The minimum effective sample size for the parameters of interest $\vec{\mu_c}$, $\vec{\mu_e}$, and $\vec{\mu_e} - \vec{\mu_c}$ was 31785.

Fitting of the algorithms to experimental data

For comparison with the participant data, we fitted the SARSA model-free algorithm and the model-based algorithm to the experimental data and generated replicated data using the fitted parameters. The parameters were obtained by fitting both algorithms to all participants (to generate

Figures 3 and 4) and the model-based algorithm to the participants in the sequential condition (to 430 perform the simulated experiments). To that end, we used a Bayesian hierarchical model, which 431 allowed us to pool data from all participants to improve individual parameter estimates. 432 The parameters of the model-based algorithm for the ith participant were α^i and β^i . They 433 were given a Beta (a_{α}, b_{α}) and $\ln \mathcal{N}(\mu_{\beta}, \sigma_{\beta}^2)$ prior distributions respectively. The hyperparameters 434 a_{α} and b_{α} were themselves given a noninformative Half-normal $(0,10^4)$ prior and the hyperparameters μ_{β} and σ_{β}^2 were given a noninformative $\mathcal{N}(0, 10^4)$ and Half-normal $(0, 10^4)$ priors respectively. The parameters of the model-free algorithm for the ith participant were α_1^i , α_2^i , λ^i , and 437 β^i . They were given a Beta $(a_{\alpha_1}, b_{\alpha_1})$, Beta $(a_{\alpha_2}, b_{\alpha_1})$, Beta $(a_{\lambda}, b_{\lambda})$ and $\ln \mathcal{N}(\mu_{\beta}, \sigma_{\beta}^2)$ prior distributions respectively. The hyperparameters a_{α_1} , a_{α_2} , a_{λ} , b_{α_1} , b_{α_2} , and b_{λ} were themselves given a 439 noninformative Half-normal $(0, 10^4)$ prior and the hyperparameters μ_{β} and σ_{β}^2 were given a noninformative $\mathcal{N}(0,10^4)$ and Half-normal $(0,10^4)$ priors respectively. We then coded the models into 441 the Stan modeling language version 2.14.0 [39, 40] and used the PyStan Python package [41] to obtain 50,000 samples of the joint posterior distribution from one chain of length 60,000 (warmup 10,000). Convergence of the chains was indicated by $\hat{R} \approx 1.0$ for all parameters. The minimum effective sample size was 1481 for all hyperparameters. The results were used to generate Figures 2 and 3.

4.7 Simulated experiments

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Given that this study's aim was to determine if working memory-dependent temporal pattern learning is necessarily model-based or can be model-free, we sought to determine if the results obtained for the sequential condition could have been generated by the model-based algorithm. To this end, we simulated 10,000 experiments wherein, in each simulated experiment, the 21 participants in the simultaneous condition were compared to a different group of 20 simulated purely-model-based agents (as replacements for the 20 human participants in the sequential condition). 453 The model-based algorithm was first fitted to the sequential condition results using the Bayesian 454 hierarchical method described above to obtain 200,000 samples of the posterior distribution from 455 four chains of length 60,000 (warmup 10,000). Convergence of the chains was indicated by $\hat{R} \approx$ 456 1.0 for all parameters. The minimum effective sample size was 16467 for all hyperparameters. 457 For each simulated experiment, a point was randomly selected from the posterior distribution of hyperparameters $(a_{\alpha}, b_{\alpha}, \mu_{\beta}, \sigma_{\beta})$ and 20 sets of algorithm parameters (α, β) were randomly generated using the selected values, i.e. $\alpha \sim \text{Beta}(a_{\alpha}, b_{\alpha}), \beta \sim \ln \mathcal{N}(\mu_{\beta}, \sigma_{\beta}^2)$. For each (α, β) parameter set, the model-based algorithm was run for 250 trials of the experimental task to generate

- results for a simulated purely-model-based agent. These simulated agents were then compared with
- the actual participants in the simultaneous condition using the same logistic regression analysis
- described above, except that, for computational efficiency, only 600 samples from one chain of 800
- samples (warmup 200) was obtained from the posterior distribution.
- The entire analysis procedure was replicated several times with differing parameter values and
- 467 prior distributions to ensure that the results and conclusions remained the same under a wide set
- of assumptions. In all cases, the results were nearly identical and supported the same conclusions.

469 4.8 Code and data availability

470 All the computer code and behavioral data used in this study are available at https://github.com/carolfs/mf wm

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475 6 Author contributions

- 476 C.F.S. and T.A.H. designed the study; C.F.S. and Y.Y. conducted the behavioral experiment;
- 477 C.F.S. performed the simulations and analyzed the data with input from T.A.H.; C.F.S., Y.Y.,
- and T.A.H. wrote the manuscript.

7 Competing financial interests

The authors declare no competing financial interests.

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