

Exploring Replay

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The normative theory of Mattar and Daw [24] suggests that hippocampal replay is a neural substrate for model-based planning. According to the theory, replay is an optimised mechanism by which information from a generative model of the world trains a model-free or reactive decision policy during offline behavioural states [32, 27]. This couples the speed of (online) model-free control with the statistical efficiency and flexibility of (offline) model-based control. However, Mattar and Daw [24]’s analysis applies when the model is known, whereas the main challenge of reinforcement learning problems is to learn what to do in the face of ignorance about the model [19, 26]. Such ignorance requires a delicate balance between exploration and exploitation when making choices. Here, we examine how replay might play a role in a form of approximately optimal exploration. We extend the theory of Mattar and Daw [24] and derive testable predictions for the patterns of exploratory replay choices one should expect, using a paradigmatic spatial navigation task as an example. Our predictions show the importance of sequence replay, and thus license a range of new experimental paradigms that should further our understanding of offline processing.

Mattar and Daw [24] consider replay as the offline activation of remembered or simulated experiences that provide additional training to model-free values learnt online. Each individual replay experience updates the model-free estimate of the long-run value of performing an action at a state in the task. Since these model-free action values determine the subject’s choices, each replay update can thus improve online behaviour. Mattar and Daw [24] show that the choice of replay state and action (which could be distal to the current location of the subject [17]) that maximizes the improvement that the subject can expect is determined by two factors: Gain and Need.

The Gain of a replay update is the local improvement in value expected for the change in policy engendered by the update. This quantifies the extra reward the subject expects to receive from the newly changed policy at the update location. By contrast, Need is a global measure of the relevance of the update state (the strength of the successor representation there [9]) under the old policy. Thus, if Need is low at the potential update state, then the estimated priority for all updates at that state will be low, since the subject does not expect to visit the update state often, and so would not benefit greatly in the long run from that policy update.

Replay in Mattar and Daw [24] allows information about reward to be propagated efficiently along sequences of actions that are known to lead to it. This form of model inversion helps a subject become proficient at exploiting its knowledge. However, subjects are typically at least partially ignorant about their environments, because of incomplete initial information, forgetting or unsignalled changes. Sufficient exploration is thus required to gain new knowledge that can subsequently be exploited (Fig 1); although the resulting potential benefits of exploration must be balanced against the costs of exploring rather than exploiting existing knowledge. The original rationale of the DYNA algorithm [32] that helped inspire Mattar and Daw [24] was that offline computations could arrange for good exploration. Here, we study how replay can play this role.

There are two coarse flavours of exploration: undirected and directed [36], along with many heuristic and approximate versions of the latter. Undirected exploration comes from introducing

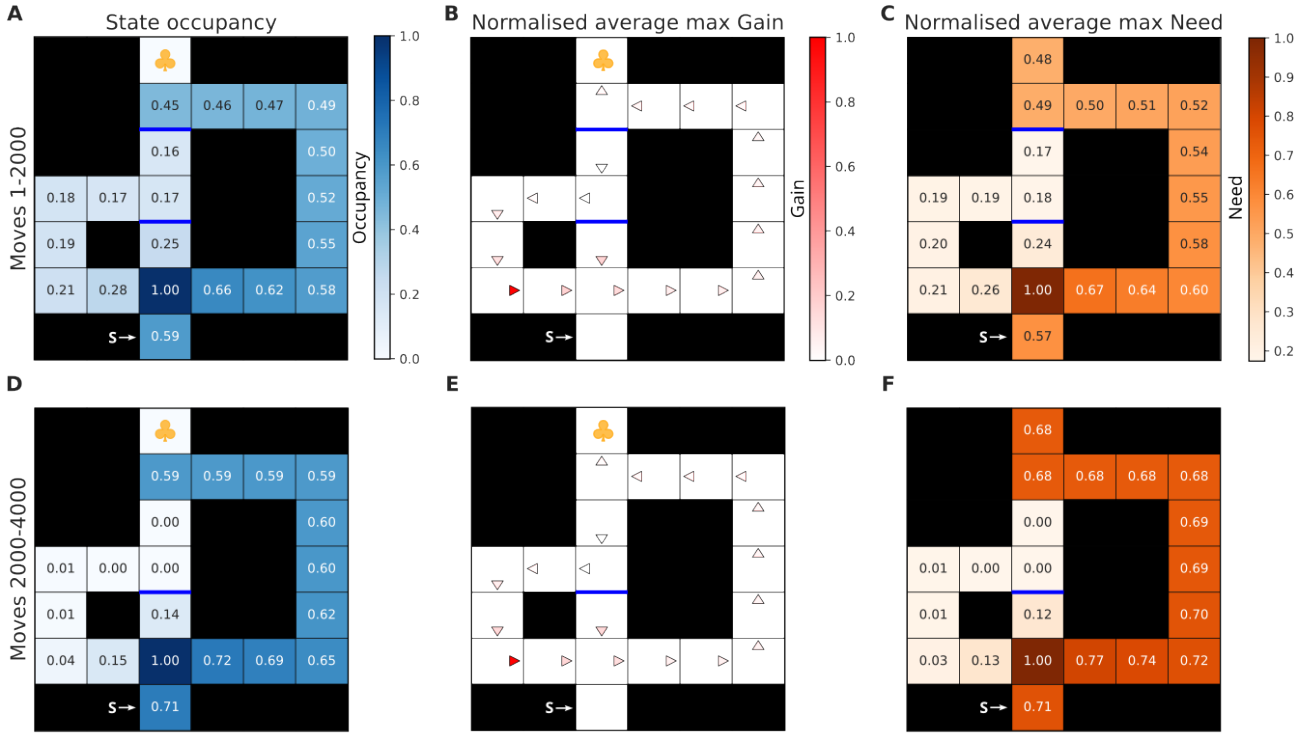


Figure 1: Exploitative replay can result in suboptimal behaviour. A) Normalised state occupancy of the subject during first 2000 moves of exploration and learning in the environment. The start state is located at the bottom (shown with the white letter 'S') and the goal state is shown with the yellow clover. The barriers are shown as opaque blue lines. Importantly, all barriers were not bidirectional, and hence could only be learnt about when attempted from an adjacent state from below. All states were visited by the subject, including those besides the barriers (darker blue corresponds to higher occupancy). B) Normalised maximal Gain that the subject estimated for the replay of each action (depicted with triangles), averaged across all 2000 moves. Only those actions for which the Gain was estimated to be positive are shown (darker red corresponds to higher Gain). The actions which the subject would replay yielded a more exploitative policy which helped the subject acquire reward at a higher rate. C) Normalised maximal Need for each state that the subject estimated, also averaged over those same 2000 moves. All values were additionally averaged over 10 simulations. Darker orange corresponds to higher Need. D-F) Same as (A-C) but for additional 2000 moves during which the top barrier was removed. Note that the estimated Gain did not change. Moreover, the state occupancy profile in D), as well as the estimated Need in F) highlight how the subject's behaviour reduced to pure exploitation. Because of the environmental change, however, this behaviour was rendered suboptimal due to the existence of a shorter path that the subject did not discover.

stochasticity into choice. Although sometimes effective [8], it is typically suboptimal. Rather, exploration should be directed to reducing the uncertainty about which actions in the environment are ultimately best [12]. One standard heuristic [32] (see also [1]) is to add a form of notional exploration bonus to the outcome of actions whose consequences are uncertain.

Optimal exploration generates bonuses by maintaining probabilistically-correct beliefs about the environment and accounting carefully for the immediate and longer term consequences of resolving the implied uncertainty [14, 11]. This amounts to performing regular optimal control, but in what is known as a belief-state decision problem in which the physical state of the subject in the environment is augmented by the subject's beliefs about the environment (in our later spatial case, how likely it thinks barriers are to have been removed). Such careful accounting is radically computationally intractable, for instance because the space of all possible beliefs is continuous, implying that the optimal policy can be very complex. We show how exploratory forms of Gain and Need (which extend the original notions to the belief-state decision problem) can generalize the use of replay to realize a limited version of this accounting offline.

Most studies of hippocampal replay have focused on navigation tasks. We therefore sought to make testable predictions for exploratory replay in a rich spatial environment inspired by Tolman [34] (and report in the supplement similar results on the simpler, theoretically more tractable, case of multi-arm bandit problems). Our maze comprises three corridors which merge onto the common

stem leading to the goal location (Fig 1). Those corridors differ in length, and thus an optimal reward-maximising agent (and rats [34]) would prefer the shortest corridor. However, either just the shortest, or all but the longest, path might possibly be blocked by barriers. The accompanying uncertainty provides the motivation for exploration.

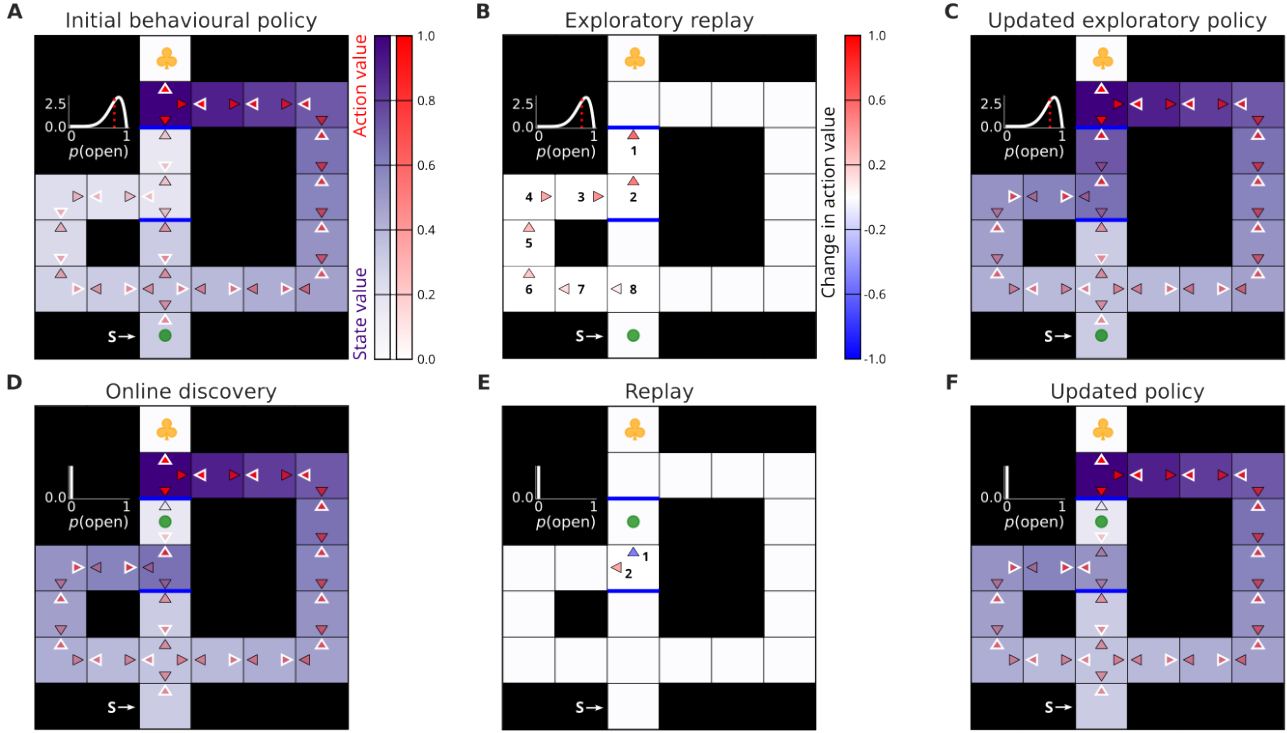


Figure 2: Exploratory replay leads to online discoveries, but potentially inadequate promulgation. A) Prior state of knowledge of the subject. The intensity of the (red-scale) colour of each action arrow shows the respective model-free Q -values. Collectively, the action values represent the subject’s model-free behavioural policy (i.e., the subject is more likely to choose actions with higher estimated Q -values – which at each state are highlighted with white outlines). Similarly, the states are coloured according to the maximal model-free Q -value at each state (which corresponds to state values, shown in purple). The inset next to the top barrier indicates the subject’s prior belief about its presence (for the other barrier, the subject was certain that the path was blocked). The red dotted line in the inset shows the expected probability that the barrier is absent. The subject itself (green dot) is located at the start state. The goal state with reward is denoted with the yellow clover. B) Changes in the subject’s model-free policy occasioned by exploratory replay updates. The numbers next to each action arrow indicate the order in which the replay updates were executed. C) New model-free policy which resulted from exploratory replay updates in B). Note how the action values now indicate that the subject should go towards the upper barrier (highlighted with white outlines). D) After pursuing the exploratory policy, the subject attempted to cross the top barrier; unfortunately, the barrier was found to be present – this is indicated by both the subject’s model-free Q -value associated with that action which was learnt online, as well as its new belief. E-F) Same as in B-C) but after the online discovery of the present barrier in D). The first replay choice of the subject correctly propagated the negative value of the present barrier to the immediately preceding state. However, as opposed to propagating this information deeper towards the start state, and hence correcting the exploratory policy in the light of the new information, the next replay choice of the subject made it more likely to visit an adjacent state which still contained the previously propagated exploration bonus, and hence had a high value that was erroneous given the subject’s new knowledge.

For exploratory Gain: suppose that the subject is at a physical location just next to a barrier and is contemplating the action that might cross over and get close to the goal. To the extent the agent is uncertain that the barrier is absent, the action will fail, leading to the belief that the barrier is there, and no Gain. However, if the agent is uncertain that the barrier is present, this action might succeed, leaving the subject in a new location, and with a new belief that the barrier is absent. This imagined outcome is associated with high Gain, because of the implied shortcut estimated, in our account, based on the high model-free values for the new location.

However, exploratory Need suffers from a chicken-and-egg problem, in that if the subject adopts the purely exploitative policy of the known-to-be-open longest path, then the Need for the potential shortcut transition is zero (as the state next to the barrier is not visited). For simplicity, we make

the approximation of including stochasticity in the subject’s behavioural policy (for instance, in the form of undirected exploration) such that Need is strictly positive for all possible belief states. This is achieved through applying a softmax behavioural policy [8].

The calculations of exploratory Gain and Need differ crucially from Mattar and Daw [24] in terms of generalization. Individual physical locations (such as those next to barriers) can be visited with different beliefs about the environment. Importantly, discovering that a barrier is present/absent is information for all belief states associated with that barrier. This requires the subject to generalise the benefit of potential discoveries across multiple belief states.

As mentioned earlier, optimally accounting for the evolution of the subject’s beliefs is woefully intractable. We therefore incorporated an approximation [10] for the estimation of exploratory Need. The subject optimally tracks how its belief will evolve up to a limited planning horizon beyond which the residual uncertainty remains fixed. This means that the subject still maintains its subjective uncertainty about the possible futures (unlike other potential approximations [6]); however, it assumes that no new knowledge can be acquired or environmental changes take place beyond its planning horizon.

We simulated behaviour in the Tolman maze and examined the replay patterns produced as a result of uncertainty about the presence of the upper barrier (Fig 2). Note that the subject has to choose which arm to pursue at a decision point remote from the potential barrier location. There is thus substantial cost for exploration: the subject has to have sufficient belief that the barrier is open – otherwise the potential benefit of exploration (i.e., discovering a shortcut) would not exceed the cost of deviating from the current behavioural policy (i.e., its current reward rate) [28].

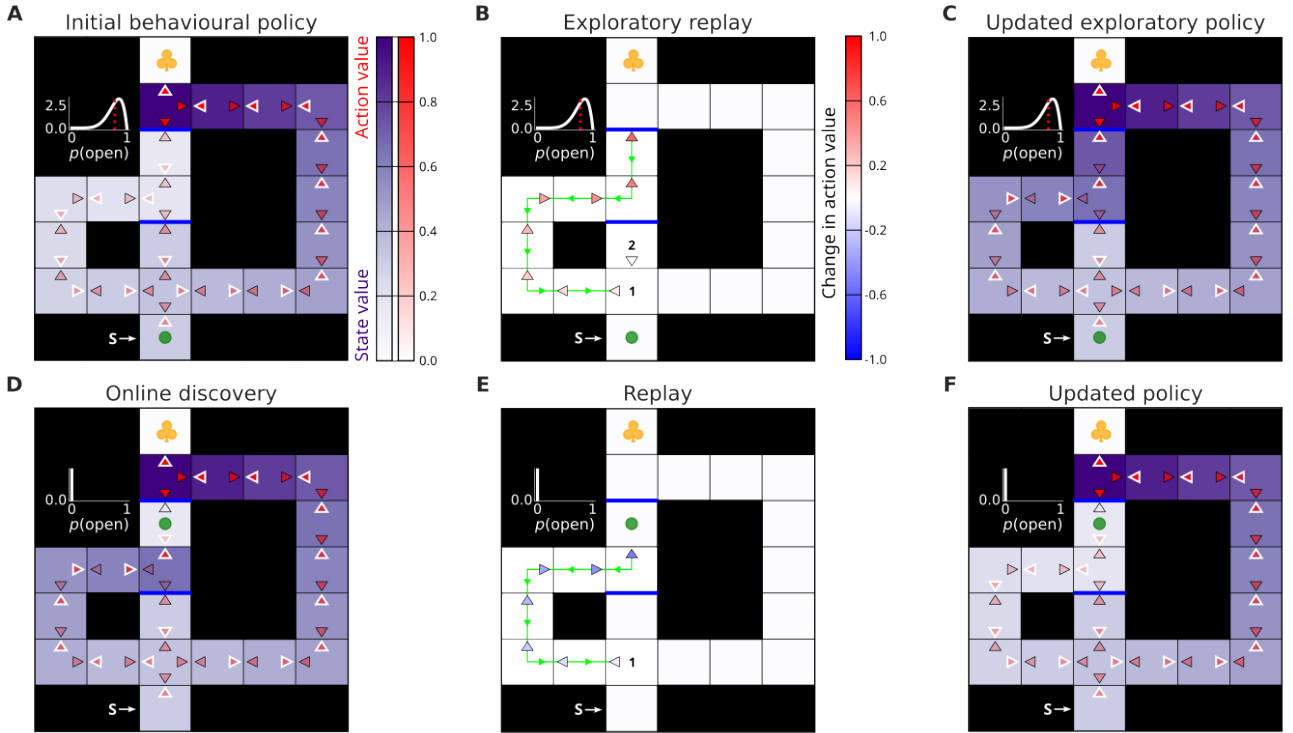


Figure 3: Sequence replay helps deep value propagation. The layout of the figure is the same as in Fig 2. A-C) Show the subject’s initial and uncertain state of knowledge, changes to the online behavioural policy occasioned by exploratory replay, and the new updated exploratory policy due to such replay, respectively. The crucial difference being that the replay in B) was a sequence event – i.e., the whole chain of actions was updated simultaneously (the actions which were updated in the replayed sequence are linked by a green line; the green triangles along that line additionally indicate the reverse direction of the replayed sequence). D-F) Again, the subject discovered the top barrier, learnt about its presence online and engaged in replay to recompile its model-free behavioural policy in the light of the negative information. Note how, in this case, sequence replay in E) resulted in deep propagation of the value of such information all the way towards the start state. The sequence replay thus enabled the subject to correct its exploratory policy appropriately as shown in F).

Here, the subject’s uncertainty resulted in consecutive replay updates which originated at the potential barrier location and progressed towards the subject’s location in a reverse manner (Fig 2A-C).

Those replays propagated the value of exploring the barrier towards the subject's current location, and the resulting new model-free behavioural policy indicated exploration was worthwhile (Fig 2C). As just discussed, the extent to which the subject was uncertain determined how large was the exploratory bonus that reached the subject's current state – and thus produced policies with different incentives for exploration (Figs S5 and S6).

Resolving uncertainty can often result in unfortunate outcomes, for instance if the barrier is found actually to be present (Fig 2D). If this happens, it is important for the subject to correct the full exploratory policy that had led to the discovery in the light of the negative information it acquired. We find that in our simulated Tolman maze, single-action replay updates do not handle this appropriately: the discovered value of the present barrier does not propagate deeply enough towards those states which had been updated with the exploratory bonus of the obsolete belief (Fig 2E-F). This is because single-action updates are myopic: the estimated benefit of a single-action update does not account for how that update can affect the benefit of potential future updates. This problem does not arise if the shortcut is found to be available, since then the replay naturally spreads the good news in backwards sequence [27].

One plausible solution is to consider the benefit of simultaneously updating a sequence of actions, as opposed to relying solely on updates at single states. This benefit combines Gain, that accumulates with the propagated policy changes (provided that all those changes result in policy improvements), as well as Need along that sequence of actions. We found that sequence replay results in deep propagation of the value of a discovered barrier, along the whole chain of actions which had previously been endowed with the exploration bonus (Fig 3).

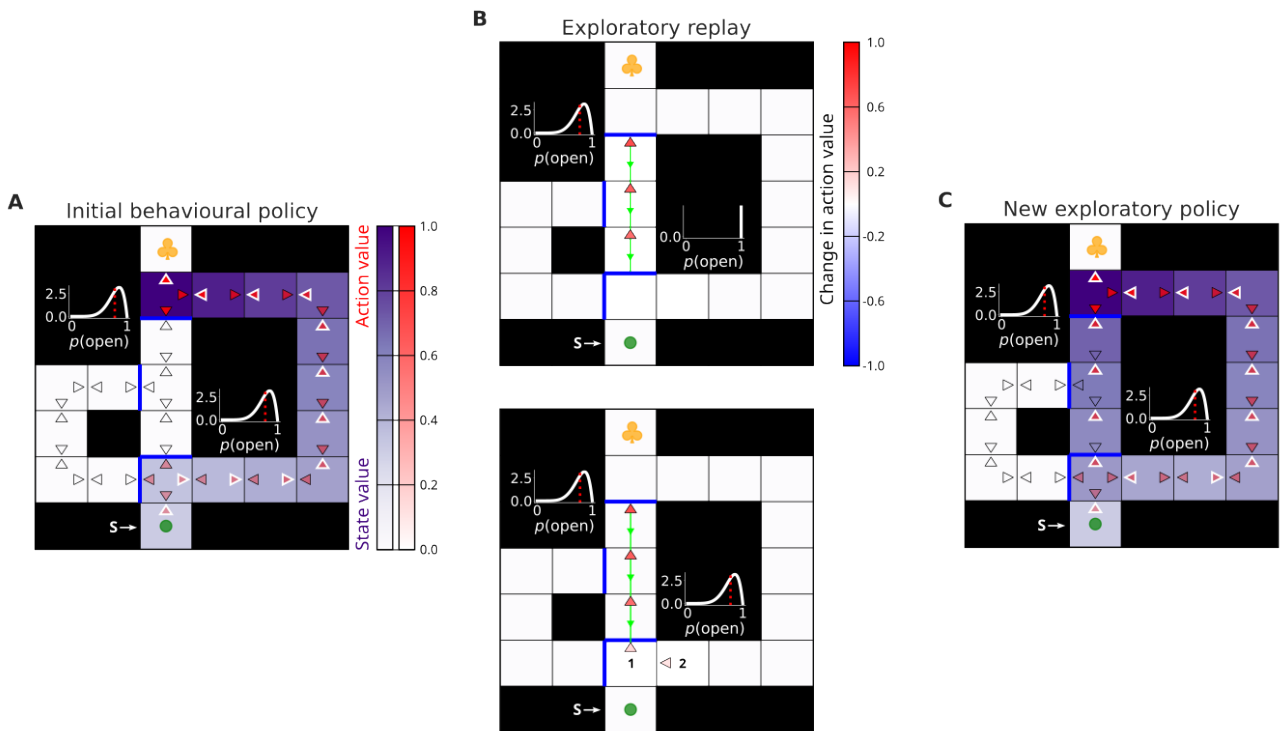


Figure 4: Replay in a blocked corridor. A) Initial state of knowledge of the subject. Note that the model-free Q -values in the blocked corridor are all initialised to 0, thus mimicking the subject's inexperience with the segment. The subject's belief state comprised its uncertainty about the presence of the top and bottom barriers that create the corridor. B) Replay choices of the subject due to its initial and uncertain state of knowledge. Note that the sequence replay event was performed across two different belief states: action updates inside the corridor (top) corresponded to a different belief state since they followed the potential transition through the bottom barrier which the subject had to first learn about (bottom). C) New exploratory policy occasioned by the replay updates in B).

There is one further aspect of the data on exploratory replay: experimental evidence implicates the hippocampus in constructing replay sequences through previously unexplored spaces [17, 29]. In our

123 account, this corresponds to replay in potential future belief states which the subject has not visited
124 yet but imagines encountering. We manipulated the barrier configuration in our maze to produce
125 a corridor segment in the central arm with both sides occluded by barriers (Fig 4). Examining the
126 replay patterns chosen by the subject due to uncertainty about the presence of both barriers revealed
127 sequence replay in the corridor. Such replay propagated the exploratory value of learning about the
128 possibility of entering the corridor (resolving uncertainty about the bottom barrier; Fig 4B bottom),
129 exiting it (learning about the top barrier; Fig 4B top) and ending up in a state close to the goal.

130 Some of the most important facets of learning in the brain involve building inverse models: this
131 characterizes bottom-up, recognition, models of sensory processing in cortex [18]; the maintenance
132 and expansion of the relationship between cortical and hippocampal representations in memory [25,
133 23, 20]; and the determination of policies that maximize reward and minimize punishment given in-
134 formation about the environment [32]. Offline processing, evident in replay, offers a way of building
135 and refining inverse models of all these forms without disturbing ongoing behaviour. However, to
136 determine good policies, it is not enough to build an inverse model based on just current information;
137 active observers have the obligation to collect new information too, and balance this against exploita-
138 tion. This obligation can be satisfied by inverting a more sophisticated model of the environment that
139 includes uncertainty; here, we showed how to conceive of (reverse) replay as performing this inverse.
140 This provided new insights into the nature and structure of offline activity – for instance surfacing the
141 importance of sequence replay, as well as predictions for new experimental paradigms.

142 1 Methods

143 We treated the (navigational) decision-making problem in our variant of the Tolman maze as a par-
144 tially observable Markov Decision Process (POMDP). The subject was designed in the spirit of the
145 DYNA architecture, such that online decisions were made according to the behavioural model-free
146 policy, and offline planning was used for additional training of the model-free controller. The sub-
147 ject was endowed with a probabilistic belief about the existence of barriers in certain locations in the
148 maze; every decision (real or imagined) therefore transitioned the subject to a new belief state which
149 comprised the subject’s physical state, as well as its updated posterior belief, which became its new
150 prior belief. For planning (replay), the subject considered how its belief state would evolve up to a
151 fixed horizon. The value of each imagined belief state was approximated with the subject’s model-free
152 Q -values at the corresponding physical location. Moreover, we considered just three possible beliefs
153 for the existence of each barrier: the initial uncertainty (which can be continuous), and either certain
154 presence or absence. The priority of each replay update was determined by the expected long-run im-
155 provement to the subject’s current belief state engendered by each potential replay update. The replay
156 updates were executed until the expected improvement was estimated to be below a fixed threshold.
157 For sequence replay updates, the maximal length of each potential sequence was limited to the dis-
158 tance from the start state to the uncertain barrier. We report a more detailed theoretical account of our
159 modelling in the Supplementary.

2 Supplementary information

Theory background

Reinforcement learning

In reinforcement learning (RL) [33], subjects learn to make appropriate decisions in order to maximize expected gains and minimize potential losses. Learning proceeds through interaction with an environment which supplies a sparse learning signal. The environment is typically formalised as a Markov Decision Process (MDP), which is a tuple $\langle \mathcal{S}, \mathcal{A}, \mathcal{P}, \mathcal{R}, \gamma \rangle$ where \mathcal{S} is the set of states, \mathcal{A} is the set of actions available at each state, $\mathcal{P} : \mathcal{S} \times \mathcal{A} \times \mathcal{S} \rightarrow [0, 1]$ is the Markov transition kernel which specifies the transition probabilities between states given an action, $\mathcal{R} : \mathcal{S} \rightarrow \mathbb{R}$ is a bounded reward function which comprises the learning signal, and $\gamma \in [0, 1)$ is the discount factor which determines the appetitiveness of delayed rewards.

The subject's behaviour in an environment is governed by its policy, $\pi : \mathcal{S} \times \mathcal{A} \rightarrow [0, 1]$, which, for every state, outputs a probability distribution over the set of available actions. At each time step, the subject interacts with its environment and receives the reward signal. The (possibly infinite) discounted collection of rewards the subject accrues along a trajectory of decisions is called the return. One main goal for a reinforcement learning subject is to predict the expected rewarding consequences of following policy π starting at a state s . This can be written as

$$V^\pi(s) = \mathbb{E}_\pi \left[\sum_{t=0}^{\infty} \gamma^t \mathcal{R}_t \mid S_0 = s \right] \quad (1)$$

A closely related task is instead to estimate the expected return for performing some action a in a given state s , in which case they are referred to as Q -functions:

$$Q^\pi(s, a) = \mathbb{E}_\pi \left[\sum_{t=0}^{\infty} \gamma^t \mathcal{R}_t \mid S_0 = s, A_0 = a \right] \quad (2)$$

The second main goal is to learn an optimal policy, π^* , which for any starting state s prescribes how to maximise the expected return:

$$\pi^* = \max_{\pi} \mathbb{E}_\pi \left[\sum_{t=0}^{\infty} \gamma^t \mathcal{R}_t \mid S_0 = s \right] \quad (3)$$

An MDP need not have a unique optimal policy. However, the optimal value function $V^{\pi^*}(s)$ and $Q^{\pi^*}(s, a)$ functions are unique. In particular, any action $a = \operatorname{argmax}_{a' \in \mathcal{A}} Q^{\pi^*}(s, a')$ can be chosen.

Model-free control

Several algorithmic approaches exist to solving the problem of optimal control in RL tasks. One popular example is Q -learning [35], which is an important and widely used algorithm for learning the optimal Q^{π^*} -function. It belongs to a more general class of model-free temporal difference algorithms which, after every experienced interaction with the environment, successively update their value function estimates based on the encountered reward prediction errors. Specifically for Q -learning, the update rule at iteration n is:

$$Q^{n+1}(s, a) \leftarrow Q^n(s, a) + \alpha \left[\mathcal{R}(s') + \gamma \max_{a' \in \mathcal{A}} Q^n(s', a') - Q^n(s, a) \right] \quad (4)$$

Here, the Q -value estimate is updated towards the difference (or prediction error) between the initial estimate, $Q^n(s, a)$, and the sum of the observed reward at the next state reached and the discounted maximal Q^n -value at that state, $\mathcal{R}(s') + \gamma \max_{a' \in \mathcal{A}} Q^n(s', a')$, weighted by the learning rate, α . Note that the action that optimises $Q^{n+1}(s, a')$ at s might be different from the one used in equation 4 that optimized $Q^n(s, a')$

The Q^{n+1} -values themselves can be used to determine a policy, for instance:

$$\pi^{n+1}(s, a) = \frac{e^{\beta Q^{n+1}(s, a)}}{\sum_{a' \in \mathcal{A}} e^{\beta Q^{n+1}(s, a')}} \quad (5)$$

where $\beta > 0$ is an inverse temperature parameter that controls how deterministic is π^{n+1} . Since $\pi^{n+1}(s, a)$ favours actions with higher Q^{n+1} -values, it tends to be better than $\pi^n(s, a)$ in terms of expected return. The remaining stochasticity is a crude method for arranging a mix of exploration and exploitation.

Model-based control

A different solution is to learn a model of the environment which can then be used to perform prospective *planning* of the actions to execute. Value functions can also be acquired using the recurrent Bellman equation [4], for instance:

$$Q^{n+1}(s, a) = \sum_{s'} \mathcal{P}(s' | s, a) \left[\mathcal{R}(s') + \gamma \max_{a' \in \mathcal{A}} Q^n(s', a') \right] \quad (6)$$

Here, the recurrent relationship between the successive states allows the subject to make use of its knowledge of the transition structure of the environment (the model \mathcal{P}) to propagate the information about future rewards towards its current situation or state in the environment. If the subject does indeed know the model (also including \mathcal{R}), then various forms of planning can be used to compute the long-run consequences associated with the available actions at decision time and make a far-sighted and informed decision. Value iteration [4] is one example planning algorithm which iteratively performs synchronous updates (for all states and actions in each sweep) specified by Equation 6. Such updates are also called Bellman backups because of the application of the Bellman equation. Given a perfect model of the environment, \mathcal{P} , such procedure is guaranteed eventually to converge to the optimal value function.

DYNA and prioritized sweeping

There is evidence for the use in animals, and the utility in artificial agents, of both model-free and model-based control [15]. This poses obvious questions about their arbitration and integration [7, 3, 1]. One important suggestion for integration is that information could be transferred from the model that the model-based controller possesses into the model-free controller, so that the latter can provide better informed choices.

In RL, the most common version of this process is known as experience replay [21], and lies at the heart of many successful algorithms [31]. Although, as we will discuss later, it was originally designed for the purpose of exploration, the so-called DYNA algorithm [32] has been used to underpin this process. In DYNA, an agent learns model-free value functions online by direct experience with the environment, as well as learning the model of that environment. During offline states, DYNA uses its learnt model to sample possible transitions and rewards, which are then used to perform further training of the model-free value functions to perform a more effective form of model inversion.

Given this overall structure, it becomes natural to consider which transitions or rewards should be sampled from the model (or replayed). One important algorithmic notion is prioritized sweeping [27], in which replays are chosen in an order that effects a form of optimal improvement in the model-free value functions.

Gain and Need

Mattar and Daw [24] synthesised the ideas of DYNA and prioritised sweeping and proposed a principled, normative scheme for the ordering of planning computations. They suggested that each replay experience corresponds to a Bellman backup (Equation 6) which uses information from a generative model of the environment to update a specific model-free state-action value.

236 Mattar and Daw [24] observed that what is important about an update at a state (which could
 237 be distal from the current state of the agent) is whether it changes the subject’s behavioural policy.
 238 For example, performing a planning computation at state s_k corresponds to changing the model-free
 239 value for action a_k at that state. Such a change is significant if the agent’s behavioural policy changes
 240 at s_k ; the agent can then estimate the consequence of that change for the expected return from its
 241 current state or a start state.

242 Mattar and Daw [24] showed that the subject can calculate how a replay update to action a_k at
 243 state s_k changes the amount of reward it can obtain in the future starting from a potentially different
 244 state s . By decomposing the difference in the subject’s model-free value function estimate before and
 245 after the policy update occasioned by such replay update, $V_{\pi_{\text{new}}}(s) - V_{\pi_{\text{old}}}(s)$, Mattar and Daw [24]
 246 showed that this expression can be written as:

$$V_{\pi_{\text{new}}}(s) - V_{\pi_{\text{old}}}(s) = \sum_{x \in S} \sum_{i=0}^{\infty} \gamma^i P(s \rightarrow x, i, \pi_{\text{old}}) \times \sum_a [\pi_{\text{new}}(a | x) - \pi_{\text{old}}(a | x)] Q_{\pi_{\text{old}}}(x, a) \quad (7)$$

247 Furthermore, by assuming that each individual replay update to the model-free value of action a_k
 248 results in a policy change at a single update location, s_k , equation 7 can be simplified into the product
 249 of Gain and Need, which Mattar and Daw [24] termed the expected value of a backup (EVB $_{\pi_{\text{old}}}$):

$$\text{EVB}_{\pi_{\text{old}}}(s_k, a_k) = \underbrace{\sum_{i=0}^{\infty} \gamma^i P(s \rightarrow s_k, i, \pi_{\text{old}})}_{\text{Need}} \times \underbrace{\sum_a [\pi_{\text{new}}(a | s_k) - \pi_{\text{old}}(a | s_k)] Q_{\pi_{\text{old}}}(s_k, a)}_{\text{Gain}} \quad (8)$$

250 Gain quantifies the expected local improvement in the subject’s behavioural policy at state s_k as
 251 a result of the replay update. Thus, Gain is higher for those replay updates which result in greater
 252 policy changes at the update state. Need, on the other hand, quantifies how likely is the subject to
 253 visit the update state in the long run, given its model of the environmental transition dynamics and
 254 behavioural policy before the update.

255 In rodents, the hippocampus is a structure known to be involved in aspects of model-based control
 256 [30, 2, 5]. Mattar and Daw [24] suggested that the reactivation of sequences of behaviourally-relevant
 257 experiences during quiet wakefulness and sleep for which the hippocampus is well known [13] is an
 258 expression of this sort of prioritized replay. They thereby explained a wealth of experimental findings
 259 on the selection of replay experiences in rodents [2, 30] as well as humans [22, 3].

260 Exploration

261 As discussed in the main text, exploration in MDPs can be accomplished by the use of heuristics
 262 which estimate the amount of the subject’s (in)experience with its environment. One such celebrated
 263 heuristic is based on the ‘optimism in the face of uncertainty’ (OFU) principle which posits that actions
 264 whose outcomes are uncertain should receive a sort of exploration bonus which would encourage the
 265 subject to pursue them. Sutton [32]’s exploration bonus indeed took that form:

$$Q^{n+1}(s, a) \leftarrow Q^n(s, a) + \alpha \left[\mathcal{R}(s') + \epsilon \sqrt{\#_{(s,a)}} + \gamma \max_{a' \in \mathcal{A}} Q^n(s', a') - Q^n(s, a) \right] \quad (9)$$

266 Improved exploration in DYNA (also known as DYNA- $Q+$) was achieved by updating its model-
 267 free Q -values according to Equation 9 during offline planning. Here, $\#_{(s,a)}$ is a count-based heuristic
 268 which grows with the number of time steps since that state-action pair had last been attempted, and ϵ
 269 is a free parameter which controls the amount of influence this uncertainty bonus has on the Q -value
 270 update. By using this update rule, actions which have not been tried for an extended period of time
 271 come to look more appealing, which happens to be particularly useful in dynamic environments with
 272 unsignalled changes.

273 Note that by virtue of the Q -learning update rule (Equation 4), the exploration bonus awarded to
 274 a distal state-action pair (Equation 9) propagates towards state-actions which lead to it, hence encour-
 275 aging off-policy exploration. The bonus itself, however, is myopic, since it does not reflect the benefit
 276 of learning about the uncertain state-action in the first place.

277 Optimal exploration, on the other hand, entails a more careful evaluation of how resolving one’s
 278 uncertainty may be useful in the long-run and whether the acquired knowledge would be of any use
 279 for subsequent exploitation. Such thorough evaluation requires the subject to maintain an explicit
 280 model of its uncertainty and what possibilities abound.

281 Partial observability

282 The classical MDP formalism assumes that the subject knows the model of the environment with
 283 which it interacts. It does not, however, capture the ignorance that subjects (at least partially) face
 284 when learning about their environments. Such ignorance can be treated as a form of incomplete
 285 information which the subject can (at least to some extent) complete with experience.

286 Partially observable Markov Decision Processes (POMDPs) are a generalisation of MDPs in which
 287 the subject can lack direct access to some knowledge that is required to learn a good policy. For in-
 288 stance, the subject can be ignorant about the state it occupies because instead of perfect information
 289 from the environment it receives noisy and ambiguous observations; equally, the subject can be un-
 290 certain about the transition dynamics that govern its movement through the environment.

291 Each observation in a POMDP therefore grants the subject a piece of information which it can use
 292 to update its knowledge about the environment in an optimal manner. A sequence of observations the
 293 subject collects is formally referred to as *history*. Critically, the subject’s policy in a POMDP depends
 294 on its full history of observations, since this history determines its state of knowledge about the envi-
 295 ronment, and thereby determines the decisions it ought to make. The dependence on history violates
 296 the Markovian assumption (which requires that future transitions and rewards are statistically inde-
 297 pendent of the history, given the present state), and POMDPs are therefore not amenable to classical
 298 MDP solutions.

299 Instead of keeping track of all encountered observations the subject can maintain a sufficient statis-
 300 tic of the entire history. This sufficient statistic is called the subject’s *belief*, and it concisely summarises
 301 the knowledge that the subject has acquired. With each new observation the subject can optimally
 302 update its beliefs in the light of new information. Beliefs can be viewed as a new, subjective, state for
 303 a decision problem; they do satisfy the Markov property, and so it is possible to formulate POMDPs
 304 as MDPs where each state of the process is the subject’s belief.

305 A belief MDP is therefore formally defined as a tuple $\langle \mathcal{B}, \mathcal{A}, \mathcal{T}, \mathcal{R}, \gamma \rangle$ where \mathcal{B} is the (continuous)
 306 set of belief states, \mathcal{A} is the set of actions, $\mathcal{T} : \mathcal{B} \times \mathcal{A} \times \mathcal{B} \rightarrow [0, 1]$ is the (Markov) belief transition kernel,
 307 $\mathcal{R} : \mathcal{B} \rightarrow \mathbb{R}$ is a bounded reward function, and $\gamma \in [0, 1]$ is the discount factor. Thus, as opposed to the
 308 original MDP formulation, in belief MDPs the subject transitions through augmented belief states. For
 309 our matters, each belief state, $b = \{s \in \mathcal{S}, P(\mathcal{P})\}$, encompasses the subject’s physical location in the
 310 environment, s , as well as its probabilistic model of uncertainty, $P(\mathcal{P})$, about the presence/absence of
 311 barriers at several locations.

312 The formalism of belief MDPs permits the construction of policies which optimally trade-off ex-
 313 ploration and exploitation [16]. To see this, consider the case that the subject is uncertain about the
 314 state transition model \mathcal{P} , and therefore maintains a prior belief $P(\mathcal{P})$. Firstly, the probabilistic belief
 315 allows the subject to learn optimally upon receiving observations from the environment – in the case
 316 of transition uncertainty, by noting which state each transition leads to. This is accomplished by cal-
 317 culating a posterior belief using Bayes’ rule. For instance, after observing a transition from state s to
 318 s' , an optimal belief update corresponds to:

$$P(\mathcal{P} \mid s') = \frac{P(s' \mid \mathcal{P})P(\mathcal{P})}{\sum_{x \in \mathcal{S}} P(x \mid \mathcal{P})P(\mathcal{P})} \quad (10)$$

319 Note that a general POMDP formalism typically involves an observation function whereby the
 320 subject has no direct access to the state of the world, and it therefore receives noisy observations

which lead to uncertain state estimates. In our setting, the subject has direct access to its physical state in world; however, the transition structure is non-trivial in the sense that it can change without the subject being aware of such changes taking place. The subject’s uncertainty can result from either the subject having an explicit probabilistic belief of how the transition dynamics might change in the course of a task, or, alternatively, because of forgetting, which can be thought of as a heuristic version of the former.

Secondly, the subject can plan the future possibilities by making use of its uncertainty and allocating the prior probabilities to each of the considered outcomes. Those outcomes, in turn, result in more potential learning which the subject also accounts for by performing the same updates as in Equation 10 but for simulated futures (those transitions are governed by the belief MDP transition function, \mathcal{T}). This allows the subject to foresee the long-run consequences associated with each exploratory decision and whether it can potentially result in better future return.

Model description

Replay updates

The subject makes use of its transition model as well as the associated uncertainty to envision the possible evolution of its belief. This can be visualised as a planning tree which is rooted at the subject’s current belief state, b_ρ . The subject considers all possible actions from this root node, and adds additional nodes for each new belief state that results from applying those actions (according to the belief transition model, \mathcal{T}) – this corresponds to adding a single step horizon to the planning tree. Applying the same procedure to all nodes at the new horizon further deepens the tree and expands the planning horizon.

Similarly to physical states in MDP problems, each belief state can have an associated value which reflects how much reward the subject expects to obtain by being in that belief state and acting according to some policy. Those values, however, are initially unknown to the subject, and the reason for performing replay updates in the belief tree is to propagate the value information from future belief states to the subject’s current belief state. Since belief states are continuous, we restrict the subject’s planning horizon to a fixed depth. This means that belief states containing reward may be beyond the subject’s reach. However, the subject’s model-free system is likely to have an estimate of how valuable each physical location is. Therefore, the model-based value of each action a at every belief state $b = \{s, P(\mathcal{P})\}$ in the planning tree, which we refer to as $Q_{MB}^n(b, a)$, is initialised to the subject’s model-free estimate of the value of performing this action at the physical location in that belief state, $Q_{MF}^0(s, a)$.

When performing replay updates, the subject considers the effect of each action at every belief state in the tree rooted at its current belief state. For example, when considering the effect of action a at belief state $b = \{s, P(\mathcal{P})\}$ which attempts to cross a potential barrier, the subject accounts for the possibility of transitioning into one of two new belief states: $b'_{\text{open}} = \{s', P'_{\text{open}}(\mathcal{P})\}$, which corresponds to the fortunate outcome of discovering that the barrier is absent, and $b'_{\text{closed}} = \{s, P'_{\text{closed}}(\mathcal{P})\}$, which corresponds to the unlucky outcome of the barrier being present. The value associated with executing action a at belief state b is updated towards the estimated values of the next belief states:

$$Q_{MB}^{n+1}(b, a) = Q_{MB}^n(b, a) + \sum_{b' \in \{b'_{\text{open}}, b'_{\text{closed}}\}} \mathcal{T}(b' | b, a) \left[\mathcal{R}(b') + \gamma \max_{a' \in \mathcal{A}} Q_{MB}^n(b', a') - Q_{MB}^n(b, a) \right] \quad (11)$$

Here, the belief transition model, \mathcal{T} , describes how the subject jointly transitions through physical states and its beliefs about the barrier configuration. Moreover, for brevity, we will refer to the set of belief states that the subject can reach by applying a single action at a belief state as the children set of that belief state, denoted as $C(b, a) \in \mathcal{B}$. For the example above:

$$C(b, a) = \{b'_{\text{open}}, b'_{\text{closed}}\} \quad (12)$$

364 Gain and Need in belief space

365 We consider optimising the prioritisation of replay updates (Equation 11) in the subject’s belief space.
 366 We follow the suggestion of Mattar and Daw [24], whereby the priority of each update is determined
 367 by the expected improvement to the subject’s behaviour at its current belief state. By applying the
 368 same value decomposition as in Mattar and Daw [24], we define $\text{EVB}_{\pi_{\text{old}}}(b_k, a_k) := V_{\pi_{\text{new}}}(b_\rho) - V_{\pi_{\text{old}}}(b_\rho)$,
 369 where $V_{\pi_{\text{old}}}(b_\rho)$ is the value the subject estimates for its current belief state, b_ρ , under the old be-
 370 havioural policy before the potential update, and $V_{\pi_{\text{new}}}(b_\rho)$ is the estimated value of the subject’s cur-
 371 rent belief state under the new policy implied by the potential update. The effect of policy change
 372 engendered by a replay update to action a_k at some (potentially distal) belief state b_k can be expressed
 373 as:

$$\text{EVB}_{\pi_{\text{old}}}(b_k, a_k) = \underbrace{\sum_{b \in \mathcal{B}} \sum_{i=0}^{\infty} \gamma^i \mathcal{T}(b_\rho \rightarrow b, i, \pi_{\text{old}})}_{\text{Need}} \times \underbrace{\sum_a [\pi_{\text{new}}(a | b) - \pi_{\text{old}}(a | b)] Q_{\pi_{\text{old}}}(b, a)}_{\text{Gain}} \quad (13)$$

374 Importantly, we do not assume that the effects of replay updates are localised to individual states
 375 (as in Equation 8), which allows the subject to account for broad generalisation across multiple belief
 376 states (see below) when calculating the expected benefit of each replay update. The Gain term as-
 377 sociated with a replay update quantifies the expected local improvement in the subject’s behavioural
 378 policy at the update belief state engendered by that replay (Equation 11). Gain therefore favours those
 379 replay updates which result in large improvements to the subject’s model-free decision policy.

380 Need, similarly to Mattar and Daw [24], quantifies the frequency with which the subject expects
 381 to visit the update belief state according to its old behavioural policy, π_{old} . As discussed before, in
 382 belief MDPs, subjects engage in continual learning which means that with every visit to the same
 383 physical location the subject has a different belief about the transition model. This allows the belief
 384 space version of Need to account for all possible future learning that can take place (however, for
 385 computational purposes, we limit the subject’s horizon – see below).

386 One critical consideration is that of the dependence of Need on the old behavioural policy of the
 387 subject, π_{old} , which tends to prioritise portions of the state space the subject already expects to visit.
 388 Thus, even if the subject was informed about a distal change in the transition structure which its
 389 current policy does not prescribe to visit, Need at those locations would still be zero. It is therefore
 390 important to include stochasticity (for instance, in the form of undirected exploration) into the sub-
 391 ject’s behavioural policy which generates Need to allow for off-policy replay choices. This motivates
 392 our choice of the softmax behavioural policy which ensures that Need is positive for all potential belief
 393 states. Below we additionally explore how the subject’s behavioural policy affects its replay choices.

394 As for Mattar and Daw [24], we set a threshold on the minimal $\text{EVB}_{\pi_{\text{old}}}$ value required for an
 395 update to be executed. This threshold can be thought of as accounting for a form of opportunity cost
 396 by balancing the trade-off between planning to improve the policy and immediately acting to collect
 397 reward [28], hence helping to subject to avoid being permanently buried in thought.

398 Generalisation

399 The notable difference between our belief space decomposition and that of Mattar and Daw [24] is the
 400 inclusion in equation 13 of the outer sum over the space of beliefs, \mathcal{B} . This critical difference enables
 401 the subject to account for a broad generalisation across multiple belief states when considering the
 402 effect of a single action update at an individual belief state.

403 Each belief state in continual learning tasks (unless there is forgetting) can be visited at most once
 404 since after every transition the subject potentially acquires information, and therefore updates its prior
 405 belief which constitutes a different belief state. However, even though each belief state can be visited
 406 at most once, physical states which also comprise those belief states recur in episodic tasks. The
 407 subject can therefore expect an accumulated benefit of replay updates at single belief states. Moreover,
 408 information that the subject discovers about a potential barrier (for instance, if it is absent) is shared
 409 across all belief states associated with that barrier – since at any time it can only be present or absent.

410 In the presence of forgetting, the replay structure might be different since the subject would need
 411 to optimally account for those belief states which it expects to visit again. This, however, will depend
 412 of the specific form of forgetting, and the resulting belief states which the subject would have to
 413 represent in the planning tree. Our general formalism of replay prioritisation can account for this, but
 414 in the present work we do not consider it.

415 Sequence replay

416 Sequence replay corresponds to updating a whole sequence of consecutive actions, as opposed to
 417 performing individual greedy action updates one at a time. For example, consider two consecutive
 418 actions a_1 and a_2 at belief states b_1 and b_2 , respectively. The order in which those two replay updates
 419 are executed depends on the expected value associated with the two possibilities. In the spatial do-
 420 main (or other domains with clear ordering) one order would typically be interpreted as a reverse
 421 reactivation, and the other as forward. Moreover, the expected value of performing forward and re-
 422 verse sequence updates will, in general, differ (see below). A sequence update to the two example
 423 actions corresponds to updating one action according to:

$$Q_{MB}^{n+\frac{1}{2}}(b_1, a_1) = Q_{MB}^n(b_1, a_1) + \sum_{b' \in C(b_1, a_1)} \mathcal{T}(b' | b_1, a_1) \left[\mathcal{R}(b') + \gamma \max_{a' \in \mathcal{A}} Q_{MB}^n(b', a') - Q_{MB}^n(b_1, a_1) \right] \quad (14)$$

424 where the sum is over the set of next possible beliefs (as in equation 12). The fractional notation $n + \frac{1}{2}$
 425 emphasises the fact that within a single iteration of replay multiple actions can simultaneously be
 426 replayed in a sequence, since in the current example with two actions there are two executed updates
 427 between iterations n and $n + 1$.

428 The second action is then updated in the same way to generate Q_{MB} ; however, in the case of
 429 reverse replay, $b_1 \in C(b_2, a_2)$, and therefore the $Q_{MB}^{n+\frac{1}{2}}$ -value of one of its children beliefs $b' \in C(b_2, a_2)$
 430 will have already been updated. The size of the value update to action a_2 at belief state b_2 therefore
 431 depends on the update to action a_1 at belief state b_1 . This is also reflected in how the expected value of
 432 sequence replay is calculated – which is the reason for why the benefit of sequence replay can be larger
 433 than that of single action updates. If we define $\mathcal{M}_N = \{(b, a)_i\}_{1, \dots, N}$ as the candidate set containing N
 434 belief state-action pairs to be potentially updated in a sequence replay event, then the expected benefit
 435 of that sequence replay is calculated as:

$$\text{EVB}_{\pi_{\text{old}}}(\mathcal{M}_N) = \sum_{(b, a) \in \mathcal{M}_N} \text{EVB}_{\pi_{\text{old}}}^{n+\frac{1}{N}}(b, a) \quad (15)$$

436 Note that, in the case of reverse replay, each individual $\text{EVB}_{\pi_{\text{old}}}(b, a)$ in Equation 15 quantifies
 437 the benefit of updating action a at belief state b with a value that is propagated towards it along the
 438 sequence of actions that had also been updated. This is not the case for forward replay where each
 439 action is updated only towards the expected value of its children belief states (with the exception of
 440 cyclic domains; however, as we report below, we restrict all sequences to be acyclic); however, even in
 441 the case of forward replay the benefit of replaying the whole sequence will still, in general, be higher
 442 because of the summed benefit of all updates along the entire sequence (see below).

443 Replayed sequences can be of arbitrary lengths. Moreover, the longer the sequence, the more
 444 the estimated expected benefit will be, in general. The natural question therefore arises concerning
 445 the termination of sequences. We do not address this issue in the current work and assume that
 446 sequences link together critical decision points – in the Tolman maze, for instance, this corresponds
 447 to the sequential replay which originates at a potential barrier location and progresses towards the
 448 intersection in front of the subject’s start state.

449 Another consideration is computational: the theory that Mattar and Daw [24] proposed is norma-
 450 tive and does not prescribe how both Gain and Need can possibly be estimated in a psychologically
 451 credible way. Sequence replay is even more computationally prohibitive because of the number of
 452 potential sequences that can be replayed. In the present work, we similarly report a normative result

describing which sequences (out of all possibilities up to a fixed length) should be replayed. How the brain manages to reduce the sample complexity of sequence replay thus remains an open and challenging question which we leave to future work.

Simplified example: Bayesian bandits

Stationary, multi-arm bandit (MAB) problems offer the simplest test bed for examining exploration in belief spaces, and we therefore provide simulation results of replay prioritisation in a class of MABs. A typical MAB problem consists of a finite set of K arms, $\mathcal{A} = \{a_1, \dots, a_K\}$, which are the equivalent of actions in sequential decision-making problems. In each of the infinitely many trials, the subject is faced with a choice to pull one of the available arms. Each of the K arms, say a_k , if chosen, has a certain probability, μ_k , of paying the subject off with a binary reward (1 with probability μ_k and 0 with probability $1 - \mu_k$). One typical goal of subjects in MAB problems is to realise a sequence of arm choices so as to maximise the total discounted reward.

MAB problems are well-studied and, under certain assumptions about the reward distribution, optimal policies can be derived (such as the Gittins index [14]). Importantly, the payoff probabilities associated with each arm are initially unknown to the subject. This makes exploration in MAB problems worthwhile even if the expected return for the arm concerned is low, since if the arm is found actually to be good, then it can be consistently exploited in the future. Furthermore, MABs lack physical states, since in each trial the subject is faced with the same selection of arms irrespective of its choices in the preceding trials. The lack of physical states and the necessity of exploration makes MABs a perfect case study for our replay prioritisation, which we detail below.

We focus on a 2-arm bandit task with binary outcomes, in which on each trial, the subject has to choose between two arms, a_1 and a_2 , which have unknown payoff probabilities, μ_1 and μ_2 , respectively. The subject models its uncertainty about the payoff probability of each arm with a probabilistic prior belief which introduces subjective belief states, $b = \{p(\mu_1), p(\mu_2)\}$. Just as in the Tolman maze example considered above, a probabilistic model of uncertainty allows the subject to learn optimally about the payoff distribution of each arm after receiving feedback from the bandit in the form of a reward signal.

We model the subject's uncertainty about each arm's payoff probability using the Beta distribution. This particular parametric form is very convenient since the Beta distribution is a conjugate prior for the Bernoulli distribution (which is the reward distribution of each arm). The Beta distribution has two parameters, α and β , where α is typically interpreted as the number of success trials (received a reward of 1) and β as the number of failed trials (received a reward of 0). After N choices of arm a_k , the Bayesian update (Equation 10) to the prior distribution parameters (i.e., the subject's belief state) due to a new observation corresponds to:

$$p(\mu_k \mid \mathcal{R}_{N+1} = r) = \begin{cases} \text{Beta}(\alpha_k + 1, \beta_k), & \text{if } r = 1 \\ \text{Beta}(\alpha_k, \beta_k + 1), & \text{if } r = 0 \end{cases} \quad (16)$$

where $\alpha_k + \beta_k = N$.

The subject can make use of its model of uncertainty to plan ahead how the choice of each arm will affect its belief. We visualise this as a planning tree in Fig S1A. The tree is rooted at the subject's current belief state, b_ρ , and each action (choosing arm a_1 or a_2) can transition the subject into two new possible belief states: one which corresponds to an imagined success trial and another corresponds to an imagined failure trial. Applying actions to belief states deepens the tree and expands the subject's planning horizon. Note that the subject's planning horizon is limited to a fixed depth (Fig S1). This is because belief states are continuous, and building the entire tree of all possibilities is intractable. In our example, the subject therefore only considering how its belief will evolve up to several steps into the future.

Analogously to the Tolman maze, each belief state has an associated value. Replay updates in the tree correspond to updating the value of each belief state towards the expected value of the beliefs of its children at one horizon deeper in the tree (Equation 11). We initialise the value of each action

500 a_k in every belief state b in the tree to 0, except for the belief states at the final horizon whose values
 501 are initialised to the immediate expected payoff the subject expects to receive in that belief state by
 502 choosing action a_k , which corresponds to $\mathbb{E}_{p(\mu_k|b)} [\mu_k]$.

503 Similarly to the belief MDP, we define the priority of each individual replay update in the subject's
 504 belief space as the expected value of the associated backup (EVB). That is, for a potential replay up-
 505 date at belief state b_k to the value of action a_k , the expected value of that update, $\text{EVB}_{\pi_{\text{old}}}(b_k, a_k) :=$
 506 $V_{\pi_{\text{new}}}(b_\rho) - V_{\pi_{\text{old}}}(b_\rho)$, which quantifies the expected improvement to the value of the subject's current
 507 belief state, decomposes into the product of Gain and Need:

$$\text{EVB}_{\pi_{\text{old}}}(b_k, a_k) = \underbrace{\gamma^i \mathcal{T}(b_\rho \rightarrow b_k, i, \pi_{\text{old}})}_{\text{Need}} \times \underbrace{\sum_a [\pi_{\text{new}}(a | b_k) - \pi_{\text{old}}(a | b_k)] Q_{\pi_{\text{old}}}(b_k, a)}_{\text{Gain}} \quad (17)$$

508 The MAB instance of Gain is very similar to that of a more general belief MDP Gain discussed
 509 earlier. The crucial difference, however, is that Need does not accumulate at any individual belief
 510 state. This is because there are no physical states which can be re-visited in each episode, and each
 511 belief state in an MAB can be visited at most once (provided there is no forgetting involved) due
 512 to the continual learning nature of the bandit problem: after each new observation, the subject learns
 513 something about the bandit and thus transitions to a new belief state. This instance of Need, therefore,
 514 quantifies how likely is the subject to ever encounter the potential update belief state according to its
 515 prior belief about each arm's payoff probability, as well as its current decision policy, π_{old} .

516 We again assume a DYNA architecture whereby the subject may or may not decide to perform re-
 517 play based on the expected improvement it estimates to its current decision policy. We set a threshold,
 518 ξ , which specifies the minimal EVB required for each potential replay update to be executed.

519 Fig S1B shows an example replay update which was executed first because the subject estimated
 520 it to provide the greatest improvement to the value of its root belief state. Moreover, this example
 521 also highlights the effect of generalisation due to each individual replay update: this is visible in how
 522 the Need term changes at all other belief states as a result of the single replay update. Fig S1C shows
 523 all replay updates executed by the subject for which the estimated benefit exceeded the fixed EVB
 524 threshold. Note that only 4 replay updates resulted in the accumulation of a near-optimal value at
 525 the subject's root belief state, and that accumulated value reflected the benefit of future learning in
 526 an approximately optimal way (with respect to the subject's prior belief). We additionally simulated
 527 our subject with varying parameters (such as the softmax inverse temperature, EVB threshold, and
 528 horizon), and those results are reported in Fig S2.

529 We further investigated the effect of behavioural policy on the statistics of the subject's replay
 530 choices. This was done by randomly shuffling the true (fixed-horizon) initialised action values across
 531 all belief states before letting the subject engage in replay. This revealed that the initial state of knowl-
 532 edge of the subject (its behavioural policy) played a critical role in affecting the resulting benefit of
 533 replay (Fig S3) – which can furthermore be harmful [3]. This is visible from the wide distribution of
 534 the value of the resulting policy (Fig 3A), as well as the frequent lack of propagation of the value of
 535 distal beliefs towards the root of the tree (Fig 3B).

536 Finally, we examined the patterns of sequence and single-action replay updates (Fig S4). Our
 537 simulations indicated that the relative proportion of forward and reverse sequence replay was bi-
 538 ased towards reverse replay (Fig S4); however, there was also a significant number of forward replay
 539 sequences (1-sample t test, $t = 11.40, p \ll 0.0001$). Moreover, the total number of updated actions ap-
 540 peared to be greater with sequence replay compared to single-action replay updates (2-sample t test,
 541 $t = 2.05, p = 0.042$) which is expected given the open-loop nature of sequence replay optimisation.
 542 The full characterisation of sequence replay thus still remains an open question which we leave to
 543 future work.

544 Implementation

545 Estimation of exploratory Need

546 We used a Monte-Carlo estimator for the Need term when calculating $\text{EVB}_{\pi_{\text{old}}}$ from equation 13 for
 547 determining the priority of replay updates. The subject's belief space was discretised into its current
 548 belief state and two future possibilities for each of the uncertain barriers that they were either present
 549 or absent with certainty. Those possible belief states, moreover, could be envisioned by the subject
 550 only so long as they were within the reach of the subject's limited horizon, h . We denote this limited
 551 horizon, discretised belief space as $\text{disc}_h(\mathcal{B})$.

552 For the estimation of Need, N trajectories were simulated, all starting from the subject's current
 553 belief state $b_\rho = \{s_\rho, P(\mathcal{P})\}$, where the decisions at each encountered belief state in each simulated
 554 trajectory were governed by the subject's behavioural policy and the belief state transitions – by the
 555 expected transition model associated with the subject's belief state in the trajectory. When attempting
 556 to cross one of the uncertain barriers in a given trajectory, the next belief state was sampled according
 557 to $b' \sim \mathcal{T}(b' | b, a)$. The subject's belief about the transition dynamics in the new belief state, b' , was
 558 then updated according to what actually happened. For successful transitions (with an
 559 open barrier), the probability of that transition was set to 1 with no remaining uncertainty; similarly,
 560 for failed transitions (with a closed barrier), the probability of that transition was set to 0, also with no
 561 remaining uncertainty.

562 All simulations were run so long as γ^d , where d was the trajectory length, exceeded a fixed thresh-
 563 old, ϵ (which was always set to 10^{-5}). Each i^{th} simulated trajectory returned the smallest number of
 564 steps, $K_i(b)$, that it took to reach each encountered belief state $b \in \text{disc}_h(\mathcal{B})$ along the trajectory, as
 565 well as the non-cumulative Need upon the first encounter, $\gamma^{K_i(b)}$, associated with those belief states.

566 Finally, for each encountered belief state $b = \{s, P(\mathcal{P})\} \in \text{disc}_h(\mathcal{B})$, we estimated the Need using a
 567 second-form certainty equivalence (as mentioned in the main text). The resulting Need was averaged
 568 over the non-cumulative Need encountered in each of N simulated trajectories, which accounted for
 569 the learning and transitions through belief states within the reach of the subject's horizon, to which a
 570 certainty-equivalent Need was added with a stationary transition model of that belief state:

$$\widehat{\text{Need}}(b) = \frac{1}{N} \sum_{i=1}^N \left[\gamma^{K_i(b)} + \left[\sum_{j=K_i(b)+1}^{\infty} (\gamma \mathbb{E}_{\pi_{\text{old},b}} [P])^j \right]_{(s_\rho, s)} \right] \quad (18)$$

571 where $[\cdot]_{(i,j)}$ is a scalar value obtained by indexing the matrix by row i and column j .

572 Note that the expression $\sum_{j=0}^{\infty} (\gamma A)^j$, which corresponds to a geometric series for some matrix A ,
 573 can also be written as $(I - \gamma A)^{-1}$. In Equation 18, however, the counter for the infinite matrix sum
 574 does not start at zero. This is because for the first $K_i(b)$ steps the transition model is non-stationary
 575 due to potential learning during those first steps within the reach of the subject's horizon. After those
 576 first $K_i(b)$ steps, the subject computes the remaining of Need using the expected transition model of
 577 the final belief state in the simulated trajectory, $\mathbb{E}_{\pi_{\text{old},b}} [P]$.

578 Sequence generation

579 Sequence generation was implemented as an iterative procedure. All possible single-action updates
 580 were first generated, for belief states which were within the reach of the subject's horizon – that is, all
 581 belief states in $\text{disc}_h(\mathcal{B})$. Then, for forward sequences, all of the single-action updates were extended
 582 by applying all possible actions from the final belief state reached in those single-action updates (gov-
 583 erned by the belief transition model \mathcal{T}). This was repeated until sequences of the maximal specified
 584 length L were generated. Three important constraints we imposed on the sequence generation pro-
 585 cedure: i) physical states encountered in the sequences were not allowed to repeat, hence preventing
 586 loops; ii) each sequence was extended by an additional action only if the $\text{EVB}_{\pi_{\text{old}}}$ of the resulting se-
 587 quence exceeded the $\text{EVB}_{\pi_{\text{old}}}$ threshold; and iii) only those belief states contained in $\text{disc}_h(\mathcal{B})$ were

added to the sequences, such that the resulting sequences could not contain belief states outside of the subject’s horizon.

To generate reverse sequences, the same procedure was applied with the same imposed constraints. The only difference was the directionality of the value propagation along the action sequences. Note that the construction of reverse sequences requires an inverse belief transition model. An inverse transition model, for any given belief state b' , outputs a probability distribution over belief state-action pairs which quantifies how likely each of those are to result in a transition to b' . With our notation from Equation 12, given b' , an inverse transition model would assign zero probability to all belief state-action pairs but those for which $b' \in C(b, a)$. When generating reverse sequences, we used a forward transition model (instead of learning a separate inverse transition model) which assigned the same uncertainty for reverse transitions as for forward ones.

Simulation details

Fig 1 was generated by simulating a vanilla Mattar and Daw [24] replay subject. The subject learned model-free Q -values according to equation 4, which it then used for online control through a softmax policy. We additionally imposed forgetting on the model-free Q -values learnt by the subject, after every move made by the subject, to imitate a continual learning problem such that replay remained throughout the whole simulated experiment [3]. The aforesaid forgetting was operationalised as the exponential decay towards the initialised values controlled by a forgetting parameter:

$$Q_{MF}^n(s, a) \leftarrow (1 - \phi_{MF})Q_{MF}^n(s, a) + \phi_{MF}Q_{MF}^{\text{init}}(s, a)$$

The state-transition model of the subject, T , was initialised such that it indicated that no barriers were present and the transition probabilities indicated the true transition structure. After every transition which attempted to cross the top-most barrier, the subject updated its state-transition model as:

$$T^{n+1}(\cdot | s, a) \leftarrow T^n(\cdot | s, a) + [\mathbb{1}(s') - T^n(\cdot | s, a)]$$

where $\mathbb{1}(s')$ is a vector of the same dimension as the state space where each entry was zero except for the experienced next state, s' , for which the entry is 1. After every such update, the subject’s state-transition model probabilities associated with the uncertain barrier transition were normalised to ensure that they add up to 1:

$$T^n(\cdot | s, a) \leftarrow \frac{T^n(\cdot | s, a)}{\sum_{s' \in \mathcal{S}} T^n(s' | s, a)}$$

The subject additionally cached all observed experiences to use them in replay (we followed the same implementation protocol as in Mattar and Daw [24]). The memory buffer of the subject was updated after each corresponding online experience to account for the possible changes in the environment. The agent then engaged in replay after every move by prioritising the replay updates using equation 8 so long as the estimated $\text{EVB}_{\pi_{\text{old}}}$ exceeded the minimal improvement threshold, ξ .

The subject was simulated for the first 2000 moves in the environment shown in Fig 1A-C. For the second 2000 moves, the environment was altered to that shown in Fig 1D-F without the subject being informed about such change. Note that the barrier was not bidirectional – the subject was not allowed to learn about the barrier from the state above it (i.e., it had to approach the barrier directly from the start state). The simulations were repeated 10 times and the average results are reported. The values of the free parameters used in those simulations are reported in Table 1.

Fig 2A was generated by performing regular value iteration with a transition model which assumed that both barriers were present. The tolerance threshold for value iteration was set to 10^{-5} . The subject’s belief about the presence of the top barrier was then set to $\text{Beta}(7, 2)$, after which it was allowed to engage in replay whilst being situated at the start state. The subject prioritised replay updates (equation 11) by calculating the Gain associated with all potential replay updates at all belief states within its horizon reach according to equation 13. The subject estimated Need for all potential

| Parameter | Value | Description |
|------------------------|-------|---|
| Q_{MF}^{init} | 0 | Initialised model-free Q -values |
| α | 1 | Online learning rate |
| α_r | 1 | Replay learning rate |
| β | 10 | Inverse temperature |
| γ | 0.9 | Discount factor |
| ϕ_{MF} | 0.05 | Model-free forgetting |
| ξ | 0.001 | $\text{EVB}_{\pi_{\text{old}}}$ threshold |

Table 1: **Simulation parameters for Fig 1.**

replay updates using equation 18. Fig 2B-C show the prioritised replay updates and their order, as well as the new updated exploratory policy respectively.

For Fig 2D-E, the subject was situated at the state just below the top barrier. Its model-free Q -value for the action to cross the barrier was set to 0 to emulate the potential online discovery of the barrier being present; similarly, the subject’s belief was initialised to indicate the presence of the barrier with certainty. Accordingly, the subject’s belief was set to reflect the potential discovery of the barrier being present. The subject was then allowed to replay in the same way as described above. The values of the free parameters used in the shown simulations are reported in Table 2. In this and all subsequent tables reporting the parameter values, we highlighted the crucial parameters and their values which differed between the simulations.

| Parameter | Value | Description |
|---------------------|-------|---|
| α | 1 | Online learning rate |
| α_r | 1 | Replay learning rate |
| β | 2 | Inverse temperature |
| γ | 0.9 | Discount factor |
| α_T, β_T | 7, 2 | Beta prior parameters for the top barrier |
| h | 8 | Planning (replay) horizon |
| N | 2000 | Number of simulated trajectories |
| ξ | 0.001 | $\text{EVB}_{\pi_{\text{old}}}$ threshold |

Table 2: **Simulation parameters for Fig 2.**

Fig 3 was generated in the same way as Fig 2 but the replays that the agent was allowed to execute additionally included sequence events. The maximal sequence length, L , was constrained to be the distance between the start state and the uncertain barrier. The agent prioritised which replay updates to execute by choosing from all possible replay updates of lengths 1 through L . The online discovery was operationalised in the same way as in Fig 2, and the replay process was then repeated with the subject being situated in the new belief state. The values of the free parameters used in the shown simulations are reported in Table 3.

| Parameter | Value | Description |
|---------------------|-------|---|
| α | 1 | Online learning rate |
| α_r | 1 | Replay learning rate |
| β | 2 | Inverse temperature |
| γ | 0.9 | Discount factor |
| α_T, β_T | 7, 2 | Beta prior parameters for the top barrier |
| h | 8 | Planning (replay) horizon |
| L | 8 | Maximal sequence length |
| N | 2000 | Number of simulated trajectories |
| ξ | 0.001 | $\text{EVB}_{\pi_{\text{old}}}$ threshold |

Table 3: **Simulation parameters for Fig 3.**

Fig 4 was generated in the same way as Fig 3 except that the subject was uncertain about two barriers at the same time. The parameter values used in the shown simulations are reported in Table 4.

| Parameter | Value | Description |
|---------------------|-------|--|
| α | 1 | Online learning rate |
| α_r | 1 | Replay learning rate |
| β | 2 | Inverse temperature |
| γ | 0.9 | Discount factor |
| α_T, β_T | 7, 2 | Beta prior parameters for the top barrier |
| α_B, β_B | 7, 2 | Beta prior parameters for the bottom barrier |
| h | 6 | Planning (replay) horizon |
| L | 4 | Maximal sequence length |
| N | 2000 | Number of simulated trajectories |
| ξ | 0.001 | $\text{EVB}_{\pi_{\text{old}}}$ threshold |

Table 4: Simulation parameters for Fig 4.

Fig S1 was generated by constructing a belief tree of horizon 2 which was rooted at the subject's prior belief about the payoff probabilities of the two arms. The Q -values for all actions in all belief states were initialised to 0, except for those at the final horizon which were initialised to the expected immediate payoff according to those beliefs. Gain associated with each replay update in the tree (equation 11) was calculated according to equation 17 and Need associated with every update belief state was calculated according to equation 17.

| Parameter | Value | Description |
|---------------------|-------|---|
| α_r | 1 | Replay learning rate |
| β | 4 | Inverse temperature |
| γ | 0.9 | Discount factor |
| α_1, β_1 | 5, 3 | Beta prior parameters for arm 1 |
| α_2, β_2 | 1, 5 | Beta prior parameters for arm 2 |
| h | 2 | Planning (replay) horizon |
| ξ | 0.01 | $\text{EVB}_{\pi_{\text{old}}}$ threshold |

Table 5: Simulation parameters for Fig S1.

Fig S2 was generated by varying the subject's policy, the $\text{EVB}_{\pi_{\text{old}}}$ threshold, as well as the subject's planning horizon (all values are reported in the figure). The root value shown was taken as the expected return the subject expected at the root belief after all executed replay updates. The value of the evaluated policy was computed by evaluating the new updated policy as a result of the replay updates in the whole tree.

Fig S3 was generated in the same way as Fig S2 but the results were averaged over 200 random value initialisations in the tree. The randomisation was achieved by first performing full value iteration in the tree, and hence computing the true fixed-horizon values associated with each action in the tree. Next, those values were randomly shuffled across all belief states in the tree. Fig S3 shows the average, as well as individual replay processes in the randomised trees.

The data shown in Fig S4 was generated in the same way as for Fig S3, as well as additionally allowing the subject to perform sequence replay where the maximal sequence length was constrained to the horizon of the tree.

Fig S5 were generated in the same way as Fig 3 but the subject was initialised with a different prior belief about the presence of the barrier. In this case, the prior belief was set to Beta(2, 2).

The data in Fig S6 were generated in the same way as for Fig 3 but the subject was initialised with a range of different prior beliefs about the presence of the barrier.

3 Supplementary figures

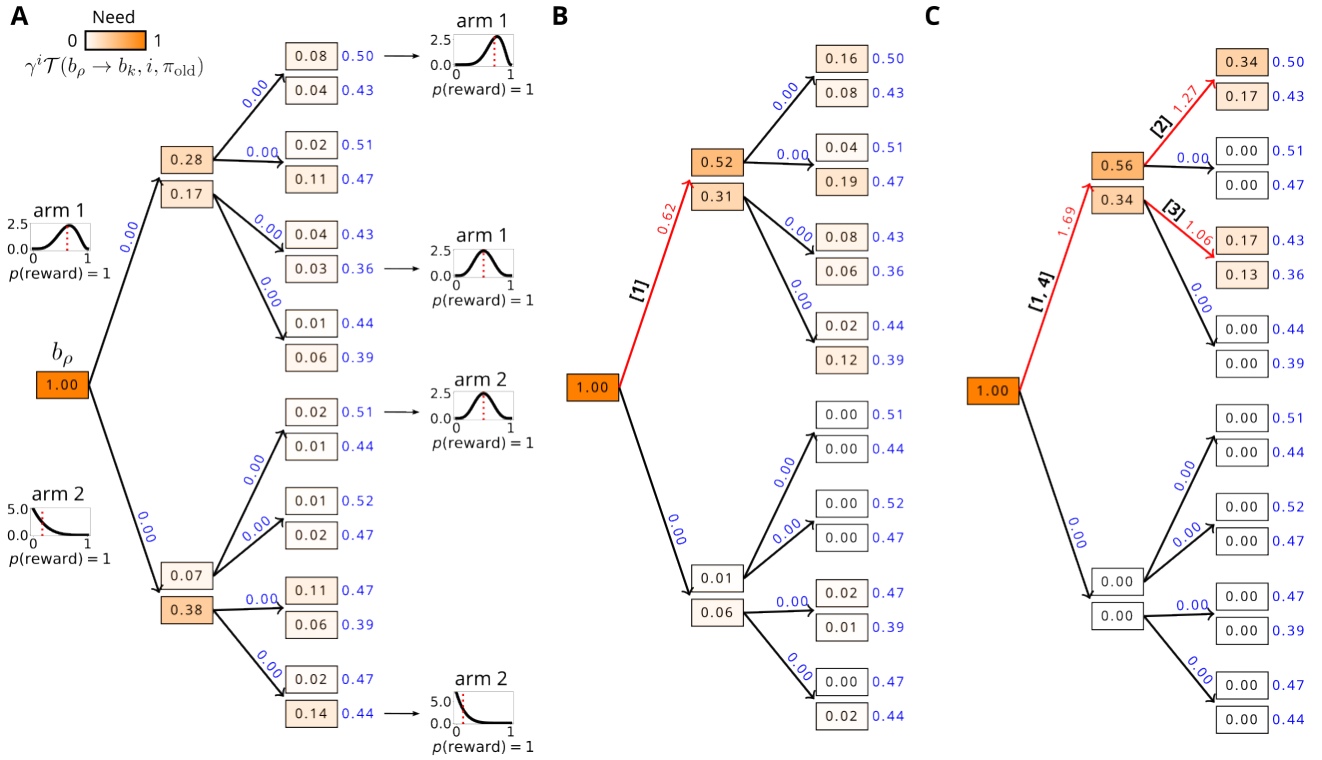


Figure S1: **Replay updates in Bandit belief space.** A) Planning tree of horizon 2. Each rectangle corresponds to a distinct belief state. The leftmost belief state, at the root of the tree, corresponds to the subject's prior belief, b_ρ . The insets next to some belief states graphically demonstrate the subject's belief about the payoff of one of the arms in those belief states (the red dotted lines show the resulting mean payoffs). For the paired belief states, the top ones always result from imagined successful outcomes (received a reward of 1), whereas the bottom ones – from imagined failed outcomes (received a reward of 0). Belief states are coloured according to their exploratory Need; moreover, Need is additionally shown with numbers in each belief state. Since the subject's behavioural policy is stochastic (softmax), all belief states have positive estimated Need (for some belief states, it is shown as 0.00 for demonstration purposes since those values were too small). The black arrows show actions available at each belief state. The top arrows always denote the choice of arm 1 and the bottom arrows – arm 2. The blue numbers above each action arrow denote the Q -values associated with each action in every belief state. B) Single replay update in the belief tree. The subject chose to update the Q -value of arm 1 at the prior belief state (the updated action arrow is highlighted in red) towards the expected value of the two belief states at the next horizon (the new updated value is highlighted in red). This replay update was executed because i) it was estimated to have the greatest EVB; and ii) the estimated EVB of this update exceeded the EVB threshold. Note the effect of generalisation of this individual replay update which is visible in how the Need that the subject calculates for all other belief states changes throughout the tree. C) All replay updates executed by the subject until the estimated benefit was calculated to be below the EVB threshold. The bold numbers in squared brackets show the order in which those updates were executed. The action values highlighted in red are the final action values updated by all shown replay updates in the tree.

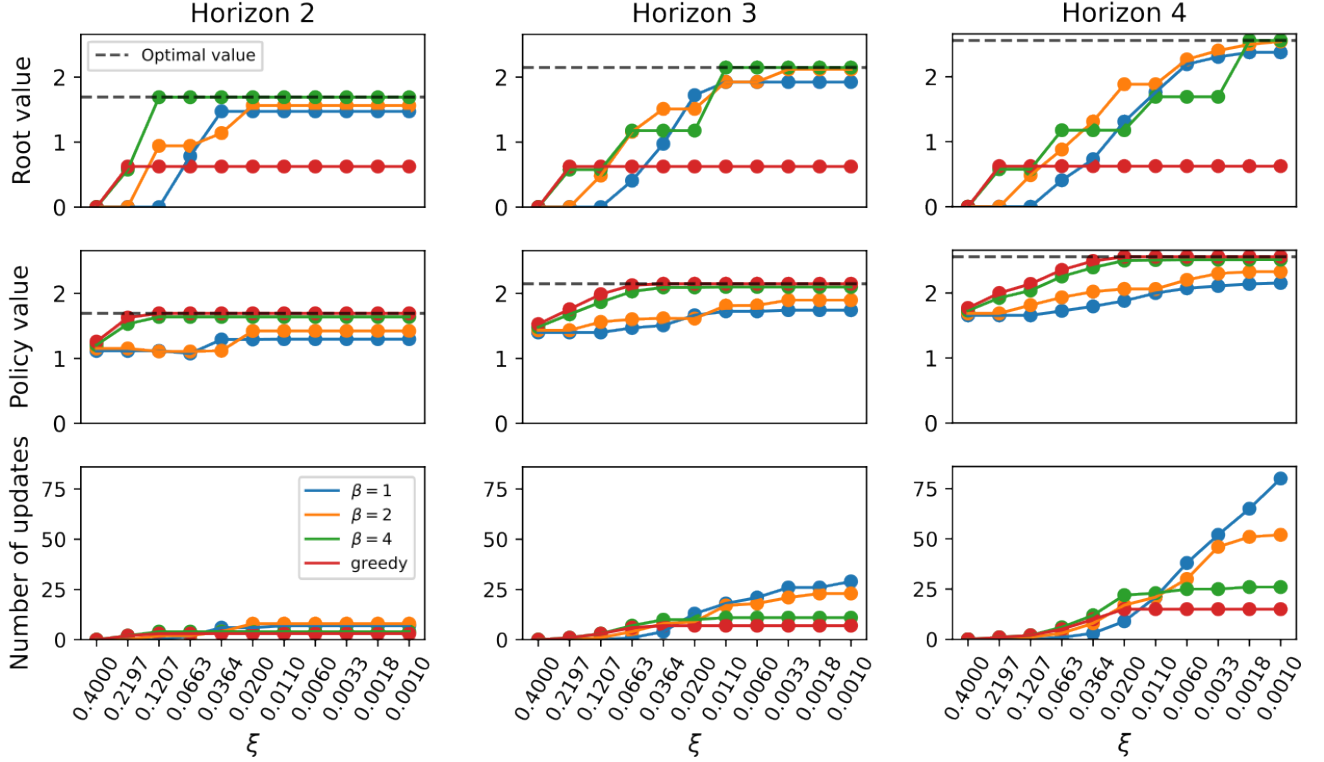


Figure S2: **Policy improvement occasioned by replay.** Top: Evolution of the value of the root belief state in the bandit task (same as in Fig S1) due to replay as a function of the EVB threshold, ξ . Middle: Evolution of the value of the policy (evaluated in the belief tree) which resulted from replay updates at different EVB thresholds. Bottom: Total number of replay updates executed for the different EVB thresholds.

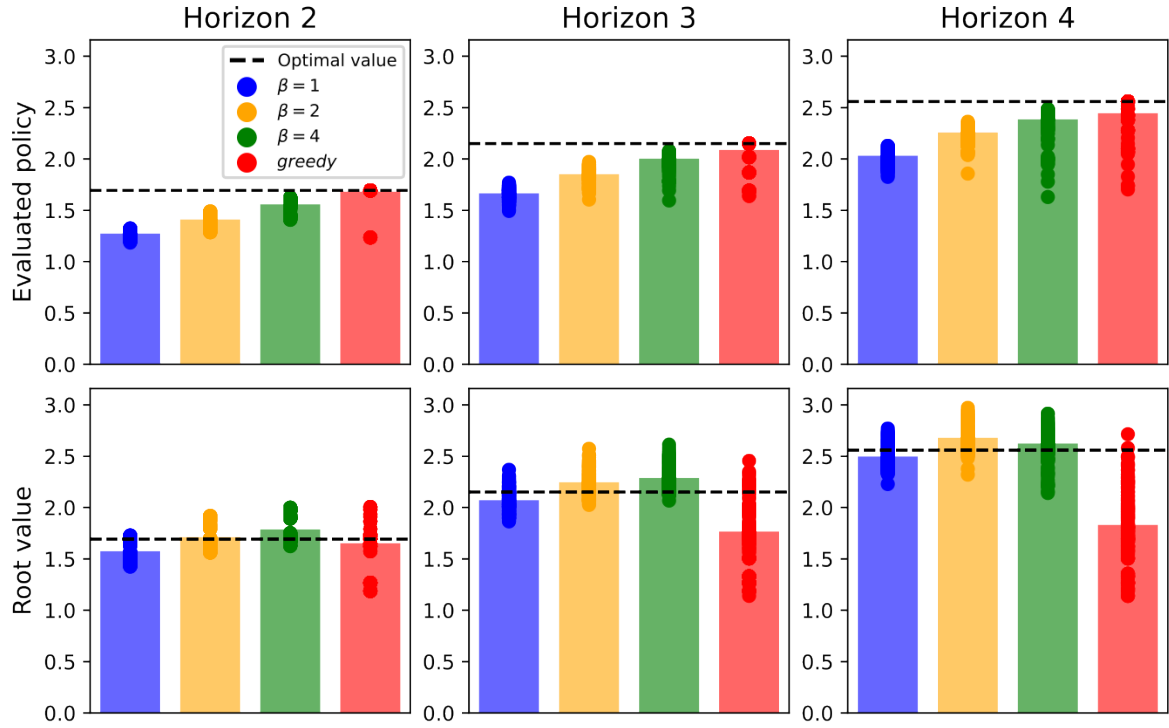


Figure S3: **Effect of initialised behavioural policy.** Top: The final value of the root belief state in the bandit task (same as in Fig S1) due to replay with a fixed EVB threshold. The initialised values of all belief states were randomised to imitate noisy initial experience (or potential changes in the bandit payoff probabilities). The bars show average root belief state values over 200 different tree initialisations. Each dot corresponds to an individual tree. Bottom: Same as above but for the value of the updated policy evaluated in the tree.

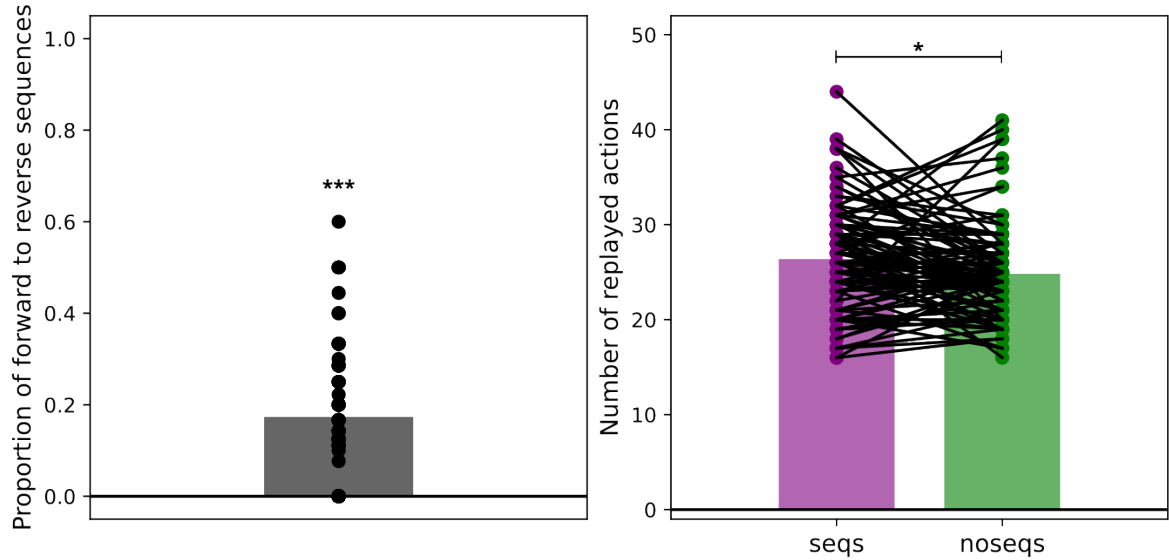


Figure S4: **Sequence replay statistics.** Left: Proportion of forward to reverse sequences replayed in the belief tree in the bandit task with the same prior belief as in Fig S1 with planning horizon set to 4. The initialised values of all belief states were randomised as in Fig S3. The bar shows average proportion over 200 different tree initialisations. Right: Average number of replayed actions in the same tree initialisations as above with and without sequence replay. *** $p < 0.001$, * $p < 0.05$.

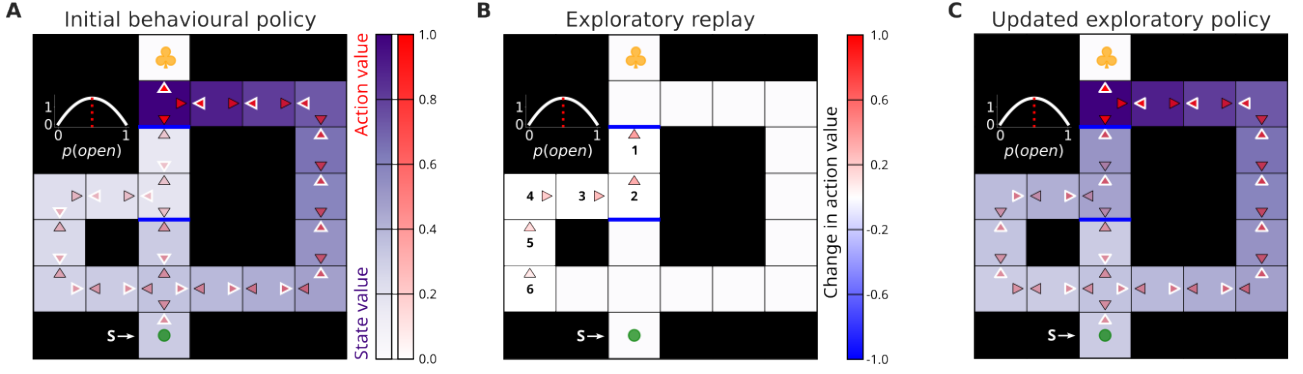


Figure S5: **Uncertainty affects replay choices and their behavioural readout.** The layout of the figure is similar to that of Fig 2. A) Prior state of knowledge of the subject. In this example, the subject's belief was more pessimistic since it indicated a lower subjective probability of the top barrier being potentially open (as evident from the expected probability the subject accorded to this possibility, shown with the red dotted line in the inset). B) The value of exploration was estimated to be lower (since the subject's belief was more pessimistic), and therefore replay did not propagate the benefit of exploration deep enough (towards the subject's location). This is in part owing to the temporal discounting which decays the benefit of exploration with travel distance. C) The updated policy still prescribed the subject to exploit the longer path (maximal Q -values at each state are again shown with white outlines), since the critical action at the junction between the different arms had not been updated by exploratory replay.

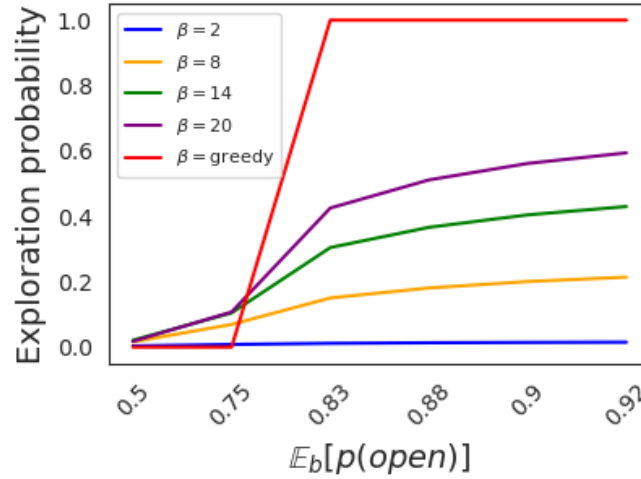


Figure S6: **Relationship between uncertainty, behavioural policy and exploration quality.** The graph shows the marginal probability of directed exploration (approaching and attempting the potential barrier in Figs 2 and 3 from the start state) as a function of the subject's uncertainty and the greediness of its behavioural policy. As the subject's belief ($\mathbb{E}[p(\text{open})]$) in the absence of the barrier increased, it became progressively more likely to engage in the act of directed exploration. The same softmax policy with inverse temperature $\beta = 2$ was used to calculate the priority of replay updates. However, applying different inverse temperature parameters (which subjects might heuristically use to arrange for offline exploration) to the resulting exploratory value function yielded policies with different incentives for exploration.

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