Novelty is not Surprise:

Exploration and learning in human sequential decision-making

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Abstract

Drivers of reinforcement learning (RL), beyond reward, are controversially debated. Novelty and surprise are often used equivocally in this debate. Here, using a deep sequential decision-making paradigm, we show that reward, novelty, and surprise play different roles in human RL. Surprise controls the rate of learning, whereas novelty and the novelty prediction error (NPE) drive exploration. Exploitation is dominated by model-free (habitual) action choices. A theory that takes these separate effects into account predicts on average 73 percent of the action choices of human participants after the first encounter of a reward and allows us to dissociate surprise and novelty in the EEG signal. While the event-related potential (ERP) at around 300ms is positively correlated with surprise, novelty, NPE, reward, and the reward prediction error, the ERP response to novelty and NPE starts earlier than that to surprise.

Introduction

Humans seek not only explicit rewards such as money or praise [1–8], but also novelty [9], an intrinsic reward-like signal linked to curiosity [9–12]. Novelty-driven exploratory actions have been interpreted in the theory of reinforcement learning as steps towards building a model of the world [13]. These world-models represent implicit knowledge that links actions to observations, such as 'if I open the door to my kitchen, I will see my fridge'. However, since the world is much more complex than any model of it, there will occasionally be a mismatch between the expectation arising from the model and the actual observation, e.g., when you return from work, the location of the fridge is suddenly empty because your room-mate has sent it off for repair. Such mismatches generate the feeling of surprise. In this study, we ask whether surprise can be distinguished from novelty and reward in human behavioral choices and in corresponding event related potentials (ERP) of the electroencephalogram (EEG).

Novelty has been shown to elicit activity of dopaminergic neurons [9, 14, 15] similar to that of the reward prediction error (RPE) [1] and has been shown to be encoded along with reward values in temporal and prefrontal areas in monkeys [16]. In psychology, novelty is considered as an intrinsic motivational signal [17, 18] and in reinforcement learning as an exploration bonus [10, 19, 20].

Surprise is triggered by the violation of expectations and manifests itself in pupil dilation [21] and EEG signals [22–24]. Whereas the RPE is a mismatch between the expected reward and the actual reward, surprise is a mismatch between an expected observation and an actual observation. Behavioral experiments [21, 25, 26] and theories [27, 28] suggest that surprise helps humans to adapt quickly to changes in the environment, potentially by modulating synaptic plasticity [29–31].

Surprise is fundamentally different from novelty; if you already know that your fridge would be fetched for repairing, the new arrangement of the kitchen without the fridge is novel but not surprising. While there is some agreement that novelty and surprise are two separate notions, it has been debated how they can be formally defined or distinguished from each other [32–34] and whether they manifest themselves differently in EEG signals [23, 24, 35]. Here, we show, via a specifically designed sequential decision task and a novel hybrid reinforcement learning model, that we can dissociate contributions of surprise from those of novelty and reward in human behavior and identify distinct corresponding ERP signatures.

Results

Experimental paradigm and human behavior

In order to distinguish between novelty, surprise, and reward, we designed an environment (cf.[5, 36]) consisting of 10 states with 4 possible actions per state plus one goal state (Fig. 1A and Fig. 1B). In the human experiments, states were represented as images on a computer screen and actions by four grey disks below the image. Before the experiment, 12 participants were shown all images of the states and were told that their task is to find the shortest path to the goal image. In each state, participants chose an action (by clicking on one of the grey disks) which brought them to the next image and then chose the next action. The episode ended when the goal image was found. Unknown to the participants, the eleven states can be classified into three types: progressing states, trap states, and a goal state (Fig. 1B). Progressing states are the 'good' states that bring participants closer to the goal whereas trap states are the 'bad' states that are off the

direct path to the goal. At each non-goal state, one of the 4 possible actions brings participants to the next progressing state, two actions bring them to one of the trap states, and one action makes them stay at the current state.

The experiment was organized in 10 episodes which, unknown to the participants, were divided into two blocks of 5 episodes each. During the 1st episode of the 1st block, participants took between 34 and 214 actions (mean 117 and std 54) until they found the goal (Fig. 1C). They then continued for another 4 episodes, each time starting in a new initial state that had been randomly chosen but kept fixed across participants. After the first episode, participants learned to reach the goal in less than 20 steps (Fig. 1C). After the end of the 5th episode, two states (state 3 and 7 in Fig. 1D) were swapped, without announcing it to the participants. Participants continued for another 5 episodes with the novel layout of the environment (2nd block, Fig. 1D). They were significantly faster in finding the goal state in the 1st episode after the swap compared to the 1st episode of the 1st block (Fig. 1C).

Because of the particular structure of the environment, trap states were encountered many times by participants during the 1st episode of the 1st block, while the states closer to the goal were less visited and hence were more novel. On the other hand, the swap in the 1st episode of the 2nd block made several transitions unexpected even though the states themselves were not novel, allowing us to study the effect of surprise independent of novelty.

Measuring Novelty and Surprise

We assume that states that are encountered frequently are experienced by participants as less novel than those encountered for the first time. We therefore define novelty of a state s as a decreasing function of the relative frequency of encountering state s compared to the total number of actions taken so far (see Methods). At the beginning of the 1st episode in block 1, all states have identical novelty. Since participants often fall into one of the trap states, novelty of trap states decreases rapidly (Fig. 2A). Hence, before the end of the 1st episode, the novelty is highest for states in the proximity of the goal (Fig. 2B). This observation suggests that seeking novel states will, in our environment, effectively lead a participant closer to the goal, even *before* the participant knows where the goal is located, i.e., before encountering the goal for the first time. When designing our model below, we will use this insight to assign novelty values to states, where novelty values influence behavioral decisions similar to reward-based values.

To navigate in such a complex environment, we assume that participants build an internal model of the environment ('world-model'), i.e., we hypothesize that participants estimate the probabilities of transitions from a given state to another state when performing a given action. With this assumption, we predict that participants are surprised in the 1st episode of the 2nd block after the swap of states 3 and 7. We define surprise as a mismatch between the observed state and the prediction of the current world-model of the participant. More precisely, our measure of surprise quantifies how 'unexpected' the next image (state s_{t+1}) is given the previous state s_t and the chosen action a_t [28] (see Methods). Our surprise measure is an increasing function of the state-prediction error [5] (see Methods) and takes high values during the first episode of the second block whenever participants encounter states 3 or 7 or transit from state 3 or 7 to another state (Fig. 3A and Fig. 3B).

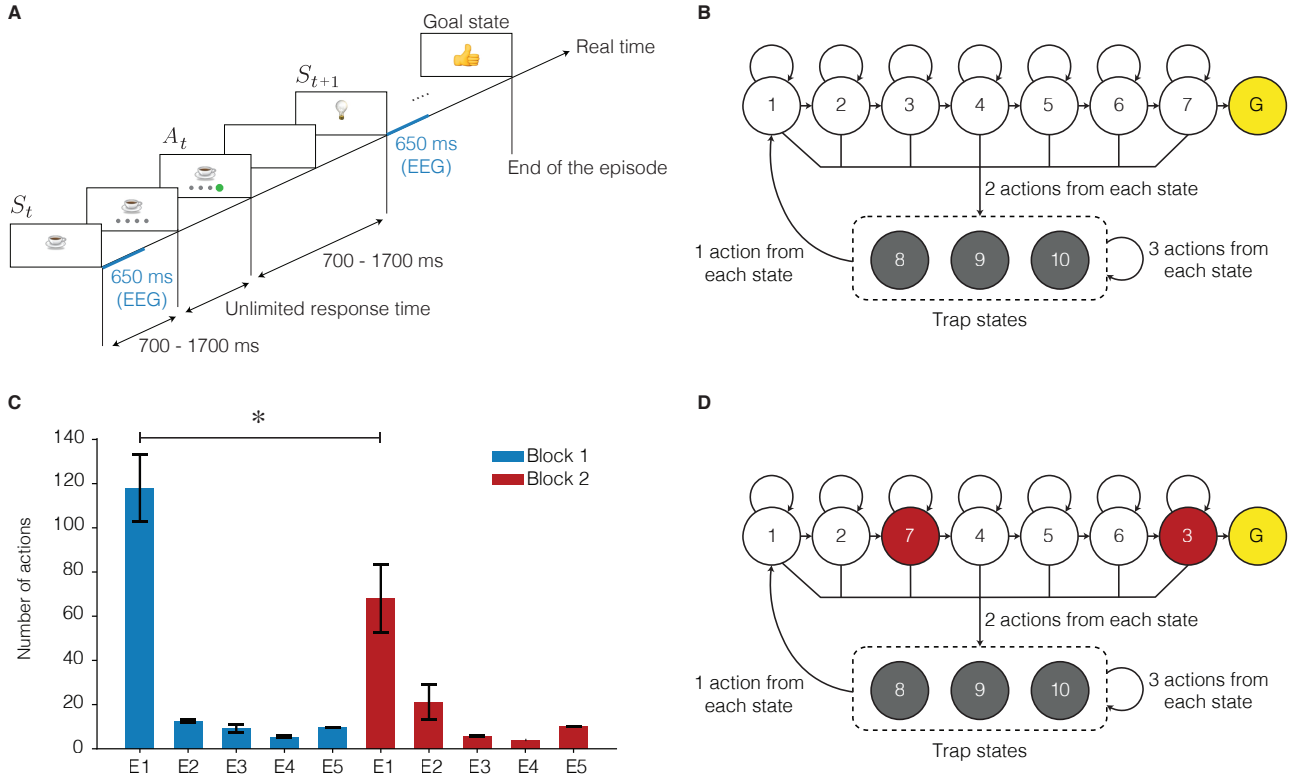

Figure 1: Experimental paradigm. **A.** After image onset, participants have to wait for 700-1700ms randomly chosen until grey disks are presented at the bottom of the image. After clicking on one disk, a blank screen is presented for another random interval of 700 to 1700ms, before the next image appears. The goal image is a 'thumb-up' image in this example. Different participants saw different images, but the underlying structure was identical for all participants. The blue lines indicate the window of EEG analysis. **B.** Structure of the environment of block 1. There are 10 states with 4 actions each plus a goal state (G). States 1-7 are *progressing states* and states 8-10 are *trap states*. For each progressing state, one action leads participants to the next progressing state, two actions lead participants to one of the trap states, and one action makes participants stay at the current state. For each trap state, three actions lead participants to one of the trap states, and one action leads participants to state 1. Not all action arrows are drawn for the trap states to simplify illustration. **C.** Average number of actions of participants during block 1 (blue) and block 2 (red): The 1st episode of the 2nd block was significantly shorter than the 1st episode of the 1st block (one-sample t-test, p-value=0.035). Error bars show the standard error of the mean. **D.** Environment used in block 2: The images presenting state 3 and state 7 (in red) were swapped. Other transitions remained unchanged.

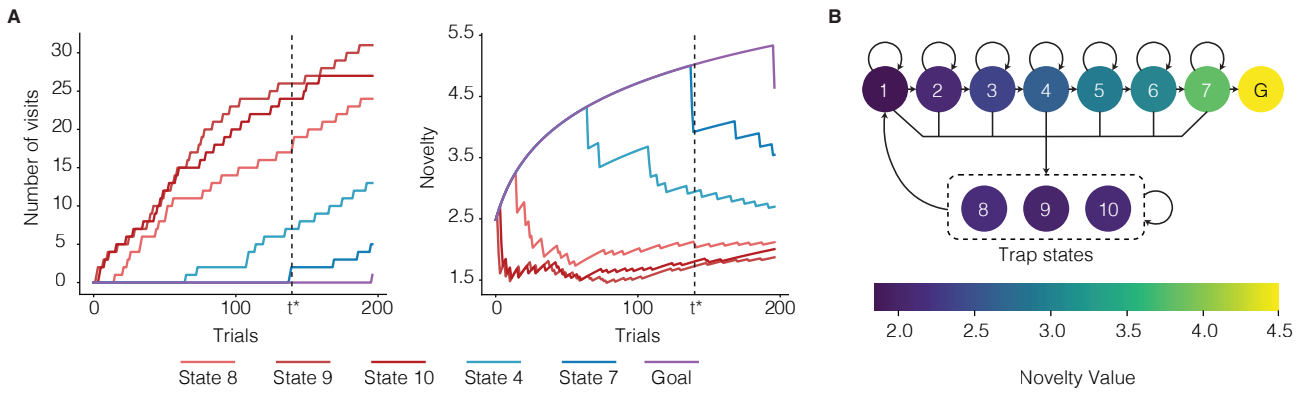

Figure 2: Novelty in episode 1 of block 1. **A.** The number of state visits (left panel) and novelty (right panel) as a function of time for one participant: The number of visits increases rapidly for the trap states and remains 0 for a long time for the states closer to the goal. Novelty of each state is defined as the negative log-frequency of observing that state (see Methods) and, hence, increases for states which are not observed as time passes. The first time participants encounter state 7 (the state before the goal state) is denoted by t^*. **B.** Average (over participants) novelty (color coded) at t^*: Novelty of each state is a decreasing function of its distance from the goal state.

The SurNoR algorithm: Distinct contributions of novelty and surprise to behavior

We hypothesize that participants use novelty to explore the environment and surprise to modulate the rate of learning. The hypothesis is formalized in the form of the Surprise-Novelty-Reward (SurNoR) algorithm and tested given the behavioral data of 12 participants (see Methods).

Novelty in SurNoR plays a role analogous to that of reward. For example, in standard Temporal-Difference (TD) Learning, the RPE, derived from reward-based Q-values, serves as a learning signal even for states a few steps away from the goal [13]. Analogously, in the SurNoR model, novelty is a reward-like signal with an associated novelty prediction error (NPE) derived from novelty-based Q-values. In the SurNoR model, the two sets of Q-values, reward-based and novelty-based, are used in a hybrid model [5, 6] that flexibly combines model-based with model-free action selection policies (Fig. 3C).

Surprise in the SurNoR model is derived from a mismatch between observations of the next state and predictions arising from the world-model that lies in the model-based branch of SurNoR. In the SurNoR algorithm, surprise is used in two different ways. First, a high value of surprise leads to a large learning rate for the update of the world-model. Second, surprise influences the learning rate of the model-free reinforcement learning branch.

We predict that, if the behavior of participants is well described by the SurNoR algorithm, they should use an action policy that attracts them to novel states, in particular during the first episode before they have found the goal. If participants do not exploit novelty, standard (potentially hybrid) reinforcement learning schemes should be sufficient to explain the behavior. Furthermore, we predict that, if the behavior of participants is well described by the SurNoR algorithm, then surprising events during the first episode of block 2 should significantly change the behavior of participants; if participants do not exploit surprise, standard hybrid models combining model-based and model-free reinforcement learning [5, 6] should be sufficient to describe the behavior.

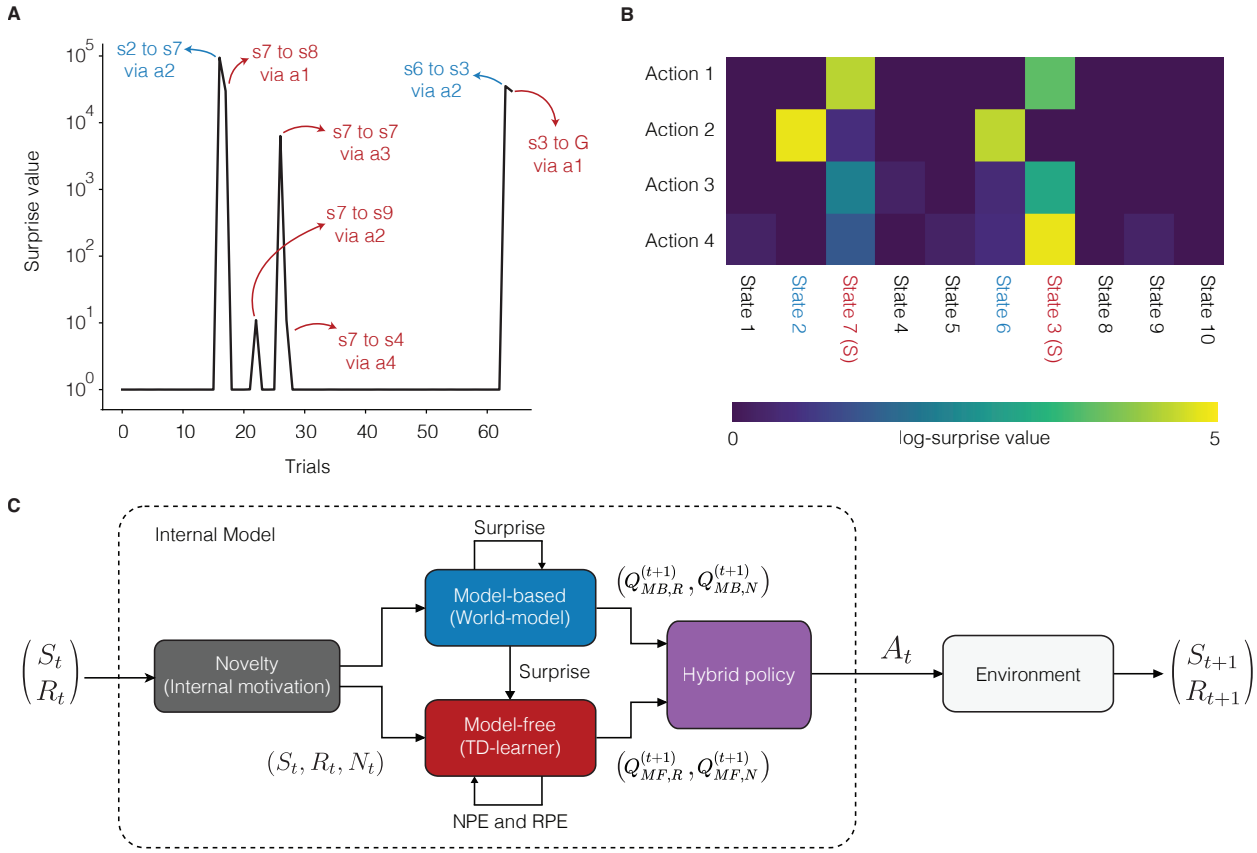

Figure 3: Surprise as a modulator of the learning rate in episode 1 of block 2. **A.** Surprise as a function of time since start of the second block for one participant: Surprise values are almost zero most of the time, because the participant has already learned the transitions in the environment during the 1st block. The surprising transitions are the ones to the swapped states (blue) and the ones from the swapped states (red). **B.** Maximal log-surprise values (yellow=large surprise) during the first episode of the second block, averaged over all participants. The swapped states are marked in red and the states before them in blue. One action from each swapped state is not surprising, i.e., the action leading participants to trap states both before and after the swap. **C.** Block diagram of the SurNoR algorithm: Information of state S_t and reward R_t at time t is combined with novelty N_t (grey block) and passed on to the world-model (blue block, implementing the model-based branch of SurNor) and TD learner (red block, implementing the model-free branch). The surprise value computed by the world-model modulates the learning rate of both the TD-learner and the world-model. The output of each block is a pair of Q-values i.e, Q-values for estimated reward $Q_{MF,R}$ and $Q_{MB,R}$ as well as for estimated novelty $Q_{MF,N}$ and $Q_{MB,N}$. The hybrid policy (in purple) combines these values.

Both surprise and novelty are needed to explain behavior

To test whether all elements of SurNoR (i.e., surprise, novelty, and hybrid policy) are necessary for explaining behavior or whether a simpler or an alternative model would have the same explanatory power, we compared 12 alternative algorithms with SurNoR: 4 model-based (MB), 4 model-free (MF), and 3 hybrid (Hyb) algorithms plus a null model based on a random choice (RC) of actions. Seven out of these 12 algorithms use surprise (+S), and five use novelty (+N, see Supplementary Material). Given the behavioral data of all 12 participants, we estimated the log-evidence of all 13 algorithms (including SurNoR) by their cross-validated maximum log-likelihood (see Methods). Comparison of the algorithms' log-evidences (Fig. 4A) shows that SurNoR explains human behavior significantly better than its alternatives. In addition, a Bayesian model selection approach with random effect [37] indicates that the SurNoR algorithm outperforms the alternatives with an Exceedance Probability of 0.99 (Fig. 4B and Methods).

The 1st episode of the 1st block is optimal to study how novelty influences behavior (middle panel in Fig. 4A). Our results show that all algorithms with novelty-seeking (+N) explain the behavior significantly better than models with random exploration strategy (RC) or optimistic initialization (MB+S+OI, MF+OI, and Hyb+S+OI), i.e., two classic approaches for exploration [13]. Our results also show that novelty-seeking explains behavior better than uncertainty-seeking (+U), a state-of-the-art exploration methods in reinforcement learning [38, 39]. The models with uncertainty-seeking (MB+S+U, MF+S+U, and Hyb+S+U) use surprisal (i.e., the logarithm of our surprise measure) as an intrinsic reward as opposed to models with novelty-seeking that use novelty as an intrinsic reward.

Surprise becomes important in the first episode of the 2nd block (right panel in Fig. 4A). Indeed, the SurNoR model is significantly better than a hybrid model with novelty but no surprise (Hyb+N); similarly, model-free reinforcement learning with novelty and surprise (MF+S+N) is significantly better than model-free reinforcement learning with novelty alone (MF+N, right panel in Fig. 4A). Our results show that a constant rate of learning and forgetting as implemented in standard models without surprise is not sufficient for explaining the choices of participants in the episode after the swap. Rather, the rate of learning and forgetting has to be modulated by a measure of surprise.

Overall, SurNoR is better than all 12 competing algorithms by a large margin, indicating that a combination of model-based and model-free algorithms explains behavior better than each algorithm separately, consistent with the notion of parallel, model-based and model-free, policy networks in the brain [3, 5, 6]. Going beyond these earlier studies, the results with SurNoR indicate that surprise and novelty are both necessary to explain human behavior in our task. Novelty is necessary to explain behavior during phases of exploration while surprise is necessary to explain behavior during the rapid re-adaption after a change in the environment

Individual decisions are dominated by model-free policy network

We wondered whether the SurNoR model is able to predict the individual actions of participants. Considering the most probable action of the model in a given state as the prediction of a participant's next action in that state, we found that the SurNoR algorithm predicted the correct action in the 1st episode of the 1st block with an accuracy of 51±3% (3-fold cross validated, mean and standard error of the mean over 12 participants, see Methods - Fig. 4C). Note that this accuracy is achieved in the absence of any a-priori preference of actions at initialization and is significantly higher than the accuracy rate of the naive random exploration strategy (25%,

chance level); SurNoR's predictions are also significantly better than the predictions of directed exploration through optimistic initialization (OI) of values or uncertainty-seeking policy (U) in a model-free, model-based, or a hybrid RL algorithm without a novelty preference. Models with OI could at best predict 36±3% of the actions (for MB+S+OI), and the uncertainty-seeking strategy could at best predict 46±3% (for Hyb+S+U); one-sample t-test p-values for comparing their accuracy rates versus SurNoR's are 0.0025 and 0.01, respectively. A crucial difference between OI and novelty-based exploration is that OI prefers those actions that have been less frequently chosen in the past, while novelty-seeking prefers actions that lead the agents to novel states, even if these are a few actions ahead and the outcome of the current action is known. Uncertainty-seeking is similar to OI because the uncertain actions are also those that have been less frequently chosen in the past.

Similarly, in the 1st episode of block 2, when participants are confused because of the swap of states 3 and 7, the SurNoR algorithm predicts $56 \pm 3\%$ of the actions of the 12 participants (Fig. 4C). In the remaining episodes 2-5 of the two blocks, the SurNoR algorithm predicts $89 \pm 2\%$ of the action choices (Fig. 4C). Most of these actions move participants closer to the goal. The intrinsic uncertainty of action choices with the SurNoR model can be estimated from the entropy of the action choice probabilities across the four possible actions (Fig. 4C). Uncertainty decreases during the first three episodes as participants become familiar with the environment, but it jumps back to higher values after the swap of states at the beginning of block 2.

The SurNoR model combines a model-free with a model-based learning component (Fig. 5B), and we wanted to analyze the relative importance of each of the two components in explaining the action choices of participants. We therefore fitted the parameters of the SurNoR algorithm to the behavior of 12 participants (see Methods). In order to evaluate the relative importance of the two components, we normalized the Q-values of both branches and determined the relative weight of each branch (see Methods) during episode 1 and episodes 2-5 of each block (Fig. 5D). We find that the model-free branch dominates the actions. Thus the world-model is of secondary importance for action selection and is mainly used to detect surprising events. In order to quantify the influence of surprise on learning, we plot the learning rate (of the model-free Q-values $Q_{\mathrm{MF,R}}$ and $Q_{\mathrm{MF,N}}$) as a function of surprise (Fig. 5A). We find that non-surprising events lead to a small learning rate of 0.06 whereas highly surprising events induce a learning rate that is more than 8 times higher (Fig. 5A and Fig. 5C) indicating that surprise strongly influences the update of model-free Q-values.

In conclusion, the SurNoR algorithm is able to predict individual actions with a high accuracy: it predicts $63 \pm 2\%$ of all actions and $74 \pm 3\%$ of the actions after the first time finding the goal. A detailed analysis of our results suggests that participants (i) rely on propagation of novelty information via NPE in the first episode, (ii) base their decisions mainly on the model-free learner, and (iii) use surprise to modulate the learning rate.

EEG correlates with novelty and surprise

Since surprise and novelty turned out to be important components of SurNoR in explaining the participants' behavior, we wondered whether both are reflected in the ERP. We first performed a grand correlation analysis in which we pooled the more than 2500 trials of 10 participants together after normalizing their ERPs to unit energy (see Methods; two participants were excluded because of noise artifacts in the recordings). We then computed the correlation of the ERP amplitudes, for

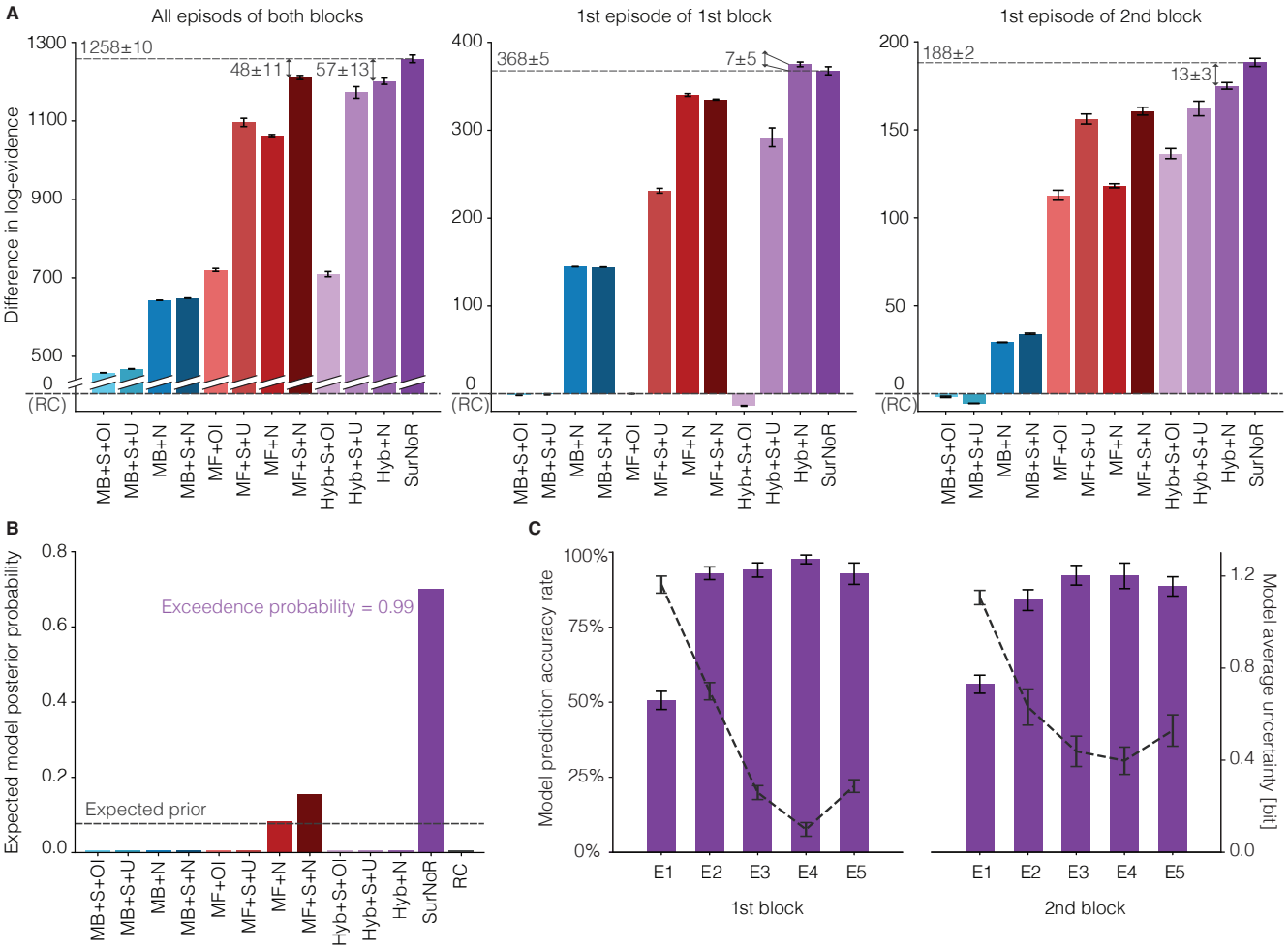

Figure 4: Model comparison of model-based (MB, blue bars), model-free (MF, red bars), and hybrid algorithms (Hyb and SurNoR, purple bars). Exploratory behavior is either induced by optimistic initialization (+OI), uncertainty-seeking (+U), unbiased random action choices ('RC'), or novelty-seeking (+N); e.g., model-based with novelty seeking is denoted as MB+N. SurNoR and the model-free or hybrid algorithms annotated with '+S' use surprise to modulate the learning rate of the model-free TD learner; SurNoR and all algorithms annotated with '+S' use surprise modulation also during model building (see Methods). **A.** Difference in log-evidence (with respect to 'RC') for the algorithms for all episodes of both blocks (left panel), the 1st episode of the 1st block (middle), and the 1st episode of the 2nd block (right panel). High values indicate good performance; differences greater than 3 or 10 are considered as significant or strongly significant, respectively (see Methods); a value of 0 corresponds to random action choices (RC). The random initialization of the parameter optimization procedure introduces a source of noise, and the small error bars indicate the standard error of the mean over different runs of optimization (Methods, statistical model analysis). **B.** The expected posterior model probability [37] given the whole dataset (Methods) with random effect assumption on the models. **C.** Accuracy rate of actions predicted by SurNoR (left scale and purple bars: mean and standard error of the mean across participant) and the average uncertainty of SurNoR (right scale and dashed grey curve: entropy of action choice probabilities).

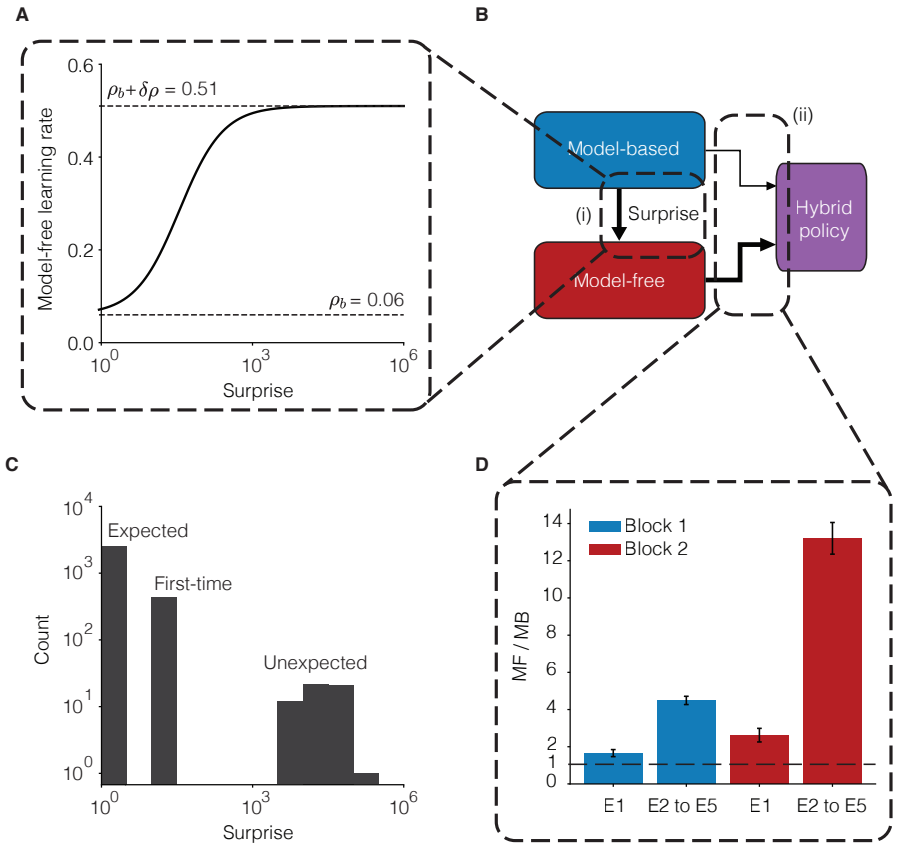

Figure 5: Model-based surprise modulates model-free learning. **A.** The learning rate of the model-free branch as a function of the model-based surprise, after fitting parameters to the behavior of all participants (see Eq. 2 in Methods). The model-free learning rate for highly surprising transitions is more than 8 times greater than the one for expected transitions. **B.** Three modules from the block diagram of Fig. 3C. There are two types of interactions between the model-based and the model-free branches of SurNoR: (i) The model-based branch modulates the learning rate of the model-free branch and (ii) the weighted (arrow thickness) outputs of the model-based and the model-free branches influence action selection (hybrid policy). **C.** The histogram of surprise values across all trials of 12 participants. The distribution is multimodal with high surprise for the unexpected transitions in episode 1 of block 2, medium surprise for whenever a transition is experienced for the first time, and low surprise for the expected transitions (expected). **D.** The relative importance of model-free (MF) compared to model-based (MB) in the weighting scheme of the hybrid policy during different episodes. Vertical axis: dominance of model-free (see Methods). Values larger than one (dashed line) indicate that the model-free branch dominates action selection. Error-bars indicate standard error of the mean.

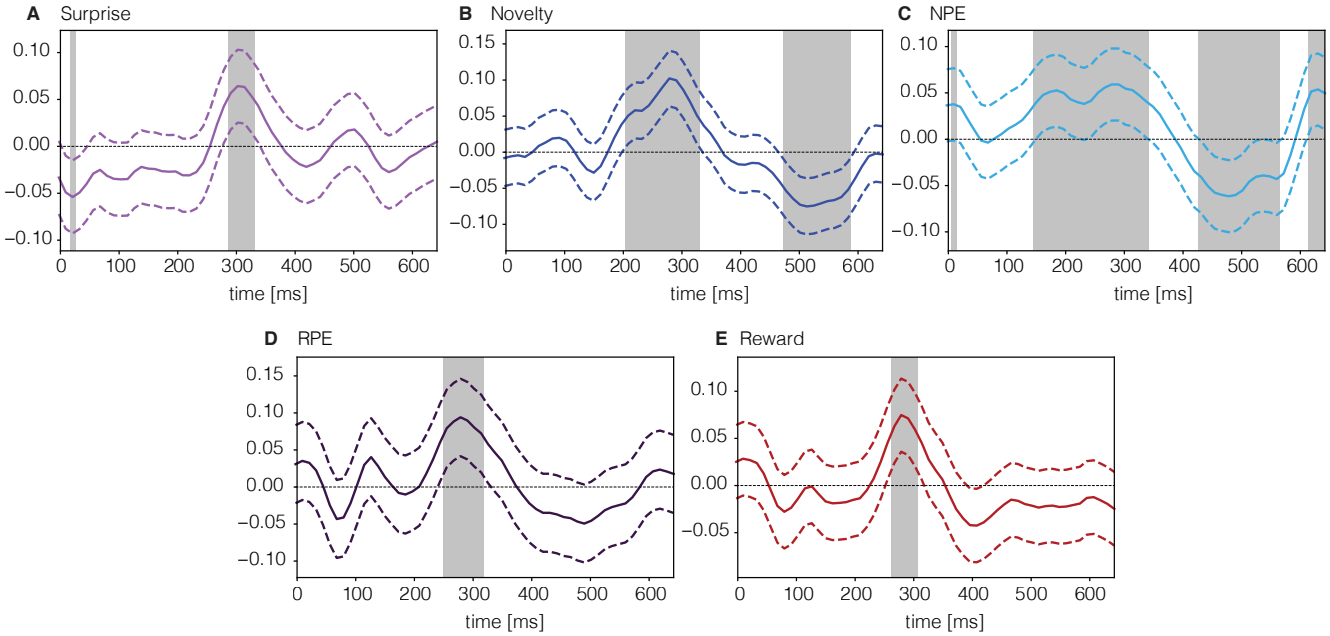

Figure 6: Grand correlation analysis of normalized ERPs over all 2524 trials of 10 participant. The dashed lines show confidence intervals. Shaded areas indicate intervals of significant correlations (FDR controlled by 0.1, one-sample t-test). Correlations of ERP with **A.** Surprise, **B.** Novelty, **C.** NPE, **D.** RPE (computed after excluding the trials from the 1st episode of the 1st block during which RPE is equal to 0) and **E.** Reward.

each time point after the trial onset, with the model variables 'Surprise', 'Novelty', 'Reward, 'NPE', or 'RPE' (capital initial letters indicate the 5 model variables). We find that Surprise, Reward, and RPE show significant positive correlations with the ERP amplitudes at around 300ms after stimulus onset (Fig. 6), in agreement with the well known correlation of the P300 amplitude with Surprise [24, 40, 41] and the well known correlation of the Feedback-Related Negativity (FRN) component with RPE [42, 43]. Moreover, compared to Surprise, Novelty and NPE have a broader positive correlation window with the ERP starting at around 200ms and ending at around 320ms after stimulus onset, and a second window with significant negative correlations with the ERP from around 450ms to 550ms. Thus Novelty and NPE have an ERP signature that is distinct from that of Surprise, Reward, or RPE (Fig. 6).

Second, we wondered how much of the variations in the ERP amplitudes could be explained by a linear combination of our five model variables, i.e., Suprise, Novelty, NPE, RPE, and Reward. We performed a trial-by-trial multivariate linear regression (MLR), separately for each participant. To be able to identify the separate contributions of each model variable to the regression, we needed to decorrelate them from each other. As expected from the design of the experiment, the cross-correlations between the normalized (zero mean and unit variance) sequences of Surprise, Novelty, and NPE are negligible (see Supplementary Material); however, the sequences of Reward and RPE are highly correlated with each other, mainly because Reward and RPE are both high at the goal state. Using principal components analysis over Reward and RPE, we find R_+ (the sum of RPE and Reward) and R_- (their difference) as their decorrelated combinations (see Methods). We then extracted the components of Surprise, Novelty, and NPE orthogonal to R_+ and R_- (see Methods). The resulting variables, denoted by an index $\perp$, are each orthogonal to R_+ and R_-, while staying

very similar to the original signals, e.g., $\text{Surprise}_\perp$ is highly correlated with Surprise, and $\text{NPE}_\perp$ is highly correlated with NPE (see Supplementary Material).

For each participant, we consider the normalized $\text{Surprise}_\perp$, $\text{Novelty}_\perp$, $\text{NPE}_\perp$, R_+, and R_- as explanatory variables in order to predict the ERP amplitude at a given time point. We find 4 time intervals with an encoding power (the adjusted R-squared, see Methods) significantly greater than zero (one-sample t-test, FDR controlled by 0.1, Fig. 7A and B; note that adjusted R-squared can take negative values, e.g., see baseline in Fig. 7A). The 1st time window is around 193 ± 5ms; the P300 component can be linked to the 2nd time window which spans from 286 to 321 ± 5ms; since the 3rd time interval is long (from 392 to 487 ± 5ms), we split it into two time windows of equal size (W3a and W3b in Fig. 7B); and the last window extends from 532 to 574 ± 5ms.

To study the contribution of surprise and novelty to encoding power, we focus on these time windows and compute the average of the regression coefficients of all explanatory variables in each time window (Fig. 7C). Our results show that in the the second time window (286 to 321 ± 5ms), $\text{Surprise}_\perp$, $\text{Novelty}_\perp$, $\text{NPE}_\perp$, and R_+ all have a significant positive coefficient in MLR (Fig. 7C, 2nd panel, FDR controlled by 0.1). While the coefficients for $\text{Surprise}_\perp$, $\text{NPE}_\perp$, and R_+ sharply peak at around 300ms, the coefficient for $\text{Novelty}_\perp$ has a broader peak starting at around 200ms (Fig. 7B) with a close to significant positive value during the 1st time window. This observation suggests that positive correlations of novelty with the ERP potentially extend from the 1st time window to the 2nd one, in agreement with our grand correlation analysis.

While consistent with previous studies of surprise in the ERP [23, 24, 40, 41], our results indicate that $\text{Surprise}_\perp$ and $\text{Novelty}_\perp$ contribute each separately to the ERP components at around 300ms. Furthermore, we find that $\text{NPE}_\perp$ is yet another independent contributor to these components. As expected from previous studies [42, 43], R_+ also shows a positive correlation with the ERP amplitude at around 300ms. While the multivariate analysis based on five explanatory variables showed significance in the later time windows (Fig. 7A), individual contributions of $\text{Surprise}_\perp$ or $\text{Novelty}_\perp$ or $\text{NPE}_\perp$ alone remained below significance level even though $\text{Novelty}_\perp$ had a close to significant negative coefficient in the last window (Fig. 7C).

To summarize, the grand correlation analysis yields time windows of significance for Novelty and NPE that start 50 to 100ms *before* those of Surprise or Reward, indicating distinct contributions. Moreover, $\text{Novelty}_\perp$ and $\text{NPE}_\perp$ explain a significant fraction of the variations of the ERP at around 300ms that is not explained by $\text{Surprise}_\perp$ and R_+ alone. Importantly, NPE has significant correlations both in the grand correlation analysis and in the analysis of variations, consistent with our earlier finding that NPE is important to explain behavior.

Discussion

Combining a deep sequential decision-making task with the SuNorR model, an augmented reinforcement learning algorithm, we were able to extract the contributions of surprise, novelty, and reward to human behavior. We found that the human brain (i) uses surprise to modulate learning in changing environments and (ii) uses novelty as an intrinsic motivational drive to explore the world. Moreover, the model variables Suprise, Novelty, NPE, Reward, and RPE could well explain variations of the EEG amplitudes on a trial-by-trial basis.

As expected from previous theoretical [27–29, 31, 44] and experimental work [21, 25, 26], our results suggest that the human brain uses surprise to modulate the learning of its world-model.

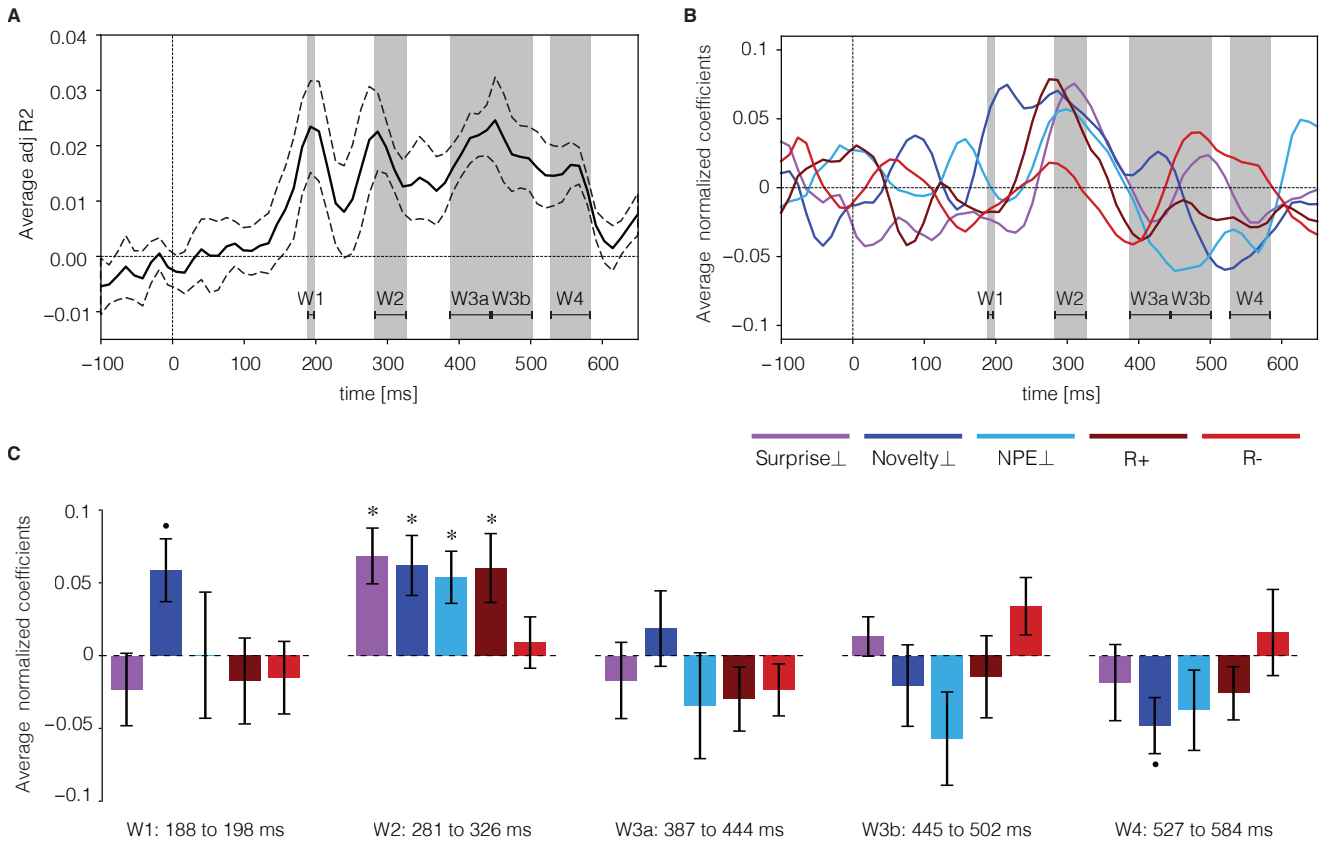

Figure 7: ERP variations explained by trial-by-trial and participant-by-participant multivariate linear regression analysis. Surprise$_\perp$ (magenta), Novelty$_\perp$ (dark blue), NEP$_\perp$ (light blue), R_+ (brown) and R_- (red) were used as explanatory variables, and the ERP amplitude at each time point was considered as the response variable. **A.** Encoding power (adjusted R-squared values) averaged over 10 participants (dashed lines show the standard error of the mean) at each time point. Shaded areas and horizontal lines indicate four time intervals (W1, ..., W4) of significant encoding power (FDR controlled by 0.1, one-sample t-test, only for the time-points after the baseline). The 3rd time interval has been split into two time windows of equal length for the analysis in C. **B.** The value of model coefficients (averaged over participants) for Surprise$_\perp$, Novelty$_\perp$, NEP$_\perp$, R_+, and R_- as a function of time. Errors are not shown to simplify the illustration. **C.** In each of the 5 time windows, the coefficients plotted in B have been averaged over time. Error bars show the standard error of the mean (across participants). Asterisks shows significantly non-zero values (FDR controlled by 0.1 for each time window, one-sample t-test). The Novelty$_\perp$ coefficients in the 1st and the last time windows (dot) have p-values of 0.03 and 0.04, respectively, which are not significant after FDR correction. In the second time window, Surprise$_\perp$, Novelty$_\perp$, NEP$_\perp$, and R_+ have significantly positive coefficients.

Rather unexpectedly, however, our results indicate that humans hardly use their world-model to plan behavior; instead they mainly rely on model-free TD learning with eligibility traces to choose their next actions. Importantly, although the surprise signal is triggered by a mismatch between an observation and the predictions of the world-model, the modulatory effect of surprise is not limited to readjusting the world-model but also used to modulate the learning rate of model-free TD-learning. Following the common interpretations of model-based reinforcement learning algorithms as descriptions of human planning behavior and model-free reinforcement learning algorithms as descriptions of human habitual behavior [3, 5, 6], our results suggest that (i) in the absence of surprise, humans prefer habitual behavior (potentially to reduce computational costs of decision-making [45]) and (ii) errors in their world-model make them reconsider their habitual behavior. Our results extend findings that humans use hybrid policies in two-stage decision tasks [3, 5] to the case of deep sequential decision tasks in the presence of abrupt changes. The dominance of model-free behavior in such deep tasks does not exclude that humans used model-based planning in shallow tasks that are easily comprehensible thanks to a spatial arrangement of states or explicit instructions [46].

In the SurNoR model, surprise measures how 'unexpected' the next event is, conditioned on the current state and the chosen action; in contrast, novelty measures how 'rare' the next event is, independent of our expectations derived from a world-model. Our results show that exploration based on novelty-seeking (as opposed to random exploration [47] or uncertainty-seeking [38, 39]) can explain human behavior in our sequential decision-making task better than all tested alternative models. The presence of trap states in our behavioral paradigm makes novelty an 'internally rewarding' signal that helps participants to avoid 'traps'. In general, an agent's desire for seeking novel events depends on its inductive biases [9]. Following the idea of information search in active sampling [17], we speculate that whether novelty is an informative cue (e.g., about the location of the goal) or not must be itself inferred by participants through the exploration procedure. Formulating and testing such a hypothesis is an interesting direction for future studies.

In contrast to published exploration strategies which give preference to those actions for which the outcome is most uncertain, i.e., those that have been tried least [38, 39, 47, 48], exploration based on novelty-seeking gives preference to actions that ultimately lead the agent to previously unvisited or less visited states, even if the agent is perfectly sure about the transition to the next state. Since, in the SurNoR model, Novelty is treated completely parallel to an external Reward, TD-learning based on NPE along with eligibility traces rapidly diffuses information about novel states to far-away non-novel states just as TD-learning based on RPE along with eligibility traces rapidly diffuses information about rewarding states to far-away non-rewarding states. Importantly, we found that NPE is a variable that has explanatory power for the ERP which adds to, and is different from, the explanatory power provided by Reward, RPE, or Surprise. The manifestation of a separate NPE signal in neural activities may open a new door for further developments of theories and experiments on novelty-driven activity of dopaminergic neurons and other neuromodulators [14, 15, 49, 50].

The SurNoR algorithm suggests that participants treat novelty and reward as separately estimated values - as opposed to adding them into a single value estimator [12, 19, 20]. This separation enables participants to rapidly switch from exploration to exploitation, once they have found the goal. Based on this insight, we make the following prediction: if participants find a goal state, but expect a second more rewarding goal state, they will continue to explore and potentially spend a large amount of time in a novelty-rich segment of an extended version of the environment of Fig. 1

- see Supplementary materials.

Our EEG analysis shows that variables of the SurNoR model can significantly explain the variations of ERP amplitudes in several time-windows: Surprise, Novelty, NPE, and Reward/RPE all significantly contribute to the encoding power in the time-window around 300ms. The positive contributions of Novelty, Surprise, and Reward and RPE in this time-window are consistent with previous studies of the P300 and the FRN component [23, 24, 35, 40–43]; whereas in earlier studies contributions of Novelty, Surprise, and Reward were often mixed together [23, 24, 35, 40–43], we have shown here separate, additive contributions of these three variables as well as a further contribution of NPE. Our results of the grand correlation analysis show that the effect of Novelty appears in ERPs earlier (at around 200ms) than the correlations with the other variables; moreover, contributions of Novelty are distinct from those of Surprise in the time window after 400ms.

In conclusion, surprise and novelty are conceptually distinct concepts that give rise to different temporal components in the ERP. Our results suggest that humans use novelty-seeking for efficient exploration and surprise for a rapid update of both their internal world-model and their 'model-free' habitual responses.

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Author Contributions

MHH, HAX and WG designed the experiment. HAX performed the experiments. AM designed the model and performed the data analysis. HAX and MPL developed preliminary models and data analysis. AM, HAX, MHH and WG wrote the paper.

Competing Interests statement

The authors declare no competing interests.

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Methods

Experimental setup

Stimuli were presented on an LCD screen that was controlled by a Windows 7 PC. Experiments were scripted in MATLAB using the Psychophysics Toolbox [1].

Participants

14 paid participants joined the experiment. Two participants quit the experiment, hence, we analysed data for 12 participants (5 females, aged 20-26 years, mean = 22.8, sd = 1.7). All participants were right-handed and naive to the purpose of the experiment. All participants had normal or corrected-to-normal visual acuity. All participants provided written consent. The experiment was approved by the local ethics committee.

Stimuli and general procedure

Before starting the experiment, we showed the participants the goal image that they were required to find on a computer screen. Next, participants were presented, in random order, all the other images that they may encounter during the experiment. Thereafter, participants clicked the 'start' button to start the experiment. At each trial, participants were presented an image (state) and four grey disks below the image. Clicking on one of the disks (action) led participants to a subsequent image; for details of timing see Fig. 1A. Participants clicked through the environment until they found the goal state which finished the episode. An episode n started at a random state $i(n)$ which was the same for all participants; we set $i(1) = 6$, $i(2) = 9$, $i(3) = 4$, $i(4) = 5$, and $i(5) = 8$.

EEG recording and processing

EEG signals were recorded using an ActiveTwo Mk2 system (BioSemi B.V., The Netherlands) with 128 electrodes at a 2048Hz sampling rate. Two participants were excluded from EEG analysis because of their noisy and low quality signals caused by substantial movements during the experiment. Data were band pass filtered from 0.1Hz to 40Hz and down sampled to 256Hz. EEG data were recorded with a Common Mode Sensor (CMS) and re-referenced using the common average referencing method. We used EEGLAB [2] toolbox in MATLAB to perform the EEG preprocessing. We extracted EEG trials from 200ms before to 700ms after the state onset. Trials in which the change in voltage at any channel exceeded 35 μV per sampling point were discarded. Eye movements and electromyography (EMG) artefacts were removed by using independent component analysis (ICA). The baseline activity was removed by subtracting the mean calculated over the interval from 200ms to 0ms before the state onset. EEG data of selected prefrontal electrodes (Fz, F1, F2, AFz, FCz) were averaged for ERP analysis. We further smoothed (moving averaging with the window of length 50ms) and downsampled (to the sampling rate of 1 sample per 11.7ms) ERPs. Data were analyzed during the time window from 0 to 650ms after state onset (blue interval in Fig. 1A). For multivariate regression analysis, a 100ms-baseline was also included for sanity check. As a result, each trial (from 100ms before to 650ms after the onset of the state) consisted of 65 time points.

SurNoR algorithm

We present a more detailed formulation and the psudocode of the SurNoR algorithm in Supplementary Material. Here we outline the algorithm in brief.

We formally define the **Novelty** of a state s at time t as $-\log p_N^{(t)}(s)$, where $p_N^{(t)}(s)$ is the empirical frequency of encountering the state s until time t. When observing the image corresponding to state s at time $t+1$, after taking action A_t, the novelty N_{t+1} is treated as an internal novelty-reward, completely analogous to the treatment of external rewards in reinforcement learning. This analogy between external reward and novelty is inspired by earlier experimental studies [3–5]. As a result, at time $t+1$, agents receive three signals: the next state S_{t+1}, the external reward R_{t+1} (i.e., the indicator of whether S_{t+1} is the goal state or not), and the Novelty N_{t+1} (indicated as the output of the grey block in Fig. 3A).

The SurNoR algorithm has two branches, i.e., a model-based and a model-free one, which are interacting with each other (Fig. 3A, blue and the red blocks). The **model-based branch** computes the Bayes-factor Surprise $\mathbf{S}_{\mathrm{BF}}^{(t+1)} \propto 1/p(S_{t+1}|S_t, A_t)$ [6] where $p(S_{t+1}|S_t, A_t)$ is the probability of observing S_{t+1} by taking action A_t in state S_t as estimated from the current world-model. Note that we directly plotted $1/p(S_{t+1}|S_t, A_t)$ as the surprise value in Fig. 3A, Fig. 3B, and Fig. 5C. As an aside we note that since the state prediction error [7] is defined as $SPE_{t+1} = 1 - p(S_{t+1}|S_t, A_t)$, the Bayes-factor Surprise can be written as $\mathbf{S}_{\mathrm{BF}}^{(t+1)} \propto 1/(1 - SPE_{t+1})$. While the definition of Bayes-factor Surprise is motivated by a Bayesian inference for volatile environments [6], $\mathbf{S}_{\mathrm{BF}}$ is in our experimental setting a monotone function of Shannon Surprise and hence comparable to previous studies [8–10].

The value $\mathbf{S}_{\mathrm{BF}}^{(t+1)}$ is used in the model-based branch to update the world-model by the Variational SMiLe algorithm [6], a learning rule with surprise-modulated learning rate designed for volatile environments with abrupt changes [6]; see Supplementary Material for details. The learning rate modulation is implemented through an adaptation factor

$$\gamma_{t+1} = m\mathbf{S}_{\mathrm{BF}}^{(t+1)}/(1 + m\mathbf{S}_{\mathrm{BF}}^{(t+1)}), \tag{1}$$

with $m \geq 0$ a free parameter related to the volatilily of the environment. The updated world-model is then used to update a pair of Q-values, i.e., $Q_{\mathrm{MB,R}}^{(t+1)}$ for Reward and $Q_{\mathrm{MB,N}}^{(t+1)}$ for Novelty, by solving the corresponding Bellman equations with a variant of prioritized sweeping [11–13] (see Supplementary Material for details).

The **model-free branch** computes Reward and Novelty prediction errors, RPE_{t+1} and NPE_{t+1}. As usual, RPE is defined as $RPE_{t+1} = R_{t+1} + \lambda_R V_{\mathrm{MF,R}}(S_{t+1}) - Q_{\mathrm{MF,R}}(S_t, A_t)$, where λ_R is the discount factor for reward, and $V_{\mathrm{MF,R}}(S_{t+1}) = \max_a Q_{\mathrm{MF,R}}(S_{t+1}, a)$ is the value of the state S_{t+1}. Analogously, NPE is defined as $NPE_{t+1} = N_{t+1} + \lambda_N V_{\mathrm{MF,N}}(S_{t+1}) - Q_{\mathrm{MF,N}}(S_t, A_t)$, where λ_N is the discount factor for novelty, and $V_{\mathrm{MF,N}}(S_{t+1}) = \max_a Q_{\mathrm{MF,N}}(S_{t+1}, a)$ is the novelty value of the state S_{t+1}.

A Surprise-modulated TD-learner with eligibility traces is used for updating the two separate sets of Q-values, i.e., $\Delta Q_{\mathrm{MF}}^{(t+1)}(s, a) = \rho_{t+1} e^{(t+1)}(s, a) PE_{t+1}$, where $e^{(t+1)}$ is the eligibility trace, PE_{t+1} is the prediction error (i.e., either RPE_{t+1} or NPE_{t+1}) and

$$\rho_{t+1} = \rho_b + \gamma_{t+1}\delta\rho \tag{2}$$

is the surprise-modulated learning rate with parameters ρ_b for the baseline learning rate and $\delta\rho$ for the effect of Surprise.

Finally, actions are chosen by a hybrid policy using a softmax function of a linear combination of the values $Q^{(t+1)}_{\mathrm{MF,R}}$, $Q^{(t+1)}_{\mathrm{MF,N}}$, $Q^{(t+1)}_{\mathrm{MB,R}}$, and $Q^{(t+1)}_{\mathrm{MB,N}}$ (the purple block in Fig. 3.A), similar, but not identical to [7, 14]. The weight of $Q^{(t+1)}_{\mathrm{MF,N}}$ and $Q^{(t+1)}_{\mathrm{MB,N}}$ and is non-zero only in the 1st episodes of blocks 1 and 2. Overall, the SurNoR algorithm has 18 free parameters.

Statistical model analysis and fit to behavior

In addition to SurNoR, we considered 12 alternative algorithms with 0 to 18 free parameters (Supplementary Material). For each algorithm, we used 3-fold cross-validation and computed its maximum log-likelihood for each participant, similar to existing methods [15]: (i) we divided participants into 3 folds each consisting of four participants; (ii) for participant i, we estimated the parameters of the algorithm by maximizing the likelihood function of the folds which did not include participant i; and (iii) we computed the log-likelihood for participant i using the estimated parameters. The maximization procedure was done by coordinate ascent (using grid search for each coordinate); we repeated the procedure until convergence starting from 25 different random initial points. We further repeated the whole process 4 times to have an estimation of the variability resulting from random initialization of the optimization procedure. The error bars in Fig. 4A are calculated using these 4 samples.

Similar to studies in economics and statistics [16–19], we considered, for each participant and each algorithm, the cross-validated maximum log-likelihood (averaged over the 4 repetitions) as the log-evidence [20]. The sum (over participants) of the log-evidences for each algorithm is shown in Fig. 4A - see [21] for a tutorial on the topic. As a convention, differences greater than 3 or 10 are considered as significant or strongly significant, respectively [20–22]. The model posterior and exceedance probabilities in Fig. 4B are computed by using the participant-wise log-evidences (averaged over the 4 repetitions) and following the Bayesian model selection method of [23] (available in SPM12 toolbox for MATLAB). We used a Dirichlet distribution with parameters equal to 1 over the number of models (1/13) as the prior distribution. This choice of prior is equivalent to stating that the prior information is worth as much as the observation coming from a single participant [20]; it is also a default choice of prior in the VBA toolbox [24].

The accuracy rate and the uncertainty in Fig. 4C are computed by the same cross-validation procedure. We define accuracy as the ratio of the number trials with correctly predicted actions to the total number of trials; for a given trial, whenever the action taken by the participant had the maximum probability under the policy but shared with other $n-1$ (e.g., 2) actions, we counted that trial as $1/n$ (e.g., 0.333) correctly predicted. With this procedure, the accuracy rate of the random choice algorithm is 25%. We define the uncertainty of one participant in an episode as the average of the entropy of his or her policy over all trials of that episode. Both the accuracy rate and the uncertainty were computed for each participant separately, but only the mean and the standard error across participants are reported in Fig. 4C.

For EEG analysis, we only considered the SurNoR algorithm (i.e., the winner of statistical model selection). To have the same set of parameters for all participants, we fitted our model to the whole behavioral data set (overall 3047 actions) by maximizing total log-likelihood - similar to [14]. For each of 100 random initialization points, maximization was implemented as coordinate ascent until convergence (using grid search for each coordinate). Amongst the 5 local maxima with high but not significantly (< 3) different log-evidence, we kept the model which had the greatest encoding power in multivariate regression analysis of EEG. The fitted parameters are reported in

in Supplementary Material.

The plots in Fig. 5 corresponds to this set of parameters. Since the softmax operator of the hybrid policy has a free scale parameter, the effective weight of each branch of the hybrid policy in Fig. 5A (i.e., model-free and model-based) is computed as the fitted weight of each component times its average difference in Q-values. For example, ω_{MF}^{eff} is equal to $\omega_{MF} \times \langle \Delta Q_{MF} \rangle$, where ω_{MF} is the weight of model-free Q-values in the hybrid policy and $\langle \Delta Q_{MF} \rangle$ is the average (over trials) of the difference between Q_{MF} of the best and the worst actions. The weight ω_{MB}^{eff} for the model-based branch is defined analogously. The dominance of the model-free branch is defined as $\omega_{MF}^{\text{eff}}/\omega_{MB}^{\text{eff}}$.

EEG Analysis

Participant-based regression analysis

Given N trials (across all episodes of both blocks) of a given participant, the matrix X_{raw} for this participant is an N by 5 matrix whose rows correspond to trials and whose columns correspond to normalized model variables (i.e., Surprise, Novelty, NPE, RPE, and Reward). For example, if the sequence of reward prediction error values for this participant is $z_{1:N}$, then one column of the matrix X_{raw} is equal to $(z_{1:N} - \mu_z)/\sigma_z$ where μ_z is the mean and σ_z is the standard deviation of $z_{1:N}$, and one row of the matrix X_{raw} is equal to the normalized values of Surprise, Novelty, NPE, RPE, and Reward for one trial. We constructed the feature matrix X from X_{raw} by applying the following steps: (i) we put 2 columns of X to be equal to normalized Reward plus RPE and Reward minus RPE, calling them R_+ and R_-, respectively; since Reward and RPE were normalized, their sum and difference correspond to their principal components (Supplementary Material); (ii) we orthogonalized each of the other variables to R_+ and R_-. For example, $\text{NPE}_\perp$ is NPE minus its projection on R_+ and R_-, followed by a renormalization step (see Supplementary Material).

For each trial, time of the ERP is measured with respect to the image onset. For a given time point, we defined the target vector y as an N dimensional vector whose elements are equal to the normalized (zero mean, unit variance) amplitude of ERPs at that particular time point in different trials. Since we have 65 time points, the response matrix Y is a N by 65 matrix. We then performed multivariate linear regression (MLR) by considering $\hat{y} = X\beta$ as an estimation of y and found β by ordinary least squared error minimization. The encoding power for a single time point and for the given participant was calculated as adjusted R-squared [25]. Note that adjusted R-squared can in principle be negative - which is the case for our regression analysis over baseline in Fig. 7A.

Fig. 7A shows the mean and the standard error of the mean of the encoding power over participants and for each time-point. The threshold for rejecting the null hypothesis is computed using the Benjamini and Hochberg algorithm [20] for controlling false discovery rate (FDR) by 0.1. Fig. 7B shows the average (over participants) of β values as a function of time. For Fig. 7C we first average the β values over time within each time window, and then evaluate their mean and their standard error of the mean (over participant). The FDR correction was done separately for each time window.

Grand correlation analysis

Similar to the approach of [26], we pooled all trials of all participants together, i.e., we concatenated X_{raw}s and Ys for different participants. However, before concatenation, to remove the difference

in the between-participant variations of ERPs energy (i.e., 2nd moment), we divided ERPs of each participant by the overall squared-energy of that participant's ERPs, i.e., we replaced Y by $Y/\sqrt{\mathbb{E}[Y^2]}$. The correlations in Fig. 6 are computed between columns of concatenated X_{raw}s and concatenated Ys. For RPE, we removed the trials corresponding to 1st episodes of the 1st blocks because RPEs are exactly equal to zero.

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