

Merits of curiosity: a simulation study

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Abstract

‘Why are we curious?’ has been among the central puzzles of neuroscience and psychology in the past decades. Recent ‘top-down’ theories have hypothesized that curiosity, as a desire for some *intrinsically generated rewards* (e.g., novelty), is the *optimal* solution for survival in *complex environments* where we have evolved. To formalize and test this hypothesis, however, it is necessary to understand the relationship between (i) intrinsic rewards (as drives of curiosity), (ii) optimality conditions (as objectives of curiosity), and (iii) environment structures. Here, we demystify this relationship through a systematic simulation study. We first propose an algorithm for generating environments that capture key abstract features of different real-world situations. Then, within these environments, we simulate different artificial agents seeking six representative intrinsic rewards (novelty, surprise, information gain, empowerment, MOP and SPIE) and evaluate their performance regarding three potential objectives of curiosity (environment exploration, model accuracy and uniform state visitation). Our results show that the comparative performance of each intrinsic reward is highly dependent on the structural features of environments and the objective under consideration; this indicates that ‘optimality’ in the top-down theories of curiosity needs a precise formulation of the curiosity objective and the environment structure. Nevertheless, we found that agents seeking a combination of novelty and information gain always achieve a close-to-optimal performance; this proposes novelty and information gain as two principal axes of curiosity-driven behavior. These results, collectively, pave the way for the further development of computational models of curiosity and design of theory-informed experimental paradigms.

31 Introduction

32 Curiosity drives humans and animals to explore their environment and acquire knowledge about
33 what appears to be new, puzzling, or strange (Berlyne, 1966; Gottlieb and Oudeyer, 2018; Kidd
34 and Hayden, 2015; Modirshanechi et al., 2023b): Human babies prefer playing with toys that
35 have surprising features (e.g., a car that passes through a solid wall) over normal toys (Stahl and
36 Feigenson, 2015), monkeys look at novel visual stimuli longer than those they have seen before
37 (Ghazizadeh et al., 2016; Ogasawara et al., 2022), rats prefer to explore mazes with complex
38 structures than those with simple layouts (Montgomery, 1954), and mice have a higher breathing
39 frequency when sniffing a new odor than a familiar one (Morrens et al., 2020). Mysteriously,
40 the drive of curiosity can even occasionally overwrite primary needs such as for safety or food
41 (FitzGibbon et al., 2020), e.g., human adults take the risk of receiving an electric shock only to
42 know the secret of a magic trick (Lau et al., 2020), and monkeys give up juice rewards in return
43 for the *information of future* reward (Bromberg-Martin et al., 2024). These observations have
44 been among the central puzzles of neuroscience and psychology in the past decades¹, yet curiosity
45 and its neuronal underpinning have remained mysterious and debated (see Forss et al. (2024);
46 Modirshanechi et al. (2023b); Monosov (2024); Poli et al. (2024) for recent reviews).

47 From a theoretical perspective, there are two principal questions regarding curiosity: ‘Why are
48 humans and animals curious?’ and ‘What are they exactly curious about?’ (Modirshanechi et al.,
49 2023b). Modern theoretical attempts to address these questions use intrinsically motivated Re-
50 inforcement Learning (RL) framework (Baldassarre and Mirolli, 2013; Barto, 2013) and describe
51 curiously-driven actions as those directed towards seeking an *intrinsically* generated ‘reward’ signal
52 (Modirshanechi et al., 2023b; Murayama, 2022; Murayama et al., 2019; Oudeyer, 2018; Poli et al.,
53 2024). In this framework, the answer to the ‘What’ question is given by the *intrinsic* reward (e.g.,
54 novelty or surprise of observations) that best describes the exploratory actions of a curious agent,
55 as opposed to the *extrinsic* reward (e.g., the monetary or nutritional value of observations) that
56 describes the exploitative actions (Aubret et al., 2019; Ladosz et al., 2022; Oudeyer and Kaplan,
57 2009). Given an intrinsic reward signal, the answer to the ‘Why’ question is often given by quan-
58 tifying the benefits of the intrinsically motivated actions in terms of the agent’s ability in, e.g.,
59 finding valuable sources of extrinsic reward (Gershman and Niv, 2015; Pathak et al., 2017; Singh
60 et al., 2010a), gaining knowledge about the environment structure (Dubey and Griffiths, 2019), or
61 unsupervised learning of complex skills (Mendonca et al., 2021; Oudeyer and Kaplan, 2009; Sekar
62 et al., 2020).

63 In several experimental paradigms, intrinsically motivated RL algorithms have been successful
64 in addressing the ‘What’ question and describing curiosity-driven and exploratory actions of hu-
65 man participants by considering novelty (Modirshanechi et al., 2023d; Xu et al., 2021), surprise
66 (Kobayashi et al., 2019), information gain (Horvath et al., 2021; Nelson, 2005), progress rate (Poli
67 et al., 2022; Ten et al., 2021a), or empowerment (Brändle et al., 2023; Klyubin et al., 2005) as the
68 intrinsic reward signal. However, these studies do not address the paradoxical observation that the
69 choice of intrinsic reward differs between different experimental paradigms (Modirshanechi et al.,
70 2023b). A potential solution has been proposed by the ‘top-down’ models of curiosity (Modir-
71 shanechi et al., 2023b) that consider curiosity as the optimal mechanism for reaching a particular
72 objective (the ‘Why’ of curiosity), e.g., finding the most valuable sources of extrinsic rewards in
73 a class of environments (Alet et al., 2020; Dubey and Griffiths, 2019; Singh et al., 2010a; Zheng

¹The seminal 1966 paper of Daniel Berlyne on curiosity (Berlyne, 1966) starts with the sentence ‘Animals spend much of their time seeking stimuli whose significance raises problems for psychology.’

74 et al., 2020b). Instead of directly answering the ‘What’ question, these models characterize (i)
75 the objective of curiosity and (ii) the class of environments where the curious agent lives. The
76 ‘What’ of curiosity is determined by the reward signal reaching this objective in the specified class
77 of environments. Hence, the observation that the ‘What’ of curiosity is experiment-dependent can
78 be because of differences in the optimal strategies for reaching the curiosity objective in different
79 experiments (Dubey and Griffiths, 2019, 2020). To advance our theoretical understanding of cu-
80 riosity, it is hence necessary to understand the relationship between different (i) intrinsic rewards,
81 (ii) objectives of curiosity, and, importantly, (iii) environment classes.

82 In this study, we aim to demystify this relationship. Specifically, we first design an algorithm for
83 generating various environments with principally different characteristics, e.g., number of states,
84 stochasticity of transitions, distribution of between-state connections, etc. We then formally define
85 three performance measures as potential objectives of curiosity: (i) how fast a curious agent
86 discovers all states of its environment, (ii) how accurately it learns the structure of the environment,
87 and (iii) how uniformly it explores all the states. We then simulate different curious agents and
88 quantify the merits of six representative intrinsic rewards (novelty, surprise, information gain,
89 empowerment, maximum occupancy principle, and successor-predecessor intrinsic exploration) for
90 maximizing these performance measures in different environments.

91 We show that, almost always, seeking information gain is the best strategy for the first two
92 performance measures, whereas seeking novelty is the best strategy for the third. Building upon
93 this observation, we show that an agent that seeks a combination of information gain and novelty
94 can reach a close to the best performance for all three performance measures and in all classes
95 of environments. This finding proposes information gain and novelty as two principal axes of
96 curiosity-driven behavior (consistent with recent experimental findings, e.g., Dubey and Griffiths
97 (2019); Monosov (2024); Poli et al. (2022)). Importantly, however, our results show that the relative
98 performance of different intrinsic rewards is highly dependent on the structure of the environment.
99 Finally, we show that our environment-generating algorithm proposes a novel approach to designing
100 experimental paradigms where seeking different intrinsic rewards results in maximally different
101 exploration strategies. These paradigms can be used in future experimental studies of curiosity in
102 humans and animals (e.g., as in Modirshanechi et al. (2023d)).

103 Results

104 General framework

105 To study the behavior of curious agents, we use the intrinsically motivated RL framework. In this
106 framework, each curious agent learns to navigate an environment represented by discrete states
107 and transitions, where states represent specific locations within the environment, and transitions
108 describe the agent’s movement from one state to another as a result of its actions. Each transition
109 is associated with a reward signal that guides the agent’s action selection. Traditional RL relies
110 on fixed, external rewards to shape the agent’s behavior (Sutton and Barto, 2018). In contrast,
111 intrinsically motivated RL uses internal reward signals that are non-stationary and evolve based
112 on the agent’s experience (Barto, 2013; Singh et al., 2010b). These intrinsic rewards encourage
113 the agent to explore and learn from the environment without relying on external rewards.

114 We assume that the agent starts with no prior knowledge of the structure of the environment and
115 builds a model of the environment by interacting with it. Specifically, we assume that the agent

116 uses Bayesian inference (similar to Liakoni et al. (2022); Meyniel et al. (2016); Xu et al. (2021)) to
 117 estimate each transition probability $P(s'|s, a)$ (i.e., the probability of reaching state s' from state s
 118 by taking action a) for every state s , action a , and the next state s' . As a result, the agent counts
 119 transitions and constructs its environment model as

$$120 \quad \hat{P}^{(t)}(s'|s, a) = \frac{C_{s,a \rightarrow s'}^{(t)} + \epsilon}{C_{s,a}^{(t)} + |S| \cdot \epsilon}, \quad (1)$$

121 where S denotes the set of all states, $|S|$ denotes the number of states, t is the current time step,
 122 $C_{s,a \rightarrow s'}^{(t)}$ is the count of the transition $s, a \rightarrow s'$ up to time t , and $C_{s,a}^{(t)}$ is the number of times action
 123 a has been taken from state s up to time t . The parameter $\epsilon > 0$ acts as a prior, preventing unseen
 124 transitions from being assigned a probability of zero (see **Hyper-parameters selection** for details).
 125 Then, using its model of the environment, the agent computes Q-value $Q(s, a)$ as an estimate of
 126 the expected future intrinsic rewards that the agent can collect, by taking action a at state s . The
 127 Q-values consider both immediate rewards and discounted future rewards and can be computed
 128 by solving the Bellman optimality equations (Sutton and Barto (2018))

$$129 \quad Q^{(t)}(s, a) = \sum_{s' \in S} \hat{P}^{(t)}(s'|s, a) \left(R^{(t)}(s, a, s') + \lambda \max_{a' \in A} Q^{(t)}(s', a') \right), \quad (2)$$

130 where $R^{(t)}(s, a, s')$ is the intrinsic reward for transitioning from s to s' via action a , determined
 131 by the agent’s intrinsic motivation (detailed in **Intrinsic motivations detailed**), and $\lambda \in [0, 1]$
 132 represents the discount factor for the Q-values. The discount factor λ determines how much the
 133 agent values the future reward compared to the immediate rewards. These Q-values are updated
 134 using prioritized sweeping (Moore and Atkeson, 1993) with 100 iterations after each observed
 135 transition to iteratively converge to a solution of the Bellman equation.

136 At each time t , the agent’s behavior in state s is described by the action policy $\pi_s^{(t)}$ which assigns
 137 probability $\pi_s^{(t)}(a)$ to selecting action a . We assume that the agent uses the Softmax of the Q-values
 138 as its action policy:

$$139 \quad \pi_s^{(t)}(a) = \frac{e^{\beta Q^{(t)}(s, a)}}{\sum_{a'} e^{\beta Q^{(t)}(s, a')}} \in [0, 1], \quad (3)$$

140 where β is the Softmax inverse temperature (Sutton and Barto, 2018). This implies that the agent
 141 will strongly favor one action if it is clearly better than the others (i.e., if it has a much higher
 142 Q-value than the other actions), but the agent will choose all actions with almost equal probability
 143 if they all seem equally rewarding (i.e., if they have a similar Q-value).

144 **Intrinsic motivations**

145 We consider six types of intrinsic motivation, each defined by a reward function $R^{(t)}(s, a, s')$ that
 146 determines the Q-values (Eq. 2) and, accordingly, specifies the agent’s action-policy (Eq. 3). Our
 147 first four choices of intrinsic rewards are well-established in the psychological literature (i.e., novelty
 148 (Modirshanechi et al., 2023d; Xu et al., 2021), surprise (Kobayashi et al., 2019), information gain
 149 (Horvath et al., 2021; Nelson, 2005) and empowerment (Brändle et al., 2023; Klyubin et al., 2005)),
 150 whereas the other two has been proposed only recently (Maximum Occupancy Principle (MOP)
 151 (Ramírez-Ruiz et al., 2024) and Successor-Predecessor Intrinsic Exploration (SPIE) (Yu et al.,
 152 2024)). In this section, we provide a brief and conceptual overview of each intrinsic motivation;

153 see [Intrinsic motivations detailed](#) for more detailed formulation and further theoretical analyses.

154 **(i) Novelty** rewards the agent for exploring rarely encountered states. Specifically, for a transi-
155 tion $s, a \rightarrow s'$, the agent receives a reward that is a decreasing function of the observation frequency
156 of s' , i.e., the less frequently the agent has visited s' , the more rewarded it feels by visiting s' .

157 **(ii) Surprise** rewards the agent for experiencing unlikely transitions and encourages exploration
158 of actions with uncertain or unexpected outcomes. Specifically, for a transition $s, a \rightarrow s'$, the agent
159 receives a reward that is a decreasing function of $\hat{P}^{(t)}(s'|s, a)$ ([Eq. 1](#)), i.e., the less the agent expects
160 to visit s' (conditioned on s and a), the more reward it feels by visiting s' (after taking a in s).

161 **(iii) Information gain** rewards the agent for reducing (the epistemic) uncertainty about the
162 environment by acquiring new information. The reward for observing a transition $s, a \rightarrow s'$ is
163 determined by the size of update of the agent’s model of the environment, quantified using the
164 KL divergence of the updated model from the previous model, i.e., the more the agent updates its
165 estimated probabilities ([Eq. 1](#)) after transition $s, a \rightarrow s'$, the more rewarded it feels.

166 **(iv) Empowerment** rewards the agent for achieving states where its actions lead to a *diverse*
167 set of *predictable* outcomes. The reward for observing a transition $s, a \rightarrow s'$ is the empowerment
168 value of s' , defined in [Intrinsic motivations detailed](#), i.e., the more ‘options’ the agent has at state
169 s' , the more it feels rewarded by visiting s' .

170 **(v) MOP** can be seen as a regularized surprise that rewards the agent for experiencing unlikely
171 transitions but also for maintaining a high-entropy policy. As a result, it motivates the agent to
172 explore a wide range of states and actions and have diverse trajectories. The reward for observing
173 a transition $s, a \rightarrow s'$ is a decreasing function of both $\hat{P}^{(t)}(s'|s, a)$ and $\pi_s^{(t)}(a)$. Details on how the
174 policy is computed and integrated into the reward definition can be found in [Intrinsic motivations](#)
175 [detailed](#).

176 **(vi) SPIE** rewards the agent for visiting rare states as well as those that are critical for reaching
177 isolated regions. Specifically, the reward for observing a transition $s, a \rightarrow s'$ is determined by the
178 difficulty for the agent to reach s' from all other states except s . This encourages visiting s' if it is
179 easy to reach from s but difficult from the other states; this is the case, e.g., if s' is in an isolated
180 region or if s is a bottleneck state. Here, a state s' is considered difficult to reach from a state s if
181 the agent rarely visits s' shortly starting from s .

182 Performance measures

183 While intrinsic motivations guide the agent’s immediate and local behavior, they do not necessarily
184 specify the long-term goal of curiosity. On the other hand, the curiosity outcome can be evaluated
185 only after a series of actions and across the whole environment, hence it remains unclear what
186 are the benefits of seeking different intrinsic rewards for a curious agent. To answer this question
187 and quantify the merits of seeking different intrinsic rewards (the ‘What’ of curiosity), we define
188 three performance measures that capture the potential ideal outcomes for a curious agent (the
189 ‘Why’ of curiosity). Our definitions are inspired by previous literature and common intuition on
190 the purpose of curiosity:

191 **Measure 1: Environment exploration.** Curiosity is closely linked to exploration (Kashdan
192 et al., 2009; Modirshanechi et al., 2023b; Voss and Keller, 2013). Hence, one key goal of a curious
193 agent can be to reach and visit all states in an environment. We measure the success of an agent,
194 concerning this goal, by the fraction of unvisited states after a certain number of steps. A successful
195 agent minimizes this fraction.

196 **Measure 2: Model accuracy.** Curiosity is often associated with gaining knowledge (Schmitt
197 and Lahroodi, 2008; Szumowska and Kruglanski, 2020) and refining internal models (Pisula, 2009;
198 Poli et al., 2024; Schmidhuber, 2010). Hence, another main goal of a curious agent can be to build
199 the most accurate model of its environment. In our case, the internal model refers to the agent’s
200 estimation of the transition probabilities, which should closely approximate the true transition
201 probabilities. We measure the success of an agent, concerning this goal, as the difference between
202 the estimated transition probabilities $\hat{P}(s'|s, a)$ and the ground truth after a certain number of
203 steps, using Root Mean Squared Error (RMSE). A successful agent minimizes this difference.

204 **Measure 3: Uniform state visitation.** It has been hypothesized that one main goal of curios-
205 ity is to find valuable sources of ‘extrinsic’ rewards (Bellemare et al., 2016; Modirshanechi et al.,
206 2023b; Pathak et al., 2017). However, since the world is inherently changing (Liakoni et al., 2021;
207 Nassar et al., 2010), the successful discovery of sources of rewards requires balanced and frequent
208 visitation of all states. Hence, another main goal of a curious agent can be to achieve an even
209 distribution of visits across the individual states, in order to avoid a disproportionate concentra-
210 tion in certain regions (similarly to Nedergaard and Cook (2023); Tolguenec et al. (2024)). This
211 is also in line with observations that repetitive experiences induce boredom in humans (Geiwitz,
212 1966) and motivate them to seek new stimuli (Bench and Lench, 2013, 2019). A curious agent
213 should similarly avoid staying in the same region for too long. We measure the success of an agent,
214 concerning this goal, as the difference between the agent’s state visitation frequency and the uni-
215 form distribution (using RMSE) after a certain number of steps. A successful agent minimizes this
216 difference.

217 Environment generation

218 To systematically study the link between intrinsic rewards and curiosity objectives, we need a
219 procedure for generating diverse environments with realistic features. In curiosity research, exper-
220 imental paradigms are typically unique and hand-crafted, lacking standardized multi-step environ-
221 ments. Our goal in this section is to propose an environment generation algorithm that replicates
222 the main relevant features of real-world environments as well as the environments commonly used
223 in the experimental studies of curiosity (Fig. 1). Common environment structures in experimen-
224 tal studies of curiosity are mazes (Behrens et al., 2018; Kosoy et al., 2020; Tolman, 1948) and
225 grid worlds (Botvinick et al., 2009; Dayan, 1993; de Tinguy et al., 2024; Piray and Daw, 2021;
226 Singh et al., 2010a; Yu et al., 2024; Zheng et al., 2020b). These serve as the foundation for our
227 generation algorithm. Additionally, some studies have highlighted the relevance of long-range con-
228 nections (Viswanathan et al., 2016), sinks states (Modirshanechi et al., 2023d; Xu et al., 2021)
229 and stochasticity (Mehlhorn et al., 2015; Modirshanechi et al., 2023d). Moreover, the number
230 of available options has been shown to have an impact on human behavior (Fasolo et al., 2009;
231 Mehlhorn et al., 2015; Scheibehenne et al., 2010). Taking these observations into account, our
232 algorithm generates environments in three main steps (see Supplementary Section **Environment**
233 **generation** for details): (i) It creates a maze with a branching structure, (ii) it integrates grid-like

234 rooms within the maze, and finally, assigns each room to one (and exactly one) of the following
235 properties:

- 236 • **Sink:** If a room is assigned to be a sink, then the algorithm introduces additional one-way
237 connections from other parts of the environment *to this room*. A sink room is easy to reach
238 from the rest of the environment. As a result, naive exploration strategies may struggle to
239 navigate the entire environment without repeatedly falling into the sink. In video games, the
240 starting point often acts as a sink state, as dying resets the player to the start. In real life,
241 laying on a couch, watching TV, or scrolling on social media can be seen as sink states, as
242 they are easy to engage in and may prevent agents from exploring other possibilities.
- 243 • **Source:** If a room is assigned to be a source, then the algorithm introduces additional one-
244 way connections *from this room* to other parts of the environment. From a source room, it is
245 easy to quickly reach any region of the environment. States in a source room have in general
246 more available options than the rest of the environment. Real-life examples of source states
247 are situations with a wide range of choices, which include being at an airport, choosing a
248 dish at a restaurant, buying a house, planning a vacation, or moving to a new city.
- 249 • **Stochastic:** If a room is assigned to be stochastic, then transitions within the room are
250 partly random. Specifically, when an agent selects an action a from a state s within a
251 stochastic room, there is a fixed probability that the action will result in the agent moving to
252 a random neighbor of s in the room instead of the intended destination of a . Unpredictability
253 is common in everyday life, such as when watching TV, interacting with others, or engaging
254 in activities where outcomes are not always certain (e.g., gambling or investing in the stock
255 market).
- 256 • **Neutral:** If a room is assigned to be neutral, then none of the aforementioned modifications
257 are applied to the room.

258 The algorithm receives, as input, a few parameters that specify the properties of the generated
259 environments, such as the number of states, the number of intersections and rooms, the room
260 sizes, the distribution of room types, and the intensity of the room properties. All parameters are
261 described in the Supplementary Material (Table 1).

262 **Environment types**

263 Using our environment generation algorithm, we can create various types of environments. We
264 focus on five types for most of our results, namely Neutral, Sink, Source, Stochastic and Mixed
265 environments. Since the process is non-deterministic, many distinct environments can be produced
266 within each type, but they are expected to exhibit similar properties. The environment types
267 considered are detailed in Supplementary Table 1. In summary, each environment contains 100
268 states, including 4 rooms of 16 states each. Neutral environments contain 4 neutral rooms. Sink
269 environments feature one sink room with 50 additional incoming connections. Source environments
270 contain one source room with 50 additional outgoing connections. Stochastic environments include
271 one stochastic room where actions lead to a random neighbor within the room. Finally, Mixed
272 environments consist of one neutral room, one sink room (with 50 incoming connections), one
273 source room (with 50 outgoing connections), and one stochastic room.

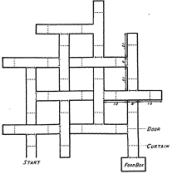
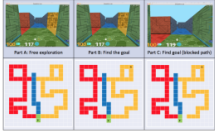
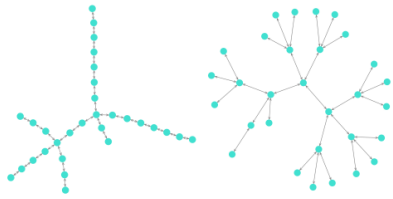
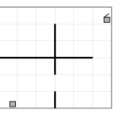
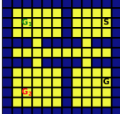
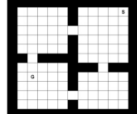
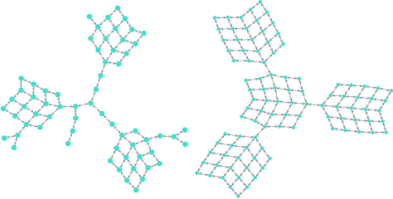

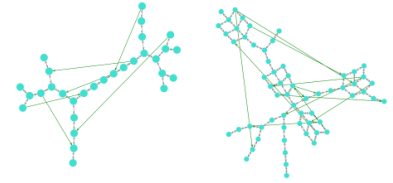
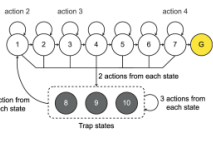
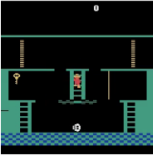
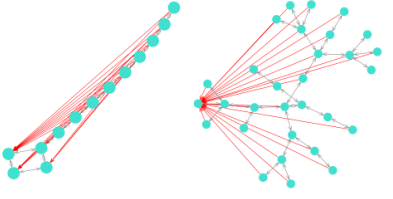
	Exemplar environments in the literature	Similar generated environments
Mazes	  <p>Tolman et al., 1948 Kosoy et al., 2010</p>	
Grid worlds	   <p>Singh et al., 2010 Yu et al., 2024 Botvinick et al., 2009</p>	
Long-range connections	 <p>Viswanathan et al., 2016</p>	
Sink states	  <p>Xu et al., 2021 Matusch et al., 2021</p>	

Figure 1: Comparison of environments from the exploration and curiosity literature with similar environments generated by our algorithm. The generated environments shown in the figure are exemplar realization that exhibit similar properties to the literature examples. However, due to the stochastic nature of the generation process, different instances with the same properties could also be produced. Blue nodes represent states, and edges indicate possible actions to transition between states. Gray edges are bidirectional. Green edges (originating from a source room) and red edges (leading to a sink room, see [Environment generation](#)) are unidirectional. Mazes are common in multi-step navigation tasks (Kosoy et al., 2020; Tolman, 1948) and are represented by complex, branching structures. Grid worlds, another common task type (Botvinick et al., 2009; Singh et al., 2010a; Yu et al., 2024), feature regular, grid-like structures. Long-range connections, highlighted as interesting in the literature (Viswanathan et al., 2016), are environments with states that have distant connections. Sink states are those that are easy to reach but hard to escape (Xu et al., 2021), similar to challenging game environments like Montezuma’s Revenge (Matusch et al., 2020) where the starting state acts as a sink state since dying resets the player to the start.

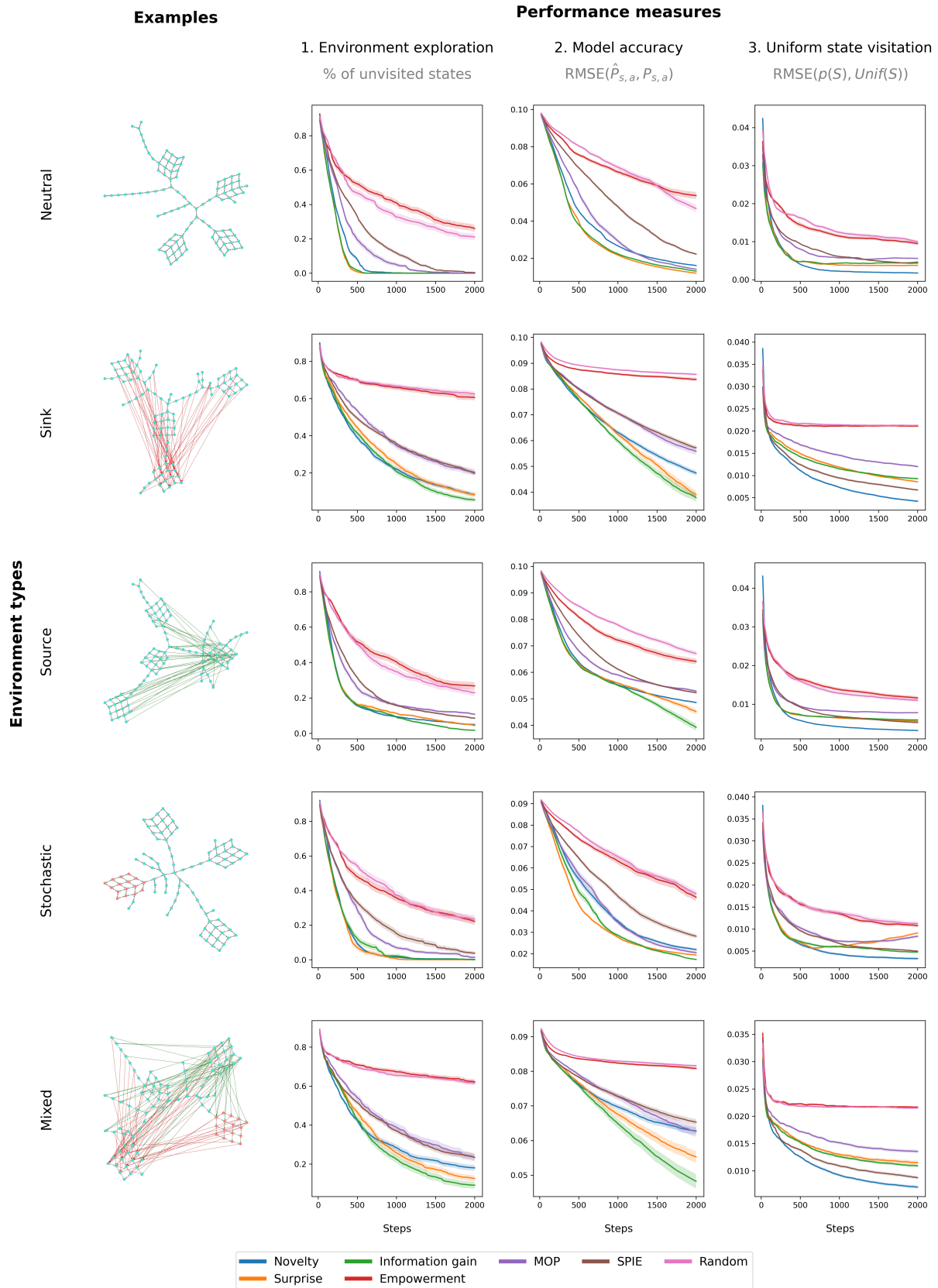


Figure 2: (Caption on the following page.)

Figure 2: Results for six intrinsic motivations (+ random), five environment types and three performance measures. Each subplot corresponds to the combination of one environment type and one performance measure. An exemplar environment is shown for each type. Blue nodes represent deterministic states, while red nodes correspond to stochastic states. The performance of each intrinsic motivation was evaluated over 50 different instances of each environment type, with the average displayed and the shaded areas representing the standard error of the mean. The first 2000 steps of simulation are shown. For performance measure 1, the y-axis represents the percentage of unvisited states. For measure 2, it displays the RMSE between the estimated transition probabilities and the ground truth. For measure 3, it shows the RMSE between the state visitation frequencies and the uniform distribution. In each case, a desirable performance is represented by a lower curve. In each case, the hyperparameter β was optimized for the first 500 steps only. **Environment types:** Neutral environments contain 4 neutral rooms. Sink environments contain one sink room with 50 additional connections leading to it. Source environments contains one source room with 50 additional connections originating from it. Stochastic environments include one stochastic room. Mixed environments consist of one neutral room, one sink room, one source room, and one stochastic room.

274 Performance analysis across different environments and measures

275 To quantify the merits of seeking different intrinsic rewards in different environments, we sim-
 276 ulated model-based reinforcement learning agents and measured their performance (defined in
 277 **Performance measures**) in our five environment types (specified in **Environment types**).

278 Overall, we observe that the novelty-seeking agents (blue in **Fig. 2**) consistently have the best
 279 performance according to Measure 3 (uniform state visitation; **Fig. 2**, right) and are competitive
 280 on Measure 1 (environment exploration; **Fig. 2**, left), except in the Mixed environments. On the
 281 other hand, agents seeking Surprise (orange in **Fig. 2**) or Information Gain (green in **Fig. 2**) excel
 282 on Measures 1 and 2 (**Fig. 2**, left and middle) but perform consistently worse than novelty-seeking
 283 agents for Measure 3 (**Fig. 2**, right). Interestingly, agents seeking Empowerment (red in **Fig. 2**)
 284 perform poorly across all scenarios; this is essentially because they avoid unknown regions, which
 285 are perceived as non-empowering due to uncertainty. As a result, they avoid further exploration
 286 of the environment and remain in where they initially explored. Agents seeking either of the two
 287 recently proposed intrinsic rewards, MOP and SPIE (purple and brown in **Fig. 2**, respectively),
 288 perform worse than agents seeking surprise, information-gain, or even novelty on Measures 1 and
 289 2. However, SPIE sometimes outperforms surprise and information-gain on Measure 3, while MOP
 290 is only better than random agents (pink in **Fig. 2**) and those seeking Empowerment on Measure 3.

291 While the performance of agents seeking each intrinsic reward is fairly consistent across multiple
 292 environments of the same kind (Supplementary **Fig. 7**), it varies strongly between environments of
 293 different types (different rows of **Fig. 2**). Different environment types affect performance in distinct
 294 ways: Neutral environments offer a good reference point. As sink rooms are challenging to escape,
 295 it is also more challenging to explore Sink environments than Neutral environments. As a result,
 296 Sink environments can more vividly show the differences in the performance of different agents
 297 (particularly for Measure 3; **Fig. 2**, row 2, column 3). On the other hand, in Source environments,
 298 building an accurate model of the environment (Measure 2) requires agents to repeatedly visit the
 299 source room to test all actions. This benefits Surprise and Information Gain agents, which are
 300 attracted to unknown actions, but is specifically detrimental for Novelty as it discourages state
 301 revisitation (**Fig. 2**, row 3, column 2). Interestingly, in Stochastic environments, Surprise and MOP

302 tend to stay in the stochastic room after learning sufficiently about the environment, resulting in
303 poor performance on Measure 3 (Fig. 2, row 4, column 3, see **Intrinsic motivations detailed** for a
304 formal explanation of this asymptotic behavior), whereas the other algorithms do not show such an
305 excessive attraction to stochasticity. Mixed environments combine features of previous types but
306 display different behaviors. Notably, Novelty performs worse in these environments on measures 1
307 and 2 compared to others.

308 To go beyond the comparison across environment types, we next evaluated the impact of specific
309 environment parameters on agent performance. Specifically, we manipulated the branching rate
310 and the number of sink connections (Fig. 3) in an environment inspired by Xu et al. (2021).
311 Specifically, we considered a class of environments with 100 states, where 4 states built a single
312 *sink* room, i.e., 96 states were neutral and outside of the room. In this setting, the branching rate
313 influences how these 96 states are arranged. At a branching rate of 0, the states are arranged in a
314 straight line, whereas at a branching rate of 1, the states are arranged in a tree-like structure (see
315 examples in Fig. 3a). Importantly, the performance of different algorithms drastically changes as
316 the branching rate increases from 0 to 1 (Fig. 3a). Novelty and SPIE, initially top performers at a
317 branching rate of 0, become among the worst as the branching rate increases to 1 in the first two
318 measures. This could be explained by the tendency of novelty-seeking agents to choose actions
319 that are known to lead to a relatively novel state, s , rather than taking an unknown action in some
320 situations (where the expected novelty of the unknown action might be less than that of s). As
321 a result, novelty-seeking agents may not explore all possible actions and could miss large parts of
322 the environment, especially when the branching rate is 1. Similarly, increasing the number of sink
323 connections generally benefits Novelty and SPIE comparatively to other motivations (Fig. 3b). This
324 shows that the structure of the environment has a great influence on the comparative performance
325 of intrinsic motivations, indicating that results from experiments in one specific environment may
326 not generalize well to others. For example, in an environment very similar to the case with a
327 branching rate of 0, Xu et al. (2021) found that Novelty to be dominant drive of human exploration.
328 Whether this result is environment-independent can be, for example, tested by repeating the same
329 experimental task in an environment with a branching rate of 1 (see Modirshanechi et al. (2023d)
330 for an alternative replication of the results of Xu et al. (2021)).

331 **Novelty and information gain as two main axes of curiosity**

332 In the previous section, we saw that agents seeking different intrinsic rewards exhibit a diverse
333 range of performance in different environment types. However, we also observed that the best
334 performing intrinsic reward, for every environment type or performance measure, is either Novelty
335 or Information Gain (Fig. 2 and Fig. 3). Specifically, by integrating over time (Fig. 4), we observe
336 that Information Gain outperforms all other motivations in environment exploration (Measure 1)
337 and model accuracy (Measure 2), whereas Novelty is the best reward signal in achieving uniform
338 state visitation (Measure 3).

339 These results propose that Novelty and Information Gain are two key drives of exploration. To
340 further this proposition, we simulated model-based RL agents that use a linear combination of
341 Novelty and Information Gain as the reward signal (Fig. 5). Interestingly, we observe that, by
342 even having a fixed and equal weight for Novelty and Information Gain ($\alpha = 0.5$ in (Fig. 5)),
343 these ‘hybrid’ RL agents reached close-to-optimal performance in all environment types and for
344 all performance measures (Fig. 5). This implies that an agent that can adaptively and on demand
345 fine-tune its reward function will always reach the best performance (see Modirshanechi et al.

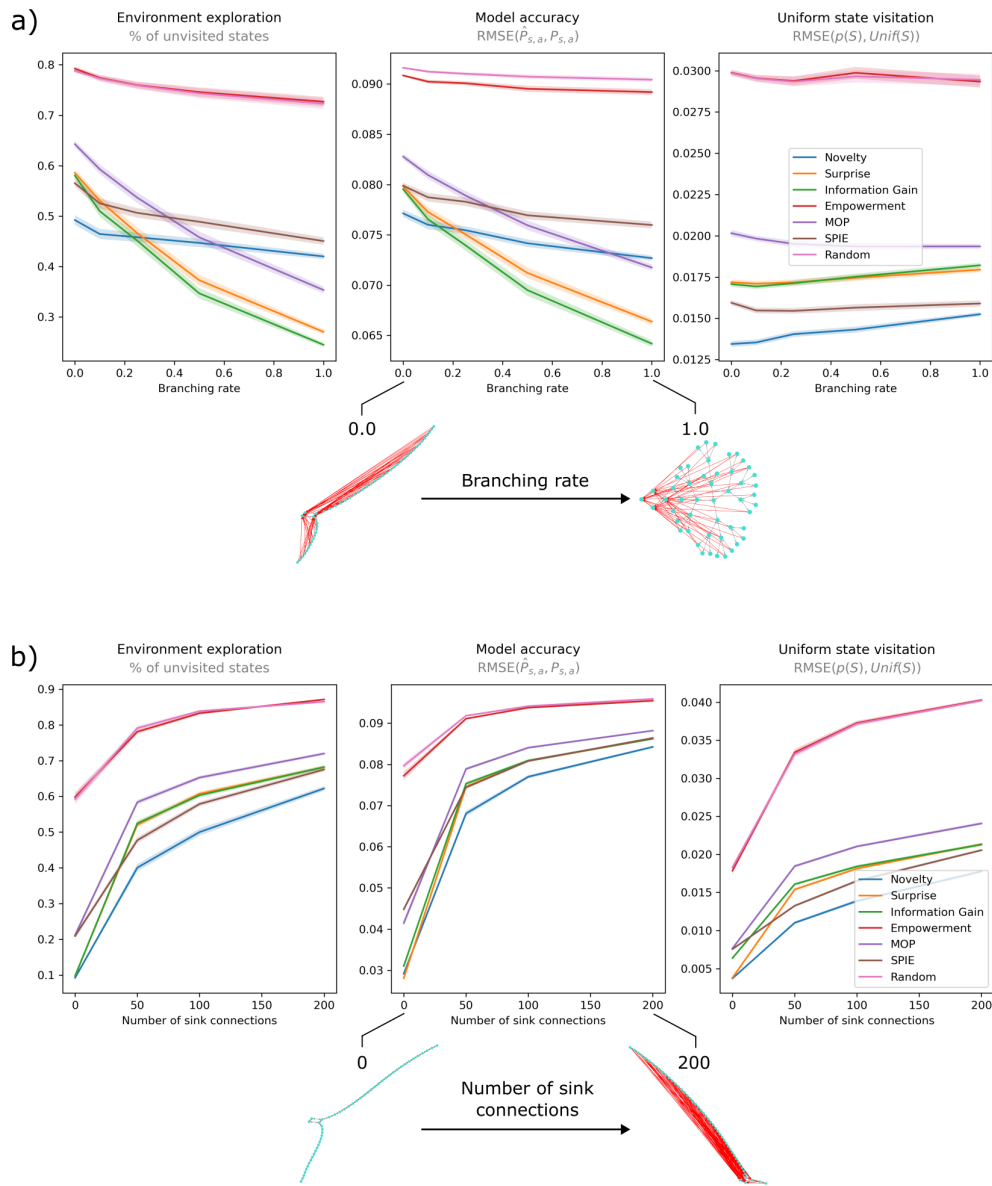


Figure 3: Performance variation of each intrinsic motivation as a single environment parameter is changed. The environment, inspired by Xu et al. (2021), contains one sink (trap) room with 4 states and 96 other states. The parameters used to generate the environments can be found in Table 1. The exemplar environments shown are smaller versions (50 states), for illustration purposes. To compute the score for a given environment, we run the agent as in Fig. 2 and calculate the area under the curve (AUC) of each measure over 2000 steps of simulations. The score for each environment type is obtained by averaging this value over 50 environment instances. (a) The parameter changed is the branching rate: at a branching rate of 0, the states are arranged in a straight line, while at a branching rate of 1, each state has multiple actions leading to distinct parts of the environment. In each case, 100 additional connections lead to the sink. (b) The parameter changed is the number of sink connections, while the branching rate is fixed to 0.

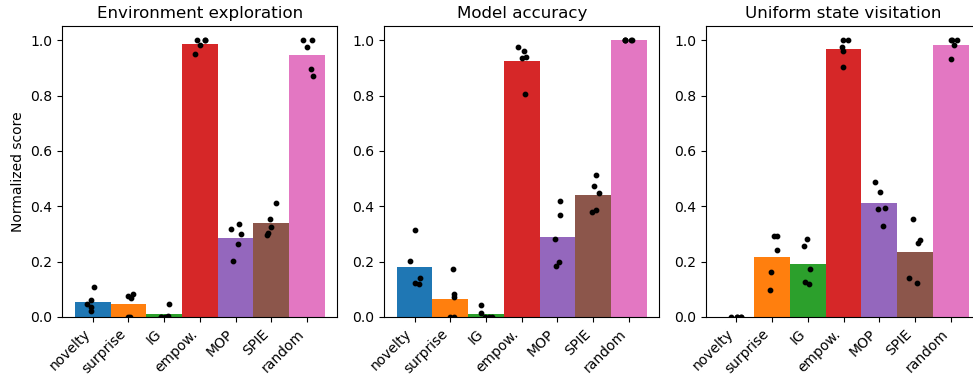


Figure 4: Average normalized score across environments for each intrinsic motivation, calculated as follows: for each setup (environment and measure), the score of each intrinsic motivation is computed as the area under the curve of Fig. 2. These scores are normalized, setting the best-performing intrinsic motivation to 0 and the worst to 1. Each dot represents the score on one environment type, and the average score over all environments is displayed. The same experiment was conducted using the KL divergence instead of RMSE for measure 2 and 3. The results are very similar and can be found in Supplementary Fig. 8.

346 (2023c) for a discussion). Importantly, this observation supports the hypothesis that Novelty and
 347 Information Gain are fundamental axes of curiosity, with each providing distinct benefits (in line
 348 with recent experimental studies on humans (Dubey and Griffiths, 2019; Monosov, 2024; Poli et al.,
 349 2022)).

350 Dissociating intrinsic motivations

351 To gain further insights into how different intrinsic motivations influence exploratory behavior,
 352 we analyzed exploration patterns of agents seeking different intrinsic rewards within the Mixed
 353 environment type (environments with one sink, one source, one stochastic, and one neutral room;
 354 see Environment types).

355 Specifically, we quantified the proportion of time that agents spend in different rooms of the
 356 environments (Fig. 6). Agents with a random policy predominantly remain in the sink room
 357 due to the difficulty of escaping it through random actions. Novelty-driven agents, on the other
 358 hand, quickly achieve a near-uniform state visitation frequency. Agents seeking SPIE follow the
 359 same trend as Novelty-seeking agents, but they learn more slowly than Novelty. After sufficient
 360 learning, Surprise-driven agents mostly spend time in the stochastic room, which has the highest
 361 transition uncertainty. Agents seeking MOP behave similarly to Surprise-driven agents, but they
 362 lean closer to random agents – as MOP also rewards policy entropy. As observed before (Fig. 2),
 363 agents driven by Information Gain learn effectively, but they eventually trend towards the random
 364 policy (as Information Gain converges to zero; see Intrinsic motivations detailed). Different from
 365 all other agents, Empowerment-driven agents do not explore the environment sufficiently to even
 366 discover all four rooms; they mainly stay within known regions (unknown regions are expected to
 367 be non-empowering due to uncertainty) which is most of the time the sink room as it acts like an
 368 attractor. However, once agents driven by Empowerment know the transition probabilities of the
 369 entire environment (i.e., are aware of the properties of all four rooms), they spend most of their
 370 time in the source room, which offers the highest empowerment.

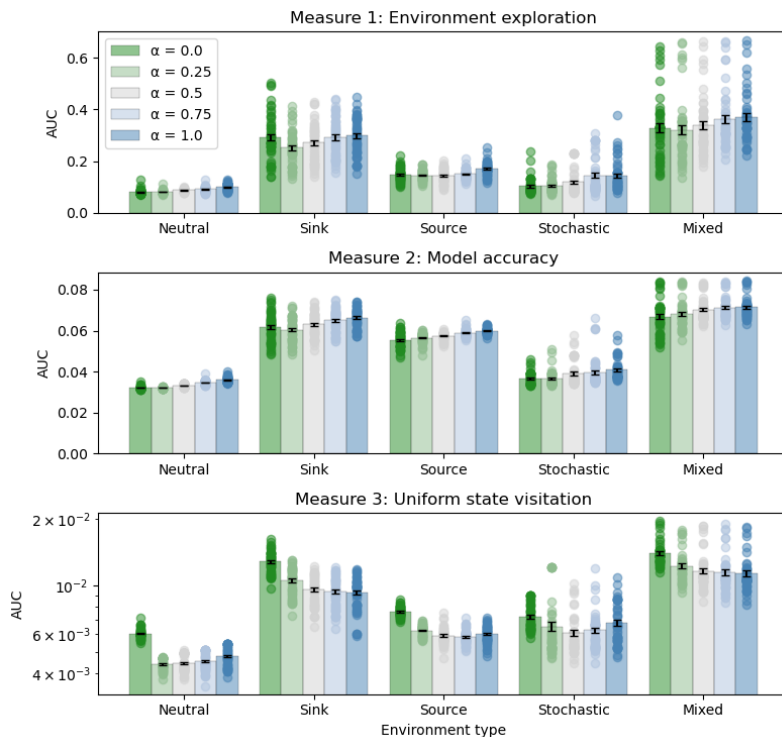


Figure 5: Combination of Information Gain and Novelty. At each step, the agent receives a weighted combination of information gain and novelty rewards, as $\alpha \cdot \text{Nov} + (1 - \alpha) \cdot \text{IG}$. In green, the agent is fully motivated by information gain; in blue, it only receives novelty rewards. For each value of α , the parameter β was optimized separately as in [Hyper-parameters selection](#). The agents were run similarly as for [Fig. 2](#), and the Area Under the Curve (AUC) after 2000 steps is reported. The results are averaged over 50 different instances of each environment type. The error bars represent the standard error of the mean. For each measure, a desirable performance is represented by a lower bar.

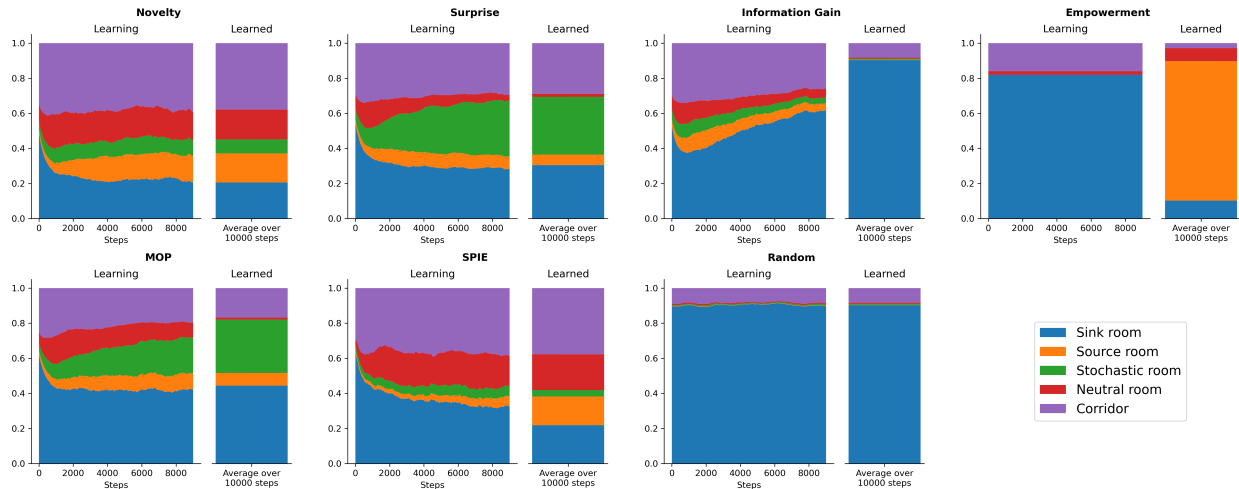


Figure 6: Proportion of time spent in each region of the environment. Agents were run in the Mixed environment (see [Environment types](#)) for 10’000 steps. Each room contains 16 states, and the corridor contain 36 states. In the ”Learning” phase, agents start without knowledge of the environment and build a model of it, as in previous experiments. The evolution of the proportion of time spent in each region during learning is shown, with a window average of 1000 steps. In the ”Learned” phase, the experiment is repeated but the agent’s model of the environment is fixed to the ground truth to assess for asymptotic behavior. The proportion of time spent is averaged over the 10’000 steps. Both phases are repeated 50 times and averaged. To allow for a fair comparison, the hyperparameter β is computed as $\frac{1}{std(r)}$ where $std(r)$ is the standard deviation of the intrinsic reward r computed over 10’000 steps under a random policy. The behavior of each intrinsic motivation in the ”Learned” case corresponds to the expected asymptotic behavior, derived from the reward formulation in [Intrinsic motivations detailed](#).

371 Overall, these results show that our environment generation algorithm can help to differentiate
 372 and highlight essential features of various intrinsic motivations. The different exploration patterns
 373 confirm that different intrinsic motivations lead to unique behaviors, even within the same en-
 374 vironment. This suggests that our algorithm for environment generation can be used to design
 375 experiments where behavioral differences between agents seeking different intrinsic rewards are
 376 most easily detectable. These experiment designs can be used for identifying exploration strate-
 377 gies in both humans and animals.

378 Discussion

379 In this study, we aimed to answer key questions about curiosity-driven behavior in humans and
 380 animals using simulated agents. Using a new environment generation algorithm, we assessed how
 381 different intrinsic motivations affect exploration in various environments. Our results show three
 382 main points: First, the performance of curiosity-driven agents depends highly on the structure
 383 of their environment. Second, information gain and novelty are the two most effective drivers
 384 of curiosity; information gain helps with exploring and understanding environments better, while
 385 novelty encourages a more even exploration of the environment. Third, different intrinsic moti-
 386 vations produce different exploratory patterns. Our environment generator creates settings where
 387 these differences are clear, making it easy to dissociate between different intrinsic motivations.

388 Our contributions can be summarized in two main points, which are developed in the following

389 paragraphs: (i) we demonstrate the significant impact of environment structure on the performance
390 of curious agents, and (ii) we introduce an environment generator to facilitate experimental design
391 across multiple domains.

392 Our first main contribution is the evidence that environment structure significantly affects the
393 performance of curious agents. Most recent studies on human curiosity use one or a few environ-
394 nments (Brändle et al., 2023; Horvath et al., 2021; Kobayashi et al., 2019; Poli et al., 2022; Ten
395 et al., 2021b) to test hypotheses and draw conclusions. Interestingly, the conclusions often vary
396 between experiments, suggesting that humans do not seek the same curiosity signals in all sce-
397 narios. We address this inconsistency by showing how the environment’s structure influences the
398 expected results. An optimal curious agent should not display the same behavior across different
399 experiments. This may suggest that the simple strategies exhibited by humans in experiments are
400 part of a more complex strategy with different assumptions about the task. While the importance
401 of environment structure in exploration behavior has been acknowledged (Mehlhorn et al., 2015),
402 it has to our knowledge not been highlighted with such precision and significance.

403 Our second major contribution is our proposed environment generation algorithm. This algorithm
404 offers several advantages: (i) It simplifies the design of environments to test specific hypotheses.
405 For instance, if we want to determine whether an agent (e.g., a human participant) behaves more
406 similarly to novelty-seeking or surprise-seeking agents, the environment generator provides a rig-
407 orous framework for creating an environment that clearly distinguishes between the two. (ii) The
408 algorithm allows for the creation of diverse environments to test agents in various scenarios while
409 keeping a common ground for comparison. It helps isolate key parameters that significantly impact
410 behavior. In many fields, it is common to use multiple environments to test a method, but these
411 environments are often either very similar to one another (Kosoy et al., 2020; Yu et al., 2023; Zheng
412 et al., 2020a), lacking generalization, or very different (Matusch et al., 2021; Piray and Daw, 2021;
413 Singh et al., 2010b), making comparisons and interpretation difficult due to a lack of common
414 ground. A parameterized environment representation helps generate various environments while
415 maintaining a common basis for comparison. Additionally, the stochastic nature of the algorithm
416 smooths out minor environmental details, ensuring that only relevant features significantly impact
417 the results. For instance, in a fixed environment, we cannot be certain that observed results are
418 due to the main feature of interest rather than an unrelated detail. With a stochastic environment
419 generator, such details can be averaged out, ensuring that only relevant features significantly im-
420 pact the results after multiple runs. (iii) The environment generator can serve as a valuable tool in
421 other domains. For instance, it can be used for benchmarking in different areas, such as comparing
422 model-based versus model-free approaches, or for developing and testing meta-learning algorithms.
423 This flexibility enhances its utility across various research contexts, making it a powerful tool for
424 experimental design and evaluation.

425 We used model-based RL to assess curiosity-driven behavior. It remains to be explored whether
426 our findings hold true in other setups, such as model-free RL. Additionally, we did not consider
427 scenarios where external rewards are present alongside intrinsic rewards. While it is expected
428 that combining these two reward types would produce intuitive results, our simulations focused
429 exclusively on intrinsic rewards, leaving this aspect unexplored. Another limitation is that all envi-
430 ronments in our study were static, with no modifications occurring during the agent’s navigation.
431 Certain scenarios or hypotheses may require dynamic environments to better reflect real-world
432 complexities. Furthermore, while our environment generation algorithm is expressive, it may not
433 capture all real-life scenarios. It serves as an initial step that can be supplemented with additional

434 factors that researchers find relevant. Future research should address these limitations.

435 Our findings are aligned with the intuition that humans adapt their exploration strategies to the
436 task. Future studies could investigate the conditions under which this adaptation occurs. Such
437 research could help clarify how people balance their curiosity-driven exploration with the specific
438 goals of a task.

439 In conclusion, our study increases the understanding of curiosity by clarifying the roles of different
440 intrinsic motivations and how they affect exploration behavior in different kinds of environments.
441 Our environment generator is a tool for future research, specifically: experiment design, algorithm
442 testing, and meta-learning.

443 Methods

444 Intrinsic motivations detailed

445 We consider six intrinsic motivations: novelty, surprise, information gain, empowerment, Maximum
446 Occupancy Principle, and Successor-Predecessor. Each is described below.

447 Novelty

Novelty, as intrinsic motivation, rewards the agent for exploring unusual states—those encountered infrequently (Aubret et al., 2019; Bellemare et al., 2016; Ostrovski et al., 2017). We use the same mathematical formulation as Xu et al. (2021). We define the observation frequency of a state s as

$$p_N^{(t)}(s) = \frac{C_s^{(t)} + 1}{\sum_{s'} C_{s'}^{(t)} + |S|}$$

where $C_s^{(t)}$ represents the number of times state s has been encountered up to time t . The novelty of a state s is then expressed as a decreasing function of the observation frequency :

$$R_{Novelty}^{(t)}(s) = -\log p_N^{(t)}(s)$$

448 *Asymptotic behavior:* Let $P_\pi(s)$ be the long-term observation frequency achieved by a fixed policy
449 π . The expected *average* novelty reward at each step for an agent following π is asymptotically
450 equal to

$$451 \mathbb{E}_{s \in S}[R_{Novelty}] = \sum_s P_\pi(s) \cdot R_{Novelty}(s) \quad (4)$$

$$452 = -\sum_s P_\pi(s) \cdot \log(P_\pi(s)) \quad (5)$$

$$453 = \mathcal{H}(P_\pi), \quad (6)$$

454 where $\mathcal{H}(P_\pi)$ is the entropy of the state observation frequency. As discount factor λ gets close
455 to 1, the policy π that maximizes Q-values in Eq. 2 becomes the same as the policy π that
456 maximizes $\mathbb{E}_{s \in S}[R_{Novelty}]$ (Puterman, 1994). Hence, an agent focused on maximizing this reward
457 will, intuitively and for large discount factors, adopt a policy π that increases the entropy of the
458 state observation frequency. This should result in a close to uniform state visitation (Measure 3
459 in Performance measures).

460 Surprise

Surprise, as intrinsic motivation, rewards the agent when observing transitions that were anticipated to be unlikely. We follow (Achiam and Sastry, 2017; Barto et al., 2013) and define the surprise of a transition as its Shannon surprise or surprisal (mod, 2022; Modirshanechi et al., 2023a):

$$R_{Surprise}^{(t)}(s, a, s') = -\log \hat{P}^{(t)}(s'|s, a)$$

461 Here, $\hat{P}^{(t)}(s'|s, a)$ represents the estimated probability of the transition. Higher intrinsic rewards
462 are granted for transitions the agent considers improbable.

463 *Asymptotic behavior:* Over time, the estimated transition probabilities $\hat{P}(s'|s, a)$ should converge
 464 to the true probabilities $P(s'|s, a)$. The expected surprise reward obtained for taking an action a
 465 in state s is

$$\mathbb{E}_{s' \in S}[R_{Surprise}(s, a, \cdot)] = \sum_{s'} \hat{P}(s'|s, a) \cdot R_{Surprise}(s, a, s') \quad (7)$$

$$= - \sum_{s'} \hat{P}(s'|s, a) \cdot \log(\hat{P}(s'|s, a)) \quad (8)$$

$$\stackrel{\approx}{\underset{t \rightarrow \infty}{\approx}} - \sum_{s'} P(s'|s, a) \cdot \log(P(s'|s, a)) \quad (9)$$

$$= \mathcal{H}(S'|s, a), \quad (10)$$

470 where $\mathcal{H}(S'|s, a)$ is the entropy of the next state distribution given action a in state s . This implies
 471 that, in the long run, the agent will prefer actions that lead to stochastic (uncertain) outcomes, as
 472 deterministic actions will eventually yield no reward. Therefore, after learning sufficiently about
 473 the environment, the surprise-seeking agent will focus on stochastic areas of the environment.

474 Information gain

Information gain, as intrinsic motivation, rewards the agent based on the amount of information
 it acquires, equivalent to the decrease of uncertainty in the knowledge that the agent has of the
 environment (Itti and Baldi, 2009; Oudeyer and Kaplan, 2009; Storck et al., 1995). We use the
 formulation also referred to as Postdictive surprise (mod, 2022; Kolossa et al., 2015; Modirshanechi
 et al., 2023a). Following a transition, the agent updates its environment model, and the intrinsic
 reward is determined by the difference between the updated and previous models. In mathematical
 terms:

$$R_{IG}^{(t)}(s, a, s') = KL \left(\hat{P}^{(t)}(\cdot |s, a) \parallel \hat{P}^{(t+1)}(\cdot |s, a, s_{t+1} = s') \right)$$

475 Where KL is the Kullback-Liebler divergence (Kullback, 1997). Here, $\hat{P}^{(t)}(\cdot |s, a)$ and $\hat{P}^{(t+1)}(\cdot |s,$
 476 $a, s_{t+1} = s')$ are the estimated probability distributions over next states before and after observing
 477 the transition $s, a \rightarrow s'$, respectively.

478 *Asymptotic behavior:* Over time, the estimated transition probabilities $\hat{P}(s'|s, a)$ will converge to
 479 the true probabilities $P(s'|s, a)$. Therefore, the information gain reward $R_{IG}^{(t)}(s, a, s')$ for every
 480 transition will tend to 0 as $t \rightarrow \infty$. This implies that the agent will converge to the uniformly
 481 random policy.

482 Empowerment

483 Empowerment is a measure of the degree of control or influence an agent has over its environment
 484 from a particular state (Klyubin et al., 2005; Salge et al., 2013). It's a way to quantify how much
 485 an agent can affect or change its surroundings (i.e. the future observed state) based on its actions
 486 from that state. Formally, the empowerment of a state s is defined as the channel capacity of
 487 the actuation channel, i.e. the maximum potential information transmission between the agent's
 488 actions and the subsequent impact of these actions after a certain duration. Here we consider

489 1-step empowerment, which is defined as:

$$490 \quad E^{(t)}(s) = \max_{p(a)} I(S'; A|s) \quad (11)$$

$$491 \quad = \max_{p(a)} (\mathcal{H}(S') - \mathcal{H}(S'|A)) \quad (12)$$

$$492 \quad = \max_{p(a)} (\mathcal{H}(A) - \mathcal{H}(A|S')) \quad (13)$$

493 where A and S' are random variable for the action and next state, respectively. There are multiple
 494 ways to intuitively understand this formula. Examining eq.12, we note that in order to maximize
 495 empowerment, we aim to maximize the entropy of the next state S' , implying a diversity of potential
 496 next states. Simultaneously, we seek to minimize $\mathcal{H}(S'|A)$, to reduce stochasticity in the process.
 497 This conceptually aligns with the desire to have control over the destination when selecting an
 498 action. An alternative interpretation is found in eq.13. To maximize empowerment, we want to
 499 maximize $\mathcal{H}(A)$ to enable numerous possible actions, while minimizing $\mathcal{H}(A|S')$ to account for
 500 the fact that multiple actions may lead to the same state. Essentially, this seeks to maximize
 501 the count of *effective* actions—those leading to diverse outcomes. In each case, we consider the
 502 maximum over all possible action distributions $p(a)$. For an agent driven by empowerment as
 503 intrinsic motivation, we set $R_{Empowerment}^{(t)}(s, a, s') = E^{(t)}(s')$.

504 *Asymptotic behavior:* An agent driven by empowerment will seek out states with a large number
 505 of available options, as these states offer the most control. In the long run, the agent’s estimation
 506 of the transition probabilities will converge to the true probabilities. Therefore, the agent will tend
 507 to stay in the most empowering regions of the environment (e.g. source states) and avoid reaching
 508 isolated areas with fewer options.

509 Maximum Occupancy Principle (MOP)

510 Introduced in Ramírez-Ruiz et al. (2024), MOP as intrinsic motivation considers that the goal of
 511 an agent’s behavior is to maximize the occupancy of future action-state paths. The agent aims to
 512 maximize the return

$$513 \quad R_{MOP}(s, a, s') = -\log \left(\pi^{\alpha_{MOP}}(a|s) \hat{P}^{\beta_{MOP}}(s'|s, a) \right) \quad (14)$$

514 Where the subscript (t) has been omitted for clarity. An agent motivated by MOP is expected to
 515 favor high entropy policies and highly stochastic regions of the environment. In our experiments,
 516 we set $\alpha_{MOP} = \beta_{MOP} = 1$ to give equal weights to these two aspects. Unlike for other intrinsic
 517 motivations, we do not compute the policy by applying softmax on Q-values. Instead, we use
 518 a modified version of value iteration as in Moreno-Bote and Ramirez-Ruiz (2023); Ramírez-Ruiz
 519 et al. (2024) to consider the optimal policy at every step.

520 *Asymptotic behavior:* As detailed in Ramírez-Ruiz et al. (2024), MOP aims to find a policy π that
 521 maximizes the value function $V_\pi(s)$ defined as

$$522 \quad V_\pi(s) = \alpha \mathcal{H}(A|s) + \beta \sum_a \pi(a|s) \mathcal{H}(S'|s, a) + \gamma \sum_{a, s'} \pi(a|s) P(s'|s, a) V_\pi(s'), \quad (15)$$

523 where $\mathcal{H}(A|s)$ is the policy in state s , and $\mathcal{H}(S'|s, a)$ is the entropy of the next state distribution
 524 given action a in state s . The first term favors states with multiple available actions, the second

term encourages to experience stochastic transition and the last term accounts for the value of the next state. The agent will aim to reach the states where $V_\pi(s)$ is highest. Therefore, after learning sufficiently about the environment, we expect the agent to spend most of its time in stochastic areas and regions with many actions.

Successor-Predecessor Intrinsic Exploration (SPIE)

SPIE was introduced in Yu et al. (2024). Instead of only rewarding the agent for discovering new states like Novelty, SPIE also rewards it for visiting states that lead to isolated regions. The key idea is to use both forward-looking (successor) and backward-looking (predecessor) information to identify and navigate critical or "bottleneck" states. The reward is defined based on the successor representation (SR), which measures how often one state is expected to be visited in the future with the current policy, given that the agent is currently in a specific state. The reward is defined as:

$$R_{SPIE}^{(t)}(s, a, s') = \hat{M}^{(t)}[s, s'] - \|\hat{M}^{(t)}[\cdot, s']\|_1 \quad (16)$$

where $\hat{M}^{(t)}[s, s']$ is the learned SR for the state s' given state s , and $\|\hat{M}^{(t)}[\cdot, s']\|_1$ is the sum of the SRs of s' from all states. Intuitively, the reward is high when state s' is difficult to reach from all states except s . Therefore, if s is a bottleneck state, the reward is high, encouraging the agent to visit such states. Unlike the original paper, we do not approximate the matrix $\hat{M}^{(t)}[s, s']$ using an online TD-learning rule. Instead, we compute it exactly after each observed transition using the agent's environment model.

Asymptotic behavior: Yu et al. (2024) argues that the behavior of SPIE is non-trivial, even when the matrix M is known or fixed. However, since the reward is higher for rarely encountered states, we expect the agent to reach a close to uniform state visitation.

Hyper-parameters selection

The framework described in **General framework** contains three hyper-parameters: ϵ , λ and β . The parameter ϵ is a small positive constant added to transition counts to prevent zero probabilities for unseen transitions, λ is the discount factor that determines the weight of future rewards compared to immediate rewards, and β is the Softmax inverse temperature parameter that influences the randomness of the action selection based on the Q-values.

In all experiments, we set $\epsilon = 1/n$ and $\lambda = \sqrt[n/2]{0.5}$ where n is the number of states in the environment, so that a future reward that is $n/2$ step away is discounted to half its value. On the other hand, β is optimized in a more complex manner. Each combination of intrinsic motivation, performance measure, and environment type is referred to as a setup. The inverse temperature β was optimized separately for each setup. For instance, in Fig. 2, with 6 intrinsic motivations, 3 performance measures, and 5 environment regimes, there are 90 setups, requiring 90 optimized values for β . The optimization process for each setup is as follows: First, we generate 50 environments based on the chosen type. Then, we find the value of β that gives the best score using grid search. To compute the score for a specific choice of β , we run an agent for 500 steps on each environment. We evaluate the performance measure every 100 steps and calculate the average, resulting in a score for each environment. The overall score is calculated as the average score across the 50 environments.

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569 Author Contributions

570 Competing Interests statement

571 The authors declare no competing interests.

572 Code and data availability

573 All code and data needed to reproduce the results reported in this manuscript will be made publicly
574 available after publication acceptance.

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825 Supplementary Material

826 Environment generation

827 All the parameters used for generating environments are described in Table 1. The environments
828 are generated in three steps:

- 829 1. Maze generation: a maze is generated with a given number of states and branching rate. The
830 branching rate determines the number of intersections in the environment. The algorithm
831 for generating the maze is defined in Algorithm 1.
- 832 2. Room integration: some states in the maze are transformed into rooms. A room is a square
833 grid, with each state having four actions to navigate up, down, left or right whenever these
834 actions are available (when the state is not on a border). Neighbors of a transformed state
835 are connected to the middle of the room borders (maximum 4 neighbors, one for each side
836 of the square room). Parameters determine the fraction of states that are transformed into
837 rooms and the size of the rooms.
- 838 3. Room properties: Each room is assigned one of sink, source, stochastic or neutral. For
839 each sink room, we iteratively sample a state u in the room and a state v outside the room
840 uniformly at random, and connect v to u . We repeat until the desired number of edges
841 has been added. For each source room, we do the same process but inverse the direction of
842 connections. The transition dynamics inside stochastic rooms are altered as follows: when
843 an agent selects an action a from a state s within a the room, there is a fixed probability
844 that the action will result in the agent moving to a random neighbor of s in the room instead
845 of the intended destination of a . Finally, neutral rooms do not receive any modification.

Algorithm 1 Algorithm to generate the initial maze

Require: $n > 0$, $\text{branch_rate} \in [0, 1]$

$Q \leftarrow$ empty queue

ENQUEUE($Q, 1$)

$\text{next_state} \leftarrow 2$

while $\text{next_state} \leq n$ **do**

$\text{cur_state} \leftarrow$ DEQUEUE(Q)

CONNECT($\text{cur_state}, \text{next_state}$)

CONNECT($\text{next_state}, \text{cur_state}$)

$\text{rand} \in [0, 1]$ uniformly at random

if $\text{rand} < \text{branch_rate}$ **and** $n_{\text{neighbors}}(\text{cur_state}) < 4$ **then**

ENQUEUE($Q, \text{cur_state}$) ▷ The current state is put back in the Queue if it does not
already have 4 neighbors

end if

ENQUEUE($Q, \text{next_state}$)

$\text{next_state} += 1$

end while

Parameter	Range	Short description	Environment types					
			Neutral	Sink	Source	Stochastic	Mixed	Trap (Fig. 3)
n_s	$[1, \infty]$	Number of states in the initial maze.	40	40	40	40	40	97
branch rate	$[0,1]$	Probability of creating a new intersection when adding a state.	0.2	0.2	0.2	0.2	0.2	$0 \rightarrow 1$
n_{room}	$[0, n_s]$	Number of rooms.	4	4	4	4	4	1
room size	$[1, \infty]$	Size of the side of rooms.	4	4	4	4	4	2
p_{sink}	$[0,1]$	Fraction of sink rooms.	0	0.25	0	0	0.25	1
p_{source}	$[0, 1 - p_{\text{sink}}]$	Fraction of source rooms.	0	0	0.25	0	0.25	0
$p_{\text{stochastic}}$	$[0, 1 - p_{\text{sink}} - p_{\text{source}}]$	Fraction of stochastic rooms.	0	0	0	0.25	0.25	0
$n_{\text{edges per sink}}$	$[0, \infty]$	Number of additional connection leading to each sink room.	0	50	0	0	50	$0 \rightarrow 200$
$n_{\text{edges per source}}$	$[0, \infty]$	Number of additional connection originating from each source room.	0	0	50	0	50	0
uncontrollability	$[0,1]$	Probability for an action taken in a stochastic room to lead to a random neighbor instead of the expected destination.	0	0	0	1	1	0

Table 1: Summary of all environment parameters used in the generation process. The right side shows the environment types considered with the corresponding parameter values.

846 **Robustness of results**

847 **Robustness to change of metrics**

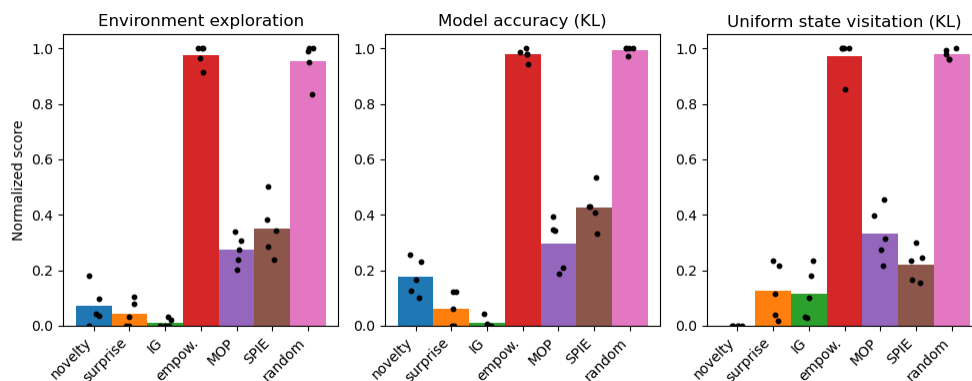
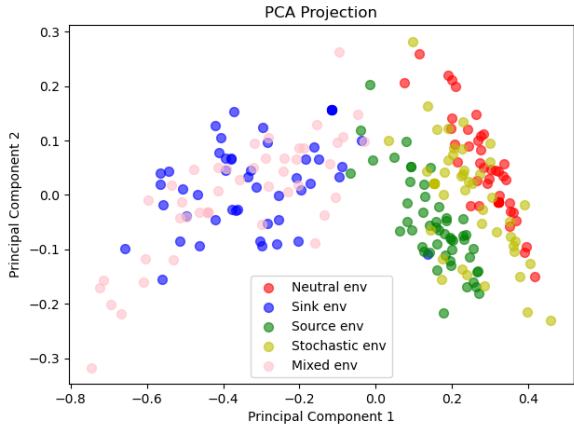
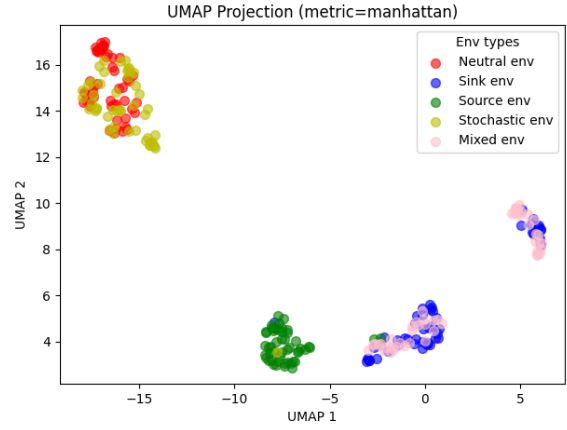


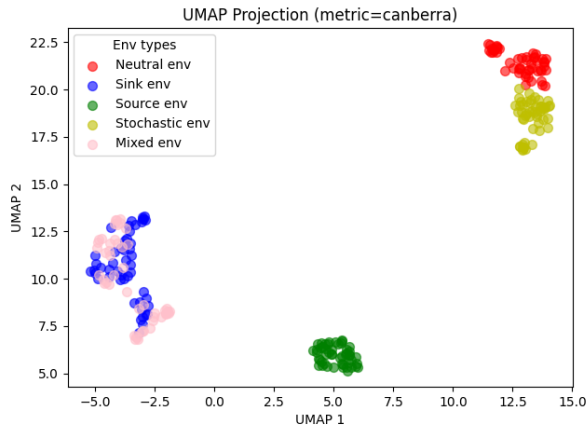
Figure 8: Average normalized score across environments for each intrinsic motivation, computed as in Fig. 4, but using the KL divergence instead of RMSE for measure 2 and 3. The results are very similar and the same conclusions can be drawn.



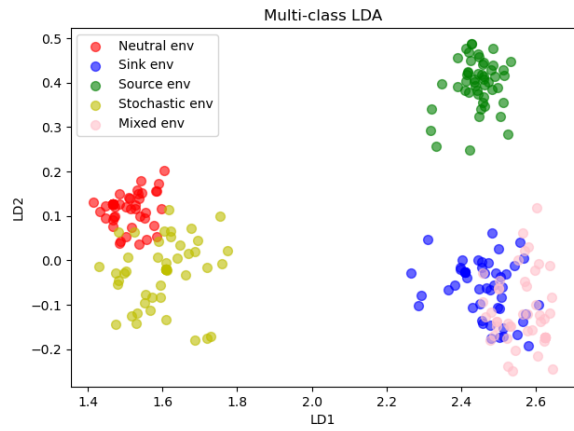
(a) PCA



(b) UMAP with Manhattan distance



(c) UMAP with Canberra distance



(d) Multi-class Linear Discriminant Analysis (LDA)

Figure 7: Consistency of performance within each environment type. The environment types are described in [Environment types](#). Various projections of performance vectors for each environment are shown. Each dot corresponds to one environment sampled from one of the given types. For each such sample, a vector of performance is created as follows: we run each intrinsic motivation for 2000 steps and calculate the Area Under the Curve for each performance measure (same curve as in [Fig. 2](#)). For each environment, we obtain a performance vector of size $(n_{IM} \cdot n_{measures}) = (6 \cdot 3)$ where n_{IM} is the number of intrinsic motivations and $n_{measures}$ is the number of measures. (a) We apply PCA and display the top two principal components. (b)-(c) We use UMAP with Manhattan and Canberra distances. (d) We apply multi-class LDA. Clusters are observed in each method. Sink and Mixed environments consistently overlap, probably due to the presence of sink rooms in both cases. Neutral and Stochastic environments are also close, but remain distinguishable in (c) and (d). This similarity is probably due to the fact that a stochastic room doesn't change the environment dynamics as much as sink and source rooms.