Explaining Reinforcement Learning with Shapley Values: Theory and Algorithms

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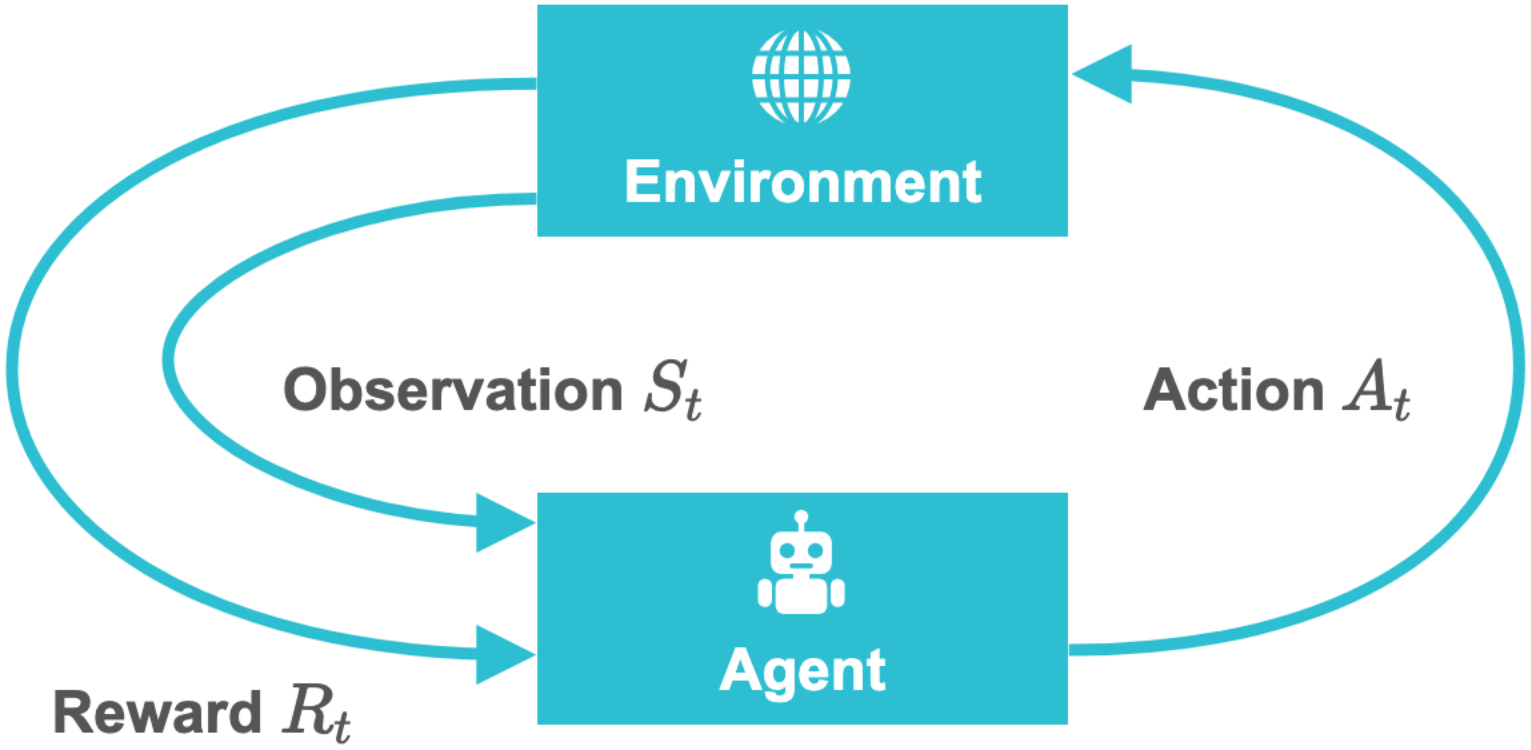
What is Reinforcement Learning?



Learn a policy $\pi : \mathcal{S} \to \Delta(\mathcal{A})$ that maps each observation to a probability distribution over actions, **maximising the expected return** [14]:

$$\mathbb{E}[G_t] = \mathbb{E}\left[\sum_{k=0}^{\infty} \gamma^k R_{t+k+1}\right]$$

What Can Reinforcement Learning Do?

Atari [7]

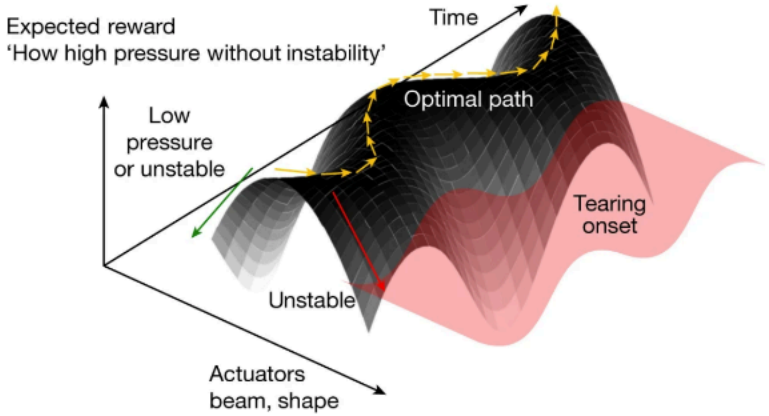
AlphaGo [9, 12, 21]

StarCraft II [17]

Gran Turismo [36]

Matrix Multiplication [32]

Stratospheric Balloons [18]



Nuclear Fusion Reactor Control [31, 39]

Reinforcement learning agents do not explain their actions.

Understanding Agent-Environment Interactions

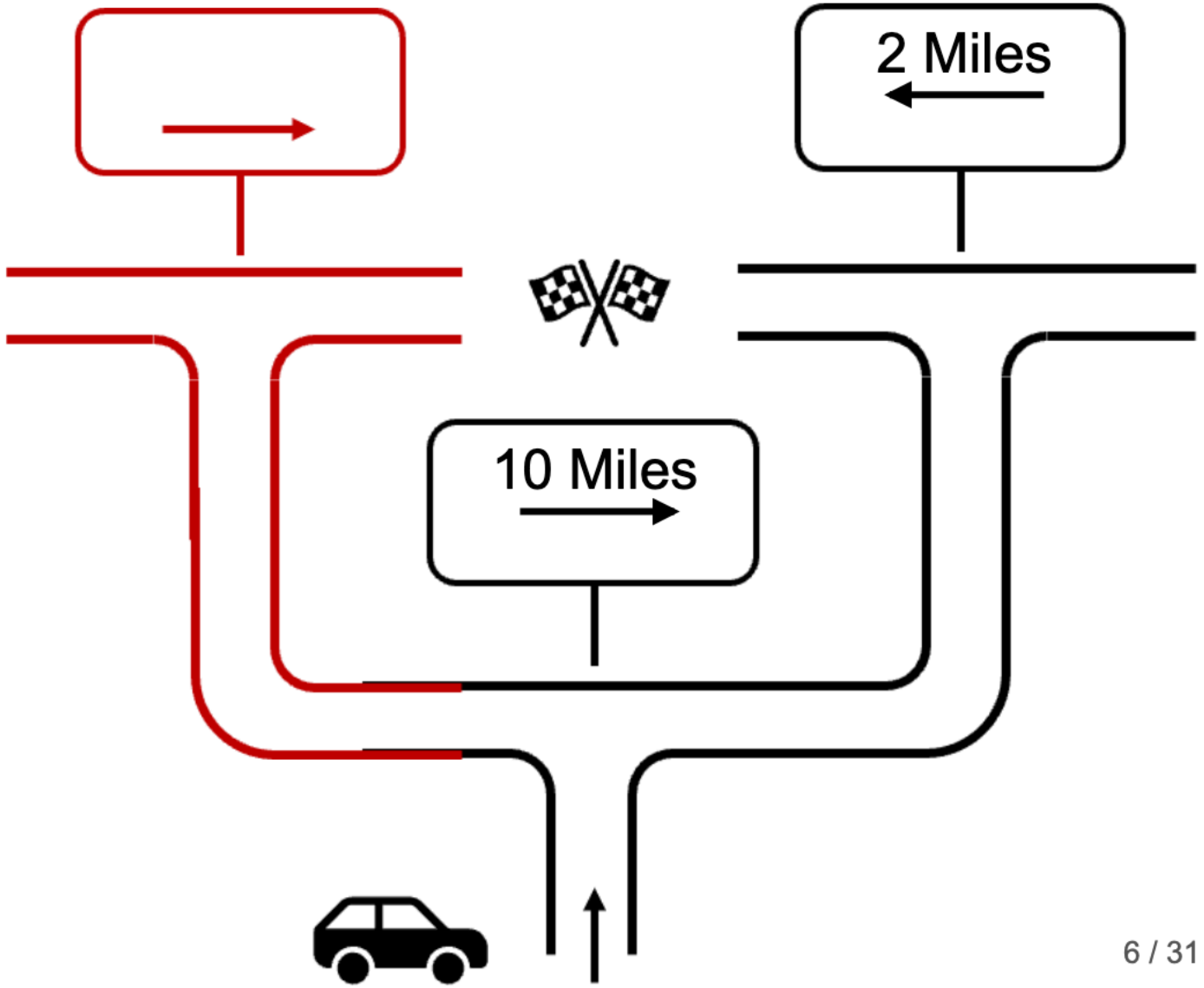
Certain features of an agent's observations influence how they interact with their environment.

Contribution: A theoretical and computational framework for explaining agent-environment interactions using the influence of features.

Beechey, D., Smith, T.M. and Şimşek, Ö., 2023, July. Explaining reinforcement learning with Shapley values. In *International Conference on Machine Learning* (pp. 2003-2014). PMLR.

What Needs Explaining?

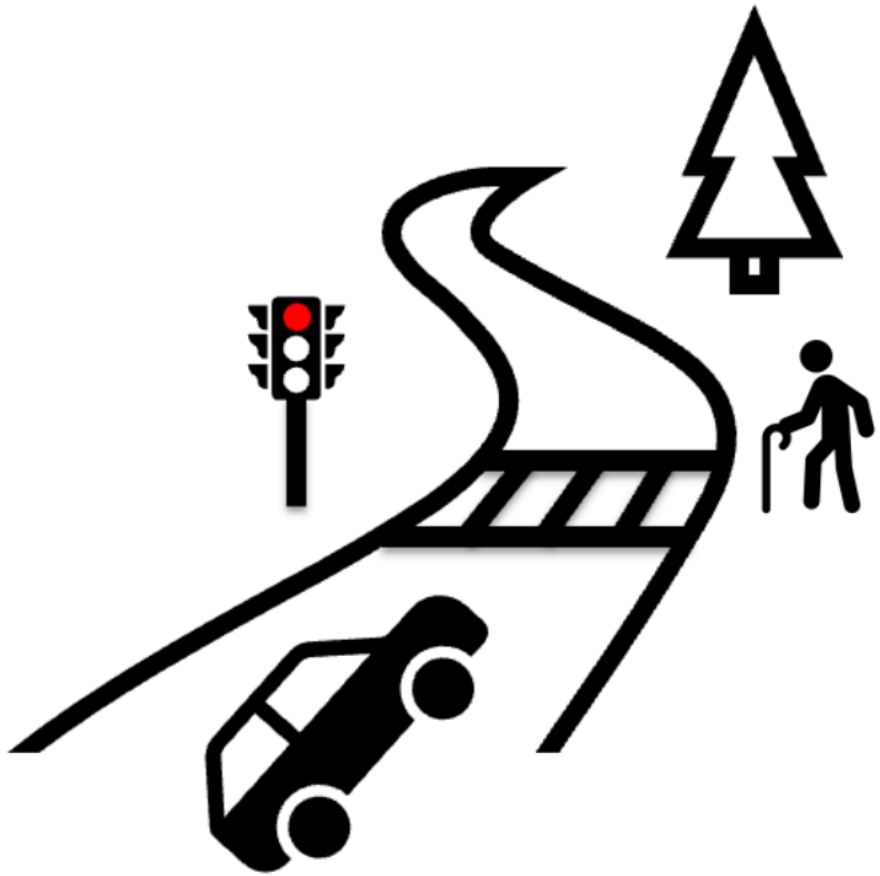
- Behaviour
- Outcomes
- Predictions



Computing Feature Influence

Compute the influence of features by observing the effect of their removal.

Features are interdependent; removing one feature does not properly capture its contribution.



The Contribution Assignment Problem

A **cooperative game** is a set of players $\mathcal{F}$ and a characteristic function $v(\mathcal{C}) : 2^{|\mathcal{F}|} \to \mathbb{R}$.

How to assign the contribution $\phi_i(v)$ of player i to the outcome of the game $(\mathcal{F}, v)$? [1]

$$\phi_i(v) = \sum_{\mathcal{C} \subseteq \mathcal{F} \setminus \{i\}} \frac{|\mathcal{C}|!\,(|\mathcal{F}| - |\mathcal{C}| - 1)!}{|\mathcal{F}|!} \left(v(\mathcal{C} \cup \{i\}) - v(\mathcal{C})\right)$$

Shapley Value Axioms

$$\phi_i(v) = \sum_{\mathcal{C} \subseteq \mathcal{F} \setminus \{i\}} \frac{|\mathcal{C}|!\,(|\mathcal{F}| - |\mathcal{C}| - 1)!}{|\mathcal{F}|!} \left(v(\mathcal{C} \cup \{i\}) - v(\mathcal{C})\right)$$

Shapley values $\phi_i(v)$ are the **unique solution** to the contribution assignment problem that satisfies four axioms of fair contribution. [1]

Efficiency: $v(\mathcal{F}) = v(\emptyset) + \sum_{i \in \mathcal{F}} \phi_i(v).$

Symmetry: $\phi_i(v) = \phi_j(v)$ if $v(\mathcal{C} \cup \{i\}) = v(\mathcal{C} \cup \{j\}) \;\; \forall \mathcal{C} \subseteq \mathcal{F} \setminus \{i, j\}.$

Nullity: $\phi_i(v) = 0$ if $v(\mathcal{C} \cup \{i\}) = v(\mathcal{C}) \;\; \forall \mathcal{C} \subseteq \mathcal{F} \setminus \{i\}.$

Linearity: $\phi_i(\alpha u + \beta v) = \alpha \phi_i(u) + \beta \phi_i(v).$

Shapley Values for Explaining Reinforcement Learning (SVERL)

Beechey, D., Smith, T. and Şimşek, Ö., 2025. A Theoretical Framework for Explaining Reinforcement Learning with Shapley Values. arXiv preprint arXiv:2505.07797.

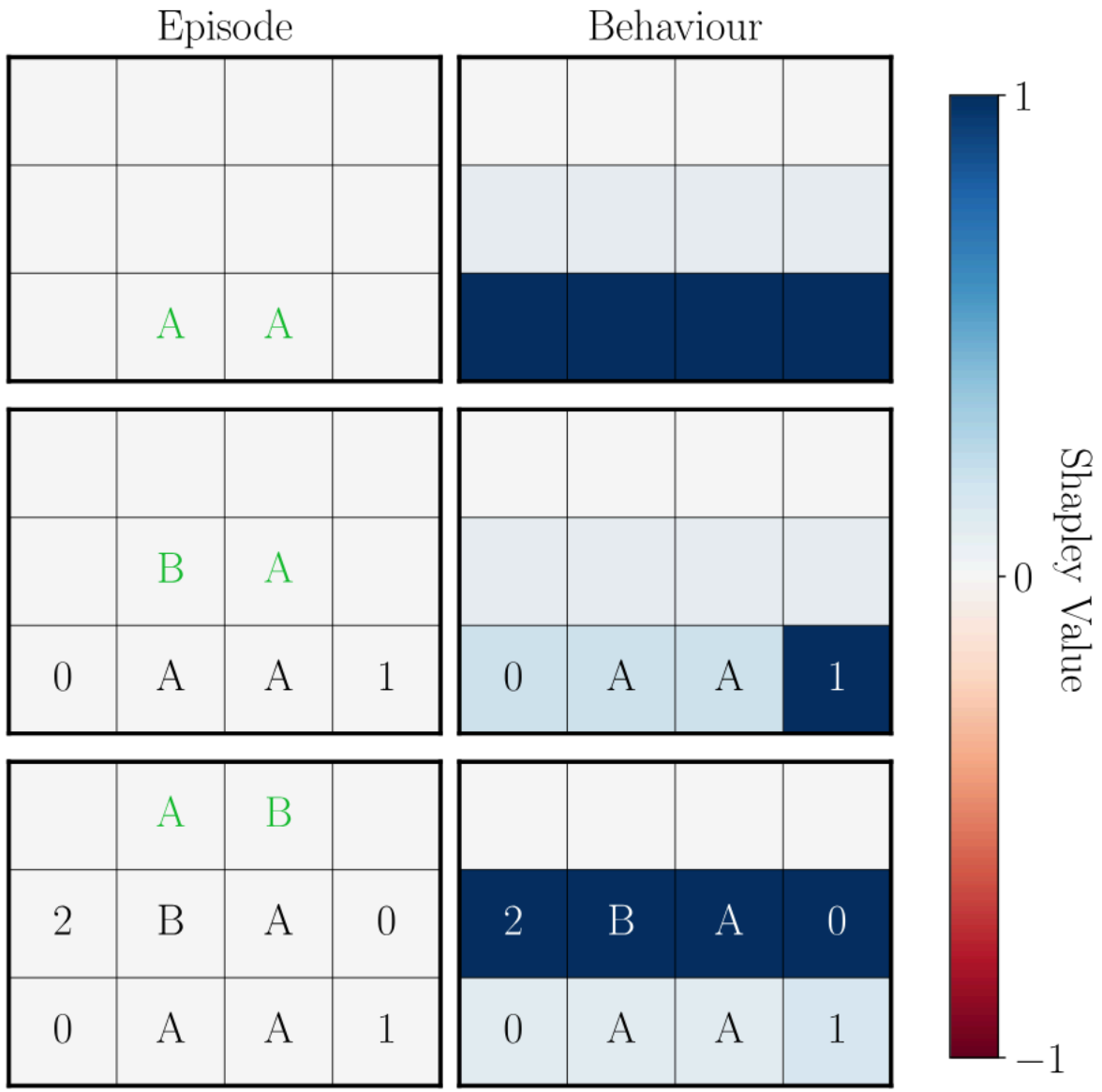
A collection of cooperative games played by the values of the features an agent observes, whose outcomes are different aspects of agent-environment interactions.

Explaining Behaviour. The contribution of feature values to the probability of selecting action a in state s.

A cooperative game played by the values of the features at state s, whose outcome $\tilde{\pi}_s^a : 2^{|\mathcal{F}|} \to [0,1]$ is the probability of selecting action a at state s when only the values of features $\mathcal{C}$ are known.

$$\tilde{\pi}_s^a(\mathcal{C}) = \mathbb{E}\left[\pi(S,a) \mid S_{\mathcal{C}} = s_{\mathcal{C}}\right] = \sum_{s' \in \mathcal{S}^+} p^\pi(s' \mid s_{\mathcal{C}})\, \pi(s',a)$$

Explaining Behaviour in Mastermind



A collection of cooperative games played by the values of the features an agent observes, whose outcomes are different aspects of agent-environment interactions.

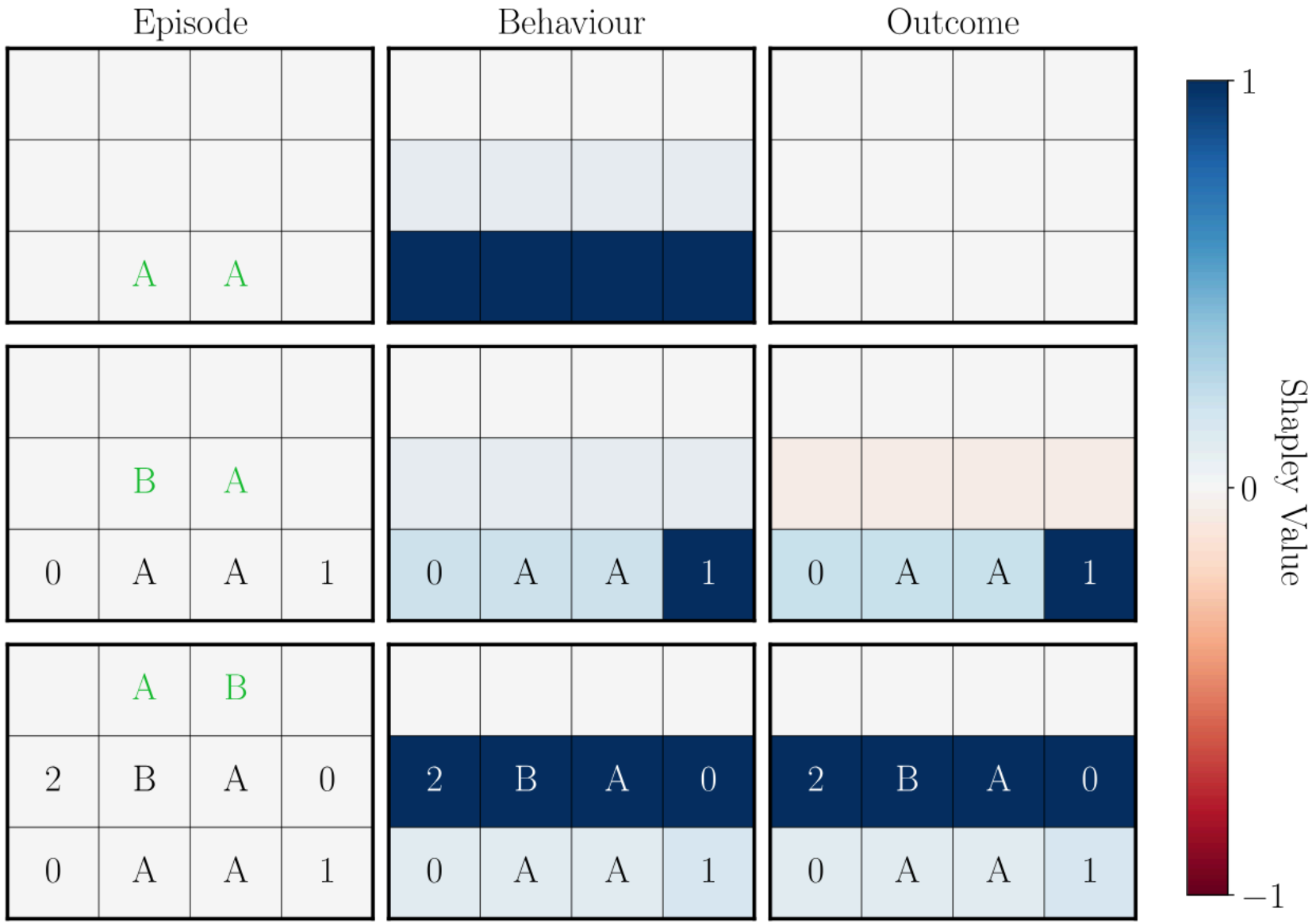
Explaining Behaviour. The contribution of feature values to the probability of selecting action a in state s.

Explaining Outcomes. The contribution of feature values to the expected return $v^{\pi}(s)$.

A cooperative game played by the values of the features at state s, whose outcome $\tilde{v}_s^\pi : 2^{|\mathcal{F}|} \to \mathbb{R}$ is the expected return from state s when policy π has access to only the values of features in $\mathcal{C}$.

$$\tilde{v}_s^\pi(\mathcal{C}) = \mathbb{E}_\mu \left[G_t \mid S_t = s \right], \quad \text{where} \quad \mu(s_t, a_t) = \begin{cases} \tilde{\pi}_{s_t}^{a_t}(\mathcal{C}) & \text{if } s_t = s, \\ \pi(s_t, a_t) & \text{otherwise.} \end{cases}$$

Explaining Outcomes in Mastermind



A collection of cooperative games played by the values of the features an agent observes, whose outcomes are different aspects of agent-environment interactions.

Explaining Behaviour. The contribution of feature values to the probability of selecting action a in state s.

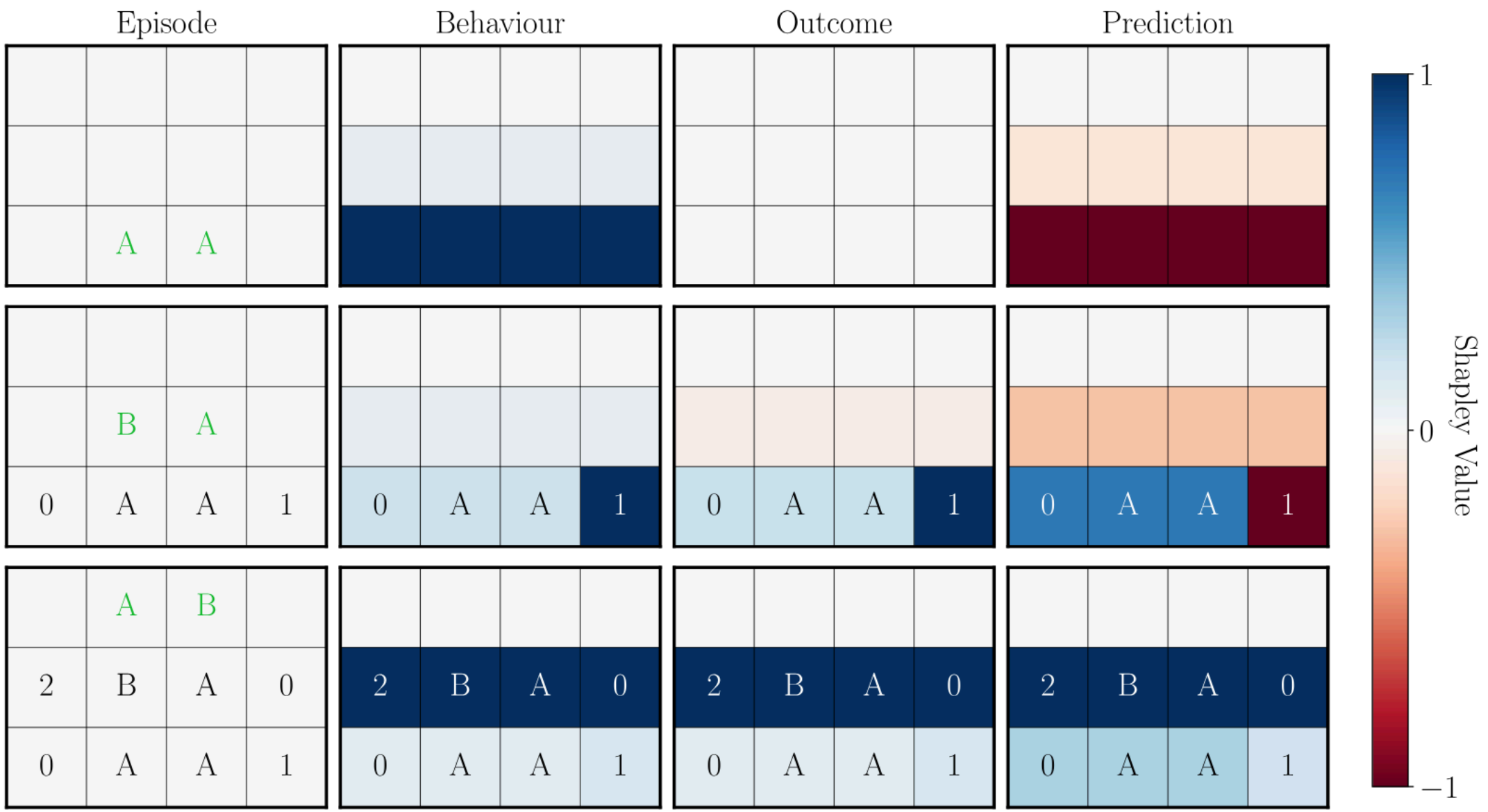
Explaining Outcomes. The contribution of feature values to the expected return $v^{\pi}(s)$.

Explaining Predictions. The contribution of feature values to the predicted expected return $\hat{v}^{\pi}(s)$.

A cooperative game played by the values of the features at state s, whose outcome $\hat{v}_s^\pi : 2^{|\mathcal{F}|} \to \mathbb{R}$ is the predicted expected return using only the feature values $s_\mathcal{C}$.

$$\hat{v}_s^\pi(\mathcal{C}) = \mathbb{E}\left[\hat{v}^\pi(S) \mid S_\mathcal{C} = s_\mathcal{C}\right] = \sum_{s' \in \mathcal{S}^+} p^\pi(s' \mid s_\mathcal{C})\, \hat{v}^\pi(s')$$

Explaining Predictions in Mastermind



Feature Importance Methods

Gradients [10] Perturbation [13, 20] Attention [15] LIME [8]

Shapley Values in Supervised Learning

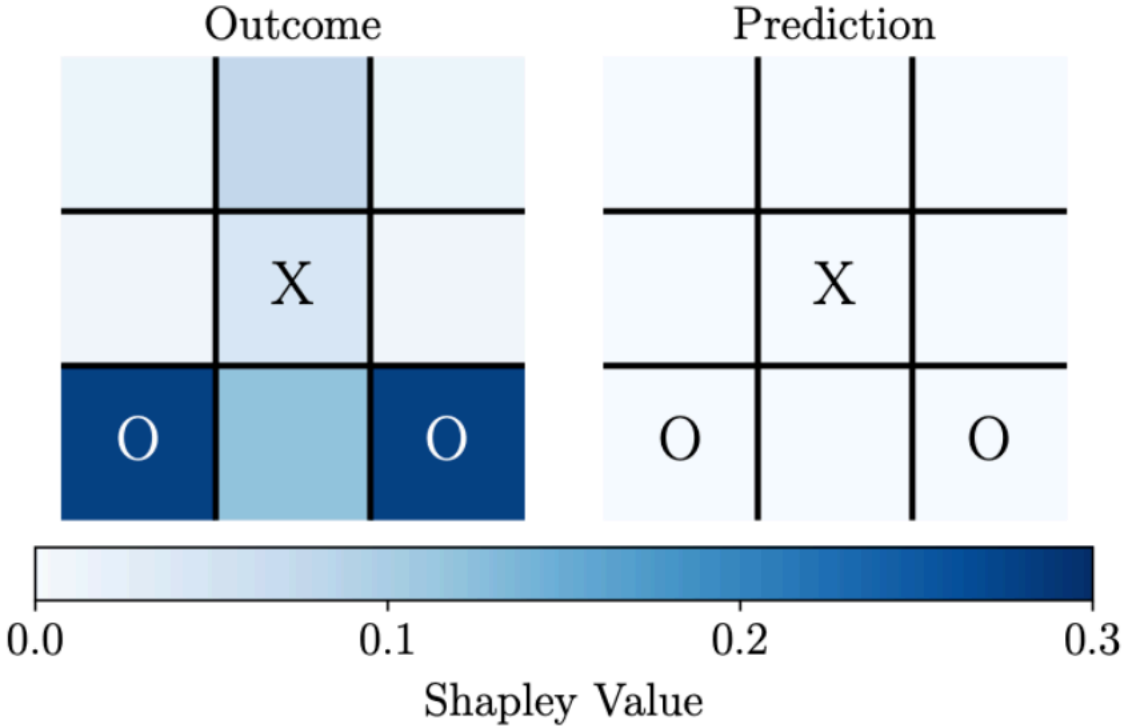
Feature attribution [4, 5, 6, 24, 25, 33, 38]

SHAP [11]

Shapley Values in Reinforcement Learning

SHAP applied to the value function [23, 29, 30]

SHAP applied to the policy [16, 19, 22, 26, 27, 28, 34, 35]



Approximating Shapley Explanations in Reinforcement Learning (FastSVERL)

Beechey, D. and Şimşek, Ö., 2025. Approximating Shapley explanations in reinforcement learning. In *Advances in Neural Information Processing Systems*.

Computing SVERL Exactly is Intractable

Shapley values sum over every subset of features:

$$\phi_i(\tilde{\pi}_s^a) = \sum_{\mathcal{C} \subseteq \mathcal{F} \setminus \{i\}} \frac{|\mathcal{C}|!\,(|\mathcal{F}| - |\mathcal{C}| - 1)!}{|\mathcal{F}|!} \left(\tilde{\pi}_s^a(\mathcal{C} \cup \{i\}) - \tilde{\pi}_s^a(\mathcal{C})\right)$$

$2^{|\mathcal{F}|-1}$ **subsets**

Each characteristic value is an expectation over the state space:

$$\tilde{\pi}_s^a(\mathcal{C}) = \mathbb{E}\left[\pi(S, a) \mid S_\mathcal{C} = s_\mathcal{C}\right] = \sum_{s' \in \mathcal{S}^+} p^\pi(s' \mid s_\mathcal{C})\, \pi(s', a)$$

$|\mathcal{S}|$ **states**

$$\mathcal{O}\left(2^{|\mathcal{F}|} \cdot |\mathcal{S}|\right)$$ **per explanation**

Approximating the Characteristic Function

The characteristic function is an expectation over the state space:

$$\tilde{\pi}_s^a(\mathcal{C}) = \mathbb{E}\left[\pi(S, a) \mid S_{\mathcal{C}} = s_{\mathcal{C}}\right] = \sum_{s' \in \mathcal{S}^+} p^\pi(s' \mid s_{\mathcal{C}})\, \pi(s', a)$$

Learn a model $\hat{\pi}(s, a \mid \mathcal{C}; \beta)$ that masks the features outside $\mathcal{C}$ [25]:

$$\mathcal{L}(\beta) = \mathop{\mathbb{E}}_{p^\pi(s)} \mathop{\mathbb{E}}_{\mathrm{Unif}(a)} \mathop{\mathbb{E}}_{p(\mathcal{C})} \left|\pi(s, a) - \hat{\pi}(s, a \mid \mathcal{C}; \beta)\right|^2$$

It **cannot** recover $\pi(s, a)$ from partial input, so it learns the average of $\pi(s', a)$ over the states sharing those values: the characteristic function.

Approximating the Shapley Values

$$\phi_i(\tilde{\pi}_s^a) = \sum_{\mathcal{C} \subseteq \mathcal{F} \setminus \{i\}} \frac{|\mathcal{C}|!\,(|\mathcal{F}| - |\mathcal{C}| - 1)!}{|\mathcal{F}|!} \left(\tilde{\pi}_s^a(\mathcal{C} \cup \{i\}) - \tilde{\pi}_s^a(\mathcal{C})\right)$$

Shapley values also solve a weighted least-squares problem [2, 11].

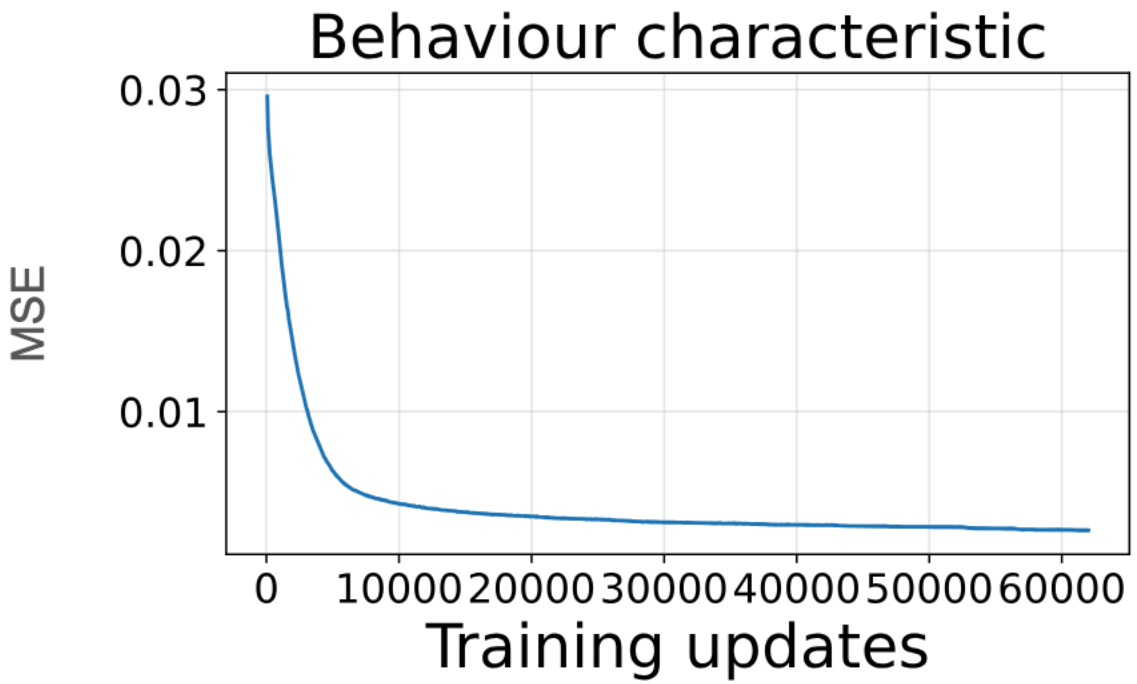
Learn a model $\hat{\phi}(s, a; \theta)$ that predicts every feature's contribution at once [33]:

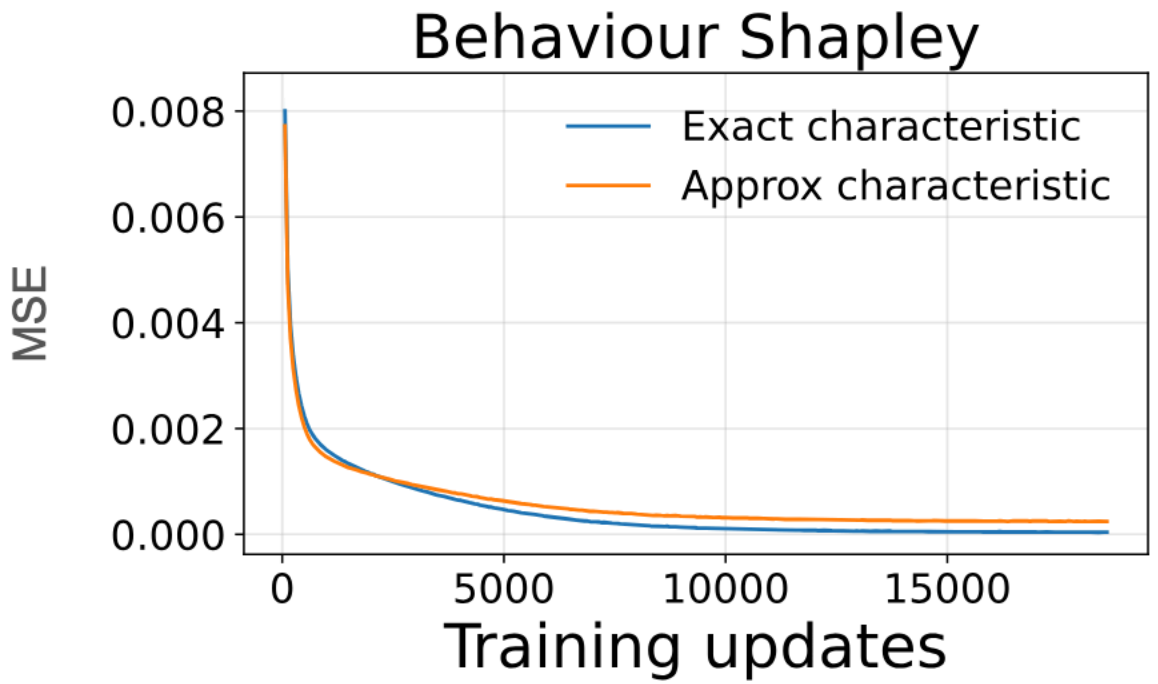
$$\mathcal{L}(\theta) = \mathop{\mathbb{E}}_{p^\pi(s)} \mathop{\mathbb{E}}_{\mathrm{Unif}(a)} \mathop{\mathbb{E}}_{p(\mathcal{C})} \left| \tilde{\pi}_s^a(\mathcal{C}) - \tilde{\pi}_s^a(\emptyset) - \sum_{i \in \mathcal{C}} \hat{\phi}^i(s, a; \theta) \right|^2$$

The cost is amortised: train once, then read off an explanation for any state. [33, 38]

How Well Does It Approximate?

Mastermind: 100,000+ states, 15 features, 27 actions.





Training the Shapley model on approximate characteristic values carries that error through.

Learning to Explain Off-Policy

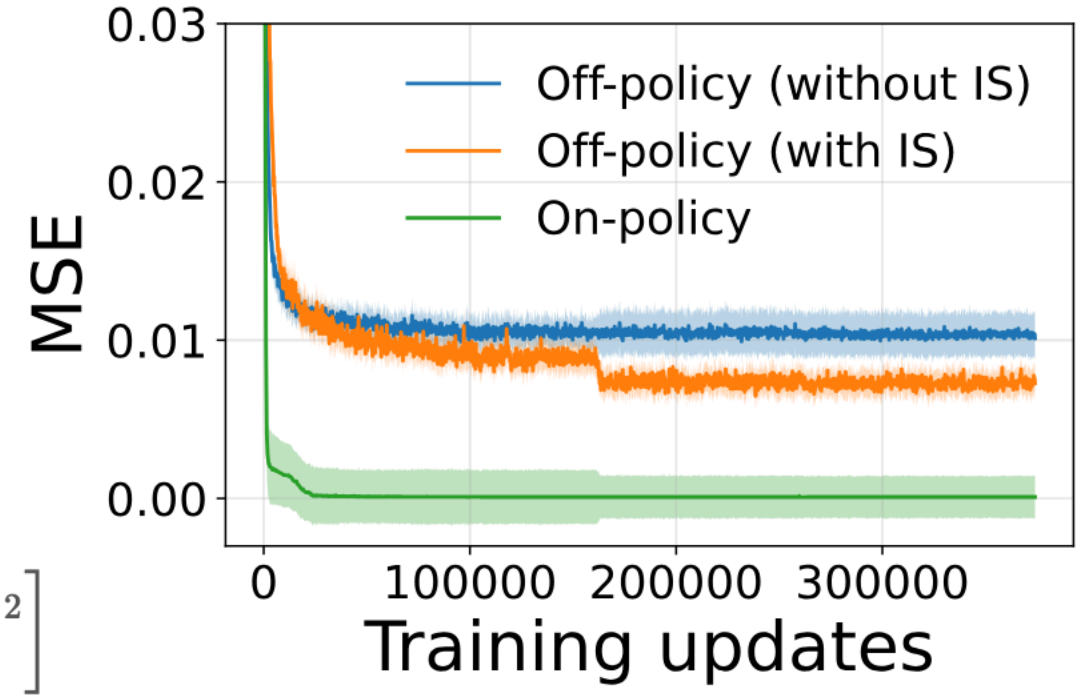
Take the behaviour characteristic loss:

$$\mathcal{L}(\beta) = \mathop{\mathbb{E}}_{p^{\pi}(s)} \mathop{\mathbb{E}}_{\text{Unif}(a)} \mathop{\mathbb{E}}_{p(\mathcal{C})} |\pi(s,a) - \hat{\pi}(s,a \mid \mathcal{C};\beta)|^2$$

What if we cannot collect states from the policy we are explaining?

Draw states from the agent's own history, and reweight [3]:

$$\mathcal{L}(\beta) \approx \mathop{\mathbb{E}}_{(s_t,a_t)\sim\mathcal{B}} \mathop{\mathbb{E}}_{p(\mathcal{C})} \left[\frac{\pi(s_t,a_t)}{\pi_t(s_t,a_t)} \cdot |\pi(s_t,a_t) - \hat{\pi}(s_t,a_t \mid \mathcal{C};\beta)|^2 \right]$$

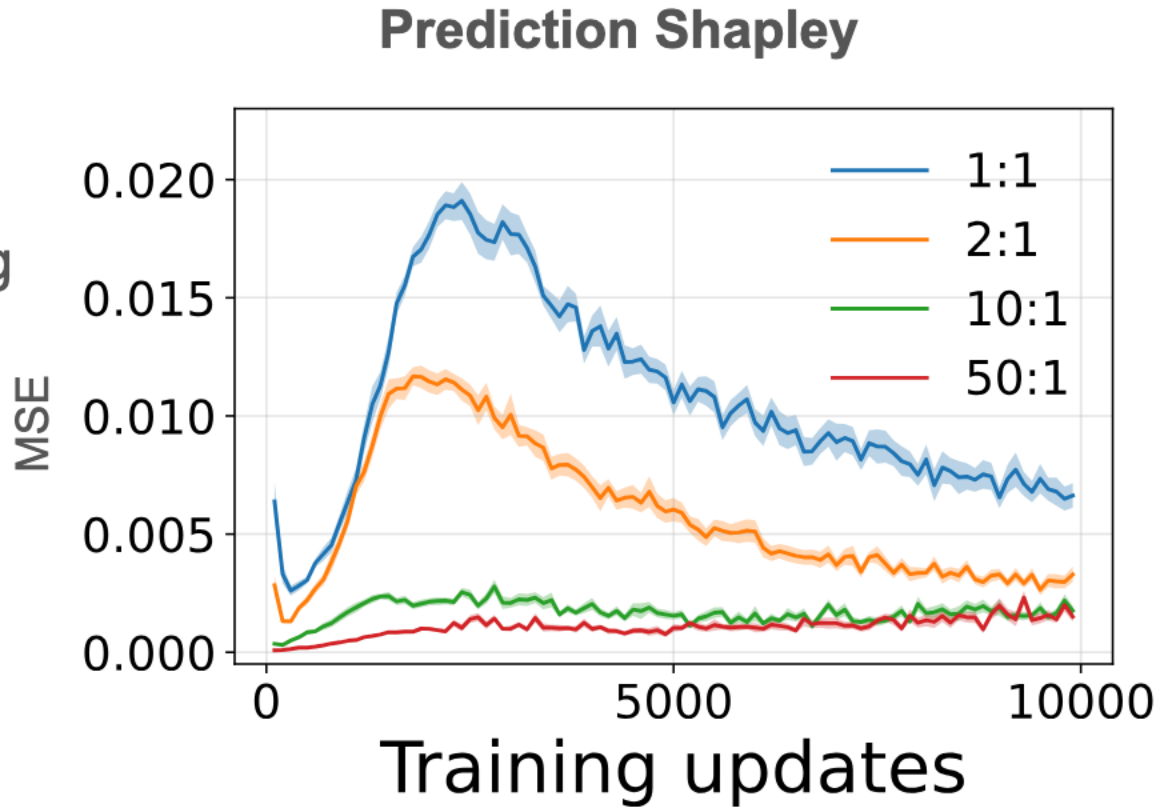


Continuously Learning to Explain

Explanations must track the agent's continuously changing policy.

Train the explanation models alongside it, using the same interaction data.

Error spikes when the policy shifts. More updates per policy update keeps them aligned.



Explaining Behaviour in Mastermind

Guess	Clue 1	Pos 1	Pos 2	Pos 3	Pos 4	Clue 2
6						
5		C	C	C	B	
4	2	B	C	C	C	2
3	2	C	B	C	C	2
2	0	C	C	C	C	3
1	0	A	A	C	A	1

3-letter alphabet. Over 2.8×10^{11} states, 36 features.

The recent guesses are enough to deduce the code is some combination of B, C, C, C.

The unused slots contribute nothing, recovering the nullity axiom.

Thank You for Listening!

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Shapley Values for Explaining Reinforcement Learning (SVERL) [37, 40]

Explaining behaviour · Explaining outcomes · Explaining predictions

How to approximate SVERL in large-scale domains [41]

Parametric approximations of explanations

Learnt off-policy from the agent's own history

Continually adapt to evolving agent behaviour

Interesting directions

A real-world application of SVERL · User studies

Website: djeb20.github.io

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