Meta-trained agents implement Bayes-optimal agents

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Abstract

Memory-based meta-learning is a powerful technique to build agents that adapt fast to any task within a target distribution. A previous theoretical study has argued that this remarkable performance is because the meta-training protocol incentivises agents to behave Bayes-optimally. We empirically investigate this claim on a number of prediction and bandit tasks. Inspired by ideas from theoretical computer science, we show that meta-learned and Bayes-optimal agents not only behave alike, but they even share a similar computational structure, in the sense that one agent system can approximately simulate the other. Furthermore, we show that Bayes-optimal agents are fixed points of the meta-learning dynamics. Our results suggest that memory-based meta-learning might serve as a general technique for numerically approximating Bayes-optimal agents—that is, even for task distributions for which we currently don’t possess tractable models.

1 Introduction

Within the paradigm of learning-to-learn, memory-based meta-learning is a powerful technique to create agents that adapt fast to any task drawn from a target distribution [1–6]. In addition, it has been claimed that meta-learning might be a key tool for creating systems that generalize to unseen environments [7]. This claim is also partly supported by studies in computational neuroscience, where experimental studies with human subjects have shown that fast skill adaptation relies on task variation [8, 9]. Due to this, understanding how meta-learned agents acquire their representational structure and perform their computations is of paramount importance, as it can inform architectural choices, design of training tasks, and address questions about generalisation and safety in artificial intelligence.

Previous theoretical work has argued that agents that fully optimise a meta-learning objective are Bayes-optimal by construction, because meta-learning objectives are Monte-Carlo approximations of Bayes-optimality objectives [10]. This is striking, as Bayes-optimal agents maximise returns (or minimise loss) by optimally trading off exploration versus exploitation [11]. The theory also makes a stronger, structural claim: namely, that meta-trained agents perform Bayesian updates “under the hood”, where the computations are implemented via a state machine embedded in the memory dynamics that tracks the sufficient statistics of the uncertainties necessary for solving the task class.

Here we set out to empirically investigate the computational structure of meta-learned agents. However, this comes with non-trivial challenges. Artificial neural networks are infamous for their hard-to-interpret computational structure: they achieve remarkable performance on challenging tasks, but the computations underlying that performance remain elusive. Thus, while much work in explainable machine learning focuses on the I/O behaviour or memory content, only few investigate the internal dynamics that give rise to them through careful bespoke analysis—see e.g. [12–18].
To tackle these challenges, we adapt a relation from theoretical computer science to machine learning systems. Specifically, to compare agents at their computational level [19], we verify whether they can approximately simulate each other. The quality of the simulation can then be assessed in terms of both state and output similarity between the original and the simulation.

Thus, our main contribution is the investigation of the computational structure of RNN-based meta-learned solutions. Specifically, we compare the computations of meta-learned agents against the computations of Bayes-optimal agents in terms of their behaviour and internal representations on a set of prediction and reinforcement learning tasks with known optimal solutions. We show that on these tasks:

- Meta-learned agents behave like Bayes-optimal agents (Section 4.1). That is, the predictions and actions made by meta-learned agents are virtually indistinguishable from those of Bayes-optimal agents.
- During the course of meta-training, meta-learners converge to the Bayes-optimal solution (Section 4.2). We empirically show that Bayes-optimal policies are the fixed points of the learning dynamics.
- Meta-learned agents represent tasks like Bayes-optimal agents (Section 4.3). Specifically, the computational structures correspond to state machines embedded in (Euclidean) memory space, where the states encode the sufficient statistics of the task and produce optimal actions. We can approximately simulate computations performed by meta-learned agents with computations performed by Bayes-optimal agents.

2 Preliminaries

Memory-based meta-learning  Memory-based meta-learners are agents with memory that are trained on batches of finite-length roll-outs, where each roll-out is performed on a task drawn from a distribution. The emphasis on memory is crucial, as training then performs a search in algorithm space to find a suitable adaptive policy [20]. The agent is often implemented as a neural network with recurrent connections, like an RNN, most often using LSTMs [4, 21], or GRUs [22]. Such a network computes two functions $f_w$ and $g_w$ using weights $w \in W$,

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\begin{align*}
    y_t &= f_w(x_t, s_{t-1}) \quad \text{(output function)} \\
    s_t &= g_w(x_t, s_{t-1}) \quad \text{(state-transition function)}
\end{align*}
$$

that map the current input and previous state pair $(x_t, s_{t-1}) \in \mathcal{X} \times \mathcal{S}$ into the output $y_t \in \mathcal{Y}$ and the next state $s_t \in \mathcal{S}$ respectively. Here, $\mathcal{X}$, $\mathcal{Y}$, $\mathcal{S}$, and $W$ are all vector spaces over the reals $\mathbb{R}$. An input $x_t \in \mathcal{X}$ encodes the instantaneous experience at time $t$, such as e.g. the last observation, action, and feedback signal; and an output $y_t \in \mathcal{Y}$ contains e.g. the logits for the current prediction or action probabilities. RNN meta-learners are typically trained using backpropagation through time (BPTT) [23, 24]. For fixed weights $w$, and combined with a fixed initial state $s_0$, equations (1) define a state machine. This state machine can be seen as an adaptive policy or an online learning algorithm.

Bayes-optimal policies as state machines  Bayes-optimal policies have a natural interpretation as state machines following [1]. Every such policy can be seen as a state-transition function $g$, which maintains sufficient statistics (i.e., a summary of the past experience that is statistically sufficient to implement the prediction/action strategy) and an output function $f$, which uses this information to produce optimal outputs (i.e., the best action or prediction given the observed trajectory) [10]. For instance, to implement an optimal policy for a multi-armed bandit with (independent) Bernoulli rewards, it is sufficient to remember the number of successes and failures for each arm.

Comparisons of state machines via simulation  To compare the policies of a meta-trained and a Bayes-optimal agent in terms of their computational structure, we adapt a well-established methodology from the state-transition systems literature [26, 30]. Specifically, we use the concept of simulation to compare state machines.

3 More precisely, a Mealy machine [25, 27].
Formally, we have the following. A *trace* in a state machine is a sequence $s_0x_1s_1 \cdots x_Ts_T$ of transitions. Since the state machines we consider are deterministic, a given sequence of inputs $x_1, \ldots, x_T$ induces a unique trace in the state machine. A deterministic state machine $M$ *simulates* another machine $N$, written $N \preceq M$, if every trace in $N$ has a corresponding trace in $M$ on which their output functions agree. More precisely, $N \preceq M$ if there exists a function $\phi$ mapping the states of $N$ into the states of $M$ such that the following two conditions hold:

- (transitions) for any trace $s_0x_1s_1 \cdots x_Ts_T$ in $N$, the transformed trace $\phi(s_0)x_1\phi(s_1)\cdots\phi(s_T)$ is also a trace in $M$;
- (outputs) for any state $s$ of $N$ and any input $x$, the output of machine $N$ at $(x, s)$ coincides with the output of machine $M$ at $(x, \phi(s))$.

Intuitively, this means there is a consistent way of interpreting every state in $N$ as a state in $M$, such that every computation in $N$ can be seen as a computation in $M$. When both $M \preceq N$ and $N \preceq M$ hold, then we consider both machines to be computationally equivalent.

### 3 Methods

#### 3.1 Tasks and agents

**Tasks** Since our aim is to compare against Bayes-optimal policies, we consider 10 prediction and 4 reinforcement learning tasks for which the Bayes-optimal solution is analytically tractable. All tasks are episodic ($T = 20$ time steps), and the task parameters $\theta$ are drawn from a prior distribution $p(\theta)$ at the beginning of each episode. A full list of tasks is shown in Figure 4 and details are discussed in Appendix A.

In prediction tasks the goal is to make probabilistic predictions of the next observation given past observations. All observations are drawn i.i.d. from an observational distribution. To simplify the computation of the optimal predictors, we chose observational distributions within the exponential family that have simple conjugate priors and posterior predictive distributions, namely: Bernoulli, categorical, exponential, and Gaussian. In particular, their Bayesian predictors have finite-dimensional sufficient statistics with simple update rules [31–33].

In reinforcement learning tasks the goal is to maximise the discounted cumulative sum of rewards in two-armed bandit problems [34]. We chose bandits with rewards that are Bernoulli- or Gaussian-distributed. The Bayes-optimal policies for these bandit tasks can be computed in polynomial time by pre-computing *Gittins indices* [35, 34, 36]. Note that the bandit tasks, while conceptually simple, already require solving the exploration versus exploitation problem [37].

**RNN meta-learners** Our RNN meta-learners consist of a three-layer network architecture: one fully connected layer (the encoder), followed by one LSTM layer (the memory), and one fully connected layer (the decoder) with a linear readout producing the final output, namely the parameters of the predictive distribution for the prediction tasks, and the logits of the softmax action-probabilities for the bandit tasks respectively. The width of each layer is the same and denoted by $N$. We selected $N = 32$ for prediction tasks and $N = 256$ for bandit tasks. Networks were trained with BPTT [23, 24] and Adam [38]. In prediction tasks the loss function is the log-loss of the prediction. In bandit tasks the agents were trained to maximise the return (i.e., the discounted cumulative reward) using the Impala [39] policy gradient algorithm. See Appendix B.2 for details on network architectures and training.

#### 3.2 Behavioral analysis

The aim of our behavioural analysis is to compare the input-output behaviour of a meta-learned (RNN) and a Bayes-optimal agent ($O_{opt}$). For prediction tasks, we feed the same observations to both agent

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Note that the (effective) network capacity needs to be large enough to at least represent the different states required by the Bayes-optimal solution. However, it is currently unknown how to precisely measure effective network capacity. We thus selected our architectures based on preliminary ablations that investigate convergence speed of training. See Appendix D.3 for details.
types and then compute their dissimilarity as the sum of the KL-divergences of the instantaneous predictions averaged over $K$ trajectories, that is,

$$d(\text{Opt, RNN}) = \frac{1}{K} \sum_{k=1}^{K} \sum_{t=1}^{T} D_{\text{KL}}(\pi_{k,t}^{\text{Opt}} \parallel \pi_{k,t}^{\text{RNN}}).$$

(2)

Bandit tasks require a different dissimilarity measure: since there are multiple optimal policies, we cannot compare action probabilities directly. A dissimilarity measure that is invariant under optimal policies is the empirical reward difference:

$$d(\text{Opt, RNN}) = \frac{1}{K} \sum_{k=1}^{K} \sum_{t=1}^{T} (r_{k,t}^{\text{Opt}} - r_{k,t}^{\text{RNN}})$$

(3)

where $r_{k,t}^{\text{Opt}}$ and $r_{k,t}^{\text{RNN}}$ are the empirical rewards collected during one episode. This dissimilarity measure only penalises policy deviations that entail reward differences.

### 3.3 Convergence analysis

In our convergence analysis we investigate how the behaviour of meta-learners changes over the course of training. To characterise how a single RNN training run evolves, we evaluate the behavioural dissimilarity measures (Section 3.2), which compare RNN behaviour against Bayes-optimal behaviour, across many checkpoints of a training run. Additionally we study the RNN behaviour across multiple training runs, which allows us to characterise convergence towards the Bayes-optimal solution. For this we use several RNN training runs (same architecture, different random initialisation), and at fixed intervals during training we compute pairwise behavioural distances between all meta-learners and the Bayes-optimal agent. The behavioural distance is computed using the Jensen-Shannon divergence for prediction tasks and the absolute value of the cumulative regret for bandits. We visualise the resulting distance matrix in a 2D plot using multidimensional scaling (MDS) [40].

### 3.4 Structural analysis

We base our structural analysis on the idea of simulation introduced in Section 2. Since here we also deal with continuous state, input, and output spaces, we relax the notion of simulation to approximate simulation:

- **(Reference inputs)** As we cannot enumerate all the traces, we first sample a collection of input sequences from a reference distribution and then use the induced traces to compare state machines.

- **(State and output comparison)** To assess the quality of a simulation, we first learn a map $\phi$ that embeds the states of one state machine into another, and then measure the dissimilarity. To do so, we introduce two measures of dissimilarity $D_s$ and $D_o$ to evaluate the state and output dissimilarity respectively. More precisely, consider assessing the quality of a state machine $M$ simulating a machine $N$ along a trace induced by the input sequence $x_1 \cdots x_T$. Then, the quality of the state embedding $D_s$ is measured as the mean-squared-error (MSE) between the embedded states $\phi(S_N) \subset S_M$ and the states $S_M$ of $M$ along the trace. Similarly, the quality of the output simulation $D_o$ is measured as the dissimilarity between the outputs generated from the states $S_N$ and $\phi(S_N)$ along the trace, that is, before and after the embedding respectively.

In practice, we evaluate how well e.g. a meta-learned agent simulates a Bayes-optimal one by first finding an embedding $\phi$ mapping Bayes-optimal states into meta-learned states that minimises the state dissimilarity $D_s$, and then using said embedding to compute the output dissimilarity $D_o$. The mapping $\phi$ is implemented as an MLP—see details in Appendix C. We use (2) and (3) as output dissimilarity measures $D_o$ in prediction and bandit tasks respectively.

Our approach is similar in spirit to [41], but adapted to work in continuous observation spaces.

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5 The Jensen-Shannon divergence is defined as $D_{\text{JS}}(X \parallel Y) = \frac{1}{2}(D_{\text{KL}}(X \parallel M) + D_{\text{KL}}(Y \parallel M))$, where $M$ is the mixture distribution $(X + Y)/2$. 

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4 Results

4.1 Behavioral Comparison

To compare the behavior between meta-learned and Bayes-optimal agents, we contrast their outputs for the same inputs. Consider for instance the two agents shown in Figure 1. Here we observe that the meta-learned and the Bayes-optimal agents behave in an almost identical manner: in the prediction case (Figure 1a), the predictions are virtually indistinguishable and approach the true probabilities; and in the bandit case (Figure 1b) the cumulative regrets are essentially the same whilst the policy converges toward pulling the best arm.

(a) Categorical-variable prediction task. Bottom row shows observations, middle row shows predictions of the meta-learner (solid) and the Bayes-optimal predictor (dashed), that converge towards the environment’s true values (shaded bars). Top-row shows the likelihood of the observation under the predictive distribution.

(b) 2-armed Bernoulli-bandit task. Bottom row shows inputs (action-reward pairs). Middle row shows action probabilities for meta-learner (solid) and expected arm payoffs as shaded bars. Action probabilities of the Bayes-optimal agent are not shown as it acts deterministically, selecting actions according to the highest Gittins index per time step. Top row shows cumulative regret for both agent-types.

Figure 1: Illustrative behavioral comparison of a meta-learned agent and the Bayes-optimal agent on 3 episodes (same environment random seed for both agents). Meta-learned agents were trained with only 20 time-steps; thus these results illustrate that the RNN generalizes to 30 time-steps.

To quantitatively assess behavioral similarity between the meta-learners and the Bayes-optimal agents, we use the measures introduced in Section 3.2, namely (2) for prediction tasks and (3) for bandit tasks. For each task distribution, we averaged the performance of 10 meta-learned agents. The corresponding results in Figure 4a show that the trained meta-learners behave virtually indistinguishably from the Bayes-optimal agent. Results for reduced-memory agents, which cannot retain enough information to perform optimally, are shown in Appendix D.7.

4.2 Convergence

We investigate how the behavior of meta-learners changes over the course of training. Following the methodology introduced in Section 3.3 we show the evolution of behavior of a single training run (top-left panels in Figure 2a, 2b). These results allow us to evaluate the meta-learners’ ability to pick up on the environment’s prior statistics and perform Bayesian evidence integration accordingly. As training progresses, agents learn to integrate the evidence in a near-optimal manner over the entire course of the episode. However, during training the improvements are not uniform throughout the episode. This ‘staggered’ meta-learning, where different parts of the task are learned progressively, resembles results reported for meta-learners on nonlinear regression tasks in [42].

Recall that the regret is invariant under optimal policies.
We also compared behavior across multiple training runs (top-right panels in Figure 2a,b). Overall the results indicate that after some degree of heterogeneity early in training, all meta-learners converge in a very similar fashion to the Bayes-optimal behavior. This is an empirical confirmation of the theoretical prediction in [10] that the Bayes-optimal solution is the fixed-point of meta-learner training. Appendix D.5 shows the convergence results for all tasks.

4.3 Structural Comparison

In this section we analyze the computational structure of the meta-learner who uses its internal state to store information extracted from observations required to act.

Following the discussion in Section 3.4, we determine the computational similarity of the meta-learning and Bayes-optimal agents via simulation. Our analysis is performed by projecting and then whitening both the RNN state (formed by concatenating both the cell- and hidden-states of the LSTM) and the Bayes-optimal state onto the first \( n \) principal components, where \( n \) is the dimensionality of the Bayes-optimal state/sufficient statistics. We find that these few components suffice to explain a large fraction of the variance of the RNN agent’s state—see Appendix D.2. We then regress an MLP-mapping \( \phi \) from one (projected) agent state onto the other and compute \( D_s \) and \( D_o \). Importantly, this comparison is only meaningful if we ensure that both agents were exposed to precisely the same input history. This is easily achieved in prediction tasks by fixing the environment random seed. In bandit tasks we ensure that both agents experience the same action-reward pairs by using the trained meta-learner to generate input streams that are then also fed into the Bayes-optimal agent.

Figure 3 illustrates our method for assessing the computational similarity. We embedded the state space of the Bayes-optimal agent into the state space of the meta-learned agent, and then we calculated the output from the embedded states. This embedding was also performed in the reverse direction. Visual inspection of this figure suggests that the meta-learned and the Bayes-optimal agents perform similar computations, as the panels resemble each other both in terms of states and outputs. We observed similar results for all other tasks (Appendix D.5). In contrast, we have observed that the computational structure of untrained meta-learners does not resemble the one of Bayes-optimal agents (Appendix D.1).

The quantitative results for the structural comparison for all tasks across 10 repetitions of meta-training are shown in Figure 4. We find that for the trained meta-learner state-dissimilarity \( D_s \) is low in almost all cases. In bandit tasks, \( D_s \) tends to be slightly larger in magnitude which is somewhat expected since the RNN-state dimensionality is much larger in bandit tasks. Additionally there is often no significant difference in \( D_s \) between the untrained and the final agent—we suspect this to be an artefact of a reservoir effect [43] (see Discussion). The output-dissimilarity \( D_o \) is low for both

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\( ^{7} \) The embeddings were implemented as MLPs having three hidden layers with either 64 (prediction) or 256 (bandits) neurons each.
(a) Categorical prediction task with parameters drawn from Dirichlet(1, 1, 1). The colors indicate the prediction probabilities emitted in each state. Three episode rollouts are shown.

(b) Two-armed Bernoulli-bandit task with biases drawn from Beta(1, 1). The colors indicate the action-probabilities emitted in each state. Three episode rollouts are shown.

Figure 3: Structural comparison. Each sub-figure depicts: two agent state spaces, namely of the Bayes-optimal (top-left) and RNN states (bottom-right), projected onto the first two principal components; and two simulations, i.e., the learned embeddings from the RNN into the Bayes-optimal states (top-right) and from the Bayes-optimal into the RNN states (bottom-left). The scores in the simulations indicate the MSE of the learned regression. The outputs emitted in each state are color-coded. Note that the color-codings in the simulations result from evaluating the output at the (potentially high-dimensional) embedded state (see Section 3.4). White lines indicate the same three episodes as shown in Figure 1.

task types for RNN → Opt, but not in the reverse direction. This indicates that the meta-learners are very well simulated by the Bayes-optimal agents, since both the state dissimilarity $D_s$ and the output dissimilarity $D_o$ are almost negligible. In the reverse direction however, we observe that the meta-learned solutions do not always simulate the Bayes-optimal with high accuracy, as seen by the non-negligible output dissimilarity $D_o$. We believe that this is because the sufficient statistics learned by the meta-learners are not minimal.

5 Discussion and conclusions

In this study we investigated whether memory-based meta-learning leads to solutions that are behaviourally and structurally equivalent to Bayes-optimal predictors. We found that behaviorally the Bayes-optimal solution constitutes a fixed-point of meta-learner training dynamics. Accordingly, trained meta-learners behave virtually indistinguishable from Bayes-optimal agents. We also found structural equivalence between the two agent types to hold to a large extent: meta-learners are well simulated by Bayes-optimal agents, but not necessarily vice versa. This failure of simulation is most likely a failure of injectivity: if a single state in one agent must be mapped to two distinct states in another then simulation is impossible. This occurs when two trajectories lead to the same state in one agent but not another (for instance if exchangeability has not been fully learned). We suspect that RNN meta-learners represent non-minimal sufficient statistics as a result of training. For instance, for Bernoulli prediction tasks the input sequences heads-tails-heads, and tails-heads-heads induce the same minimal sufficient statistics and thus lead to precisely the same internal state in the Bayes-optimal agent, but might lead to different states in the RNN agent. From a theoretical point of view this is not unexpected, since there is no explicit incentive during RNN training that would force representations to be minimal. Note that overly strong regularization can reduce the RNN’s effective capacity to a point where it can no longer represent the number of states required by Bayes-optimal solution, which of course strictly rules out computational equivalence.

A related issue can be observed in bandit tasks: even untrained meta-learners show low state-dissimilarity. We hypothesize that this is due to a “reservoir effect” [33], that is the dynamics of
Figure 4: Behavioral and structural comparison for all tasks. Figure shows similarity measures across $K = 500$ episodes of length $T = 20$, and 10 different training runs of the meta-learner (bars show median over training-runs, error bars denote 5-95 quantiles). ‘init’ denotes the untrained meta-learner, ‘final’ denotes evaluation at the end of training. Numerical results are shown in Figure 7 in the Appendix. Column a: Behavioral dissimilarity between meta-learned agent and Bayes-optimal agent (see Section 4.1). Columns b & c: State- and Output-dissimilarity for $\text{RNN} \rightarrow \text{Opt}$. Columns d & e: State- and Output-dissimilarity for $\text{Opt} \rightarrow \text{RNN}$. Low values of the state- and output-dissimilarity measures (simultaneously) indicate that the state machines implemented by RNN and Opt are structurally equivalent.

Our work contributes to understanding the structure and computations implemented by recurrent neural networks. Focusing analysis on computational equivalence, as in our work, opens up the future possibility of separating different, heterogeneous agents into meaningful sets of equivalent classes, and study universal aspects of these agent-classes.

5.1 Related work

In this paper we study memory-based meta-learning through a Bayesian lens, showing that meta-learning objectives naturally induce Bayes-optimal behaviour at convergence. A number of previous works have attempted to devise new recurrent architectures to perform Bayes filtering in a number of settings, including time series prediction [44], state space modelling [45], and Kalman filtering [46]. Other previous work has attempted to improve memory-based meta-learners’ abilities by augmenting them with a memory, and using weights which adapt at different speeds [47, 48].

Another approach to meta-learning is optimiser-based meta-learning such as MAML [49]. In optimiser-based meta-learning models are trained to be able to adapt rapidly to new tasks via gradient descent. MAML has been studied from a Bayesian perspective, and shown to be a hierarchical Bayesian model [50]. Recent work suggests that solutions obtained by optimiser-based meta-learning might be more similar to those from memory-based meta-learning than previously thought [51].

In this paper we relate memory-based meta-learning to finite-state automata which track sufficient statistics of their inputs. The field of computational mechanics [52] studies predictive automata (known as $\epsilon$-machines) which track the state of a stochastic process in order to predict its future states. The states of $\epsilon$-machines are referred to as causal states, and have recently been used to augment recurrent agents in POMDPs [53]. Finite-state automata have also been considered as a model for decision-making agents in the situated automata work of Rosenschein and Kaelbling [54, 55]. The states of situated automata track logical propositions about the state of the world instead of having a probabilistic interpretation, but are naturally suited to goal-directed agents.
There is considerable work on understanding recurrent neural networks on natural language tasks [56], and in neuroscience [57–59], e.g. how relations between multiple trained models can illuminate computational mechanisms [15], and the dynamics involved in contextual processing [13]. Computational analysis of internal dynamics of reinforcement learning agents has received less attention in the literature, though there are some notable examples: a multi-agent setting [18] and Atari games [60]. Using a related formalism to our approach, the authors of [61] extract minimal finite-state machines (FSM) from the internal dynamics of Atari-agents. However their focus is on extracting small human-interpretable FSM, whereas we compare the computational structure of two agents in a fully automated, quantitative fashion.

In recent years a diverse range of tools to allow interpretability and explainability of deep networks have been developed, including saliency maps [62–67], manual dissection of individual units [17, 16, 68] and training explainable surrogate models to mimic the output of deep networks [69, 61]. Although our focus here is different - we seek to establish how a broad class of architectures behaves on a family of tasks, rather than explaining a specific network - the closest parallel is with the use of surrogate explainable models. In this case, the Bayes-optimal agent serves as an understood model, and we relate its (well-understood) behaviour to that of the meta-trained agent.

**Scope and limitations** We performed our empirical comparison on a range of tasks where optimal solutions are analytically and computationally tractable. The latter is typically no longer true in more complex tasks and domains. However, the simulation methodology used in this paper could be useful to compare agent-types against each other in more general settings, as it does not rely on either agent being Bayes-optimal. While most aspects of our methodology scale up well to more complex agents, the main difficulty is generating reference trajectories that cover a large (enough) fraction of possible experiences. Finally, our results show that when optimal policies are in the search space, and training converges to those policies, then the resulting policy will be Bayes-optimal. In more complex cases, one or both of these assumptions may no longer hold. Further study is needed to understand the kind of suboptimal solutions that are generated by meta-learning in this case.

**Conclusions** Our main contribution is to advance the understanding of RNN-based meta-learned solutions. We empirically confirm a recently published theoretical claim [10] that fully-converged meta-learners and Bayes-optimal agents are computationally equivalent. In particular, we showed that RNN meta-learners converge during training to the Bayes-optimal solution, such that trained meta-learners behave virtually indistinguishably from Bayes-optimal agents. Using a methodology related to the concept of *simulation* in theoretical computer science, we additionally show (approximate) structural equivalence of the state-machines implemented by the RNN meta-learners and the Bayes-optimal agent. Our results suggest that memory-based meta-learning will drive learned policies towards Bayes-optimal behaviour, and will converge to this behaviour where possible.

### 6 Broader Impact

Our work helps advance and verify the current understanding of the nature of solutions that meta-learning brings about (our empirical work focused on modern recurrent neural network architectures and training algorithms, but we expect the findings to qualitatively hold for a large range of AI systems that are trained through meta-learning). Understanding how advanced AI and ML systems work is of paramount importance for safe deployment and reliable operation of such systems. This has also been recognized by the wider machine-learning community with a rapidly growing body of literature in this emerging field of “Analysis and Understanding” of deep learning. While increased understanding is likely to ultimately also contribute towards building more capable AI systems, thus potentially amplifying their negative aspects, we strongly believe that the merits of understanding how these systems work clearly outweigh the potential risks in this case.

We argue that understanding meta-learning on a fundamental level is important, since meta-learning subsumes many specific learning tasks and is thought to play an important role for AI systems that generalize well to novel situations. Accordingly we expect meta-learning to be highly relevant over the next decade(s) in AI research and in the development of powerful AI algorithms and applications. In this work we also show a proof-of-concept implementation for analysis methods that might potentially allow one to separate (heterogeneous) agents into certain equivalence classes, which would allow to safely generalize findings about an individual agent to the whole equivalence class. We believe that this might open up interesting future opportunities to boost the generality of analysis methods and automatic diagnostic tools for monitoring of AI systems.
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Supplementary Material

A Task Details

There is a total of 14 tasks, out of which 10 are prediction and 4 are bandit tasks.

Prediction: The prediction tasks can be grouped according to their observational distributions:

- **Bernoulli**: The agent observes samples $x_t$ drawn from a Bernoulli distribution $Ber(\theta)$. The prior distribution over the bias $\theta$ is given by a Beta distribution $Beta(\alpha, \beta)$, where $\alpha > 0$ and $\beta > 0$ are the hyperparameters. We have three tasks with three respective prior distributions: $Beta(1, 1)$, $Beta(0.5, 0.5)$, and $Beta(1, 5)$.

- **Categorical**: The agent observes samples $x_t$ drawn from a categorical distribution $Cat(\vec{\theta})$ where $\vec{\theta} = [\theta_1, \theta_2, \theta_3]^T$. The prior distribution over the bias parameters $\vec{\theta}$ is given by a Dirichlet distribution $Dirichlet(\vec{\alpha})$, where $\vec{\alpha} = [\alpha_1, \alpha_2, \alpha_3]^T$ are the concentration parameters. We have three categorical tasks with three respective prior distributions: $Dirichlet(1, 1, 1)$, $Dirichlet(1, 1, 0.1)$, and $Dirichlet(0.5, 0.5, 0.5)$.

- **Exponential**: The agent observes samples $x_t$ drawn from an exponential distribution $Exp(\lambda)$ where $\lambda > 0$ is the rate parameter. The prior distribution over the rate parameter $\lambda$ is given by a Gamma distribution $Gamma(\alpha, \beta)$, where $\alpha > 0$ is the shape and $\beta > 0$ is the rate. We use two exponential prediction tasks: their priors are $Gamma(1, 0.5)$ and $Gamma(5, 1)$.

- **Gaussian**: The agent observes samples $x_t$ drawn from a Gaussian distribution $Normal(\mu, 1/\tau)$, where $\mu$ is an unknown mean and $\tau$ is a known precision. The prior distribution over $\mu$ is given by a Gaussian distribution $Normal(m, 1/p)$, where $m$ and $p$ are the prior mean and precision parameters. We have two Gaussian prediction tasks: their priors are $Normal(0, 1)$ and $Normal(1, 1)$ and their precisions $\tau = 1$ and $\tau = 5$ respectively.

A prediction task proceeds as follows. As a concrete example, consider the Bernoulli prediction case—other distributions proceed analogously. In the very beginning of each episode, the bias parameter $\theta$ is drawn from a fixed prior distribution $p(\theta) = Beta(1, 1)$. This parameter is never shown to the agent. Then, in each turn $t = 1, 2, \ldots, T = 20$, the agent makes a probabilistic prediction $\pi_t$ and then receives an observation $x_t \sim p(x|\theta) = Ber(\theta)$ drawn from the observational distribution. This leads to a prediction loss given by $\log(\pi_t(x_t))$, where $\pi_t(x_t)$ is the predicted probability of the observation $x_t$ at time $t$. Then the next round starts.

Bandits: As in the prediction case, the two-armed bandit tasks can also be grouped according to their reward distributions:

- **Bernoulli**: Upon pulling a lever $a \in \{1, 2\}$, the agent observes a reward sampled from a Bernoulli distribution $Ber(\theta_a)$, where $\theta_a$ is the bias of arm $a$. The prior distribution over each arm bias is given by a Beta distribution as in the prediction case. We have two Bernoulli bandit tasks: the first draws both biases from $Beta(1, 1)$, and the second from $Beta(2, 1)$ and $Beta(1, 2)$ respectively.

- **Gaussian**: Upon pulling a lever $a \in \{1, 2\}$, the agent observes a reward sampled from a Gaussian distribution $Normal(\mu, \tau)$, where $\mu$ and $\tau$ are the unknown mean and the known precision of arm $a$ respectively. As in the prediction case, the prior distribution over each arm mean is given by a Normal distribution. We have two Gaussian bandit tasks: the first with precision $\tau = 1$ and prior $Normal(0, 1)$ for both arms; and the second with precision $\tau = 1$ and prior $Normal(0, 0.1)$.

The interaction protocol for bandit tasks is as follows. For concreteness we pick the first Bernoulli bandit—but other bandits proceed analogously. In the very beginning of each episode, the arm biases $\theta_1$ and $\theta_2$ are drawn from a fixed prior distribution $p(\theta) = Beta(1, 1)$. These parameters are never shown to the agent. Then, in each turn $t = 1, 2, \ldots, T$, the agent pulls a lever $a \sim \pi_t$ from its policy at time $t$ and receives a reward $r_t \sim p(r|\theta_a) = Ber(\theta_a)$ drawn from the reward distribution. Then the next round starts. The agent’s return is the discounted sum of rewards $\sum_1^T \gamma^t r_t$ with discount factor $\gamma = 0.95$.
where the Q-value is recursively defined as

\[ Q(a|\alpha_1, \beta_1, \alpha_2, \beta_2):= 0 \]

if \( t = T \)

\[ Q(a|\alpha_1, \beta_1, \alpha_2, \beta_2) := \sum_r p(r|\alpha_r, \beta_r) \left\{ r + \max_{\alpha'} \gamma Q(a'|\alpha'_1, \beta'_1, \alpha'_2, \beta'_2) \right\} \]

if \( t < T \)  

and where \( \alpha'_1, \beta'_1, \alpha'_2, \beta'_2 \) are the hyperparameters for the next step, updated in accordance to the action taken and the reward observed. Computing (6) naively is computationally intractable. Instead, one can pre-compute Gittins indices in polynomial time, and use them as a replacement for the Q-values in (6) [35, 34, 36]. In particular, we have used the methods presented in [36] to compute Gittins indices for the Bernoulli- and Gaussian-distributed rewards.

### B Agent Details

#### B.1 Bayes-optimal agents

Our Bayes-optimal agents act and predict according to the standard models in the literature. We briefly summarize this below.

**Prediction:** A Bayes-optimal agent makes predictions by combining a prior with observed data to form a posterior belief. Consider a Bernoulli environment that generates observations according to a Bernoulli law, then the agent keeps track of one (\( \alpha, \beta \)) sufficient-statistic pair per arm. The optimal arm to pull next is then given by

\[ a^* = \arg \max_a Q(a|\alpha_1, \beta_1, \alpha_1, \beta_1), \]

where the Q-value is recursively defined as

\[ Q(a|\alpha_1, \beta_1, \alpha_1, \beta_1) := 0 \]

if \( t = T \)

\[ Q(a|\alpha_1, \beta_1, \alpha_1, \beta_1) := \sum_r p(r|\alpha_r, \beta_r) \left\{ r + \max_{\alpha'} \gamma Q(a'|\alpha'_1, \beta'_1, \alpha'_2, \beta'_2) \right\} \]

if \( t < T \)  

and where \( \alpha'_1, \beta'_1, \alpha'_2, \beta'_2 \) are the hyperparameters for the next step, updated in accordance to the action taken and the reward observed. Computing (6) naively is computationally intractable. Instead, one can pre-compute Gittins indices in polynomial time, and use them as a replacement for the Q-values in (6) [35, 34, 36]. In particular, we have used the methods presented in [36] to compute Gittins indices for the Bernoulli- and Gaussian-distributed rewards.

| Observation          | Prior                  | Update                     | Posterior Predictive |
|----------------------|------------------------|----------------------------|----------------------|
| Bernoulli(\( \theta \)) | Beta(\( \alpha, \beta \)) | \( \alpha \leftarrow \alpha + x; \beta \leftarrow \beta + (1 - x) \) | Bernoulli(\( \frac{\alpha}{\alpha + \beta} \)) |
| Categorical(\( \hat{\theta} \)) | Dirichlet(\( \alpha_1, \alpha_2, \alpha_3 \)) | \( \alpha_x \leftarrow \alpha_x + 1 \) | Categorical(\( \sum \alpha_i \)) |
| Normal(\( \mu, 1/\tau \)) | Normal(\( m, 1/p \)) | \( m \leftarrow \frac{\mu m + x \tau}{\mu + \tau}; \ p \leftarrow p + \tau \) | Normal(\( m, \frac{1}{p} + \frac{1}{\tau} \)) |
| Exponential(\( \lambda \)) | Gamma(\( \alpha, \beta \)) | \( \alpha \leftarrow \alpha + 1, \beta \leftarrow \beta + x \) | Lomax(\( \alpha, \beta \)) |

**Table 1: Prediction rules for Bayes-optimal agents**
B.2 RNN agents

Prediction: We trained agents on the prediction tasks (episode length $T = 20$ steps) using supervised learning with a batch size of 128 using BPTT unroll of 20 timesteps, and a total training duration of 1.7 steps. We used the Adam optimizer with learning rate $10^{-4}$, parameters $\beta_1 = 0.9$, $\beta_2 = 0.999$, and gradients clipped at magnitude 1. Networks were initialised with weights drawn from a truncated normal with standard deviation $1/\sqrt{N_{in}}$, where $N_{in}$ is the size of the input layer. We use the following output-parametrization: Bernoulli-predictions - single output corresponding to the log-probability of observing “heads”; Categorical predictions - 3-D outputs corresponding to prediction logits; Normal predictions - 2 linear outputs, one for mean and one for log-precision; Exponential predictions - 2 linear outputs, one for $\log \alpha$ and one for $\log \beta$.

Bandit: We trained the reinforcement learners on bandit tasks (episode length $T = 20$ steps) with the Impala algorithm [39] using a batch size of 16 and discount factor $\gamma = 0.95$ for a total number of 1e8 training steps. The BPTT unroll length was 5 timesteps, and the learning rate was $2.5 \times 10^{-5}$. We used an entropy penalty of 0.003 and value baseline loss scaling of 0.48; i.e., the training objective was $L_{VTrace} + 0.003L_{Entropy} + 0.48L_{Value}$. We used the same initialisation scheme as for the prediction tasks. RNN outputs in all bandit tasks were 2-dimensional action logits (one for each arm). Bandit agents are trained to minimize empirical (“sampled”) cumulative discounted rewards. For our behavioral and output dissimilarity measures we report expected reward instead of sampled reward (using the environment’s ground-truth parameters to which the agent does not have access to)—this reduces the impact of sampling noise on our estimates.

C Structural Comparison Details

We implement the map $\phi$ from RNN agent states $S_N$ to optimal agent states $S_M$ using an MLP with three hidden layers, each of size 64 (prediction tasks where the RNN state is 64-dimensional) or 256 (bandit tasks where the RNN state is 512-dimensional), with ReLu activations. We first project the high-dimensional RNN agent state space down to a lower-dimensional representation using PCA. The number of principal components is set to match the dimension of the minimal sufficient statistics required by the task. We trained the MLP using the Adam optimiser with learning rate 0.001, $\beta_1 = 0.9$, $\beta_2 = 0.999$ and batch size 200. The training set consisted of data from 500 roll-outs—all results we report were evaluated on 500 held out test-trajectories.

State dissimilarity $D_s$ is measured by providing the same inputs to both agents (same observations in prediction tasks, and action-reward pairs from a reference trajectory in bandit tasks), and then taking the mean-squared error between the (PCA-projected) original states and the mapped states (compare Figure 4 in the main paper). Output dissimilarity is computed by comparing the output produced by the original agent with the output produced after projecting the original agent state into the “surrogate” agent and evaluating the output. Note that the last step requires inverting the PCA projection in order to create a “valid” state in the surrogate agent. For the optimal agent the PCA is invertible since its dimensionality is the same as the agent’s state (i.e., the PCA on the optimal agent simply performs a rotation and whitening). On the RNN agent, we use the following scheme: we construct an invertible PCA projection as well, which requires having the same number of components as the internal state’s dimensionality. Then, to implant a state from the Bayes-optimal agent the first $n$ components are set according to the mapping $\phi$, all other principal components are set to their mean-value (across 500 episodes).

D Additional Results

D.1 PCA for untrained meta-learner

Figure 5 shows the principal component projection and approximate simulation (mapping the state of one agent onto the other and computing the resulting output) for meta-learner after random initialization, without any training. Results for the trained agent (at the end of the training run) are shown in Figure 3 in the main paper.

The reference trajectory is always generated from the fully trained RNN agent—also when analyzing RNN agents during training.
(a) Categorical-variable prediction task
Dirichlet(1, 1, 1). Colors indicate the output-probabilities (=posterior predictive dist.) for the corresponding state. Lines correspond to the three episodes shown in Figure [1]. Dimensionality of $s_t^{rnn}$ is 64. MLP-regressor $\phi$ has three hidden layers with 64 neurons each.

(b) 2-armed Bernoulli-bandit task $\sim$ Beta(1, 1). Colors indicate the output-probabilities (=action probabilities) for the corresponding state. Lines correspond to the three episodes shown in Figure [1]. Dimensionality of $s_t^{rnn}$ is 512. MLP-regressor $\phi$ has three hidden layers with 256 neurons each.

Figure 5: Structural comparison for untrained agent (compare Figure [3] in main paper). Each sub-figure shows:
(i - top left) Projection of Bayes-optimal state onto first two principal components, (iv - bottom right) projection of RNN state onto first two principal components, (ii - top right) learned regression from (iv) to (i), (iii - bottom left) learned regression from (i) to (iv). Scores in panels (ii) and (iii) indicate the mean-squared-error (MSE) of the learned regression (map $\phi$ was trained on training data, plots and numerical results show evaluation on held-out test-data—500 data-points for training and test respectively).

D.2 Variance explained by PC projections

Table [2] shows the variance explained when projecting the RNN state onto the first $n$ principal components, which is the first step of our structural analysis ($n$ is the dimensionality of the tasks’ minimal sufficient statistics, and is between 2 and 4 dimensions)—see Section 4.3. Numbers indicate the variance explained by projecting 500 trajectories of length $T = 20$ onto first $n$ principal components. Large number indicate that most of the variance in the data is captured by the PCA projection, which is the case for us in all tasks.

D.3 Preliminary architecture sweeps

The meta-learners in our main experiments are three-layer RNNs (a fully connected encoder, followed by an LSTM layer and a fully connected decoder). Each layer has the same width $N$ which was selected by running preliminary architecture sweeps (on a subset of tasks), shown in Figure D.3. Generally we found that smaller RNNs suffice to successfully train on the prediction tasks compared to the RNN tasks. For instance a layer-width of 3 would suffice in principle to perform well on the prediction tasks (not that the maximum dimensionality of the minimal sufficient statistics is also exactly 3). However, we found that the smallest networks also tend to require more iterations to converge, with more noisy convergence in general. We thus selected $N = 32$ for prediction tasks (leading to a 64-dimensional RNN state, which is the concatenation of cell- and hidden-states) as a compromise between RNN-state dimensionality, runtime-complexity and iterations required for training to converge robustly (in our main experiments we train prediction agents for $1e7$ steps, and bandit agents for $1e8$ steps). Using similar trade-offs we chose $N = 256$ for bandit tasks (leading to a 512-dimensional RNN state).
Table 2: Variance of RNN-state explained by PCA projection.

| Task                  | at initialization | after training |
|-----------------------|-------------------|----------------|
| Beta(1, 1)            | 0.98              | 0.94           |
| Beta(0.5, 0.5)        | 0.98              | 0.92           |
| Beta(1, 5)            | 0.98              | 0.96           |
| Dirichlet(0.5, 0.5, 0.5) | 0.93             | 0.96           |
| Dirichlet(1, 1, 1)    | 0.93              | 0.95           |
| Dirichlet(1, 1, 0.1)  | 0.94              | 0.96           |
| Gamma(1, 0.5)         | 0.95              | 0.97           |
| Gamma(5, 1)           | 0.97              | 0.96           |
| Normal(0, 1)          | 0.95              | 0.88           |
| Normal(1, 1)          | 0.97              | 0.94           |

Bandits

| Task                  | at initialization | after training |
|-----------------------|-------------------|----------------|
| Beta(1, 1)            | 0.97              | 0.96           |
| Beta(2, 1), Beta(1, 2)| 0.98              | 0.97           |
| Normal(0, 1)          | 0.94              | 0.92           |
| Normal(0, 0.1)        | 0.95              | 0.90           |

(a) Subset of prediction tasks. Lines show difference between RNN and Bayes-optimal log-loss, averaged over 10 training runs.

(b) Bandit tasks. Lines show mean reward computed over the last 10k steps (rolling average) for a single training run.

Figure 6: Architecture sweeps.

D.5 Structural comparison

We report the structural comparison plots for all the tasks. These were generated using the same methodology as in Figure 3. Figures 8, 9, and 10 show the comparisons for the prediction of discrete observations, prediction of continuous observations, and bandits respectively.

D.6 Convergence analysis - additional results

Convergence plots for all our tasks (except the two exponential prediction tasks, where the KL-divergence estimation for the Lomax distribution can cause numerical issues that lead to bad visual results) are shown in Figure 11 and Figure 12. Note that our agents were trained with episodes of 20 steps, and the figures show how agents generalize when evaluated on episodes of 30 steps.
D.4 Behavioral and structural comparison

Figure 7: Behavioral and structural comparison for all tasks—same as Figure 4 in main paper. Figure shows dissimilarity measures across 500 episodes of length $T = 20$, and 10 different training runs of the meta-learner. ‘init’ denotes the untrained meta-learner, ‘final’ denotes evaluation at the end of training. Colored bars show median across training runs (also given as numerical values on y-axis), error bars denote 5-95 quantiles (bold numbers indicate that upper end of ‘final’ error bar is strictly lower than lower end of ‘init’ error bar), vertical grey ticks indicate mean values (across training runs). (a) Behavioral dissimilarity between meta-learned agent and Bayes-optimal agent (see Section 4.1). (b), (c) State- and Output-dissimilarity for $\text{RNN} \rightarrow \text{Opt}$. (d), (e) State- and Output-dissimilarity for $\text{Opt} \rightarrow \text{RNN}$. 

(a) 

(b) 

(c) 

(d) 

(e)
Figure 8: Structural comparison I. Prediction probabilities are color-coded.
D.7 Reduced-memory agents

In order to understand outcomes when the optimal policy is not in the search space we investigated the performance of a series of reduced-memory baselines. These were implemented with purely feedforward architectures, which observed a context window of the previous $k$ timesteps (padded for $t < k$), rather than with an LSTM. Short context windows dramatically impaired performance, and the degree to which longer context windows allowed for improved performance was strongly task-dependent. In some cases (Dirichlet and high-precision Gaussian), extending the context window to match the episode length almost completely recovers performance, whereas in other cases performance plateaus.

Figure 9: Structural comparison II. The predicted means are color-coded.
Figure 10: Structural comparison III (bandit tasks). Action probabilities are color-coded.

(a) $\theta_1, \theta_2 \sim \text{Beta}(1, 1)$

(b) $\theta_1 \sim \text{Beta}(2, 1), \theta_2 \sim \text{Beta}(1, 2)$

(c) $\mu_1, \mu_2 \sim \text{Normal}(0, 1)$

(d) $\mu_1, \mu_2 \sim \text{Normal}(0, 0.1)$
Figure 11: Convergence plots for our prediction tasks, showing 10 steps of generalisation (demarcated by grey dashed line).
Figure 12: Convergence plots for bandit tasks, showing 10 steps of generalisation (demarcated by grey dashed line).

(a) Prediction tasks.
(b) Bandit tasks

Figure 13: Performance as a percentage of LSTM agent score for reduced-memory baselines. Solid line is mean over 20 trials, shaded area shows standard error of the mean over 20 repetitions. Reduced-memory baselines are feedforward agents trained with a fixed-width context of past observations. Adjusting the context width scales the amount of history the agent can use when computing a prediction/action decision.