## Learning to select computations

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#### Abstract

Efficient use of limited computational resources is essential to intelligence. Selecting computations optimally according to rational metareasoning would achieve this, but rational metareasoning is computationally intractable. Inspired by psychology and neuroscience, we propose the first learning algorithm for approximating the optimal selection of computations. We derive a general, sample-efficient reinforcement learning algorithm for learning to select computations from the insight that the value of computation lies between the myopic value of computation and the value of perfect information. We evaluate the performance of our method against two state-of-theart methods for approximate metareasoning-the meta-greedy heuristic and the blinkered policy-on three increasingly difficult metareasoning problems: metareasoning about when to terminate computation, metareasoning about how to choose between multiple actions, and metareasoning about planning. Across all three domains, our method achieved near-optimal performance and significantly outperformed the meta-greedy heuristic. The blinkered policy performed on par with our method in metareasoning about decision-making, but it is not directly applicable to metareasoning about planning where our method outperformed both the meta-greedy heuristic and a generalization of the blinkered policy. Our results are a step towards building self-improving AI systems that can learn to make optimal use of their limited computational resources to efficiently solve complex problems in real-time.

#### Introduction

The human brain is the best example of an intelligent system we have so far. One feature that sets it apart from current AI is its remarkable computational efficiency, which enables people to effortlessly solve intractable computational problems for which artificial intelligence either under-performs humans or requires superhuman computing power and training time (Lake et al. 2016). For instance, to defeat Garry Kasparov 3.5–2.5, Deep Blue had to evaluate 200 000 000 positions per second, whereas Kasparov was able to perform at almost the same level by evaluating only 3 positions per second (Campbell, Hoane, and Hsu 2002; IBM Research 1997). This ability to make efficient use of limited computational resources is the essence of intelligence (Russell and Wefald 1991b). People accomplish this feat by being very

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selective about when to think, what to think about, choosing computations adaptively, and terminating deliberation when its expected benefit falls below its cost (Gershman, Horvitz, and Tenenbaum 2015; Lieder and Griffiths 2017; Payne, Bettman, and Johnson 1988).

The theory of rational metareasoning was developed to recreate such intelligent control over computation in machines (Russell and Wefald 1991a; Hay et al. 2012). In principle, rational metareasoning can be used to always select those computations that make optimal use of the agent's finite computational resources. Unfortunately, the computational complexity of exact rational metareasoning is prohibitive (Hay et al. 2012). Recent research suggests that the human mind circumvents this computational challenge by learning to select computations through metacognitive reinforcement learning (Krueger, Lieder, and Griffiths 2017; Lieder and Griffiths 2017; Wang et al. 2017). Concretely, people appear to learn to predict the value of alternative cognitive operations from features of the task, their current belief state, and the cognitive operations themselves. If humans learn to metareason through metacognitive reinforcement learning, then it should be possible to build intelligent systems that learn to metareason as efficiently as people.

In this paper, we propose the first algorithm for learning how to metareason and evaluate it against existing methods for approximate metareasoning on three increasingly more complex problems. We find that our learning algorithm performs significantly better than previous approximations to rational metareasoning and conclude with a discussion of future directions towards self-improving AI systems and potential applications.

#### **Background**

## Metareasoning

If reasoning seeks an answer to the question "what should I do?", metareasoning seeks an answer to the question "how should I decide what to do?". The theory of rational metareasoning (Russell and Wefald 1991a; Russell and Subramanian 1995) frames this problem as selecting computations so as to maximize the sum of the rewards of resulting decisions minus the costs of the computations involved. Concretely, one can formalize reasoning as a metalevel Markov decision process (metalevel MDP) and metareasoning as solving that

$$M_{\text{meta}} = (\mathcal{B}, \mathcal{A}, T_{\text{meta}}, r_{\text{meta}}) \tag{1}$$

is a Markov decision process (Puterman 2014) where the actions  $\mathcal A$  are cognitive operations, the states  $\mathcal B$  encode the agent's beliefs, and the transition function  $T_{\rm meta}$  describes how cognitive operations change the beliefs.  $\mathcal A$  includes computations  $\mathcal C$  that update the belief, as well as a special metalevel action  $\bot$  that terminates deliberation and initiates acting on the current belief. A belief state b encodes a probability distribution over parameters  $\theta$  of a model of the domain. The parameters  $\theta$  determine the utility of acting according to a policy  $\pi$ , that is  $U_\pi^{(\theta)}$ . For one-shot decisions,  $U_\pi^{(\theta)}$  is the expected reward of a taking a single action. In sequential decision-problems,  $U_\pi^{(\theta)}=V_\pi^{(\theta)}(s)$  is the expected sum of rewards the agent will obtain by acting according to policy  $\pi$  if the environment has the characteristics encoded by  $\theta$ . Since b encodes the agent's belief about  $\theta$ , its subjective utility  $\hat{U}_\pi^{(b)}$  of acting according to  $\pi$  is  $\mathbb{E}_{\theta \sim b}[U_\pi^{(\theta)}]$ . The metalevel reward function  $r_{\rm meta}$  captures the cost of

The metalevel reward function  $r_{\text{meta}}$  captures the cost of thinking (Shugan 1980) and the external reward r the agent expects to receive from the environment. The computations  $\mathcal C$  have no external effects, thus they always incur a negative reward  $r_{\text{meta}}(b,c) = -\text{cost}(c)$ . In the problems studied below, all computations that deliberate have the same cost, that is  $\text{cost}(c) = \lambda$  for all  $c \in \mathcal C$  whereas  $\text{cost}(\bot) = 0$ . An external reward is received only when the agent terminates deliberation and makes a decision based on the current belief state b. To reduce the variance of this reward signal, the metalevel reward of terminating deliberation is defined as the expectation of the external reward, that is

$$r_{\text{meta}}(b, \perp) = \max_{\pi} \hat{U}_{\pi}^{(b)} = \max_{\pi} \mathbb{E}_{\theta \sim b} \left[ U_{\pi}^{(\theta)} \right].$$
 (2)

Early work on rational metareasoning (Russell and Wefald 1991a) defined the optimal way to select computations as maximizing the value of computation (VOC), that is

$$\arg\max_{c} \text{VOC}(c, b), \tag{3}$$

where VOC(c,b) is the expected improvement in decision quality that can achieved by performing computation c in belief state b and continuing optimally minus the cost of the optimal sequence of computations (Russell and Wefald 1991a). When no computation has positive value, the policy terminates computation and executes the best object-level action, thus  $VOC(\bot,b)=0$ . Using the formalism of metalevel MDPs (Hay et al. 2012), this definition can be rewritten as

$$VOC(c,b) = Q_{\text{meta}}^{\star}(b,c) - r_{\text{meta}}(b,\perp), \tag{4}$$

and the optimal selection of computations can be expressed as the optimal metalevel policy  $\pi_{\text{meta}}^{\star}(b) = \arg\max_{c} Q_{\text{meta}}^{\star}(b,c)$ .

#### Approximations to rational metareasoning

Previous work (Russell and Wefald 1991a; Lin et al. 2015) has approximated rational metareasoning by the metagreedy policy

$$\pi_{\text{greedy}}(b) = \arg\max_{c} \text{VOC}_1(b, c),$$
(5)

where

$$VOC_1(c, b_t) = \mathbb{E}\left[r_{\text{meta}}(B_{t+1}, \perp)|b_t, c_t\right] + r_{\text{meta}}(b_t, c) - r_{\text{meta}}(b_t, \perp), \tag{6}$$

is the myopic value of computation (Russell & Wefald, 1991). This is optimal when the improvement from each additional computation is less than that from the previous one but deliberates too little when this assumption is violated.

Hay et al. (2012) approximated rational metareasoning by combining the solutions to smaller metalevel MDPs that formalize the problem of deciding how to decide between one object-level action and the expected return of its best alternative. While this *blinkered* approximation is more accurate than the meta-greedy policy it is also significantly less scalable and not directly applicable to metareasoning about planning.

It has been proposed that people approximate optimally selecting individual computations by metareasoning over a small subset of all possible sequences of computations (Milli, Lieder, and Griffiths 2017). The solution to this simplified problem can be approximated efficiently (Lieder and Griffiths 2017), but this approximation neglects the sequential nature of selecting individual computations.

To our knowledge these are the main approximations to rational metareasoning. Hence, to date, there appears to be no accurate and scalable method for solving general metalevel MDPs.

#### Metalevel reinforcement learning

It has been proposed that metareasoning can be made tractable by learning an approximation to the value of computation (Russell and Wefald 1991a). However, despite some preliminary steps in this direction (Harada and Russell 1998; Lieder et al. 2014; Lieder, Krueger, and Griffiths 2017) and related work on meta-learning (Smith-Miles 2009; Schaul and Schmidhuber 2010; Thornton et al. 2013; Wang et al. 2017), learning to approximate bounded optimal information processing remains an unsolved problem in artificial intelligence.

Previous research in cognitive science suggests that people circumvent the intractability of metareasoning by learning a metalevel policy from experience (Lieder and Griffiths 2017; Cushman and Morris 2015; Krueger, Lieder, and Griffiths 2017). At least in some cases, the underlying mechanism appears to be model-free reinforcement learning (RL) (Cushman and Morris 2015; Krueger, Lieder, and Griffiths 2017; Wang et al. 2017). This suggests that model-free reinforcement learning might be a promising approach to solving metalevel MDPs. To our knowledge, this approach is yet to be explored in artificial intelligence. Here, we present a proof-of-concept that near-optimal metalevel policies can be learned through metalevel RL.

# A metalevel RL algorithm for selecting computations

According to rational metareasoning, one should continue to reason until none of the available computations has a positive VOC. Until then, one should always choose the computation that confers the highest improvement in decisionquality net its cost. While the improvement in decision quality contributed by a computation c under the optimal continuation is generally intractable to compute, it can be bounded. Figure 1 illustrates that if the expected decision quality improves monotonically with the number of computations, then the improvement achieved by the optimal sequence of computations should lie between the advantage of deciding immediately after the first computation over making a decision without it (Russell & Wefald, 1991) and the benefit of obtaining perfect information about all actions (Howard 1966). The former is given by the myopic value of information<sup>1</sup>, that is

$$VOI_{1}(c, b_{t}) = \mathbb{E}_{B_{t+1}|b_{t}, c} \left[ \max_{\pi} \hat{U}_{\pi}^{(B_{t+1})} \right] - \max_{\pi} \hat{U}_{\pi}^{(b)}. \quad (7)$$

The latter is given by the value of perfect information about all actions, that is

$$VPI_{all}(b) = \mathbb{E}_{\theta \sim b} \left[ \max_{\pi} U_{\pi}^{(\theta)} \right] - \max_{\pi} \hat{U}_{\pi}^{(b)}. \tag{8}$$

In problems with many possible actions, this upper bound can be very loose, and the VOC may be closer to the value of knowing the value functions of the policies  $\Pi_c$  about whose returns the computation c is informative, that is

$$VPI_{A}(b,c) = \mathbb{E}_{\theta \sim b} \left[ \max \left( \mathcal{U}_{c}^{(\theta)} \cup \hat{\mathcal{U}}_{\neg c}^{(b)} \right) \right] - r_{\text{meta}}(b, \perp), \tag{9}$$

where  $\mathcal{U}_c^{(\theta)} = \{U_\pi^{(\theta)} \colon \pi \in \Pi_c\}$  are the unknown utilities of the policies that computation c is informative about, and  $\hat{\mathcal{U}}_{\neg c}^{(b)} = \{\hat{U}_\pi^{(b)} \colon \pi \notin \Pi_c\}$  is the set of the expected utilities of all policies that c is not informative about. This definition

<sup>&</sup>lt;sup>1</sup>The VOI<sub>1</sub> defined here is equal to the myopic VOC defined by Russell and Wefald (1991) plus the cost of the computation.

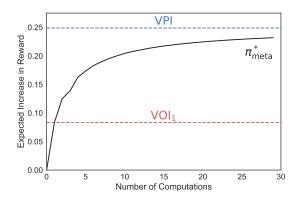


Figure 1: Expected performance in metareasoning about how to choose between three actions increases monotonically with the number of computations, asymptoting at the value of perfect information (VPI). Consequently, the value of executing a single computation must lie between the myopic value of information (VOI<sub>1</sub>) and the VPI.

generalizes the value of perfect information about a single action (Dearden, Friedman, and Russell 1998) to policies.

Critically, the myopic value of information (VOI<sub>1</sub>), the VPI about all actions, and the VPI<sub>A</sub> can all be computed efficiently or efficiently approximated by Monte-Carlo integration (Hammersley 2013). Our method thus approximates the expected improvement in decision quality gained by a computation by linearly interpolating between its myopic VOI and the value of perfect information, that is

$$VOC(c,b) \approx w_1 \cdot VOI_1(c,b) + w_2 \cdot VPI_{all}(b) + w_3 \cdot VPI_A(b,c) - w_4 \cdot cost(c),$$
(10)

with the constraints that  $w_1, w_2, w_3 \in [0, 1]$ ,  $w_1 + w_2 + w_3 = 1$ , and  $w_4 \in [1, h]$  where h is an upper bound on how many computations can be performed. Below we propose an algorithm through which the agent can learn these weights from experience.

Since the VOC defines the optimal metalevel policy (Equation 3), we can approximate the optimal policy by plugging in our VOC approximation (Eq. 10) into Equation 3. This yields

$$\pi_{\text{meta}}(b; \mathbf{w}) = \arg \max_{c} \left\{ w_1 \cdot \text{VOI}_1(c, b) + w_2 \cdot \text{VPI}_{\text{all}}(b) + w_3 \cdot \text{VPI}_A(b, c) - w_4 \cdot \text{cost}(c) \right\}.$$
(11)

The parameters  $\mathbf{w}$  of this policy are estimated by maximizing the expected return  $\mathbb{E}\left[\sum_t r_{\text{meta}}(b_t, \pi_{\text{meta}}(b_t; \mathbf{w}))\right]$ . Together with the constraints on the weights stated above, this effectively reduces the intractable problem of solving metalevel MDPs to a simple 3-dimensional optimization problem. There are many ways this optimization problem could be solved. Since estimating the expected return for a given weight vector can be expensive, we use Bayesian optimization (BO) (Mockus 2012) to optimize the weights in a sample efficient manner.

The novelty of our approach lies in leveraging machine learning to approximate the solution to metalevel MDPs and in the discovery of features that make this tractable. As far as we know, our method is the first general approach to metalevel RL.

In the following sections, we validate the assumptions of our approach, evaluate its performance on increasingly complex metareasoning problems, compare it to existing methods, and discuss potential applications.

#### **Evaluation of the method in simulations**

We evaluate how accurately our method can approximate rational metareasoning against two state-of-the-art approximations—the meta-greedy policy and the blinkered approximation—on three increasingly difficult metareasoning problems: deciding when to stop thinking, deciding how to decide, and deciding how to plan.

#### 1. Metareasoning about when to stop deliberating

How long should an agent deliberate before answering a question? Our evaluation mimics this problem for a binary prediction task (e.g., "Will the price of the stock go up or

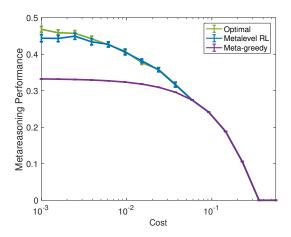


Figure 2: Results of performance evaluation on the problem of metareasoning about when to terminate deliberation.

down?"). Every deliberation incurs a cost and provides probabilistic evidence  $X_t \sim \operatorname{Bernoulli}(p)$  in favor of one outcome or the other. At any point the agent can stop deliberating and predict the outcome supported by the majority of its deliberations so far. The agent receives a reward of +1 if its prediction is correct, or incurs a loss of -1 if it is incorrect. The goal is to maximize the expected reward of this one prediction minus the cost of computation.

**Metalevel MDP:** We formalize the problem of deciding when to stop thinking as a metalevel MDP  $M_{\text{meta}} = (\mathcal{B}, \mathcal{A}, T_{\text{meta}}, r_{\text{meta}})$  where each belief state  $(\alpha, \beta) \in \mathcal{B}$  defines a beta distribution over the probability p of the first outcome. The metalevel actions  $\mathcal{A}$  are  $\{c_1, \bot\}$  where  $c_1$  refines the belief by sampling, and  $\bot$  terminates deliberation and predicts the outcome that is most likely according to the current belief. The transition probabilities for sampling are defined by the agent's belief state, that is  $T_{\text{meta}}((\alpha,\beta),c_1,(\alpha+1,\beta)) = \frac{\alpha}{\alpha+\beta}$  and  $T_{\text{meta}}((\alpha,\beta),c_1,(\alpha,\beta+1)) = \frac{\beta}{\alpha+\beta}$ . Predicting (executing  $\bot$ ) always transitions to a terminal state. The reward function  $r_{\text{meta}}$  reflects the cost of computation ( $r_{\text{meta}}(b,c_1)=-\lambda$ ) and the probability of making the correct prediction ( $r_{\text{meta}}(b,\bot)=+1\cdot p_{\text{correct}}(\alpha,\beta)-1\cdot (1-p_{\text{correct}}(\alpha,\beta))$ ) where  $p_{\text{correct}}(\alpha,\beta)=\max\{\frac{\alpha}{\alpha+\beta},\frac{\beta}{\alpha+\beta}\}$ ). We set the horizon to h=30, meaning that the agent can perform at most 30 computations before making a prediction.

Since there is only one object-level action (i.e., to predict the outcome that appears most likely) the VPI about all actions is identical to the VPI for a single action. When reporting on this problem, we will thus not distinguish between them and use the term VPI instead. For the same reason, the blinkered approximation is equivalent to solving the problem exactly.

**Evaluation procedure:** We evaluated the potential of our method in two steps: First, we performed a regression analy-

sis to evaluate whether the proposed features are sufficient to capture the value of computation. Second, we tested whether the proposed features are sufficient to learn a near-optimal metalevel policy. The metalevel RL agent learns the weights w of the policy defined in Equation 11 that maximize expected return through Gaussian process Bayesian optimization. We ran 500 iterations of optimization, estimating the expected return of the policy entailed by the probed weight vector by its average return across 2500 episodes. The performance of learned policy was evaluated on an independent test set of 3000 episodes.

To perform these evaluations, we first established the ground truth by solving the metalevel MDP with backward induction (Puterman 2014).

**Results:** First, linear regression analyses confirmed that three simple features (VOI $_1(c,b)$ , VPI(c,b), and cost(c)) are sufficient to capture between 90.8% and 100.0% of the variance in the value of computation for performing a simulation (VOC $(b,c_1)$ ) across different states b depending on the cost of computation. Concretely, as the cost of computation increased from 0.001 to 0.1 the regression weights shifted from 0.76  $\cdot$  VPI + 0.46  $\cdot$  VOI $_1$  - 4.5  $\cdot$  cost to 0.00  $\cdot$  VPI+1.00  $\cdot$  VOI $_1$ -1.00  $\cdot$  cost and the explained variance increased from 90.8% to 100.0%. The explained variance and the weights remained the same for costs greater than 0.1. Supplementary Figure 1 illustrates this fit for  $\lambda$  = 0.02.

Second, we found that the VOI $_1$  and the VPI features are sufficient to learn a near-optimal metalevel policy. As shown in Figure 2, the performance of metalevel RL policy was at most 5.19% lower than the performance of the optimal metalevel policy across all costs. The difference in performance was largest for the lowest cost  $\lambda=0.001$  (t(2999)=3.75, p=0.0002) and decreased with increasing cost so that there was no statistically significant performance difference between our method and the optimal metalevel policy for costs greater than  $\lambda=0.0025$  (all p>0.15). The policy learned with BO performed between 6.78% and 35.8% better than the meta-greedy policy across all costs where the optimal policy made more than one observation (all p<0.0001) and 20.3% better on average  $(t(44999)=42.4, p<10^{-15})$ .

#### 2. Metareasoning about decision-making

How should an agent allocate its limited decision-time across estimating the expected utilities of multiple alternatives? To evaluate how well our method can solve this kind of problem, we evaluate it on the *Bernoulli metalevel probability model* introduced by Hay et al. (2012). This problem differs from the previous one in two ways. First, instead of having only a single object-level action (i.e., make a prediction), there are now  $k \geq 2$  object-level actions. Second, instead of making a prediction and being rewarded for its accuracy, the agent chooses an action  $a_i$  and receives a payoff that is sampled from its outcome distribution, that is  $r(s,a_i) \sim \text{Bernoulli}(\theta_i)$  where  $\theta_i$  is the action's unknown reward probability. This problem differs from the standard multi-armed bandit problem in two ways: First, the agent

takes only a single object-level action and thus receives only one external reward. Second, the agent is equipped with a simulator that it can use to estimate the reward probabilities  $\theta_1, \dots, \theta_k$  via sampling; simulated outcomes do not count towards the agent's reward, but each simulation has a cost.

Metalevel MDP: The Bernoulli metalevel probability model is a metalevel MDP  $M_{\mathrm{meta}} = (\mathcal{B}, \mathcal{A}, T_{\mathrm{meta}}, r_{\mathrm{meta}}, h)$ where each belief state b defines k Beta distributions over the reward probabilities  $\theta_1, \dots, \theta_k$  of the k possible actions. Thus b can be represented by  $((\alpha_1, \beta_1), \dots, (\alpha_k, \beta_k))$  where  $b(\theta_i) = \text{Beta}(\theta_i; \alpha_i, \beta_i)$  for all  $1 \leq i \leq K$ . For the initial belief state  $b_0$  these parameters are  $\alpha_i = \beta_i = 1$  for all  $1 \leq i \leq k$ . The metalevel actions  $\mathcal{A}$  are  $\{c_1, \ldots, c_k, \perp\}$ where  $c_i$  simulates action  $a_i$  and  $\perp$  terminates deliberation and executes the action with the highest expected return, that is action  $\arg\max_i \frac{\alpha_i}{\alpha_i + \beta_i}$ . The metalevel transition probabilities  $(T_{\mathrm{meta}}(b_t,c_i,b_{t+1}))$  encode that performing computation  $c_i$  increments  $\alpha_i$  with probability  $\frac{\alpha_i}{\alpha_i+\beta_i}$ and increments  $\beta_i$  with probability  $\frac{\beta_i}{\alpha_i + \beta_i}$ . The metalevel reward function  $r_{\mathrm{meta}}(b,c)$  is  $-\lambda$  for  $c \in \{c_1,\cdots,c_k\}$  and  $r_{\mathrm{meta}}(b,\perp) = \max_i \frac{\alpha_i}{\alpha_i + \beta_i}$ . Finally, the horizon h is the maximum number of metalevel actions that can be performed and the last metalevel action has to be to terminate deliberation and take action ( $\perp$ ).

Evaluation procedure: We evaluated our method on Bernoulli metalevel probability problems with k $\{2, \dots, 5\}$  object-level actions, a horizon of h = 25, and computational costs ranging from  $10^{-4}$  to  $10^{-1}$ . We evaluated the performance of metalevel RL against the optimal metalevel policy and three alternative approximations: the meta-greedy heuristic (Russell and Wefald 1991a), the blinkered approximation (Hay et al. 2012), and the metalevel policy that always deliberates as much as possible. We trained the metalevel RL policy with Bayesian optimization as described above, but with 100 iterations of 1000 episodes each. To combat the possibility of overfitting, we evaluated the average returns of the five best weight vectors over 5000 more episodes and selected the one that performed best. The optimal metalevel policy and the blinkered policy were computed using backward induction (Puterman 2014). We evaluated the performance of each policy by its average return across 2000 episodes for each combination of computational cost and number of object-level actions.

**Results:** An analysis of variance confirmed that these four methods differed significantly in their performance  $(F(4,279932)=123078.5,p<10^{-15})$ . We found that the policy obtained by metalevel RL attained 99.2% of optimal performance (0.6540 vs. 0.6596, t(1998)=-6.98,p<0.0001) and significantly outperformed the meta-greedy heuristic  $(0.60, t(1998)=86.9, p<10^{-15})$  and the full-deliberation policy  $(0.20, t(1998)=475.2, p<10^{-15})$ . The performance of our method (0.6540) and the blinkered approximation (0.6559) differed by only 0.29%.

Figure 3b shows the metareasoning performance of each method as a function of the number of options. We found that our method's performance scaled well with the size of the decision problem. For each number of options, the relative performance of the different methods was consistent with the results reported above.

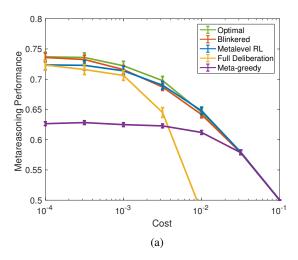
Figure 3a shows the methods' average performance as a function of the cost of computation. An ANOVA confirmed that the effect of the metareasoning method differed across different costs of computation (F(24, 279932)) $64401.4, p < 10^{-15}$ ). Our method outperformed the metagreedy heuristic for costs smaller than 0.03 (all  $p < 10^{-15}$ ), and the full-deliberation policy for costs greater than 0.0003 (all p < 0.005). For costs below 0.0003, the blinkered policy performed slightly better than our method (all p < 0.0005). For all other costs both methods performed at the same level (all p > 0.1), with the exception of the cost  $\lambda = 0.01$ , for which our method outperformed the blinkered approximation (t(1998) = 3.2, p = 0.001). Additionally, for costs larger than 0.01, our method's performance becomes indistinguishable from the optimal policy's performance (all p > 0.24).

Finally, as illustrated in Supplementary Figure 2, we found that our metalevel RL algorithm learned surprisingly quickly, usually discovering near-optimal policies in less than 10 iterations.

#### 3. Metareasoning about planning

Having evaluated our method on problems of metareasoning about how to make a one-shot decision, we now evaluate its performance at deciding how to plan. To do so, we define the Bernoulli metalevel tree, which generalizes the Bernoulli metalevel probability model by replacing the oneshot decision between k options by a tree-structured sequential decision problem that we will refer to as the object-level MDP. The transitions of the object-level MDP are deterministic and known to the agent. The reward associated with each of  $K = 2^{h+1} - 1$  states in the tree is deterministic, but initially unknown;  $r(s, a, s_k) = \theta_k \in \{-1, 1\}$ . The agent can uncover these rewards through reasoning at a cost of  $-\lambda$ per reward. When the agent terminates deliberation, it executes a policy with maximal expected utilty. Unlike in the previous domains, this policy entails a sequence of actions rather than a single action.

**Metalevel MDP:** The Bernoulli metalevel tree is a metalevel MDP  $M_{\text{meta}} = (\mathcal{B}, \mathcal{A}, T_{\text{meta}}, r_{\text{meta}})$  where each belief state b encodes one Bernoulli distribution for each transition's reward. Thus, b can be represented as  $(p_1, \cdots, p_K)$  such that  $b(\theta_k = 1) = p_k$  and  $b(\theta_k = -1) = 1 - p_k$ . The initial belief  $b_0$  has  $p_k = 0.5$  for all k. The metalevel actions are defined  $\mathcal{A} = \{c_1, \cdots, c_K, \bot\}$  where  $c_k$  reveals the reward at state k and  $\bot$  selects the path with highest expected sum of rewards according to the current belief state. The transition probabilities  $T_{\text{meta}}(b_t, c_k, b_{t+1})$  encode that performing computation  $c_k$  sets  $p_k$  to 1 or 0 with equal probability (unless  $p_k$  has already been updated, in which case  $c_k$  has no effect). The metalevel reward func-



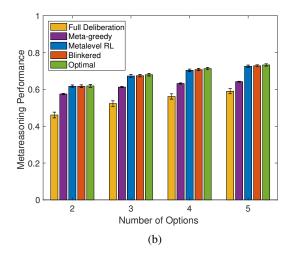


Figure 3: (a) Metareasoning performance as a function of the cost of computation. Error bars enclose 95% confidence intervals. (b) Metareasoning performance (i.e. expected reward of chosen option minus cost of the decision process) of alternative methods on the Bernoulli metalevel probability model as a function of the number of actions. Error bars enclose 95% confidence intervals.

tion is defined  $r_{\text{meta}}(b,c) = -\lambda$  for  $c \in \{c_1, \cdots, c_K\}$ , and  $r_{\text{meta}}\left((p_1, \cdots, p_k), \bot\right) = \max_{\mathbf{t} \in \mathcal{T}} \sum_{k \in \mathbf{t}} \mathbb{E}\left[\theta_k \mid p_k\right]$  where  $\mathcal{T}$  is the set of possible trajectories through the environment, and  $\mathbb{E}\left[\theta_k \middle| p_k\right] = 2p_k - 1$  is the expected reward attained at state  $s_k$ .

The recursively blinkered policy The blinkered policy of Hay et al. (2012) was defined for problems where each computation informs the value of only one action. This assumption of "independent actions" is crucial to the efficiency of the blinkered approximation because it allows the problem to be decomposed into one independent subproblem for each action. When there are few computations associated with each action, each subproblem can be efficiently solved.

Critically, the Bernoulli metalevel tree violates the assumption of independent actions. This is because here "actions" are policies, and the reward at each state affects the values of all policies visiting that state. One can still apply the blinkered policy in this case, approximating the value of a computation  $c_k$  by assuming that future computations will be limited to  $\mathcal{E}_{c_k}$ , the set of computations that are informative about any of the policies the initial computation is relevant to. However, for large trees, this only modestly reduces the size of the initial problem. This suggests a recursive generalization: Rather than applying the blinkered approximation once and solving the resulting subproblem exactly, we recursively apply the approximation to the resulting subproblems. Finally, to ensure that the subproblems decrease in size monotonically, we remove from  $\mathcal{E}_{c_k}$  the computations about rewards on the path from the agent's current state to the state  $s_k$  inspected by computation  $c_k$  and call the resulting set  $\mathcal{E}'_{c_k}$ . Thus, we define the recursively blinkered policy as  $\pi^{\rm RB}(b) = \arg\max_c Q^{\rm RB}(b,c)$ 

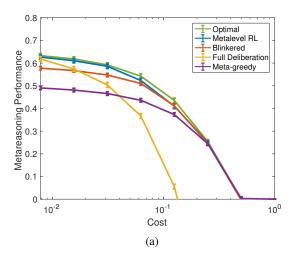
with 
$$Q^{\mathrm{RB}}(b_t, \perp) = r_{\mathrm{meta}}(b_t, \perp)$$
 and 
$$Q^{\mathrm{RB}}(b_t, c_t) = \mathbb{E}\left[r_{\mathrm{meta}}(b_t, c_t) + \max_{c_{t+1} \in \mathcal{E}'_{c_t}} Q^{\mathrm{RB}}(B_{t+1}, c_{t+1})\right] \tag{12}$$

**Evaluation procedure:** We evaluated each method's performance by its average return over 5000 episodes for each combination of tree-height  $h \in \{2, \cdots, 6\}$  and computational cost  $\lambda \in \{2^{-7}, \cdots, 2^0\}$ . To facilitate comparisons across planning problems with different numbers of steps, we measured the performance of meta-level policies by their expected return divided by the tree-height.

We trained the metalevel RL policy with Bayesian optimization as described above, but with 100 iterations of 1000 episodes each. To combat the possibility of overfitting, we evaluated the average returns of the three best weight vectors over 2000 more episodes and selected the one that performed best.

For metareasoning about how to plan in trees of height 2 and 3, we were able to compute the optimal metalevel policy using dynamic programming. But for larger trees, computing the optimal metalevel policy would have taken significantly longer than 6 hours and was therefore not undertaken.

**Results:** We first compared our method with the optimal policy for  $h \in \{2,3\}$ , finding that it attained 98.4% of optimal performance  $(0.367 \text{ vs. } 0.373, t(159998) = -2.87p < 10^{-15})$ . An ANOVA of the performance of the approximate policies confirmed that the metareasoning performance differed significantly across the four methods we evaluated  $(F(3,799840) = 4625010; p < 10^{-15})$ , and that the magnitude of this effect depends on the height of the tree  $(F(12,799840) = 1110179, p < 10^{-15})$  and the cost of computation  $(F(21,799840) = 1266582, p < 10^{-15})$ .



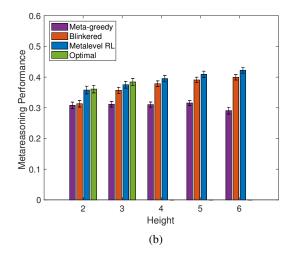


Figure 4: (a) Metareasoning performance as a function of computation cost on a Bernoulli tree of height three. Metareasoning performance is the average reward earned per object-level state visited. (b) Metareasoning performance as a function of tree height. The optimal policy is only shown for heights at which it can be computed in under six hours. The full observation policy is not shown because its performance is negative for all heights.

Across all heights and costs, our method achieved a metareasoning performance of 0.392 units of reward per object-level action, thereby outperforming the meta-greedy heuristic (0.307, t(399998) = 72.84,  $p < 10^{-15}$ ), the recursively blinkered policy (0.368, t(399998) = 20.77,  $p < 10^{-15}$ ), and the full-deliberation policy (-1.740, t(399998) = 231.18,  $p < 10^{-15}$ ).

As shown in Figure 4a, our method performed nearoptimally across all computational costs, and its advantage over the meta-greedy heuristic and the tree-blinkered approximation was largest when the cost of computation was low, whereas its benefit over the full-deliberation policy increased with increasing cost of computation.

Figure 4b shows that the performance of our method scaled very well with the size of the planning problem, and that its advantage over the meta-greedy heuristic increased with the height of the tree.

#### **Discussion**

We have introduced a new approach to solving the foundational problem of rational metareasoning: metalevel RL. This approach applies algorithms from RL to metalevel MDPs to learn a policy for selecting computations. Our results show that metalevel RL can outperform the state of the art methods for approximate metareasoning. While we illustrated this approach using a policy search algorithm based on Bayesian optimization, there are many other RL algorithms that could be used instead, including policy gradient algorithms, actor-critic methods, and temporal difference learning with function approximation.

Since our method approximates the value of computation as a linear combination of the myopic VOI and the value of perfect information, it can be seen as a generalization of the meta-greedy approximation (Lin et al. 2015; Russell and Wefald 1991b). It is the combination of these

features with RL that makes our method tractable and powerful. Metalevel RL works well across a wider range of problems than previous approximations because it reduces arbitrarily complex metalevel MDPs to low-dimensional optimization problems.

Our method could be used to find the optimal algorithms that specific computational architectures should use to solve a specific class of problems as efficiently as possible. We predict that metalevel RL will enable significant advances in artificial intelligence and its applications. In the long view, metalevel RL may become a foundation for self-improving AI systems that learn how to solve increasingly more complex problems increasingly more efficiently. To facilitate this advance, future work will apply deep RL (Mnih et al. 2015) to metalevel MDPs to discover efficiently computable features for predicting the value of computation. This will overcome the limitation that computing the value of perfect information takes a non-negligible amount of time. To increase the sample efficiency of solving metalevel MDPs by deep RL, one could use the method presented here to construct shaping rewards (Ng, Harada, and Russell 1999) that make the optimal metalevel policy easier to learn (see Supplemental Material). Ongoing experimental work suggests that this approach can also be applied to accelerate how people learn cognitive skills. The current version of our method might already have merit for selecting very expensive computations, such as complex large-scale simulations, solving active learning problems, hyperparameter search, and the optimization of functions that are very expensive to evaluate. Finally, our method could also be applied to derive rational process models of human cognition.

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## Supplemental Material

### Supplementary Figures

Figure 1 illustrates that the features proposed in the Main Text are sufficient to capture the VOC. Each data point corresponds to the VOC of deliberating for a different belief state. The cost of computation was  $\lambda = 0.02$  and similar fits were obtained for other costs.

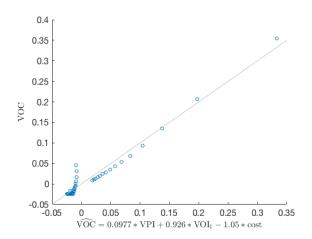


Figure 1: Linear fit of the value of computation for metareasoning about when to stop deliberating.

Figure 2 illustrates that our meta-level RL very quickly converged to near-optimal policies. This particular learning curve was observed for the 4-action meta-level probability model with a horizon of h=25 and a cost of  $\lambda=0.01$ .

#### Accelerating metalevel RL

The effectiveness of model-free RL critically depends on the reward structure. Delayed rewards are a particularly dire problem. This problem is particularly pronounced in meta-level MDPs, because the meta-level reward function is negative until the agent terminates deliberation. Previous research on model-free reinforcement learning has shown that the problem of delayed rewards can be

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ameliorated by reward shaping (Ng, Harada, and Russell 1999). Future work might therefore explore using reward-shaping to accelerate meta-level reinforcement learning.

One approach could be to use the method proposed in the main text to quickly learn a rough approximation to the meta-level value function and then use it to generate shaping rewards for a method that learns an approximation that is more accurate or can be evaluated more efficiently. This could be done as follows:

- 1. Apply the method presented in the main text to learn  $\pi_{(meta)}(b)$ .
- 2. Approximate  $Q_{\pi_{\text{meta}}}$  by regressing the returns of  $\pi_{(meta)}$  onto the features VOC<sub>1</sub>, VPI<sub>a</sub>, VPI<sub>all</sub>, cost(c), and  $r_{\text{meta}}(b, \perp)$ .
- 3. Apply the shaping theorem (Ng, Harada, and Russell 1999) to translate the resulting approximation  $\hat{Q}_{\text{meta}}$  into a modified reward function

$$r'_{\text{meta}}(b, c) = \hat{Q}_{\text{meta}}(b, c) - \max_{c} \hat{Q}_{\text{meta}}(b, c).$$
(1)

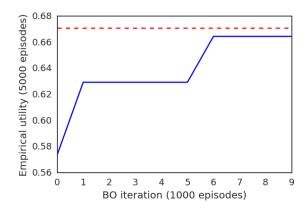


Figure 2: Learning curve of our metalevel RL method. The vertical axis shows the performance of the current best policy as a function of the number of iterations of the Bayesian optimization algorithm (horizontal axis) on an independent test set.

4. Train a different meta-level reinforcement learning algorithm on the modified reward function  $r'_{\text{meta}}$ .

## Approximating the meta-level Q-function using regression

To generate shaping rewards, we can use the policy  $\pi(b; \mathbf{w})$  learned with the method described in the main text to approximate the optimal meta-level action-value function  $Q_{\mathrm{meta}}^{\star}.$  This can be achieved by running the approximate policy starting from randomly selected (b, c)-pairs, recording the resulting returns, and regressing them on features of the (b, c)-pair that the policy started from. Recall that  $Q_{\text{meta}}^{\star}$  is the sum of the VOC and the expected reward of acting without deliberation (Equation 4 in the Main Text). Thus, assuming that we can approximate the VOC as a linear combination of the  $VOI_1$ , the  $VPI_{all}$ , the  $VPI_A$ , and cost(c), it should be possible to approximate  $Q^{\star}_{\mathrm{meta}}$  as a linear combination of these three predictors and the expected reward of acting without deliberation  $(r_{\text{meta}}(b, \perp))$ . We will illustrate this approach by regressing the Monte-Carlo estimate of the returns of  $\pi(b; \mathbf{w})$  onto these features. This leads to a simple approximation of  $Q_{\text{meta}}^{\star}$  by

$$\hat{Q}_{\text{meta}}(b, c; \mathbf{w}) = w_1 \cdot \text{VOI}_1(b, c) + w_2 \cdot \text{VPI}_{\text{all}} + w_2 \cdot \text{VPI}_A(b, c) - w_4 \cdot \text{cost}(c) + w_5 \cdot \mathbb{E} \left[ r_{\text{meta}}(b, \perp) | b \right],$$
(2)

where the weights  $\mathbf{w}$  are be estimated by linear regression.

#### **Proof-of-Concept Simulations**

As a proof-of-concept that our method could be leveraged to accelerate meta-level reinforcement learning, we show that the shaping rewards computed with this approach can accelerate tabular Q-learning on the first two metareasoning problems that we studied in the Main Text. This illustrates that our approximate method could, in principle, be used to accelerate reinforcement learning methods that converge to the optimal solution.

Learning when to terminate deliberation We first evaluate the approach on the learning when to terminate deliberation meta-MDP with a horizon of h=30 and a computational cost of  $\lambda=-0.015$ . In this problem, the VPI<sub>all</sub> and VPI<sub>A</sub> are identical, so Equation 2 reduces to

$$\hat{Q}_{\text{meta}}(b, c; \mathbf{w}) = w_1 \cdot \text{VOI}_1(b, c) + w_2 \cdot \text{VPI} - w_3 \quad (3)$$
$$\cdot \cot(c) + w_4 \cdot r_{\text{meta}}(b, \perp).$$

First, we learned  $\pi_{\text{meta}}$  using the meta-level reinforcement learning algorithm described in the Main Text. Second, we approximated  $Q_{\pi_{\text{meta}}}$  using linear regression. To do so, we ran the policy learned with meta-level reinforcement learning once for each  $((\alpha, \beta), c)$ -pair with  $1 \leq \alpha, \beta \leq 30$  and  $\alpha + \beta < 30$  and  $c \in c_1, \bot$ . We

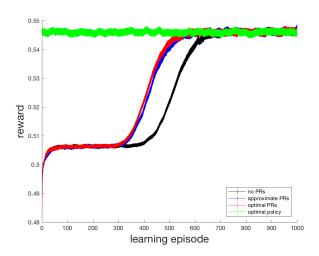


Figure 3: Shaping rewards accelerate learning when to stop deliberating. The amount of relative reward (vertical axis) increases over time at a greater rate when the agent receives shaping rewards.

then used the resulting returns to estimate the feature-weights in in Equation 3 by linear regression with the maximum likelihood method  $(w_{\rm ML})$ . We found that the resulting predictions  $\hat{Q}(b,c;w_{\rm ML})$  captured the optimal meta-level Q-function very accurately: The root-mean-squared-error between our approximation and the optimal meta-level Q-function was only 0.0103, the correlation between  $\hat{Q}_{\rm meta}$  and  $Q_{\rm meta}^{\star}$  was r=0.9995, and our approximation explained 99.9% of the variance in  $Q^{\star}$  across state-action pairs. We found that the same held true when we restricted our analysis to the meta-level Q-values of deliberating (RMSE = 0.0146, r=0.9996,  $R^2=0.999$ ) and terminating deliberation respectively (RMSE <  $10^{-15}$ , r=1.0000,  $R^2=1.0000$ ).

Third, we translated  $\hat{Q}_{\pi_{\rm meta}}$  into shaping rewards according to Equation 1 and ran 2000 simulations to determine whether they can accelerate tabular Q-learning of the meta-level policy. The agent which was given either optimal shaping rewards based on  $Q_{\text{meta}}^{\star}$ , pseudorewards based on  $\hat{Q}_{\pi_{\text{meta}}}$  (Equation 1), or no pseudorewards. The agent was trained for 1000 learning episodes with Q-values initialized to zero, a constant learning rate of 0.1, and a constant exploration rate of 0.25, and the cost of computation was set to 0.1. Figure 3 shows the performance of these three agents, with the approximate and optimal pseudoreward agents earning comparable rewards, and learning faster than the agent with no pseudorewards. All three agents eventually converge to the performance of an agent following the optimal policy, but for the agents that received pseudorewards this takes only 500 episodes instead of the 600 episodes required without pseudorewards.

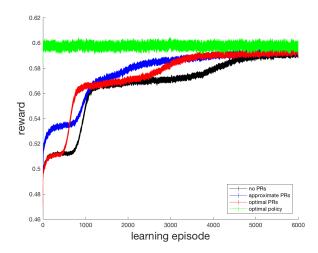


Figure 4: Shaping rewards accelerate learning how to choose between 3 options.

Metareasoning about decision-making Next, we evaluated this approach on the problem of metareasoning about decision-making described in the main text. As shown in Figure 4, the approximate pseudorewards generated with our method significantly accelerated learning compared to the control condition without pseudorewards. In the beginning the learning with approximate pseudorewards was even faster than with optimal pseudorewards, and over all both kinds of pseudoreward were about equally beneficial. This supports the hypothesis that our method can be used to accelerate meta-level RL. The cost of computation was 0.01. All other parameters were the same as in the simulations above.

#### References

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