Deep Exploration via Randomized Value Function

RLRG 2022W2 Helen Zhang



Slides partially stolen from Bingshan's OTS presentation, and Chris and Jason' MLRG in 2019, and various paper/poster/slides from authors



ABOUT ME



I am a research scientist at Google Deepmind working to solve artificial intelligence. My research focus is on decision making under uncertainty (a.k.a. reinforcement learning). I want to design autonomous agents that teach themselves to do well in any task. If we can do this, then we will be well on our way to general AI.

I completed my Ph.D. at Stanford University advised by Benjamin Van Roy. My thesis Deep Exploration via Randomized Value Functions won second place in the national Dantzig dissertation award. It takes some steps towards a practical RL algorithm that combines efficient generalization and exploration... and I'm still focused on making progress in this area!

Before coming to Stanford I studied maths at Oxford University and worked for J.P.Morgan as a credit derivatives strategist. I spent the summer of 2015 working for Google in Mountain View and, after a great internship in 2016 joined DeepMind full time in London. If you want to know more about what I'm thinking check out my blog.

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- Bandits
 - UCB
 - Thompson Sampling
- MDP
 - Least square value iteration
 - RLSVI: exploration via randomized value function
- Regret Analysis
- Practical Variants/Experiments



Exploration in Bandits

Stochastic Multi-arm Bandits



Goal: minimize regret (equivalent to maximize reward)



Upper Confidence Bound

Optimism in the face of uncertainty

- Compute the empirical mean of each arm and a confidence interval;
- Use the upper confidence bound as a proxy for goodness of arm.



"Randomly take action according to the probability you believe it is the optimal action" - Thompson 1933

An empirical MAB instance
$$\widehat{\Theta} := \left([K]; \hat{\mu}_{1,O_1(t-1)}, \hat{\mu}_{2,O_2(t-1)}, \dots, \hat{\mu}_{K,O_K(t-1)}\right)$$

Data-dependent distributions $\widetilde{\theta} := \left([K]; \widetilde{\theta}_{1,O_1(t-1)}, \widetilde{\theta}_{2,O_2(t-1)}, \dots, \widetilde{\theta}_{K,O_K(t-1)}\right)$,
where each $\widetilde{\theta}_{j,O_j(t-1)} = \mathcal{N}\left(\hat{\mu}_{j,O_j(t-1)}, \frac{3\ln(t)}{O_j(t-1)}\right)$

A sampled MAB instance $\widetilde{\Theta} := ([K]; \tilde{\mu}_{1,t}, \tilde{\mu}_{2,t}, \dots, \tilde{\mu}_{K,t})$

where each
$$\tilde{\mu}_{j,t} \sim \tilde{\theta}_{j,O_j(t-1)} \Rightarrow \tilde{\mu}_{j,t} \sim \mathcal{N}\left(\hat{\mu}_{j,O_j(t-1)}, \frac{3\ln(t)}{O_j(t-1)}\right)$$

Standard TS: behave greedy in $\widetilde{\Theta}$, pull $J_t \leftarrow \max_{j \in [K]} \widetilde{\mu}_{j,t}$





Use two events to split up the expectation:

- $E_i^{\theta}(t)$ the event that the sampled parameter is far from μ_i
- $E_i^{\hat{\mu}}(t)$ the event that the estimated mean $\hat{\mu}_i$ is from from μ_i

Posterior deviation

Empirical deviation



Exploration in MDPs



Markov Decision Processes (MDPs) provide a framework for modelling **sequential decision making**, where the environment has different states which change over time as a result of the agent's actions.

- A learning agent draws a trajectory (a sequence of state-action pairs) and try to <u>maximize cumulative reward</u>
- Bandit can be viewed as an <u>MDP with one state and K</u> actions.





- Bandit Problem
- MDP
- POMDP

Least Square Value Iteration

Adapting value-iteration with imperfect statistical knowledge and limited compute.

Algorithm	f 2 vi				
Input:	$\mathcal{M} = (\mathcal{S}, \mathcal{A}, \mathcal{R}, \mathcal{P}, \rho)$	MDP			
	$H \in \mathbb{N}$	planning horizon			
Output:	Q_H^*	optimal value function for H -period problem			
1: $Q_0^* \leftarrow 0$					
2: for h in $(0,, H-1)$ do					
3: $Q_{h+1}^*(s,a) \leftarrow \sum_{s' \in \mathcal{S}} \mathcal{P}_{s,a}(s') \left(\int r \mathcal{R}_{s,a,s'}(dr) + \max_{a' \in \mathcal{A}} Q_h^*(s',a') \right) \forall s,a \in \mathcal{S} \times \mathcal{A}$					
4: return Q_H^*					

Empirical temporal difference loss: $\mathcal{L}(\theta; \theta^{-}, \mathcal{D}) \coloneqq \sum_{t \in \mathcal{D}} \left(r_t + \max_{a' \in \mathcal{A}} \mathcal{Q}_{\theta^{-}}(s'_t, a') - \mathcal{Q}_{\theta}(s_t, a_t) \right)^2$

Regularized towards prior: $\mathcal{R}(\theta; \theta^p) \coloneqq \frac{v}{\lambda} \|\theta^p - \theta\|_2^2$.

	Algorithm 3 learn_lsvi				
	Agent:	$\mathcal{L}(\theta = \cdot; \theta^{-} = \cdot, \mathcal{D} = \cdot)$	TD error loss function		
		$\mathcal{R}(\theta = \cdot; \theta^p = \cdot)$	regularization function		
		buffer	memory buffer of observations		
		prior	prior distribution of θ		
		$H \in \mathbb{N}$	planning horizon		
	Updates:	$ ilde{ heta}$	agent value function estimate		
	1: $\tilde{ heta}_0 \leftarrow \mathbf{null}$				
	2: Data $\tilde{\mathcal{D}} \leftarrow \texttt{buffer.data}()$				
	3: Prior parameter $\tilde{\theta}^p \leftarrow \texttt{prior.mean}()$				
	4: for h in $(0,, H-1)$ do				
	5: $ \tilde{\theta}_{h+1} \leftarrow \underset{\theta \in \mathbb{R}^D}{\operatorname{argmin}} \left(\mathcal{L}(\theta; \tilde{\theta}_h, \tilde{\mathcal{D}}) + \mathcal{R}(\theta; \tilde{\theta}^p) \right)$ 6: update value function estimate $\tilde{\theta} \leftarrow \tilde{\theta}_H$				

Key idea: replace least square computation with an alternative value iteration that trains on randomly perturbed version of the data

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- Consider conventional linear regression:

Let $\theta \in \mathbb{R}^d$, prior $N(\overline{\theta}, \lambda I)$ and data $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$ for $y_i = \theta^T x_i + \epsilon_i$ with $\epsilon_i \sim N(0, \sigma^2)$ iid. Then, conditioned on \mathcal{D} , the posterior for θ is Gaussian:

$$\mathbb{E}[\theta|\mathcal{D}] = \left(\frac{1}{\sigma^2}X^T X + \frac{1}{\lambda}I\right)^{-1} \left(\frac{1}{\sigma^2}X^T y + \frac{1}{\lambda}\overline{\theta}\right),$$
$$\operatorname{Cov}[\theta|\mathcal{D}] = \left(\frac{1}{\sigma^2}X^T X + \frac{1}{\lambda}I\right)^{-1}.$$
(1)

Relies on Gaussian conjugacy and linear models, which cannot easily be extended to deep NN

Lemma 1 (Computational posterior samples). Let $f_{\theta}(x) = x^T \theta$, $\tilde{y}_i \sim N(y_i, \sigma^2)$ and $\tilde{\theta} \sim N(\bar{\theta}, \lambda I)$. Then either of the following optimization problems generate a sample $\theta \mid \mathcal{D}$ according to (1):

$$\operatorname{argmin}_{\theta} \sum_{i=1}^{n} \|\tilde{y}_{i} - f_{\theta}(x_{i})\|_{2}^{2} + \frac{\sigma^{2}}{\lambda} \|\tilde{\theta} - \theta\|_{2}^{2}, \qquad (2)$$

$$\tilde{\theta} + \underset{\theta}{\operatorname{argmin}} \sum_{i=1}^{n} \|\tilde{y}_{i} - (f_{\tilde{\theta}} + f_{\theta})(x_{i})\|_{2}^{2} + \frac{\sigma^{2}}{\lambda} \|\theta\|_{2}^{2}.$$
(3)

Proof. Note output is Gaussian, match moments.

Computationally tractable approximate posterior, drive deep exploration via randomized value functions.

Algorithm



Deep Exploration Intuition

Consider a simple MDP with 4 stats, 2 actions

Suppose we are highly uncertain about state-action pair (4, down), but are pretty sure about others.



Regret Analysis

Finite-horizon Time-inhomogeneous MDP

Assumption 2 (Finite-horizon time-inhomogeneous MDP). The state space factorizes as $S = S_0 \cup S_1 \cup S_2 \cup \cdots \cup S_{H-1}$ where $|S_0| = \cdots = |S_{H-1}| < \infty$. For any MDP $\mathcal{M} = (S, \mathcal{A}, \mathcal{R}, \mathcal{P}, \rho)$,

$$\sum_{s'\in\mathcal{S}_{t+1}}\mathcal{P}_{s,a}(s')=1 \qquad \forall t\in\{0,...,H-2\}, s\in\mathcal{S}_t, a\in\mathcal{A},$$

and

$$\sum_{s'\in\mathcal{S}}\mathcal{P}_{s,a}(s')=0\qquad\forall s\in\mathcal{S}_{H-1},\,a\in\mathcal{A}.$$

Each state $s \in S_t$ can be written as a pair s = (t, x) where $t \in \{0, ..., H-1\}$ and $x \in \mathcal{X} = \{1, ..., |S_0|\}$. Similarly, a policy $\pi : S \to \mathcal{A}$ can be viewed as a sequence $\pi = (\pi_0, ..., \pi_{H-1})$ where $\pi_t : x \mapsto \pi((t, x))$. Our notation can be specialized to this time-inhomogenous problem, writing transition probabilities as $\mathcal{P}_{t,x,a}(x') \equiv \mathcal{P}_{(t,x),a}((t+1, x'))$ and reward probabilities as $\mathcal{R}_{t,x,a,x'}(r) \equiv \mathcal{R}_{(t,x),a,(t+1,x')}(r)$. For consistency, we also use different notation for the optimal value function, writing

$$V_{\mathcal{M},t}^{\pi}(x) \equiv V_{\mathcal{M}}^{\pi}((t,x))$$

and define $V_{\mathcal{M},t}^*(x) \coloneqq \max_{\pi} V_{\mathcal{M},t}^{\pi}(x)$. Similarly, we can define the state-action value function under the MDP at timestep $t \in \{0, ..., H-1\}$ by

$$Q_{\mathcal{M},t}^*(x,a) = \mathbb{E}[r_{t+1} + V_{\mathcal{M},t+1}^*(x_{t+1}) \mid \mathcal{M}, x_t = x, a_t = a] \qquad \forall x \in \mathcal{X}, a \in \mathcal{A}$$



Average over distribution

Regret / L should converge to 0 Regret $(\mathcal{M}, \operatorname{alg}, L) = \sum_{\ell=1}^{L} \mathbb{E}_{\mathcal{M},\operatorname{alg}} \left[V^*(s_0^{\ell}) - V^{\pi^{\ell}}(s_0^{\ell})) \right]$ Bayos Pogret (alg. L) = $\mathbb{E} \left[\operatorname{Pogret}(\mathcal{M}, \operatorname{alg}, L) \right]$

BayesRegret(alg, L) = \mathbb{E} [Regret(\mathcal{M} , alg, L)].

For $|\mathcal{S}_0|$ = ... = $|\mathcal{S}_{H-1}|$ = $|\mathcal{X}|$,

 $\operatorname{BayesRegret}(\operatorname{RLSVI}_{\bar{\theta},v,\lambda},L) \leq 6H^2 \sqrt{\beta |\mathcal{X}||\mathcal{A}|L} \log_+(1+|\mathcal{X}||\mathcal{A}|HL)} \log_+\left(1+\frac{L}{|\mathcal{X}||\mathcal{A}|}\right),$

RLSVI requires a number of episodes that is just <u>linear in the number of states</u> to reach near optimal performance.

Regret Decomposition



If the function Q_0 is optimistic at an initial state x, in the sense that $\max_a Q_0(x,a) \ge \max_a Q_{\mathcal{M},0}^*(x,a)$, then regret in the episode is bounded by on policy Bellman error under $(Q_0, ..., Q_H)$.

Stochastic Optimism

Assumption 3 (Independent Dirichlet prior for outcomes).

Rewards take values in $\{0,1\}$ and so the cardinality of the outcome space is $|\mathcal{X} \times \{0,1\}| = 2|\mathcal{X}|$. For each, $(t, x, a) \in \{0, ..., H-2\} \times \mathcal{X} \times \mathcal{A}$, the outcome distribution is drawn from a Dirichlet prior

 $\mathcal{P}^{O}_{t,x,a}(\cdot) \sim \mathrm{Dirichlet}(\alpha_{0,t,x,a})$

for $\alpha_{0,t,x,a} \in \mathbb{R}^{2|\mathcal{X}|}_+$ and each $\mathcal{P}^O_{t,x,a}$ is drawn independently across (t,x,a). Assume there is $\beta \geq 3$ such that $\mathbb{1}^T \alpha_{0,t,a,x} = \beta$ for all (t,x,a).

(6.7)



Definition 2 (Stochastic optimism).

A random variable X is stochastically optimistic with respect to another random variable Y, written $X \succeq_{SO} Y$, if for all convex increasing functions $u : \mathbb{R} \to \mathbb{R}$

$$\mathbb{E}[u(X)] \ge \mathbb{E}[u(Y)]$$

Lemma 4 (Gaussian vs Dirichlet optimism). Let $Y = P^T V$ for $V \in \mathbb{R}^n$ fixed and $P \sim \text{Dirichlet}(\alpha)$ with $\alpha \in \mathbb{R}^n_+$ and $\sum_{i=1}^n \alpha_i \ge 3$. Let $X \sim N(\mu, \sigma^2)$ with $\mu \ge \frac{\sum_{i=1}^n \alpha_i V_i}{\sum_{i=1}^n \alpha_i}, \ \sigma^2 \ge 3 (\sum_{i=1}^n \alpha_i)^{-1} \operatorname{Span}(V)^2$, then $X \ge_{SO} Y$.

Bellman operator underlying RLSVI is stochastically optimistic relative to the true Bellman operator



Bellman Error



(6.4)
$$F_{\ell,t}Q(x,a) = \frac{(v/\lambda)\bar{\theta} + n_{\ell}(y)V_Q^T\hat{\mathcal{P}}_{\ell,y}^O}{(v/\lambda) + n_{\ell}(y)} + w_{\ell}(y) \quad \forall y = (t,x,a).$$

By equation (6.4), we find

$$F_{\ell,t}Q(x,a) - \mathbb{E}[F_{\mathcal{M},t}Q(x,a)|\mathcal{H}_{\ell-1}, x_1^{\ell}, a_1^{\ell}, ..., x_t^{\ell}, a_t^{\ell}] \le \frac{\beta(\|\bar{\theta}\|_{\infty} + \|V_Q\|_{\infty})}{\beta + n_{\ell}(y)} + w_{\ell}(y).$$

By Gaussian maximal inequality:

Corollary 3. For each $t \leq H$ and $\ell \leq L$

 $\mathbb{E}[w_{\ell}(t, x_t, a_t)] \leq \sqrt{2\log(|\mathcal{A}||\mathcal{X}|)\mathbb{E}[\sigma_{\ell}(t, x_t, a_t)^2]}.$

Bounding noise term

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Corollary 4. If RLSVI is applied with parameters $(\lambda, v, \overline{\theta})$ with $v/\lambda = \beta \ge 3$, $v = 3H^2$ and $\overline{\theta} = H\mathbb{1}$,

$$\mathbb{E}\left[\max_{\ell \leq L, t < H} \|V_{Q_{\ell, t+1}}\|_{\infty}\right] \leq 2H + H^2 \sqrt{2\log(1 + |\mathcal{X}||\mathcal{A}||HL)}.$$

Bounding norm of value function sampled by RLSVI

Practical Variants/Experiments

Practical Variants

- Finite buffer experience replay
- Discount factor approximating effective planning horizon
- Incremental parameter update with (batch) gradient descent
- Ensemble sampling

Algorithm 8 learn_ensemble_risvi				
Agent:	$ ilde{ heta}_1,, ilde{ heta}_K$	ensemble parameter estimates		
	$ ilde{ heta}_1^p,, ilde{ heta}_K^p$	prior samples of parameter estimates		
	$\mathcal{L}_{\gamma}(heta = \cdot ; heta^{-} = \cdot , \mathcal{D} = \cdot)$	TD error loss function		
	$\mathcal{R}(\theta = \cdot; \theta^p = \cdot)$	regularization function		
	$ensemble_buffer$	replay buffer of K -parallel perturbed data		
	α	Learning rate		
Updates:	$ ilde{ heta}$	agent value function estimate		
1: for k in $(1,, K)$ do				
2: Data $\tilde{\mathcal{D}}_k \leftarrow \texttt{ensemble_buffer[k].sample_minibatch()}$				
3: $\delta \leftarrow \text{buffer.minibatch_size} / \text{buffer.size}$				
4: $ \tilde{\theta}_k \leftarrow \tilde{\theta}_k - \alpha \nabla_{\theta \theta = \tilde{\theta}_k} \left(\mathcal{L}_{\gamma}(\theta; \tilde{\theta}_k, \tilde{\mathcal{D}}_k) + \mathcal{R}(\theta; \tilde{\theta}_k^p) \right) $				
5: update $\tilde{\theta} \leftarrow \tilde{\theta}_j$ for $j \sim \text{Unif}(1,, K)$				



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1.7

📾 Tabular: DeepSea



- Environment description:
 - State space = $N \times N$ grid.
 - Begin top left, fall one row each step.
 - Actions "left" or "right" vary per state.
 - Big reward +1 in chest.
 - \circ Small cost -0.1/N for moving "right".
- 1 policy > 0, 1 policy = 0, all others < 0.
- ... "a piece of hay in a needle-stack"
- No deep exploration $\rightarrow 2^{N}$ episodes to learn.

'Time to learn' := #episodes until AveRegret < 0.9.

- ϵ -greedy = DQN with annealing dithering.
- BS = BootDQN without explicit prior.
- BSR = BootDQN with regularize $\|\theta_k \theta_k^{\text{init}}\|$.
- BSP = BootDQN with prior, $Q_k = f_{\theta_k} + p_k$.



Figure 3: Only BSP scales to large problems. Plotting log-log suggests an empirical scaling $T_{\text{learn}} = \tilde{O}(N^3)$.

Deep Learning: Cart-Pole Swing Up

Agent begins each episode with the pole hanging down and has to learn to swing it up.

Reward structure requires deep exploration:

- Agent pays a cost for any action
- Gets reward if pole is balanced up right





Figure 16: DQN with ϵ -greedy exploration simply learns to stay motionless. Figure 17: RLSVI with 2-layer neural network is able to learn a near-optimal policy.

Thanks for listening!

And happy to hear any questions and feedbacks :)

