From Dirichlet to Rubin: Optimistic Exploration in RL without Bonuses

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     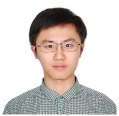  

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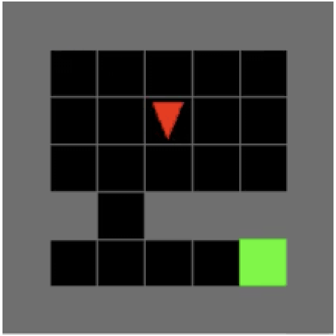
- Algorithm that can be easily extended to the deep RL setting.
  - Link between our algorithm and Bayesian bootstrap.

Bridging tabular and deep RL

Tabular setting: $S \approx 100$;



Deep RL setting: $S \approx 10^{100}$;

Is there an algorithm that at the same time

- provably optimal in tabular setting?
- practically good in Deep RL setting?

Markov Decision Process (MDP)

Tabular, episodic MDP: H horizon, S states, A actions.

Learning in MDP: at episode t, step h

- state s_h^t
- action a_h^t
- next state $s_{h+1}^t \sim p_h(\cdot|s_h^t, a_h^t)$
- reward $r_h(s_h^t, a_h^t)$ (known and bounded in $[0, 1]$)

Bellman equation policy π

$$\begin{aligned} Q_h^\pi(s, a) &= (r_h + p_h V_{h+1}^\pi)(s, a) \\ V_h^\pi(s) &= Q_h^\pi(s, \pi_h(s)) \\ V_{H+1}^\pi(s) &= 0 \end{aligned}$$

where $p_h f(s, a) = \sum_{s'} p_h(s'|s, a) f(s')$

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Optimal Bellman equation

$$\begin{aligned} Q_h^\star(s,a) &= (r_h + p_h V_{h+1})(s,a) \\ V_h^\star(s) &= \max_a Q_h^\star(s,a) \\ V_{H+1}^\star(s) &= 0 \end{aligned}$$

where $p_h f(s,a) = \sum_{s'} p_h(s'|s,a) f(s')$

Regret after T episodes: $R^T = \sum_{t=1}^{T} V_1^\star(s_1) - V_1^{\pi^t}(s_1)$

Bonus-driven exploration

Basic idea: solve Bellman equation with upper approximations.

$$\overline{Q}_h^t(s,a) = r_h(s,a) + \underbrace{\overbrace{\widehat{p}_h^t}^{\text{empirical model}} \overline{V}_{h+1}^t(s,a) + \overbrace{B_h^t(s,a)}^{\text{exploration bonus}}}_{\text{upper approximation of } p_h V_{h+1}^\star(s,a)}$$

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- Near optimal in tabular setting: $\widetilde{\mathcal{O}}(\sqrt{H^3SAT})$ regret.
- Poor empirical performance.
- Difficult scale to deep RL.

Bayes-UCBVI: From Dirichlet...

Idea: use directly an upper quantile over posterior distribution (cf. Bayes-UCB [Kaufmann et al., 2012]).

$$\overline{Q}_h^t(s,a) = r_h(s,a) + \overbrace{\mathrm{Quantile}_{\underbrace{p\sim\rho_h^t(s,a)}_{\text{Dirichlet distribution}}}}^{\text{quantile over posterior}}\big(p\overline{V}_{h+1}^t, \overbrace{\kappa}^{\text{quantile level}}\big)$$

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  - *Estimation error:* reduction to `UCBVI` [Azar et al., 2017].

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  - *Optimism:* novel anti-concentration inequality for Dirichlet weighted sum;
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- Scalable with the magic of Bayesian bootstrap!

Where do we stand: Known guarantees

Algorithm	Upper bound (non-stationary)
UCBVI [Azar et al., 2017] UCB-Advantage [Zhang et al., 2020] RLSVI [Xiong et al., 2021]	$\widetilde{\mathcal{O}}(\sqrt{H^3SAT})$
PSRL [Agrawal and Jia, 2017] BootNARL [Pacchiano et al., 2021]	$\widetilde{\mathcal{O}}(H^2S\sqrt{AT})$
Bayes-UCBVI (this paper)	$\widetilde{\mathcal{O}}(\sqrt{H^3SAT})$
Lower bound [Jin et al., 2018, Domingues et al., 2021]	$\Omega(\sqrt{H^3SAT})$

Table: Regret upper bound for episodic, non-stationary, tabular MDPs.
Green: scalable, Yellow: scalable under simplifications, Red: not scalable.

$\texttt{Bayes-UCBVI}$: ...to Rubin - Scaling up!

Given: dataset $y^1, \dots, y^n \sim \mathcal{P}$.

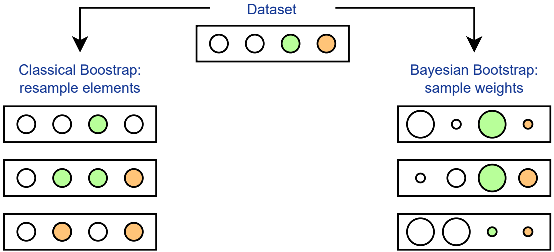
Goal: confidence interval for $\mathbb{E}_{y \sim \mathcal{P}}[y]$.

Classical Bootstrap [Efron, 1979]

- Resample $y^{1,b}, \dots, y^{n,b}$ B times;
- Compute mean estimates as $\bar{y}^b = \frac{1}{n}\sum_{i=1}^n y^{i,b}$ for all b;
- Compute quantile over $\bar{y}^b$.

Bayesian Bootstrap [Rubin, 1981]

- Sample $w^b \sim \mathcal{D}\mathrm{ir}(\underbrace{1, \dots, 1}_{n})$ B times;
- Compute mean estimates as $\bar{y}^b = \sum_{i=1}^n w^{b,i} y^i$ for all b;
- Compute quantile over $\bar{y}^b$.



Efficient implementation

- targets for Q-function estimation $y^n = r_h(s,a) + \overline{V}^t_{h+1}(s^n_{h+1})$ for visits $n = 1, \ldots, n^t$.
- prior targets $y^n = r_h(s,a) + \overline{V}^t_h(s_0)$ for prior visits $n = -n^0 + 1, \ldots, 0$.

By aggregation property and sample quantile approximation

$$\begin{aligned}\overline{Q}^t_h(s,a) &= r_h(s,a) + \mathrm{Quantile}_{p \sim \rho^t_h(s,a)}\left(p\overline{V}^t_{h+1}(s,a), \kappa\right) \\ &= \mathrm{Quantile}_{w \sim \mathcal{D}\mathrm{ir}(\underbrace{1,\ldots,1}_{n^t+n^0})}\left(\sum_{n=-n^0+1}^{n^t} w^n y^n, \kappa\right) \\ &\approx \underbrace{\mathrm{Quantile}_{b \sim \mathcal{U}\mathrm{nif}([1,B])}\left(\sum_{n=-n^0+1}^{n^t} \overbrace{w^{n,b}}^{\text{samples from Dirichlet}} y^n, \kappa\right)}_{\text{upper confidence bound by Bayesian bootstrap}} .\end{aligned}$$

Deep RL extension: `Bayes-UCBDQN`

Recall $w^{n,b} \sim \mathcal{D}\mathrm{ir}(\underbrace{1,\ldots,1}_{n^t+n^0})$

$$\overline{Q}_h^t(s,a) \approx \mathrm{Quantile}_{b\sim\mathcal{U}\mathrm{nif}([1,B])}\left(\bar{y}^b, \kappa\right)$$

where Bayesian bootstrap sample $\bar{y}^b = \sum_{n=-n^0+1}^{n^t} w^{n,b} y^n$

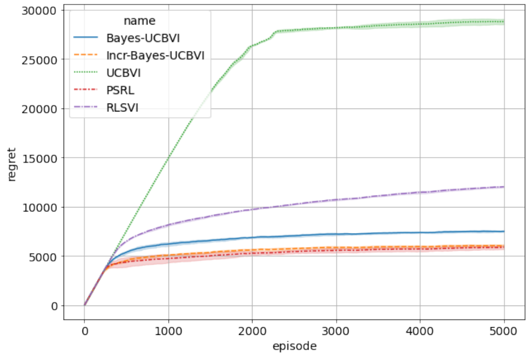
Uniform Dirichlet distribution $=$ exponential with normalization

$$\bar{y}^b = \arg\min_x \sum_{n=-n^0+1}^{n^t} z^{n,b}(x-y^n)^2$$

where $z^{n,b} \sim \mathcal{E}(1)$ i.i.d..

$\rightarrow$ Weighted regression of the targets!

Experimental results



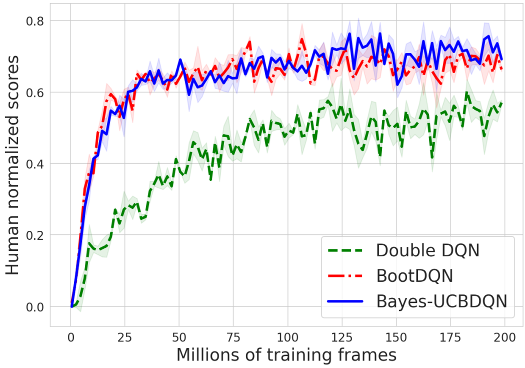


Figure: Left: Regret of `Bayes-UCBVI` and `Incr-Bayes-UCBVI` compared to baselines on grid-world with 5 rooms of size 5×5. Right: deep RL algorithms with median human normalized scores across Atari-57 games.

Takeaways

- `Bayes-UCBVI` $\rightsquigarrow$ near optimal optimistic algorithm **without bonuses**.
- New *anti-concentration* inequality for a Dirichlet weighted sum.
- `Bayes-UCBVI` scales to deep RL.

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