Notes on Fitted Q-iteration

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Let $M = (S, A, P, R, \gamma, \rho_0)$ be an MDP, where ρ_0 is the initial distribution over states.¹ Given a dataset $\{(s, a, r, s')\}$ generated from M and a Q-function class $\mathcal{F} \subset \mathbb{R}^{S \times A}$, we want to analyze the guarantee of Fitted Q-Iteration. This note is inspired by and scrutinizes the results in Approximate Value/Policy Iteration literature [e.g., 1, 2, 3] under simplification assumptions.

Setup and Assumptions

- 1. \mathcal{F} is finite but can be exponentially large.
- 2. Realizability: $Q^* \in \mathcal{F}$.
- 3. \mathcal{F} is closed under Bellman update: $\forall f \in \mathcal{F}, \mathcal{T}f \in \mathcal{F}$. (For finite \mathcal{F} , this implies realizability.)
- 4. The dataset $D = \{(s, a, r, s')\}$ is generated as follows: $(s, a) \sim \mu \times U$ (U is uniform over actions), $r \sim R(s, a)$, $s' \sim P(s, a)$. Define the empirical update $\widehat{\mathcal{T}}_{\mathcal{F}} f'$ as

$$\mathcal{L}_D(f; f') := \frac{1}{|D|} \sum_{(s, a, r, s') \in D} (f(s, a) - r - \gamma V_{f'}(s'))^2.$$

$$\widehat{\mathcal{T}}_{\mathcal{F}}f' := \underset{f \in \mathcal{F}}{\arg\min} \mathcal{L}_D(f; f'),$$

where $V_{f'}(s') := \max_{a'} f'(s', a')$. Note that by completeness, $\mathcal{T}f' \in \mathcal{F}$ is the Bayes optimal regressor for the regression problem defined in $\mathcal{L}_D(f; f')$. It will also be useful to define

$$\mathcal{L}_{\mu \times U}(f; f') := \mathbb{E}_D[\mathcal{L}_D(f; f')].$$

- 5. For any function $g: \mathcal{S} \to \mathbb{R}$, any distribution $\nu \in \Delta(\mathcal{S})$, and $p \geq 1$, define $||g||_{p,\nu} := (\mathbb{E}_{s \sim \nu}[|g(s)|^p])^{1/p}$, and let $||g||_{\nu}$ be a shorthand for $||g||_{2,\nu}$. Such norms are similarly defined for functions over $\mathcal{S} \times \mathcal{A}$.
- 6. Let η_h^{π} be the distribution of s_h under π , that is, $\eta_h^{\pi}(s) := \Pr[s_h = s \mid s_1 \sim \rho_0, \pi]$.
- 7. μ is exploratory: for a distribution $\nu \in \Delta(S)$ generated by any (non-stationary) policy at any time step (that is, any distribution ν of the form η_h^{π} where π may be non-stationary),

$$\forall s \in \mathcal{S}, \ \frac{\nu(s)}{\mu(s)} \le C.$$

¹In previous notes we have used μ for the initial distribution; for this note we will reserve μ for the data distribution.

As a consequence, $\|\cdot\|_{\nu} \leq \sqrt{C} \|\cdot\|_{\mu}$. Similarly, when we couple μ with a uniform distribution over \mathcal{A} , we have similar results for state-action distributions: $\|\cdot\|_{\nu\times\pi} \leq \sqrt{|\mathcal{A}|C} \|\cdot\|_{\mu\times U}$. See slides for example scenarios where C is naturally bounded.

- 8. Algorithm (simplified for analysis): let $f_0 \equiv \mathbf{0}$ (assuming $\mathbf{0} \in \mathcal{F}$), and for $k \geq 1$, $f_k := \widehat{\mathcal{T}}_{\mathcal{F}} f_{k-1}$.
- 9. Uniform deviation bound (can be obtained by concentration inequalities and union bound):

$$\forall f, f' \in \mathcal{F}, |\mathcal{L}_D(f; f') - \mathcal{L}_{\mu \times U}(f; f')| \leq \epsilon.$$

(Note: at the end we will show how to obtain fast rates.)

Goal Let $\hat{\pi} := \pi_{f_k}$. Derive an upper bound on $v^* - v^{\hat{\pi}}$.

Analysis

$$v^{*} - v^{\hat{\pi}} = \sum_{h=1}^{\infty} \gamma^{h-1} \mathbb{E}_{s \sim \eta_{h}^{\hat{\pi}}} [V^{*}(s) - Q^{*}(s, \hat{\pi})]$$

$$\leq \sum_{h=1}^{\infty} \gamma^{h-1} \mathbb{E}_{s \sim \eta_{h}^{\hat{\pi}}} [Q^{*}(s, \pi^{*}) - f_{k}(s, \pi^{*}) + f_{k}(s, \hat{\pi}) - Q^{*}(s, \hat{\pi})]$$

$$\leq \sum_{h=1}^{\infty} \gamma^{h-1} \left(\|Q^{*} - f_{k}\|_{1, \eta_{h}^{\hat{\pi}} \times \pi^{*}} + \|Q^{*} - f_{k}\|_{1, \eta_{h}^{\hat{\pi}} \times \hat{\pi}} \right)$$

$$\leq \sum_{h=1}^{\infty} \gamma^{h-1} \left(\|Q^{*} - f_{k}\|_{\eta_{h}^{\hat{\pi}} \times \pi^{*}} + \|Q^{*} - f_{k}\|_{\eta_{h}^{\hat{\pi}} \times \hat{\pi}} \right). \tag{1}$$

The last line contains two terms, both in the form of $\|Q^* - f_k\|_{\nu \times \pi}$. So it remains to bound $\|Q^* - f_k\|_{\nu \times \pi}$ for any $\nu \times \pi \in \Delta(\mathcal{S} \times \mathcal{A})$ that combines any $\nu \in \Delta(\mathcal{S})$ that satisfies bullet 4 with any $\pi : \mathcal{S} \to \mathcal{A}$. First a helper lemma:

Lemma 1. Define $\pi_{f,f_k}(s) := \arg \max_{a \in A} \max\{f(s,a), f_k(s,a)\}$. Then we have $\forall \nu \in \Delta(\mathcal{S})$,

$$||V_f - V_{f_k}||_{\nu} \le ||f - f_k||_{\nu \times \pi_{f, f_k}}.$$

Proof.

$$||V_f - V_{f_k}||_{\nu}^2 = \sum_{s \in \mathcal{S}} \nu(s) (\max_{a \in \mathcal{A}} f(s, a) - \max_{a' \in \mathcal{A}} f_k(s, a'))^2$$

$$\leq \sum_{s \in \mathcal{S}} \nu(s) (f(s, \pi_{f, f_k}) - f_k(s, \pi_{f, f_k}))^2 = ||f - f_k||_{\nu \times \pi_{f, f_k}}^2.$$

Now we can bound $\|Q^* - f_k\|_{\nu \times \pi}$ using Lemma 1. Define $P(\nu \times \pi)$ as a distribution over \mathcal{S} generated as $s' \sim P(\nu \times \pi) \Leftrightarrow (s,a) \sim \nu \times \pi, s' \sim P(s,a)$, and

$$\begin{split} \|f_{k} - Q^{\star}\|_{\nu \times \pi} &= \|f_{k} - \mathcal{T} f_{k-1} + \mathcal{T} f_{k-1} - Q^{\star}\|_{\nu \times \pi} \\ &\leq \|f_{k} - \mathcal{T} f_{k-1}\|_{\nu \times \pi} + \|\mathcal{T} f_{k-1} - \mathcal{T} Q^{\star}\|_{\nu \times \pi} \\ &\leq \sqrt{|\mathcal{A}|C} \|f_{k} - \mathcal{T} f_{k-1}\|_{\mu \times U} + \gamma \|V_{f_{k-1}} - V^{\star}\|_{P(\nu \times \pi)} \\ &\leq \sqrt{|\mathcal{A}|C} \|f_{k} - \mathcal{T} f_{k-1}\|_{\mu \times U} + \gamma \|f_{k-1} - Q^{\star}\|_{P(\nu \times \pi) \times \pi_{f_{k-1}, Q^{\star}}}. \end{split} \tag{\star}$$

Step (*) holds because:

$$\begin{split} \|\mathcal{T}f_{k-1} - \mathcal{T}Q^{\star}\|_{\nu \times \pi}^{2} &= \mathbb{E}_{(s,a) \sim \nu \times \pi} \left[((\mathcal{T}f_{k-1})(s,a) - (\mathcal{T}Q^{\star})(s,a))^{2} \right] \\ &= \mathbb{E}_{(s,a) \sim \nu \times \pi} \left[\left(\gamma \mathbb{E}_{s' \sim P(s,a)} [V_{f_{k-1}}(s') - V^{\star}(s')] \right)^{2} \right] \\ &\leq \gamma^{2} \, \mathbb{E}_{(s,a) \sim \nu \times \pi, s' \sim P(s,a)} \left[\left(V_{f_{k-1}}(s') - V^{\star}(s') \right)^{2} \right] \\ &= \gamma^{2} \, \mathbb{E}_{s' \sim P(\nu \times \pi)} \left[\left(V_{f_{k-1}}(s') - V^{\star}(s') \right)^{2} \right] = \gamma^{2} \, \|V_{f_{k-1}} - V^{\star}\|_{P(\nu \times \pi)}^{2}. \end{split}$$
 (Jensen)

Note that we can apply the same analysis on $P(\nu \times \pi) \times \pi_{f_{k-1},Q^*}$ and expand the inequality k times. It then suffices to upper bound $\|f_k - \mathcal{T}f_{k-1}\|_{\mu \times U}$.

$$\begin{split} \|f_k - \mathcal{T} f_{k-1}\|_{\mu \times U}^2 &= \mathcal{L}_{\mu \times U}(f_k; f_{k-1}) - \mathcal{L}_{\mu \times U}(\mathcal{T} f_{k-1}; f_{k-1}) \quad (\mathcal{L} \text{ squared loss} + \mathcal{T} f_{k-1} \text{ Bayes optimal}) \\ &\leq \mathcal{L}_D(f_k; f_{k-1}) - \mathcal{L}_D(\mathcal{T} f_{k-1}; f_{k-1}) + 2\epsilon \qquad \qquad (\mathcal{T} f_{k-1} \in \mathcal{F}) \\ &\leq 2\epsilon. \qquad \qquad (f_k \text{ minimizes } \mathcal{L}_D(\cdot; f_{k-1})) \end{split}$$

Note that the RHS does not depend on k, so we conclude that

$$||f_k - Q^*||_{\nu \times \pi} \le \frac{1 - \gamma^k}{1 - \gamma} \sqrt{2|\mathcal{A}|C\epsilon} + \gamma^k \frac{R_{\text{max}}}{1 - \gamma}.$$

Apply this to Equation (1) and we get

$$v^{\star} - v^{\pi_{f_k}} \le \frac{2}{1 - \gamma} \left(\frac{1 - \gamma^k}{1 - \gamma} \sqrt{2|\mathcal{A}|C\epsilon} + \gamma^k \frac{R_{\max}}{1 - \gamma} \right).$$

Extension: fast rate The previous bound should have $O(n^{-1/4})$ dependence on sample size n := |D|, because ϵ in bullet 6 should be $O(n^{-1/2})$ using Hoeffding's, and the final bound depends on $\sqrt{\epsilon}$. Here we exploit realizability to achieve fast rate so that the final bound is $O(n^{-1/2})$.

Define

$$Y(f;f') := (f(s,a) - r - \gamma V_{f'}(s'))^2 - ((\mathcal{T}f')(s,a) - r - \gamma V_{f'}(s'))^2.$$

Plug each $(s, a, r, s') \in D$ into Y(f; f') and we get i.i.d. variables $Y_1(f; f'), Y_2(f; f'), \dots, Y_n(f; f')$ where n = |D|. It is easy to see that

$$\frac{1}{n}\sum_{i=1}^{n}Y_{i}(f;f') = \mathcal{L}_{D}(f;f') - \mathcal{L}_{D}(\mathcal{T}f';f'),$$

so we only shift our objective \mathcal{L}_D by a f-independent constant. Our goal is to show that

$$\|\widehat{\mathcal{T}}_{\mathcal{F}}f' - \mathcal{T}f'\|_{\mu \times U}^2 \equiv \mathbb{E}[Y(\widehat{\mathcal{T}}_{\mathcal{F}}f'; f')] = O(1/n).$$

Note that this result can be directly plugged into the previous analysis by letting $f' = f_{k-1}$ (hence $\widehat{\mathcal{T}}_{\mathcal{F}} f' = f_k$), and we immediately obtain a final bound of $O(n^{-1/2})$.

To prove the result, first notice that $\forall f \in \mathcal{F}$,

$$\mathbb{E}[Y(f;f')] = \mathcal{L}_{\mu \times U}(f;f') - \mathcal{L}_{\mu \times U}(\mathcal{T}f';f') = \|f - \mathcal{T}f'\|_{\mu \times U}^2,$$

thanks to realizability and squared loss. Next we bound variance of *Y*:

$$V[Y(f; f')] \leq \mathbb{E}[Y(f; f')^{2}]$$

$$= \mathbb{E}\left[\left(\left(f(s, a) - r - \gamma V_{f'}(s')\right)^{2} - \left((\mathcal{T}f')(s, a) - r - \gamma V_{f'}(s')\right)^{2}\right)^{2}\right]$$

$$= \mathbb{E}\left[\left(f(s, a) - (\mathcal{T}f')(s, a)\right)^{2}\left(f(s, a) + (\mathcal{T}f')(s, a) - 2r - 2\gamma V_{f'}(s')\right)^{2}\right]$$

$$\leq 4V_{\max}^{2} \mathbb{E}\left[\left(f(s, a) - (\mathcal{T}f')(s, a)\right)^{2}\right]$$

$$= 4V_{\max}^{2} \|f - \mathcal{T}f'\|_{\mu \times U}^{2} = 4V_{\max}^{2} \mathbb{E}[Y(f; f')],$$

where $V_{\rm max} = R_{\rm max}/(1-\gamma)$ is a constant.

Next we apply (one-sided) Bernstein's inequality (see [4]) and union bound over all $f \in \mathcal{F}$. Let $N = |\mathcal{F}|$. For any fixed f', with probability at least $1 - \delta$, $\forall f \in \mathcal{F}$,

$$\mathbb{E}[Y(f;f')] - \frac{1}{n} \sum_{i=1}^{n} Y_i(f;f') \le \sqrt{\frac{2\mathbb{V}[Y(f;f')] \log \frac{N}{\delta}}{n}} + \frac{4V_{\max}^2 \log \frac{N}{\delta}}{3n} \qquad (Y_i \in [-V_{\max}^2, V_{\max}^2])$$

$$= \sqrt{\frac{8V_{\max}^2 \mathbb{E}[Y(f;f')] \log \frac{N}{\delta}}{n}} + \frac{4V_{\max}^2 \log \frac{N}{\delta}}{3n}.$$

Since $\widehat{\mathcal{T}}_{\mathcal{F}}f'$ minimizes $\mathcal{L}_D(\cdot;f')$, it also minimizes $\frac{1}{n}\sum_{i=1}^n Y_i(\cdot;f')$ because the two objectives only differ by a constant $\mathcal{L}_D(\mathcal{T}f';f')$. Hence,

$$\frac{1}{n}\sum_{i=1}^{n}Y_{i}(\widehat{\mathcal{T}}_{\mathcal{F}}f';f') \leq \frac{1}{n}\sum_{i=1}^{n}Y_{i}(\mathcal{T}f';f') = 0.$$

Then,

$$\mathbb{E}[Y(\widehat{\mathcal{T}}_{\mathcal{F}}f';f')] \leq \sqrt{\frac{8V_{\max}^2\mathbb{E}[Y(\widehat{\mathcal{T}}_{\mathcal{F}}f';f')]\log\frac{N}{\delta}}{n}} + \frac{4V_{\max}^2\log\frac{N}{\delta}}{3n}.$$

Solving for the quadratic formula,

$$\mathbb{E}[Y(\widehat{\mathcal{T}}_{\mathcal{F}}f';f')] \leq \left(\sqrt{2} + \sqrt{\tfrac{10}{3}}\right)^2 \frac{V_{\max}^2 \log \frac{N}{\delta}}{n}.$$

References

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