Finite-Time Bounds for Sampling-Based Fitted Dynamic Programming

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1. Problem formulation

We collected data: $\{(X_n, A_n, R_n, Y_y)_{n \le N}\}$

- Assume a generative model: $Y_n \sim p(\cdot|X_n, A_n)$
- Passively observe trajectories under behavior policy: $A_n \sim \pi_b(\cdot|X_n)$

Properties:

- Setting: Off policy batch learning with general function approximation \mathcal{F} (state space is big or continuous)
- What is known: on-policy with linear function approximation works: TD (Tsitsiklis and Van Roy, 1997), LSTD (Bradtke and Barto, 1996), off-policy batch learning with "averagers" (Gordon, 1995) is stable.
- Method: fitted value iteration or policy iteration: Very popular! Ex: LSPI (Lagoudakis and Parr, 2003), Fitted Q iterations (Ernst et al., 2005) for recent algorithms.
- **Problem:** may diverge! (famous counter-examples (Baird, 1995; Tsitsiklis and Van Roy, 1996))
- Goal: Design a policy π with near-optimal performance with high probability, ie. with proba $1 - \delta$, provide a bound on $||V^* - V^{\pi}||$ in terms of the number of samples N, the capacity of the function space \mathcal{F} , δ , ...

Approximate Value Iteration

$$V_{k+1} = \mathcal{P}TV_k,$$

where \mathcal{P} = approximation operator (eg. projection, regression, supervised learning), T = Bellman operator (i.e. $Tf(x) = \max_a [r(x, a) = \gamma \int f(y) P(dy|x, a)])$.

• **Propagation of error:** define π_k = greedy policy wrt V_k . Write $\varepsilon_k = TV_k - \mathcal{P}TV_k$ the approximation error. Then (Bertsekas and Tsitsiklis, 1996):

$$\lim \sup_{k \to \infty} ||V^* - V^{\pi_k}||_{\infty} \le \frac{2\gamma}{(1-\gamma)^2} \lim \sup_{k \to \infty} ||\varepsilon_k||_{\infty}$$
(1)

• Each step = projection:

$$V_{k+1} = \arg\min_{f \in \mathcal{F}} ||TV_k - f||$$

Statistical learning results for regression: Let g a function, μ a distribution, such that some data $(x_n, y_n)_{n \leq N}$ are collected, with $x_n \sim \mu$, and y_n is a noisy estimate of $g(x_n)$. Then the solution to the empirical least squares regression problem:

$$\arg\min_{f\in\mathcal{F}}\sum_{n}|f(x_{n})-y_{n}|^{2}$$

is close to the projection of g onto \mathcal{F} , i.e. the solution to

$$\arg\min_{f\in\mathcal{F}}||f-g||_{2,\mu},$$

when N is large. Statistical learning theory uses capacity measures (VC dimension, metric entropy) of \mathcal{F} to bound the difference between the empirical loss (learning error) and the functional loss (generalization error). The minimized error is defined in terms of L_p -norms (or variants) (eg. Neural Networks, linear regession, SVM, kernel methods, ...) but not with L_{∞} norm (except for "averagers" (Gordon, 1995) for which $||\mathcal{P}||_{\infty} \leq 1$).

• **Problem:** Dynamic Programming uses L_{∞} norms (property: $||T||_{\infty} < 1$) whereas Statistical Learning theory (and Approximation theory) uses L_p norms (property: $||\mathcal{P}||_p \leq 1$). Thus the combined operator $\mathcal{P}T$ is neither a contraction in L_{∞} nor in L_p .

Tools:

- Statistical Learning: provide bound on each sampling-based Bellman iterate
- L_p -norm analysis in DP: for the propagation of error

2. L_p analysis of AVI

We have:

Under A1,
$$\lim_{k \to \infty} \sup_{k \to \infty} ||V^* - V^{\pi_k}||_{\infty} \leq \frac{2\gamma}{(1-\gamma)^2} C(\mu)^{1/p} \lim_{k \to \infty} \sup_{k \to \infty} ||\varepsilon_k||_{p,\mu}$$
(2)

Under A2,
$$\lim_{k \to \infty} \sup_{k \to \infty} ||V^* - V^{\pi_k}||_{p,\rho} \leq \frac{2\gamma}{(1-\gamma)^2} C(\rho,\mu)^{1/p} \lim_{k \to \infty} \sup_{k \to \infty} ||\varepsilon_k||_{p,\mu}$$
(3)

where assumption A1 [concentration of the transition kernel] says that there exists $C(\mu) < \infty$ such that, for all x, a,

$$P(dy|x,a) \le C(\mu)\mu(dy)$$

(Example: if μ is the uniform measure then this assumption says that the transition probability kernel $P(\cdot|x, a)$ admits a uniformly bounded density).

And assumption A2 [concentration of the discounted future-state distributions] assumes that there exists $C(\rho, \mu) < \infty$, for all x, a,

$$(1-\gamma)^2 \sum_{t\geq 1} t\gamma^{t-1} \mathbb{P}\big(X_t \in dy | X_0 \sim \rho, A_0, A_1, \cdots \big) \leq C(\rho, \mu) \mu(dy).$$

Property: Dynamics which fail to satisfy these assumptions would probably preclude any sample-based estimation of the performance.

Where do these L_p bounds come from? Assume that for two positive vectors u and v are such that $u \leq Pv$, with P a stochastic matrix. Of course we deduce that $||u||_{\infty} \leq ||v||_{\infty}$, but moreover if ρ and μ are probability distributions such that componentwise $\rho P \leq C\mu$, with $C \geq 1$ a constant, then we deduce that

$$||u||_{p,\rho} \le C^{1/p} ||v||_{p,\mu}.$$

Indeed we have

$$\begin{aligned} ||u||_{p,\rho}^p &= \int_{x \in X} \rho(dx) |u(x)|^p &\leq \int_{x \in X} \rho(dx) \left[\int_{y \in X} P(dy|x) v(y) \right]^p \\ &\leq \int_{x \in X} \rho(dx) \int_{y \in X} P(dy|x) v(y)^p \\ &\leq C \int_{y \in X} \mu(dy) v(y)^p = C ||v||_{p,\mu}^p, \end{aligned}$$

using Jensen's inequality.

Well, in AVI, this is the case. We may prove that we have the following componentwise bound:

$$\limsup_{k \to \infty} V^* - V^{\pi_k} \le \limsup_{k \to \infty} (I - \gamma P^{\pi_k})^{-1}$$

$$\Big(\sum_{l=0}^{k-1} \gamma^{k-l} \Big[(P^{\pi^*})^{k-l} + P^{\pi_k} P^{\pi_{k-1}} \dots P^{\pi_{l+2}} P^{\pi_{l+1}} \Big] |\varepsilon_l| \Big),$$
(4)

which implies both the L_{∞} bound (1) and the L_p bounds (2) and (3).

Extension to other approximate DP methods: The L_{∞} bounds for Approximate policy iteration:

$$\lim \sup_{k \to \infty} ||V^* - V^{\pi_k}||_{\infty} \le \frac{2\gamma}{(1-\gamma)^2} \lim \sup_{k \to \infty} ||V_k - V^{\pi_k}||_{\infty}$$

and the **Bellman residual** bound:

$$||V^* - V^{\pi}||_{\infty} \le \frac{2}{1 - \gamma} ||TV - V||_{\infty}$$

have their counterpart L_p bounds too!

3. Finite sample bound on each AVI iteration

Two sources of error:

- The Bellman operator T (which makes use of an expectation over next states) needs to be estimated from samples (sampling-based Bellman operator: T)
- The projection (approximation) operators uses samples (sampling-based projection: $\hat{\mathcal{P}}$).

A single update: Draw N points $(X_i \sim \mu)_{i < N}$, and then from each of those points, for all possible actions, draw M samples of observed rewards $(R_i^{i,a})_{j\leq M}$ and next states $(Y_j^{i,a} \sim P(\cdot|X_i, a))_{j \leq M}$ using generative model. Then define the sampling based Bellman backed up values:

$$\hat{V}(X_i) = \max_a \frac{1}{M} \left[\sum_j [R_j^{i,a} + \gamma V(Y_j^{i,a})] \right]$$

and the sampling-based projection onto \mathcal{F} :

$$\hat{\mathcal{P}}\hat{T}V = \arg\min_{f\in\mathcal{F}}\sum_{i}|f(X_{i}) - \hat{T}V(X_{i})|^{p}.$$
(5)

Sample bound: We have (neglecting log N terms) with probability $1 - \delta$,

$$||\hat{\mathcal{P}}\hat{T}V - TV||_{p,\mu} \le d(TV,\mathcal{F}) + O\left\{\left(\frac{V_{\mathcal{F}}\log\delta^{-1}}{N}\right)^{1/2p} + \left(\frac{\log\delta^{-1}}{M}\right)^{1/2}\right\}$$

where $d(TV, \mathcal{F}) = \inf_{f \in \mathcal{F}} ||TV - f||_{p,\mu}$ and $V_{\mathcal{F}}$ is a capacity measure of \mathcal{F} (pseudo-dimension).

4. AVI: Putting things together

Sampling-based fitted VI: repeat K times the previous update (5): $V_{k+1} = \hat{\mathcal{P}}\hat{T}V_k$ (where either using the same set of samples throughout all iterations or regenerate a fresh set at each iteration). Then, with probability $1 - \delta$, we have:

$$||V^* - V^{\pi_K}||_{\infty} \le \frac{2\gamma}{(1-\gamma)^2} C(\rho,\mu)^{1/p} \Big[d(T\mathcal{F},\mathcal{F}) + O\Big\{ \Big(\frac{V_{\mathcal{F}}\log\delta^{-1}}{N}\Big)^{1/2p} + \Big(\frac{\log\delta^{-1}}{M}\Big)^{1/2} \Big\} \Big] + O(\gamma^K)$$

where $d(T\mathcal{F},\mathcal{F}) = \sup_{q\in\mathcal{F}} \inf_{f\in\mathcal{F}} ||Tg - f||_{p,\mu}$ is the inherent Bellman residual of \mathcal{F} .

Analysis of this result:

- This explains the counter examples of (Baird, 1995; Tsitsiklis and Van Roy, 1996) for which $d(T\mathcal{F}, \mathcal{F}) = \infty$
- Question: if the space \mathcal{F} grows, does $d(T\mathcal{F}, \mathcal{F})$ decrease?
- Answer: Yes! if the MDP is smooth (ie. P(dy|, a) and $r(\cdot, a)$ are Lipschitz)
- Thus fitted policy iteration is a sound method!
- Bias-variance tradeoff: when \mathcal{F} grows, the approximation error $d(T\mathcal{F},\mathcal{F})$ decreases (bias term) but the estimation error $O((V_{\mathcal{F}}/N)^{1/2p})$ (variance term) increases, but may be made smaller by using more samples (to avoid overfitting).

Numerical experiment: This is an optimal replacement problem (see e.g. (Rust, 1996)). We consider approximation of the value function using polynomials of degree l.



Figure 1: Approximation errors $||V^* - V_K||_{\infty}$ of the function V_K returned by samplingbased FVI after K = 20 iterations, for different values of the polynomials degree l, for N = 100, M = 10 (plain curve), N = 100, M = 100 (dot curve), and N = 1000, M = 10 (dash curve) samples. The plotted values are the average over 100 independent runs.

5. What about if we must follow a fixed policy?

We observe a plant under control (behavior policy π_b) and from those collected data $(X_t, A_t \sim \pi_b(\cdot|X_n), R_t, X_{t+1} \sim P(\cdot|X_t, A_t), \dots)$, can we design a near-optimal policy?

What are the additional assumptions?

- Exploration: The behavior policy $\pi_b > 0$ and the MDP following π_b is stationary: $X_t \sim \mu$,
- Since the samples are correlated, we need a forgetting property of the process. We assume the Markov chain (X_t) is β -mixing with exponential rate: $\sup_{t\geq 1} |\mathbb{P}(X_{t+m} \in B|X_1, \cdots, X_t) \mathbb{P}(X_{t+m} \in B)]| \leq O(e^{-bm^{\kappa}})$ (i.e. future depends weakly on the past)

Let us use fitted policy iteration (fitted Q iteration should work also...)

5.1 Policy evaluation by Bellman residual minimization

Here we use Q-functions instead of value functions.

Repeat K policy iteration steps, where at each iteration k, we find a approximation $Q_k \in \mathcal{F}$ of V^{π_k} that minimizes the norm of the Bellman residual:

$$\arg\min_{Q\in\mathcal{F}}||Q-T^{\pi_k}Q||_{2,\mu}.$$
(6)

However we need to be careful when writting a sampling-based version of that problem. Indeed, the solution to

$$\arg\min_{Q\in\mathcal{F}}\sum_{t} |Q(X_t, A_t) - [R_t + \gamma Q(X_{t+1}, \pi_k(X_{t+1}))]|^2$$
(7)

is not consistent with the solution to (6) (see eg. (Sutton and Barto, 1987), (Munos, 2003), (Lagoudakis and Parr, 2003)): the sampling-based estimate is biased.

Indeed, defining the function $h(x, a, y) = r(x, a) + \gamma Q(y, \pi_k(y))$, the problem (6) minimizes $\mathbb{E}_{(X,A)\sim\mu}[(Q(X,A) - (\mathbb{E}_{Y\sim P(\cdot|X,A)}[h(X,A,Y)])^2]$ whereas (7) is a sampled-based minimization of $\mathbb{E}_{(X,A)\sim\mu,Y\sim P(\cdot|X,A)}[(Q(X,A) - h(X,A,Y))^2]$. The difference between these quantities is the variance of h(x, a, Y), ie:

$$\mathbb{E}[(Q(x,a) - h(x,a,Y))^2] - [Q(x,a) - (\mathbb{E}[h(x,a,Y)])^2] = \operatorname{Var}[h(x,a,Y)].$$

Thus we defined the modified Bellman residual empirical minimization problem:

$$\arg\min_{Q\in\mathcal{F}} \left\{ \sum_{t} |Q(X_{t}, A_{t}) - [R_{t} + \gamma Q(X_{t+1}, \pi_{k}(X_{t+1}))]|^{2} - \arg\min_{g\in\mathcal{F}} \sum_{t} |g(X_{t}, A_{t}) - [R_{t} + \gamma Q(X_{t+1}, \pi_{k}(X_{t+1}))]|^{2} \right\}$$

which is a unbiased estimate and yields a solution consistent to the solution of (6)

Linear approximation space In case \mathcal{F} is linear, then the modified Bellman residual problem is nothing else than LSPI (Lagoudakis and Parr, 2003) which provides a finite-time performance bound for this algorithm.

Result: High probability bound on the performance loss in terms of the number of samples N and of iterations K: Under A1, with probability $1 - \delta$, we have (neglecting log N terms):

$$||V^* - V^{\pi_K}||_{\infty} \le \frac{2\gamma}{(1-\gamma)^3} \sqrt{C(\mu)} \Big[d(\mathcal{F}, T\mathcal{F}) + O\Big(\Big(\frac{[V_{\mathcal{F}} + \log(1/\delta)]^{1+1/\kappa}}{N}\Big)^{1/4}\Big) \Big] + O(\gamma^K),$$
(8)

where: $d(\mathcal{F}, T\mathcal{F}) = \sup_{g \in \mathcal{F}} \sup_{\pi} \inf_{f \in \mathcal{F}} ||T^{\pi}g - f||_{\mu}$ is the inherent Bellman error of \mathcal{F} , and $V_{\mathcal{F}}$ is a capacity measure of \mathcal{F} which depends on the pseudo-dimension and the VC-crossing dimension of \mathcal{F} (i.e. VC-dimension of $\{\{x \in X, f(x) \geq g(x)\}, f, g \in \mathcal{F}\}$).

5.2 Policy evaluation by FVI:

Repeat K times:

• Fitted policy evaluation step: find an approximation of Q^{π_k} by repeating M steps of fitted value iteration:

- Define
$$I_k \stackrel{\text{def}}{=} \{t \in [1, N], A_t = \pi_k(X_t)\}$$
.

- Define $(Q_k^m)_{0 \le m \le M}$ by: for $0 \le m < M$,

$$\begin{cases} v_t^m \stackrel{\text{def}}{=} R_t + \gamma Q_k^m(X_{t+1}, \pi_k(X_{t+1})), \text{ for all } t \in I_k \\ Q_k^{m+1} \stackrel{\text{def}}{=} \arg\min_{f \in \mathcal{F}} \sum_{t \in I_k} [f(X_t, A_t) - v_t^m]^2 \end{cases}$$

• Policy improvement step: define the new policy π_{k+1} by:

$$\pi_{k+1}(x) \stackrel{\text{def}}{=} \arg\max_{a} Q_k^M(x,a)$$

Return policy π_K .

Results: Similar to (8) with $O(\gamma^{\min(K,M)})$ instead of $O(\gamma^K)$.

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