



Towards Function Approximation Methods

Easwar Subramanian

TCS Innovation Labs, Hyderabad

Email: cs5500.2020@iith.ac.in

September 16, 2023

Overview



• Function Approximation Methods

2 Convergence of Approximation Methods



Function Approximation Methods



On the need for Function Approximators



- ▶ To solve large scale RL problems
 - ★ Game of Backgammon: 10^{20} states
 - \star Game of Go: 10^{170} states
 - \bigstar Even Atari games have large state space



 $|\mathcal{S}|$ is very large : Curse of Dimensionality



Value Function Approximators

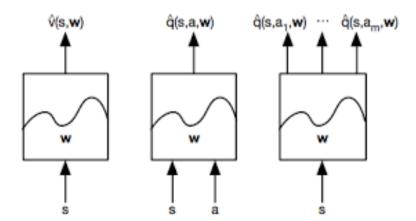


- ▶ Value function have been basically lookup tables.
- ▶ Solution for large MDP's is to use function approximators
 - ★ Generalize from seen to unseen states
- ► Function approximators could be
 - ★ Linear function approximator
 - ★ Neural networks
 - ★ Decision tree
 - **★** ···



Neural Network Approximators





Policy Evaluation Using Neural Networks



The value of a policy π is given by

$$V^{\pi}(s) = \mathbb{E}_{\pi} \left(\sum_{k=0}^{\infty} \gamma^k r_{t+k+1} | s_t = s \right)$$
$$= \mathbb{E}_{\pi} \left[r_{t+1} + \gamma V^{\pi}(s_{t+1}) | s_t = s \right]$$

Question: How do we compute the above expectations using neural networks?



 \triangleright Roll-out m trajectories from state s and observe rewards



Value Function Fitting using Monte Carlo



► Consider a MDP with a finite horizon H

$$V^{\pi}(s) \approx \frac{1}{m} \left[\sum_{j=1}^{m} \left[\sum_{k=0}^{H} \left(\gamma^{k} r_{t+k+1}^{i} | s_{t} = s \right) \right] \right]$$

- \triangleright Need to reset the simulator back to state s (Not always possible)
- ▶ Alternative : Roll-out single sample estimate (high variance, but OK)
- ▶ Collect training data for as many states as possible and regress thereafter

$$\left(s_{i}, \underbrace{\left[\sum_{k=t}^{H} \left(\gamma^{k} r_{t+k+1} | s_{t} = s\right)\right]}_{=y_{i}}\right)$$



MC Based Algorithm



Algorithm Monte Carlo Based Value Function Fitting

Initialize number of iterations N

for i = 1 to N do

Perform a roll-out from an initial state s_i (could be any state from S)

Calculate targets y_i using Monte-Carlo roll outs

$$y_i = \left[\sum_{k=0}^{H} \left(\gamma^k r_{t+k+1}^i | s_t = s_i \right) \right]$$

Form input-output pairs (s_i, y_i) (N datapoints in total)

end for

Perform supervised regression with loss function

$$L(\phi) = \frac{1}{2} \sum_{i=1}^{N} \left[V_{\phi}^{\pi}(s_i) - y_i \right]^2$$



Policy Evaluation : MC Based Algorithm



 $\blacktriangleright\,$ Needs complete sequences, suitable only for episodic tasks



Fitted V Iteration



We observe transition (s, a, r, s') at time t; Using one step look-ahead,

$$V^{\pi}(s) = \mathbb{E}_{\pi} \left[r + \gamma V^{\pi}(s') | s_t = s \right]$$

$$\approx r + \gamma V^{\pi}(s') \text{ (Bootstrap } V^{\pi})$$

Using function approximators, we get,

$$V_{\phi}^{\pi}(s) \approx r + \gamma V_{\phi}^{\pi}(s')$$

- ▶ Directly use the previous fitted value function V_{ϕ}^{π}
- ► Collect training data,

$$\left(s_i, \underbrace{r + V_{\phi}^{\pi}(s_i')}_{=y_i}\right)$$

Perform supervised regression

$$L(\phi) = \frac{1}{2} \sum_{i=1}^{N} \left[V_{\phi}^{\pi}(s_i) - y_i \right]^2$$

Fitted V Iteration: Algorithm



Algorithm Fitted V Iteration

- 1: Initialize number of iterations N
- 2: **for** j = 1 to N **do**
- 3: Sample K transitions (s, a, r, s') using policy π
- 4: **for** i = 1 to K **do**
- 5: Calculate targets y_i using one step TD approximation

$$y_i = \left[r + V_{\phi_j}^{\pi}(s_i')\right]$$

- 6: Form input-output pairs (s_i, y_i) (K datapoints in total)
- 7: end for
- 8: Perform supervised regression (Optimizer : RProp) using loss function

$$L(\phi_j) = \frac{1}{2} \sum_{i=1}^{K} \left[V_{\phi_j}^{\pi}(s_i) - y_i \right]^2$$

and get a new function approximator with new weights ϕ_{j+1}

Optimal Value Function : Control



Bellman optimality equation for V_* is given by,

$$V_*(s) \leftarrow \max_{a} \left[\sum_{s' \in \mathcal{S}} \mathcal{P}_{ss'}^a \left(\mathcal{R}_{ss'}^a + \gamma V_*(s') \right) \right] \approx \max_{a} E \left[r_{t+1} + \gamma V_*(s_{t+1}) | s_t = s \right) \right]$$

Question: How do we get a sample estimate for transition (s, a, r, s') for V_* ?

$$V(s) \approx \max_{a} [r + \gamma V(s')]$$



- \blacktriangleright To compute max over a, we need to know the outcome of all actions starting from s. Mostly not possible and costly as well.
- \blacktriangleright For model free control, we use approximators for Q and not V

Fitted Q Iteration



Bellman optimality equation for Q_*

$$Q_*(s, a) = \left| \sum_{s' \in S} \mathcal{P}_{ss'}^a \left(\mathcal{R}_{ss'}^a + \gamma \max_{a'} Q_*(s', a') \right) \right| \approx \mathbb{E} \left[r_{t+1} + \gamma \max_{a'} Q_*(s_{t+1}, a') | s_t = s, a_t = a \right]$$

- ▶ Max is inside the expectation; that's ok
- ▶ For transitions (s, a, r, s') we can compute $r + \gamma \max_{a'} Q(s', a')$
- ▶ Does not require simulating over actions
- \blacktriangleright Use the previous fitted optimal Q function Q_{ϕ}^* like in fitted V iteration
- ► Collect training data,

$$\left(s_{i}, \underbrace{r + \gamma \max_{a'} Q_{\phi}(s'_{i}, a'_{i})}_{=y_{i}}\right)$$

▶ Perform supervised regression

$$L(\phi) = \frac{1}{2} \sum_{i=1}^{N} \left[Q_{\phi}(s_i, a_i) - y_i \right]^2$$



Fitted Q Iteration : Algorithm



Algorithm Fitted Q Iteration

- 1: Initialize number of iterations N
- 2: for j = 1 to N do
- 3: Sample K transitions (s, a, r, s') using any behaviour policy μ
- 4: **for** i = 1 to K **do**
- 5: Calculate targets y_i using one step TD approximation

$$y_i = \left[r + \gamma \max_{a'} Q_{\phi_j}(s'_i, a')\right]$$

- 6: Form input-output pairs (s_i, y_i) (K Datapoints in total)
- 7: end for
- 8: Perform supervised regression (Optimizer: RProp) using loss function

$$L(\phi_j) = \frac{1}{2} \sum_{i=1}^{K} \left[Q_{\phi_j}(s_i, a_i) - y_i \right]^2$$

and get a new function approximator with new weights ϕ_{j+1}

9: end for



Convergence of Approximation Methods



On the Convergence of Fitted Iterations



Question: What can we say about the convergence of fitted iteration methods?

- ightharpoonup Does fitted V iteration converge to V^{π} ?
- ▶ Does neural fitted iteration converge to Q_* ?

Convergence in DP setup

▶ Use the fixed point equation below to define a **contraction** operator \mathcal{L} (contraction in L_{∞} norm)

$$Q_*(s, a) \leftarrow \left[\sum_{s' \in \mathcal{S}} \mathcal{P}^a_{ss'} \left(\mathcal{R}^a_{ss'} + \gamma \max_{a'} Q_*(s', a') \right) \right]$$

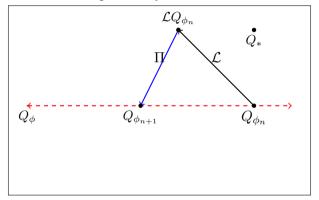
Convergence in TD setup

- ▶ State and action spaces are finite
- ► All state-action pairs are visited infinitely often
- ▶ Robbins-Monroe condition: $\sum_t \alpha_t = \infty$, $\sum_t \alpha_t^2 < \infty$

Projections and Convergence



Space of Q Functions



Convergence Guarantee For Fitted Iteration Methods



▶ Define operator $\mathcal{L}: \mathcal{Q} \to \mathcal{Q}$ such that

$$\mathcal{L}Q = r + \gamma \max_{a'} Q(s', a')$$

- ▶ Backup operator \mathcal{L} is a contraction in L_{∞} norm
- \blacktriangleright Projection operator (Π) are contractions in L_2 norm
- ▶ What about the composition $(\Pi \circ \mathcal{L})Q$?
 - \bigstar Need not be a contraction with respect to any norm

Sad Corollary

No guarantees on convergence to optimal value functions (on the manifold) exist for fitted iteration methods



Convergence of Monte Carlo Based Algorithm



Algorithm Monte Carlo Based Value Function Fitting

- 1: Initialize number of iterations N
- 2: **for** i = 1 to N **do**
- 3: Perform a roll-out from an initial state s_i (could be any state from S)
- 4: Calculate targets y_i using Monte-Carlo roll outs

$$y_i = \left[\sum_{k=0}^{H} \left(\gamma^k r_{t+k+1}^i | s_t = s_i \right) \right]$$

- 5: Form input-output pairs (s_i, y_i) (N datapoints in total)
- 6: end for
- 7: Perform supervised regression with loss function

$$L(\phi) = \frac{1}{2} \sum_{i=1}^{N} \left[V_{\phi}^{\pi}(s_i) - y_i \right]^2$$



Convergence of Monte Carlo Based Algorithm



- ▶ Step 7 is gradient descent and it will converge at least local optimum
- ▶ Important : Convergence guarantee is in the parameter space (ϕ) and not in value function space

Fitted Q Iteration



Algorithm Fitted Q Iteration

- 1: Initialize number of iterations N
- 2: for j=1 to N do
- 3: Sample K transitions (s, a, r, s') using any behaviour policy μ
- 4: **for** i = 1 to K **do**
- 5: Calculate targets y_i using one step TD approximation

$$y_i = \left[r + \gamma \max_{a'} Q_{\phi_j}(s'_i, a')\right]$$

- 6: Form input-output pairs (s_i, y_i) (K Datapoints in total)
- 7: end for
- 8: Perform supervised regression (Optimizer: RProp) using loss function

$$L(\phi_j) = \frac{1}{2} \sum_{i=1}^{K} \left[Q_{\phi_j}(s_i, a_i) - y_i \right]^2$$

and get a new function approximator with new weights ϕ_{j+1}

9: end for

Online Q learning / Incremental Q learning



Question: Can we do the gradient update for every transition (s, a, r, s')?

- ▶ We use the fitted Q iteration and set K=1
- This is also the Watkins Q-learning update (used with function approximators)

Algorithm Online Q Learning

- 1: for n=1 to N do
- Take an action a and obtain the transition (s, a, r, s') using ϵ -greedy policy
- 3: Calculate target y using one step TD approximation

$$y = \left[r + \gamma \max_{a'} Q_{\phi_n}(s', a')\right]$$

- Compute $g^{(n)} = \nabla_{\phi}(Q_{\phi_n}(s, a) y)^2$ Set $\phi_{n+1} = \phi_n \alpha g^{(n)}$
- 6: end for



Convergence Guarantee on Online Q learning



Algorithm Online Q Learning

- 1: for n=1 to N do
- Take an action a and obtain the transition (s, a, r, s') using ϵ -greedy policy
- 3: Calculate target y using one step TD approximation

$$y = \left[r + \gamma \max_{a'} Q_{\phi_n}(s', a')\right]$$

- Compute $g^{(n)} = \nabla_{\phi}(Q_{\phi_n}(s, a) y)$ Set $\phi_{n+1} \leftarrow \underbrace{\phi_n \alpha g^{(n)}}_{}$
- 6: end for
 - Take a closer look at the one step gradient

$$g^{(n)} \leftarrow \phi_n - \alpha \nabla_{\phi}(Q_{\phi}(s, a) - \underbrace{r + \gamma \max_{a'} Q_{\phi}(s', a')}_{\text{moving target}})$$



Summary: Convergence Discussion



- ▶ Projection (Π) of the backup operator (\mathcal{L}) of optimal Q function need not be a contraction in any norm
- lacktriangle Fitted V iteration or fitted Q iteration need not converge because of the moving target problem
- ▶ In online Q learning algorithm,
 - ★ Samples obtained are sequentially correlated
 - ★ Moving target problem
- ▶ Convergence guarantees exist only in tabular case