DS-GA 3001 005 | **Lecture 3**

Reinforcement Learning

Jeremy Curuksu, PhD NYU Center for Data Science jeremy.cur@nyu.edu

February 14, 2024

DS-GA 3001 RL Curriculum

Reinforcement Learning:

- Introduction to Reinforcement Learning
- Multi-armed Bandit
- Dynamic Programming on Markov Decision Process
- ► Model-free Reinforcement Learning
- Value Function Approximation (Deep RL)
- Policy Function Approximation (Actor-Critic)
- Planning from a Model of the Environment
- Examples of Industrial Applications
- Advanced Topics and Development Platforms

Dynamic Programming on Markov Decision Process

Last week:

- ightharpoonup Multi-armed Bandit with action values (ϵ -greedy)
- ► Upper Confidence Bound
- ► Bayesian Bandit

Today:

- Markov Decision Process
- Value Functions and Bellman Equations
- Dynamic Programming

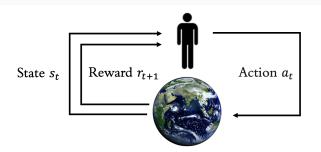
Generalization to Sequential RL

Sequential Goal-Directed Reinforcement Learning

- ► Bandit problems have only one state, but often the agent must learn different actions in different situations (states)
- Actions in turn may influence subsequent states, and through those states may influence future rewards
- To learn to make good decisions, we need assign credit for long term consequences to individual actions

Markov Decision Process

Markov Decision Process (MDP)



At each step, the agent:

- Finds itself in state s_t (from o_t)
- Executes action a_t
- ightharpoonup Receives reward r_{t+1}

The environment:

- ightharpoonup Receives action a_t
- Send reward r_{t+1}
- ► Send observation o_{t+1}

Markov Decision Process (MDP)

An MDP is a mathematical idealization of goal-directed learning from interaction with an environment

Simulating a MDP produces a sequence of n tuples (trajectory)

$$(s_t, a_t, r_{t+1}, s_{t+1})_n = (s_0, a_0, r_1, s_1, a_1, r_2, ..., s_n)$$

▶ The environment dynamics is fully characterized by the joint probability of each possible s_{t+1} and r_{t+1} as a function of the immediately preceding state and action, s_t and a_t

$$p(s', r|s, a) = p(s_{t+1} = s', r_{t+1} = r|s_t = s, a_t = a)$$

Markov property: The state must include all information from past agent-environment interactions that influence the future

$$p(s,r|s_t,a_t) = p(s,r|H_t,a_t)$$

Goals and Rewards

RL applies the reward hypothesis

- The purpose of an RL agent is formalized in term of a signal called *reward* $r_t \in \mathbb{R}$ passing from the environment to the agent
- ► The agent goal is to maximize the amount of reward it receives

Reward:

 r_t

Optimal Policy:

$$\pi_* = \operatorname*{arg\,max}_a \left(\sum r_t \right)$$

Agent goal is to maximize return G_t

G_t is the total accumulated reward from time-step t

Acting in a MDP results in returns G_t that depend on the policy:

$$G_t = r_{t+1} + r_{t+2} + r_{t+3} + \dots + r_T$$

▶ G_t can be discounted by factor $\gamma \in [0,1]$ to account for present value of future rewards (in episodic or continuing tasks)

$$G_t = r_{t+1} + \gamma r_{t+2} + \gamma^2 r_{t+3} + \dots = \sum_{k=0}^{\infty} \gamma^k r_{t+1+k}$$

- $ightharpoonup \gamma < 1 \Rightarrow$ Immediate rewards > delayed rewards
- $ightharpoonup \gamma$ close to $o \Rightarrow$ "Myopic" agent
- $ightharpoonup \gamma$ close to 1 \Rightarrow "Far-sighted" agent

Value Functions and

Bellman Equations

State Value Function $V_{\pi}(s)$

Expected return when starting in s and following π

 Rewards the agent can expect to receive in the future depend on what actions it will take. Accordingly, value functions are defined with respect to particular ways of acting (policies)

$$\forall s \in \mathcal{S}, \qquad v_{\pi}(s) \stackrel{.}{=} \underset{\pi}{\mathbb{E}}(G_t \mid s)$$

$$v_{\pi}(s) = \underset{\pi}{\mathbb{E}}(r_{t+1} + \gamma G_{t+1} \mid s)$$

$$v_{\pi}(s) = \mathbb{E}(r_{t+1} + \gamma v_{\pi}(s_{t+1}) \mid s)$$

$$v_{\pi}(s) = \sum_{a} \pi(a \mid s) \sum_{s', r} p(s', r \mid s, a) [r + \gamma v_{\pi}(s')]$$

 \triangleright $v_{\pi}(s)$ indicates how good it is to be in s when following π

Action Value Function $q_{\pi}(s, a)$

Expected return when selecting a in s and following π

The action value more directly informs on which action to take

$$\forall s \in \mathcal{S}, \qquad q_{\pi}(s, a) \doteq \underset{\pi}{\mathbb{E}}(G_t \mid s, a)$$
$$q_{\pi}(s, a) = \underset{s', f}{\mathbb{E}}(r_{t+1} + \gamma q_{\pi}(s_{t+1}, a_{t+1}) \mid s, a)$$
$$q_{\pi}(s, a) = \sum_{s', f} p(s', r \mid s, a) \left[r + \gamma \sum_{a'} \pi(a' \mid s') q_{\pi}(s', a') \right]$$

- $q_{\pi}(s,a)$ indicates how good it is to select a in s under π
- Note that $\sum_{a} \pi(a \mid s) q_{\pi}(s, a) = \mathbb{E} (q_{\pi}(s, a)) = v_{\pi}(s) \quad \forall s$

Optimal Value Functions v_* and q_*

Bellman Optimality equations

 \triangleright $v_*(s)$ is the maximum state-value function over all policies:

$$\begin{aligned} v_*(s) &\doteq \max_{\pi} v_{\pi}(s) \\ v_*(s) &= \max_{\alpha} \mathbb{E}(r_{t+1} + \gamma v_*(s_{t+1}) \mid s, a) \\ v_*(s) &= \max_{\alpha} \sum_{s', r} p(s', r \mid s, a) \left[r + \gamma v_*(s') \right] \end{aligned}$$

 $ightharpoonup q_*(s,a)$ is the maximum action-value function over all policies:

$$\begin{aligned} q_*(s,a) &\doteq \max_{\pi} q_{\pi}(s,a) \\ q_*(s,a) &= \mathbb{E}(r_{t+1} + \gamma \max_{a'} q_*(s_{t+1},a') \,|\, s,a) \\ q_*(s,a) &= \sum_{s',\,r} p(s',r \,|\, s,a) \left[r + \gamma \max_{a'} q_*(s',a') \right] \\ &\underset{\mathsf{DS-GA 3001 005}}{\text{DS-GA 3001 005}} \left[\text{Lecture 3} \right] \end{aligned}$$

Summary of Bellman equations

There are four main Bellman equations:

$$v_{\pi}(s) = \mathbb{E}(r_{t+1} + \gamma v_{\pi}(s_{t+1}) | s)$$
 (1)

$$v_*(s) = \max_{a} \mathbb{E}(r_{t+1} + \gamma v_*(s_{t+1}) | s, a)$$
 (2)

$$q_{\pi}(s,a) = \mathbb{E}(r_{t+1} + \gamma \, q_{\pi}(s_{t+1}, a_{t+1}) \, | \, s, a) \tag{3}$$

$$q_*(s,a) = \mathbb{E}(r_{t+1} + \gamma \max_{a'} q_*(s_{t+1},a') | s,a)$$
 (4)

► There are equivalences between state and action values:

$$egin{aligned} \mathbf{v}_{\pi}(\mathbf{s}) &= \sum_{a} \pi(a \,|\, \mathbf{s}) \, q_{\pi}(\mathbf{s}, a) = \mathbb{E} \left(q_{\pi}(\mathbf{s}, a)
ight) \ \mathbf{v}_{*}(\mathbf{s}) &= \max_{a} \mathbf{v}_{\pi}(\mathbf{s}) = \max_{a} q_{*}(\mathbf{s}, a) \end{aligned}$$

Policy Evaluation and Optimization

Bellman equations are used for prediction and control

Prediction: Evaluate a policy by estimating v_{π} or q_{π}

$$V_{\pi}(s) \geq V_{\pi'}(s) \iff \pi \geq \pi' \quad \forall \, s$$

Control: Improve a policy based on v_{π} or q_{π}

Example:
$$\pi_*(s,a) = \begin{cases} 1, & \text{if } a = \arg\max_a(q_*(s,a)) \\ 0, & \text{otherwise} \end{cases}$$

- ▶ **Theorem**: For any MDP, there exists an optimal policy π_* that is better than or equal to all other policies: $\pi_* \geq \pi$, $\forall \pi$
- ► There is always at least one deterministic optimal policy for any MDP. There can be multiple optimal policies

Solving Bellman Equations

Solving the RL Prediction problem

Bellman equations are linear so can in principle be solved:

$$V = R + \gamma P^{\pi}V$$
$$(I - \gamma P^{\pi}) V = R$$
$$V = (I - \gamma P^{\pi})^{-1}R$$

where:
$$v_i = v(s_i)$$
, $r_i = \mathbb{E}_{\pi}[r_t|s_i]$, $P_{ij}^{\pi} = \sum_a \pi(a \mid s_i) p(s_j \mid s_i, a)$

- Solving Bellman equations algebraically is akin to exhaustive search $(O(|s|^3))$, it can be computed only for small problems
- ► This method assumes (1) Markov property, (2) MDP dynamics is known, (3) we have enough ressources to compute the solution

Solving Bellman Equations

Solving the RL Prediction problem

Bellman equations are linear so can in principle be solved:

$$V = (I - \gamma P^{\pi})^{-1} R$$

Solving the RL Optimization problem

- Bellman optimality equations are non-linear thus can't be solved directly
- RL optimization relies on iterative solution methods
 - Dynamic Programming (use a model)
 - Monte-Carlo, Temporal Difference (use samples)

Dynamic Programming

Dynamic Programming

- DP refers to a collection of algorithms to evaluate and/or improve policies given a model of the environment as a MDP
- DP is an essential foundation: all RL methods can be viewed as attempts to achieve the same effect as DP, but with less computation and without a perfect model of the environment
- Key idea of DP is the use of value functions to organize the search for good policies
- All DP methods consist of two different parts: policy evaluation and (optionally) policy improvement
- ► All DP methods update estimates of the values of states based on estimates of the values of successor states (bootstrapping)

Policy Evaluation for a Given Policy

Estimate $v_{\pi}(s)$ of a given policy π

► Turn the Bellman equation

$$v_{\pi}(s) = \sum_{a} \pi(a \mid s) \sum_{s', r} p(s', r \mid s, a) [r + \gamma v_{\pi}(s')]$$

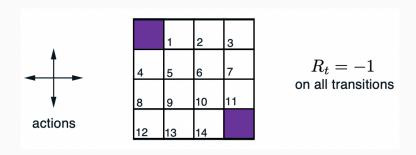
...into an update function:

► Initialize v_0 e.g., to zero, then iterate:

$$\forall s, \ V_{k+1}(s) = \sum_{a} \pi(a \mid s) \sum_{s', r} p(s', r \mid s, a) [r + \gamma V_k(s')]$$

- ▶ Whenever $v_{k+1}(s) = v_k(s)$, for all s, we have found v_{π}
- lt can be shown that $\lim_{k \to \infty} \mathsf{V}_k = \mathsf{V}_\pi$ (demonstration out of scope)

Example of Policy Evaluation



Evaluate random policy π_{random} in this 4 imes 4 gridworld

At each iteration k, loop through all states and update value estimate $v_k(s)$ of every state s for π_{random}

Example of Policy Evaluation

k = 0	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0

$$k = 3 \begin{bmatrix} 0.0 & -2.4 & -2.9 & -3.0 \\ -2.4 & -2.9 & -3.0 & -2.9 \\ -2.9 & -3.0 & -2.9 & -2.4 \\ -3.0 & -2.9 & -2.4 & 0.0 \end{bmatrix}$$

$$k = 1 \begin{array}{|c|c|c|c|c|c|}\hline 0.0 & -1.0 & -1.0 & -1.0 \\ \hline -1.0 & -1.0 & -1.0 & -1.0 \\ \hline -1.0 & -1.0 & -1.0 & -1.0 \\ \hline -1.0 & -1.0 & -1.0 & 0.0 \\ \hline \end{array}$$

$$k = 10$$

$$0.0 | -6.1 | -8.4 | -9.0$$

$$-6.1 | -7.7 | -8.4 | -8.4$$

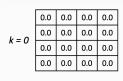
$$-8.4 | -8.4 | -7.7 | -6.1$$

$$-9.0 | -8.4 | -6.1 | 0.0$$

$$k = 2 \begin{array}{|c|c|c|c|c|c|}\hline 0.0 & -1.7 & -2.0 & -2.0 \\ \hline -1.7 & -2.0 & -2.0 & -2.0 \\ \hline -2.0 & -2.0 & -2.0 & -1.7 \\ \hline -2.0 & -2.0 & -1.7 & 0.0 \\\hline \end{array}$$

$$k = \infty \begin{bmatrix} 0.0 & -14. & -20. & -22. \\ -14. & -18. & -20. & -20. \\ -20. & -20. & -18. & -14. \\ -22. & -20. & -14. & 0.0 \end{bmatrix}$$

Example of Policy Evaluation





	0.0	-2.4	-2.9	-3.0
2	-2.4	-2.9	-3.0	-2.9
= 3	-2.9	-3.0	-2.9	-2.4
	-3.0	-2.9	-2.4	0.0
: = 3	-2.9	-3.0	-2.9	-2.

	←	←	Ţ	l
†	Ţ	\leftrightarrow	+	l
†	\leftrightarrow	Ţ	+	l
₽	\rightarrow	\rightarrow		١
				•

$$k = 1 \begin{array}{|c|c|c|c|c|c|c|}\hline 0.0 & -1.0 & -1.0 & -1.0 \\ \hline -1.0 & -1.0 & -1.0 & -1.0 \\ \hline -1.0 & -1.0 & -1.0 & -1.0 \\ \hline -1.0 & -1.0 & -1.0 & 0.0 \\\hline \end{array}$$

	↓	\leftrightarrow	\longleftrightarrow
1	\leftrightarrow	\leftrightarrow	\Leftrightarrow
\leftrightarrow	\leftrightarrow	\leftrightarrow	1
\leftrightarrow	\leftrightarrow	\rightarrow	

	0.0	-6.1	-8.4
c = 10	-6.1	-7.7	-8.4
- 10	-8.4	-8.4	-7.7
	-9.0	-8.4	-6.1

		_	_
	↓		Ţ
†	Ĺ,	Ĵ	+
†	₽	Ļ	+
₽	1	1	

$$k = 2 \begin{array}{|c|c|c|c|c|c|}\hline 0.0 & -1.7 & -2.0 & -2.0 \\ \hline -1.7 & -2.0 & -2.0 & -2.0 \\ \hline -2.0 & -2.0 & -2.0 & -1.7 \\ \hline -2.0 & -2.0 & -1.7 & 0.0 \\\hline \end{array}$$

	←	←	\leftrightarrow
1	Ĺ,	\leftrightarrow	←
+	\Rightarrow	Ļ	+
\Rightarrow		\rightarrow	

0.0	-14.	-20.	-22.
-14.	-18.	-20.	-20.
-20.	-20.	-18.	-14.
-22.	-20.	-14.	0.0

-9.0

-8.4

0.0



 $k = \infty$

Policy Improvement

Find a better policy π' given $V_{\pi}(s)$

1. For a given policy π , compute:

$$\forall \, \mathbf{S}: \, \pi'(\mathbf{S}) = \argmax_{\mathbf{a}} q_{\pi}(\mathbf{S}, \mathbf{a}) = \arg\max_{\mathbf{a}} \sum_{\mathbf{S}', \, \mathbf{r}} p(\mathbf{S}', \mathbf{r} \, | \, \mathbf{S}, \mathbf{a}) \left[\mathbf{r} + \gamma \, \mathbf{v}_{\pi}(\mathbf{S}') \right]$$

- 2. Evaluate $v_{\pi'}(s)$ as in previous slides (policy evaluation)
- 3. Repeat

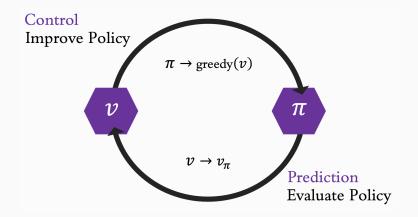
Policy Improvement Theorem:

$$\forall \, \mathsf{s}, \, \mathsf{v}_{\pi'}(\mathsf{s}) = \mathsf{max}_a \, q_\pi(\mathsf{s}, a) \geq \mathsf{v}_\pi(\mathsf{s}) \implies \pi' \; \mathsf{better} \; \mathsf{or} \; \mathsf{same} \; \mathsf{as} \; \pi$$

- When $v_{\pi'}(s) = v_{\pi}(s)$, $v_{\pi'} = \max_a q_{\pi'}(s, a)$. This is the Bellman optimality equality, thus π' is optimal.
- ▶ Thus, if $v_{\pi'}(s) \ge v_{\pi}(s)$, π' either is an improvement or is optimal

Generalized Policy Iteration

All RL methods are Generalized Policy Iteration methods



Practice: Policy Iteration Algorithm

Policy Iteration iterates multiple loops over all states to evaluate v, then loops over all states once to improve π , then repeats:

```
Initialize v(s) and \pi(s) arbitrarily for all s
1. Loop:
       \Lambda = 0
       For each s:
            v_{old} = v(s)
            v(s) = \sum_{a} \pi(a \mid s) \sum_{s',r} p(s',r \mid s,a) [(r + \gamma v(s'))]
            \Delta = \max(\Delta, |v_{old} - v(s)|)
       Stop when \Delta < \xi
2. For each s:
       \pi_{\text{old}}(s) = \pi(s)
       \pi(s) = \arg\max_{s} \sum_{s',r} p(s',r|s,a) [(r+\gamma v(s'))]
Stop if \pi_{\text{old}} \iff \pi(s), else go to step 1
```

Practice: Value Iteration Algorithm

Policy improvement with truncated policy evaluation

- Policy iteration involves policy evaluation at each iteration, which may itself require multiple loops through all states
- Is exact convergence needed, or can we stop sooner? When?
- Policy evaluation can be truncated in several ways without losing the convergence guarantees of policy iteration
- ► A special case is when policy evaluation is stopped after just one loop (one update of each state). It is equivalent to turning the Bellman optimality equation into an update function:

$$v_{k+1}(s) = \max_{a} \sum_{s',r} p(s',r \,|\, s,a) [r + \gamma v_k(s')]$$

Practice: Value Iteration Algorithm

Value Iteration truncates policy evaluation to 1 step between two (greedy) policy improvement steps while looping over all states

```
Initialize v(s) arbitrarily for all s
Loop:
        \Lambda = 0
        For each s:
             v_{old} = v(s)
             v(s) = \max_{a} \sum_{s',r} p(s',r \mid s,a) \left[ (r + \gamma v(s')) \right]
             \Delta = \max(\Delta, |v_{old} - v(s)|)
        Stop when \Delta < \xi
\pi(s) = \arg\max \sum_{s',r} p(s',r \,|\, s,a) \left[ (r + \gamma v(s')) \right]
```

Example of Value Iteration





	0	-1	-2	-3
k = 3	-1	-2	-3	-2
K – 3	-2	-3	-2	-1
	-3	-2	-1	0
	-2 -3	-3 -2	-2 -1	-1 0

	←	←	Ç
1	Ţ	\leftrightarrow	+
1	\leftrightarrow	Ţ	+
t→	\rightarrow	\rightarrow	

$$k = 1 \begin{array}{c|ccccc} 0 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 \\ \hline -1 & -1 & -1 & -1 \\ \hline -1 & -1 & -1 & 0 \end{array}$$



	0	-1	-2	-3
= 10	-1	-2	-3	-2
- 10	-2	-3	-2	-1
	-3	-2	-1	0

	←	←	\
1	Ĺ,	+	←
1	\oplus	Ļ	→
₽	\rightarrow	\rightarrow	

$$k = 2 \begin{array}{c|cccc} 0 & -1 & -2 & -2 \\ \hline -1 & -2 & -2 & -2 \\ \hline -2 & -2 & -2 & -1 \\ \hline -2 & -2 & -1 & 0 \end{array}$$

	←	←	\leftrightarrow
1	Ĺ,	\leftrightarrow	←
†	\Rightarrow	Ļ	+
\oplus	1	1	

<i>k</i> =∞	0	-1	-2	-3
	-1	-2	-3	-2
	-2	-3	-2	-1
	-3	-2	-1	0



Asynchronous Dynamic Programming

Update values in any order whatsoever...

- ▶ DP algorithms described so far loop over all states, but in practice this is often impossible (e.g., Chess has 10⁴⁰ states)
- Asynchronous DP backs up states in any order, and still converges if it continues to udpate values of all states
- Asynchronous DP makes it possible to focus DP updates onto parts of the state space that are most relevant to the agent:
 - Prioritised Sweeping: States with largest Bellman Error:

$$\max |[r_{t+1} + \gamma \hat{\mathbf{v}}(\mathbf{s}_{t+1}) \,|\, \mathbf{s}] - \hat{\mathbf{v}}(\mathbf{s})|$$

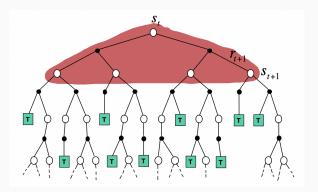
Real-time DP: Agent's real experience determines states to update, while latest values guide its decision making

Efficiency of Dynamic Programming

DP provides a well defined notion of optimality, but is often an ideal that AI agents can only approximate

- √ Asynchronous DP often exponentially faster than direct search
- √ …in particular if agent starts with good initial values or policies
- ✓ DP is iterative so can learn with limited compute resources
- √ With today's computers, DP can solve MDPs with millions of state (assuming a small number of actions)
- In most cases of practical interest, a perfect MDP model of state transitions and rewards is not available
- x In most cases of practical interest, there are far more states that there could possibly be entries in a look-up table

Efficiency of Dynamic Programming



DP often suffers from the curse of dimensionality

- ▶ DP uses full-width backups
- Even one full-depth backup can be too expensive
- Need to sample (next lecture)

Today's Takeaways

Dynamic Programming provides a foundation for RL by numerically solving the Bellman equations through GPI, which involves two processes taking place in parallel:

- Process of prediction which can learn values online at every step by bootstrapping estimates on the basis of previous estimates until they are consistent with a policy followed.
- Process of optimization which can improve the policy followed by making it greedy with respect to the latest value estimates.
- ► Both processes stabilize only when a policy has been found that is greedy with respect to its own value function.
- But Dynamic Programming needs a model of the environment.

Thank you!