Deep Learning Summer semester '24



9. Deep Reinforcement Learning

Slide credit: Slides in parts adapted from the lecture at the PRL @ FAU Erlangen-Nürnberg (K. Breininger, T. Würfl, A. Maier, V. Christlein).





- Basics of Reinforcement Learning;
- Only discrete MDPs;
- Today:

Continuous and high-dimensional MDPs!





- 1. Continuous MDPs
- 2. Approximated on-policy methods
- 3. Feature construction for linear methods
- 4. Approximated off-policy methods
- 5. Value-based deep RL DQN algorithm

Continuous MDPs - 1



Discrete MDPs:

- $\blacksquare \mathcal{M} = \langle \mathcal{S}, \mathcal{A}, \mathcal{R}, \mathcal{P}, \iota, \gamma \rangle;$
- **discrete** state space $S = \{1, \ldots, N_s\} \subseteq \mathbb{N};$
- **discrete** action space $\mathcal{A} = \{1, ..., N_a\} \subseteq \mathbb{N}$.

Continuous MDPs:

- $\blacksquare \mathcal{M} = \langle \mathcal{S}, \mathcal{A}, \mathcal{R}, \mathcal{P}, \iota, \gamma \rangle$
- **continuous** state space $S \subseteq \mathbb{R}^d$;
- discrete action space $\mathcal{A} = \{1, \dots, N_a\} \subseteq \mathbb{N};$
- or continuous action space $\mathcal{A} \subseteq \mathbb{R}^m$.

Not every problem can be formalized as a discrete MDP!





In this lecture: MDPs with continuous states, discrete actions;



In future lectures: MDPs with continuous states and actions.





- 2. Approximated on-policy methods
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Value-function approximation - 1



Value-function cannot be computed as a table;

- too many states/actions to store in memory;
- too **slow** to update each state.
- Commonly used function approximators:
 - Linear function;
 - Neural network;
 - Regression tree;
 - Gaussian process;
 - **.**...





■ Use **parametric** value function estimators where the parameters are expressed as the weight vector $w \in \mathbb{R}^d$

 $\hat{V}_{\boldsymbol{w}}(s) \approx V^{\pi}(s)$ $\hat{Q}_{\boldsymbol{w}}(s,a) \approx Q^{\pi}(s,a);$

- Parameters w are much fewer than the states (that are potentially infinite!);
- Changing weights affects the accuracy of the estimate of multiple states;
- Improving the accuracy of the value-function estimate of one state, may decrease the accuracy of the estimate of others.

Mean squared value error



Accuracy is measured as the mean squared value error:

$$\overline{\mathsf{VE}}(\boldsymbol{w}) \triangleq \sum_{s \in \mathcal{S}} \mu(s) \left[V^{\pi}(s) - \hat{V}_{\boldsymbol{w}}(s) \right]^2,$$

with the state distribution $\mu(s) \ge 0$;

- $\sum_{s} \mu(s) = 1$ weighs the importance of the estimate error for each state *s*;
- For **on-policy** algorithms, $\mu(s)$ is the fraction of time spent in state *s* while following policy π .

Value estimation with stochastic gradient descent

- Assume the **exact** value-function $V^{\pi}(s)$ is known $\forall s \in S$;
- **Goal:** find approximation with a **differentiable** estimator $\hat{V}_{w}(s)$;
- Value-function is updated each discrete time step t = 0, 1, 2, ...;
- Define weights vector $\boldsymbol{w}_t \triangleq (w_{1_t}, w_{2_t}, \dots, w_{d_t})^T$

■ A basic **step-based** update of *V*:

$$\boldsymbol{w}_{t+1} \triangleq \boldsymbol{w}_t - \frac{1}{2} \alpha \nabla \left[V^{\pi}(s_t) - \hat{V}_{\boldsymbol{w}_t}(s_t) \right]^2$$
$$= \boldsymbol{w}_t + \alpha \left[V^{\pi}(s_t) - \hat{V}_{\boldsymbol{w}_t}(s_t) \right] \nabla \hat{V}_{\boldsymbol{w}_t}(s_t)$$
(1)

where $\alpha > 0$ is the *learning rate* and

$$\nabla \hat{V}_{\boldsymbol{w}_{t}}(\boldsymbol{s}_{t}) \triangleq \left(\frac{\partial \hat{V}_{\boldsymbol{w}_{t}}(\boldsymbol{s}_{t})}{\partial w_{1}}, \frac{\partial \hat{V}_{\boldsymbol{w}_{t}}(\boldsymbol{s}_{t})}{\partial w_{2}}, \dots, \frac{\partial \hat{V}_{\boldsymbol{w}_{t}}(\boldsymbol{s}_{t})}{\partial w_{d}}\right); \quad (2)$$

Convergence to local optimum if properly decaying α .

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Semi-gradient SARSA - 1



On-policy control algorithm: approximate *Q* instead of *V*;
 Gradient descent update:

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t + \alpha \left[\boldsymbol{U}_t - \hat{\boldsymbol{Q}}_{\boldsymbol{w}_t}(\boldsymbol{s}_t, \boldsymbol{a}_t) \right] \nabla \hat{\boldsymbol{Q}}_{\boldsymbol{w}_t}(\boldsymbol{s}_t, \boldsymbol{a}_t); \tag{3}$$

One-step SARSA update:

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t + \alpha \left[r_{t+1} + \gamma \hat{Q}_{\boldsymbol{w}_t}(s_{t+1}, a_{t+1}) - \hat{Q}_{\boldsymbol{w}_t}(s_t, a_t) \right] \nabla \hat{Q}_{\boldsymbol{w}_t}(s_t, a_t).$$
(4)

Semi-gradient SARSA - 2



Algorithm Semi-gradient SARSA

- 1: **Input:** the policy π to evaluate;
- 2: **Input:** a differentiable function $\hat{Q} : S \times A \to \mathbb{R}$;
- Initialize action-value-function weights $w \in \mathbb{R}^d$ arbitrarily, e.g., w = 0; 3:

4: while true do

- 5: Initialize first state $s = s_0$ and action $a = a_0$ (e.g., ε -greedy);
- while true do 6:
- if s' is terminal then

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \alpha [r - \hat{\mathcal{Q}}_{\boldsymbol{w}}(s, a)] \nabla \hat{\mathcal{Q}}_{\boldsymbol{w}}(s, a);$$

- Terminate the episode;
- 10: end if

8: 9:

Choose action a' as a function of $\hat{Q}_{W}(s', \cdot)$ (e.g., ε -greedy); 11:

12:
$$\mathbf{w} \leftarrow \mathbf{w} + \alpha [r + \gamma \hat{Q}_{\mathbf{w}}(s', a') - \hat{Q}_{\mathbf{w}}(s, a)] \nabla \hat{Q}_{\mathbf{w}}(s, a);$$

- 13: $s \leftarrow s'$: 14:
- $a \leftarrow a'$:
- 15: end while
- 16: end while





- 2. Approximated on-policy methods
- 3. Feature construction for linear methods
- 4. Approximated off-policy methods
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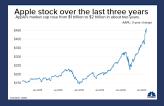
Feature construction for linear methods



- State vector contains representative features of the problem;
- For example:
 - position and angular velocity for balancing a pendulum;
 - pixels for playing a videogame;
 - stock price for finance applications.







Feature construction for linear methods



- Basic features may not be representative enough to capture complex behavior;
- Consider the pendulum example:
 - state $s = (s_1, s_2)$, with $s_1 \in \mathbb{R}$ the angular position and $s_2 \in \mathbb{R}$ the angular velocity;
 - a feature vector $\varphi(s) = (s_1, s_2)^T$ is a **poor** representation of the problem;
 - interaction between the state dimensions are not considered!
- Representative feature vectors consider all dimensions of the state and their (potentially complex) interaction;
- How to obtain good features?

Polynomial features



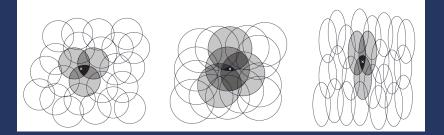
Polynomial features capture interaction among state dimensions by multiplication:

- 1st-order: $\varphi(s) = (1, s_1, s_2, s_1s_2)^T$;
- **2**nd-order: $\varphi(s) = (1, s_1, s_2, s_1s_2, s_1^2, s_2^2, s_1s_2^2, s_1^2s_2, s_1^2s_2^2)^T$;
- **...**
- The number of features grows exponentially with the number of dimensions of the state;
- Note that the approximation is still linear in the weights.

Coarse coding



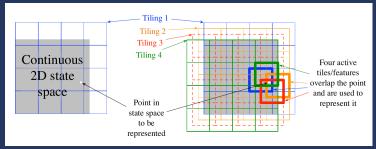
- Divide the state space in *M* different **regions**;
- The feature vector has *M* binary values;
- Given a state s, for each region, assign feature value 1 if the state is inside the region, 0 otherwise;
- 0-1 features are also called sparse.



Tile coding - 1



- Flexible and computationally efficient form of coarse coding;
- Use N tilings, each one composed of M tiles;
- The feature vector is a $N \times M$ matrix;
- The feature value is 1 if the state is **inside** a tile, 0 otherwise;

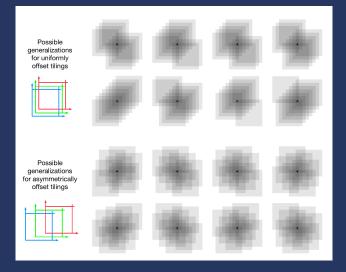


Every state has the same number of active features.

3. Feature construction for linear methods

Tile coding - 2





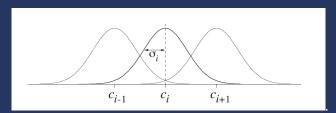
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Radial basis functions



- Generalization of coarse coding;
- Feature values are **real** numbers in [0, 1];
- The Gaussian distribution is a typical RBF with mean c_i and standard deviation σ_i

$$\varphi_i(s) = \exp\left(-\frac{\|s-c_i\|^2}{2\sigma_i^2}\right); \tag{5}$$

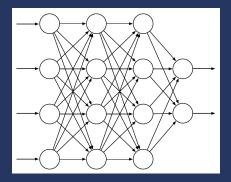


Neural networks



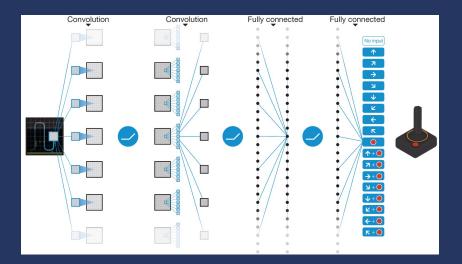
What if constructing features by hand is difficult or impractical?

- Use neural networks!
 - Automatically extract features in hidden layers;
 - Enable processing high-dimensional data.



Deep neural networks









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Semi-gradient off-policy TD(0)

Recall: perform importance sampling to change the expectation from a **target** policy π to the **behavioral** distribution *b*;

Define the *importance sampling ratio*

$$\rho_t = \frac{\pi(a_t|s_t)}{b(a_t|s_t)};$$
(6)

■ The one-step semi-gradient off-policy TD(0) update is

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t + \alpha \rho_t \delta_t \nabla \hat{V}_{\boldsymbol{w}_t}(\boldsymbol{s}_t); \tag{7}$$

where, e.g., $\delta_t = r_{t+1} + \gamma \hat{V}_{w_t}(s'_t) - \hat{V}_{w_t}(s_t)$.



Off-policy divergence



- Updating value functions following the on-policy distribution is important for convergence;
- The distribution of updates does not match the on-policy distribution;
- Off-policy algorithms with approximation can diverge!

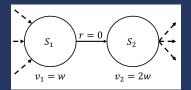
Example of off-policy divergence - 1



- Consider this transition as part of a bigger MDP;
- Consider **w**₀ = [w₀] = [10];
- Suppose $\gamma \approx 1$ and $\alpha = 0.1$;
- Step 1:

■ Take the transition, update *w*_t:

$$\begin{split} \delta_0 &= r_1 + \gamma \hat{V}_{w_0}(s_2) - \hat{V}_{w_0}(s_1) \\ &= 0 + \gamma 2w_0 - w_0 \\ &= (2\gamma - 1)w_0 \approx 10 \\ w_1 &= w_0 + \alpha \rho_0 \delta_0 \nabla \hat{V}_{w_0}(s_1) \\ &= w_0 + \alpha \cdot 1 \cdot (2\gamma - 1)w_0 \cdot 2 \\ &= (1 + \alpha (2\gamma - 1))w_0 \approx 11 \end{split}$$

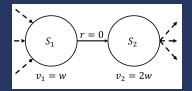


Example of off-policy divergence - 2



Step 2: Take the transition, update w_t:

$$\begin{split} \delta_1 &= r_2 + \gamma \hat{V}_{w_1}(s_2) - \hat{V}_{w_1}(s_1) \\ &= 0 + \gamma 2w_1 - w_1 \\ &= (2\gamma - 1)w_1 \approx 11 \\ w_2 &= w_1 + \alpha \rho_1 \delta_1 \nabla \hat{V}_{w_1}(s_1) \\ &= w_1 + \alpha \cdot 1 \cdot (2\gamma - 1)w_1 \cdot 1 \\ &= (1 + \alpha(2\gamma - 1))w_1 \approx 12... \end{split}$$

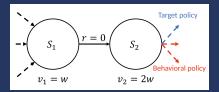


The value of the updated parameter **diverges** if $1 + \alpha(2\gamma - 1) > 1$.



Example of off-policy divergence - 3

- Divergence happens because the distribution of update is different from the on-policy distribution;
- w is updated only during the given transition, not after;



The deadly triad



Instability and divergence arise for methods based on the following elements:

- function approximation;
- bootstrapping;
- off-policy training.
- Can we get rid of one of them without disadvantages?
 - function approximation is necessary to **scale** to large problems;
 - bootstrapping is important for data efficiency;
 - off-policy training is essential for learning from heterogeneous experience.

Batch reinforcement learning



Up to now, we have seen mostly online RL algorithm;
 Batch (a.k.a., Offline) RL methods use a previously collected dataset of transitions:

$$\mathcal{D} = \langle s_i, a_i, r_i, s'_i \rangle_{i=1}^T.$$
(8)

Fitted *Q***-Iteration**



Given a dataset $D = \langle s_i, a_i, r_i, s'_i \rangle_{i=1}^T$, solve a sequence of regression problems;

Stability guarantees hold for particular regression methods:

- regression trees;
- kernel averaging.

Algorithm FQI

- 1: **Input:** dataset of transitions $\mathcal{D} = \langle s_i, a_i, r_i, s'_i \rangle_{i=1}^T$;
- 2: **Input:** N = 0, an initial $\hat{Q}_N(s, a) = 0$;
- 3: while true do
- 4: $N \leftarrow N+1;$
- 5: Build training set $\mathcal{T} = \{\langle s_i, a_i, r_i + \gamma \max_{a \in \mathcal{A}} \hat{Q}_{N-1}(s'_i, a) \rangle\}_{i=1}^T$;
- 6: Use regression algorithm to build $\hat{Q}_N(s, a)$;
- 7: end while





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High-dimensional RL problems - 1



- Dimension of state and action space is **critical** in RL;
- Curse of dimensionality: theoretical and practical issues arising from high-dimensional problems;
- The RL methods we discussed can only handle low-dimensional problems.



How to enable RL to solve more complex problems?

High-dimensional RL problems - 2



- **High**-dimensional problems have a state space S with:
 - Impractically large number of discrete values (e.g., each pixel of an image has an integer value ∈ [0, 255]);
 - More than 8 10 dimensions (e.g., position and velocity of joints for a robot).
- The action space *A* could be either **discrete** or **continuous**:
 - commands to a videogame;
 - torque to joints of a robot.



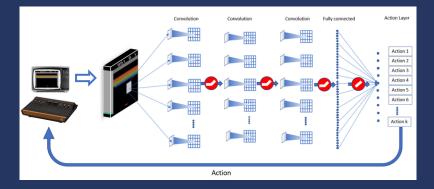


5. Value-based deep RL - DQN algorithm

Deep neural networks for RL



High-dimensional state/action spaces can be handled with deep neural networks and the use of deep learning techniques.



Deep Q-Learning - 1



Recall the definition of action-value function:

$$Q_{\pi}(s,a) = \mathbb{E}_{\pi}\left[\sum_{t} \gamma^{t} r_{t+1} \middle| s_{0} = s, a_{0} = a\right]; \qquad (9)$$

- Suppose the state space S is high-dimensional;
- Goal: approximate the action-value function using a deep neural network with parameters θ:

$$\hat{Q}(s,a;\theta) \approx Q_{\pi}(s,a).$$
 (10)

Deep Q-Learning - 2



Minimize the loss

$$\mathcal{L}_{i}(\theta_{i}) = \mathbb{E}_{(s,a,r,s')\sim\mathcal{D}}\left[\left(r + \gamma \max_{a'} \hat{Q}(s',a';\theta_{i}) - \hat{Q}(s,a;\theta_{i})\right)^{2}\right];$$
(11)

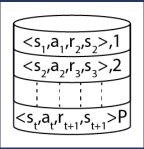
Problems:

- this loss contains bootstrapping, off-policy, and of course function approximation → deadly triad!
- an offline dataset of transitions is assumed unavailable due to the complexity of the problems → we cannot use offline algorithms (e.g., FQI);
- data have to be collected online → training neural networks in online RL can lead to catastrophic forgetting.

5. Value-based deep RL - DQN algorithm

Deep Q-Learning - Replay buffer





Collect and store past transitions to reuse them for update;

- Store transitions in queue, a.k.a. **replay buffer**, of finite capacity;
- Off-policy updates allow to reuse transitions out of the sampling distribution;
- Reduces the negative impact of distribution shift.

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Deep *Q***-Learning - Target network**



- Keep a copy of the neural network updating it periodically;
- Every *C* steps, the weights θ of the online network are **copied** in the target network as θ' and kept fixed for the next *C* steps;
- The copy of the neural network, the target network, is used to compute the target of the mean squared TD-error

$$\mathcal{L}_{i}(\theta_{i}) = \mathbb{E}_{(s,a,r,s')\sim\mathcal{D}}\left[\left(r + \gamma \max_{a'} \hat{Q}(s',a';\theta') - \hat{Q}(s,a;\theta_{i})\right)^{2}\right];$$
(12)

Avoids instability due to function approximation.

5. Value-based deep RL - DQN algorithm



Deep *Q*-Learning - Minibatch updates

At each step, uniformly sample a minibatch of N transitions from the replay buffer

$$\mathcal{L}_{i}(\theta_{i}) = \sum_{i=1}^{N} \left[\left(r_{i} + \gamma \max_{a'} \hat{Q}(s'_{i}, a'; \theta') - \hat{Q}(s_{i}, a_{i}; \theta_{i}) \right)^{2} \right]; \quad (13)$$

Improves efficiency w.r.t. training on all transitions.

5. Value-based deep RL - DQN algorithm

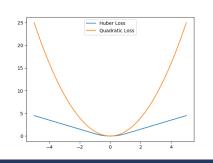
Deep *Q*-Learning - Reward and target clipping



Clip reward between -1 and 1;
 Clip the error term of the update

 r + γ max_{a'} Q̂(s', a'; θ') - Q̂(s, a; θ) between -1 and 1;

 It is sufficient to use Huber loss!



Improve stability of the optimization.

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Deep *O*-Learning - Pseudocode



Algorithm Deep O-Learning

- 1: Initialize replay buffer D to capacity N;
- 2: Initialize action-value function \hat{O} with random weights θ ;
- Initialize target action-value function weights $\theta' = \theta$; 3:

while true do 4:

- 5: Initialize state *s*₀;
- 6: for t = 1, ..., T do
- 7: Sample action a_t with ε -greedy using \hat{O} ;
- 8: Execute a_t and observe reward r_t and s'_t ;
- 9: Store transition (s, a, r, s') in \mathcal{D} ;
- Uniformly sample minibatch of *M* transitions $\langle s_i, a_i, r_i, s'_i \rangle_{i=1}^M$ from *D*; 10:
- 11:
- $y_i = \begin{cases} r_i & \text{if episode terminates at step } i+1\\ r_i + \gamma \max_{a'} \hat{Q}(s'_i, a'; \theta') & \text{otherwise} \end{cases}$ Perform gradient descent step on $\left(y_i \hat{Q}(s_i, a_i; \theta)\right)^2$ w.r.t. weights θ ; 12:
- 13: Every C steps do $\theta' = \theta$:
- 14: end for

15: end while

5. Value-based deep RL - DQN algorithm

Deep *Q*-Learning - Applications



DQN is a powerful algorithm

- https://www.youtube.com/watch?v=W2CAghUiofY
- https://www.youtube.com/watch?v=XMo0899Nz7o
- https://www.youtube.com/watch?v=V1eYniJ0Rnk

But this comes at a cost!

- Requires many samples;
- Highly sensitive to hyperparameter tuning;
- High computation time.





How to handle continuous Markov Decision Processes;
How to build features for linear value function approximation;
How to handle high-dimensional Markov Decision Processes;
Deep *Q*-Network algorithm.