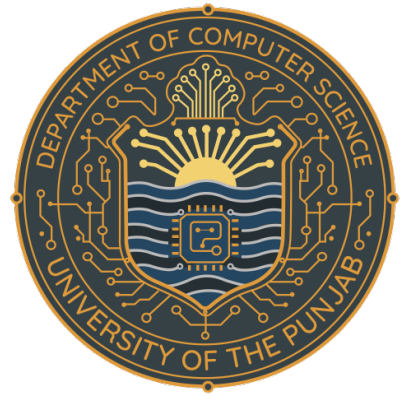
CS-566 Deep Reinforcement Learning

Deep Value-Based Agents



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From Tabular to Deep Agents

- So far, we have studied **tabular methods** such as
  - Monte Carlo Sampling
  - SARSA
  - Q-learning
- These methods work well for **small, discrete environments**.
- But what happens when the state space becomes huge or continuous?

Main Challenge

Create an **agent algorithm** that can learn a good policy *by interacting with the world*, even in large, high-dimensional environments.

The Next Step: Deep Reinforcement Learning

- From now on, our agents will be **deep learning agents**.
- We combine:

$$\text{Reinforcement Learning (decision making)}$$
$$+ \text{ Deep Learning (function approximation)}$$
$$\Rightarrow \text{Deep Reinforcement Learning (DRL)}$$

- DRL allows us to handle:
  - Large or continuous state spaces
  - Complex perceptual inputs (e.g., images, audio)
  - High-dimensional control problems

Motivation: Beyond Toy Problems

- Simple grid worlds or taxi environments are **toy problems**.
- Real-world domains:
  - Robotics
  - Autonomous driving
  - Game playing (e.g., Go, Chess, Atari)
  - Financial decision-making
- These involve thousands or millions of states and actions.

Key Question

How can we scale from a small tabular $Q(s, a)$ to a powerful **neural-network-based** $Q_\theta(s, a)$?

From Tables to Parameterized Functions

Tabular Methods

- Store $Q(s, a)$ in a lookup table
- Feasible for small, discrete spaces
- Example: Taxi world with 500 states

Deep Methods

- Use a neural network $Q_\theta(s, a)$
- θ are trainable weights
- Approximates the value function for unseen states

Goal

Transform:

$$V, Q, \pi \quad \rightarrow \quad V_\theta, Q_\theta, \pi_\theta$$

so that our agent can generalize to **large or continuous spaces**.

Core Questions in Deep Value-Based RL

- How can we use deep learning for large-scale sequential decision-making?
- How do we represent the value or policy functions with neural networks?
- How can we train these networks stably and efficiently?
- What challenges arise from using non-linear function approximators?

From Supervised to Reinforcement Learning

- **Deep supervised learning**[1] uses a *static dataset* $\{(x_i, y_i)\}$.
- The goal is to approximate a function $f_\theta(x)$ such that:

$$\theta^* = \arg\min_\theta \mathcal{L}(f_\theta(x_i), y_i)$$

  where $\mathcal{L}$ is a loss function.
- The labels y_i are **fixed, static targets**.
- Learning proceeds via gradient descent until the loss converges.

Key Idea

Supervised learning optimizes against **known, static truths**.

[1] See Appendix B of Plaat's book

Bootstrapping as a Minimization Process

- In reinforcement learning, **bootstrapping** plays a similar role.
- The agent learns from the difference between successive estimates:

$$\delta_t = r_{t+1} + \gamma\, V(s_{t+1}) - V(s_t)$$

- This **temporal difference (TD) error** acts like a loss term that we try to minimize.
- Over time, this process converges to the true value functions:

$$V^*(s), \quad Q^*(s, a)$$

Analogy

Supervised learning: minimize $(y - \hat{y})^2$
Reinforcement learning: minimize $(r + \gamma V(s') - V(s))^2$

The Challenge: Moving Targets

- In Q-learning, the data samples are **not static**.
- The agent's actions generate new experience tuples:

$$(s_t, a_t, r_{t+1}, s_{t+1})$$

- The target in the loss function,

$$y_t = r_{t+1} + \gamma \max_a Q_\theta(s_{t+1}, a),$$

  changes as the network parameters θ change!
- Hence, the **target itself moves** during training.

Consequence

The Q-network tries to predict targets that depend on itself — this creates potential instability and divergence.

Dynamic Data and Policy Coupling

- Unlike supervised learning, RL samples depend on the current policy π_θ.
- Thus, as π_θ improves, the distribution of states and rewards changes.
- The agent is both:
  - The **generator** of its own data, and
  - The **learner** from that data.
- This circular dependency makes convergence hard.

Moving Target Problem

$$y_t(\theta) = r_{t+1} + \gamma \max_a Q_\theta(s_{t+1}, a)$$

depends on θ itself — our target moves every time we update the network.

Stability: The Central Challenge of Deep RL

- Finding stable learning algorithms for moving targets took years of research.
- The key innovations:
  - **Experience Replay:** breaks correlation between consecutive samples.
  - **Target Networks:** stabilize the moving target by freezing parameters temporarily.
  - **Careful learning rate tuning.**

Why It's Hard

The optimization landscape is **non-stationary** and **self-referential**.

Connecting the Three Worlds

Aspect	Supervised Learning	Tabular Q-learning	Deep Q-learning
Data source	Static dataset	Sampled from environment	Sampled, stored, replayed
Targets	Fixed labels	Bootstrapped rewards	Moving bootstrapped rewards
Function type	$f_\theta(x)$	Table $Q(s, a)$	Network $Q_\theta(s, a)$
Loss	$\mathcal{L}(y, \hat{y})$	TD Error	TD Error with moving target
Stability	High	Moderate	Low (requires tricks)

Summary

Deep Q-learning generalizes Q-learning to large problems by using deep networks, but inherits instability from its **bootstrapped, moving-target** nature.

Overview of Supervised Training

- In supervised deep learning, training minimizes a loss function between predicted outputs and known targets.
- The dataset is **static** — both inputs and labels remain fixed throughout training.
- The optimization aims to approximate a target function through repeated forward and backward passes.

Typical Supervised Learning Algorithm

```
def train_sl(data, net, alpha=0.001):          # train classifier
    for epoch in range(max_epochs):            # an epoch is one
        pass
        sum_sq = 0                        # reset to zero for each
            pass
        for (image, label) in data:
            output = net.forward_pass(image) # predict
            sum_sq += (output - label)**2 # compute error
        grad = net.gradient(sum_sq)           # derivative of error
        net.backward_pass(grad, alpha)        # adjust weights
    return net
```

Typical Supervised Learning Algorithm

- The main components are:
  1. **Input dataset:** static pairs of inputs and target labels.
  2. **Forward pass:** compute network predictions.
  3. **Loss computation:** measure prediction error.
  4. **Backward pass:** compute gradients and update parameters.

Goal: minimize the loss function over the dataset to find parameters that best fit the data.

Structure of the Training Loops

- Training typically involves a **double loop:**
  1. **Outer loop:** controls the number of epochs.
  2. **Inner loop:** iterates through each example (or minibatch) of the dataset.
- In each epoch:
  - Perform a forward approximation using current parameters.
  - Compute the loss and its gradient.
  - Adjust the parameters via backpropagation.

Inner Loop Dynamics

- The **inner loop** provides samples to the forward computation of:
  - Output value
  - Loss value
  - Gradient computation
- The **backward pass** then adjusts the parameters accordingly.
- The dataset is static, so each epoch processes the same data repeatedly until convergence.

Independence and Sampling of Data

- Each training sample is assumed to be **independent** of the others.
- Samples are typically selected with **equal probability**.
- For example:
  - After an image of a white horse is sampled,
  - The probability that the next image is a black grouse or a blue moon remains equally (un)likely.
- This independence ensures that learning is based purely on the data distribution, not temporal correlations.

Key Characteristics of Supervised Training

- Static dataset $\Rightarrow$ fixed ground-truth targets.
- Independent samples $\Rightarrow$ no temporal dependencies.
- Objective $\Rightarrow$ minimize loss over dataset to achieve best approximation of the target function.
- The learning process is stable because:
  - Targets do not change during training.
  - Gradients are computed against fixed labels.

Introduction to Bootstrapping Q-Values

- Q-learning is a foundational reinforcement learning (RL) algorithm.
- Unlike supervised learning, RL chooses its training examples **dynamically** through interaction with the environment.
- The algorithm learns by **bootstrapping** — updating estimates based partly on other learned estimates.
- For convergence, every state must eventually be sampled by the environment[2].

[2] Christopher JCH Watkins. 'Learning from Delayed Rewards'. PhD thesis. King's College, Cambridge, 1989.

Challenges of Large State Spaces

- In small environments, it is feasible for all states to be visited repeatedly.
- However, for large or continuous state spaces:
  - This condition no longer holds.
  - Many states may never be visited.
  - Therefore, convergence to the true value function is not guaranteed.
- This motivates the use of **function approximation** (e.g., deep networks) in modern RL.

Structure of the Q-Learning Algorithm[3]

- As with supervised training, Q-learning consists of a **double loop:**
  1. **Outer loop:** Controls the number of episodes.
  2. **Inner loop:** Iterates through steps within an episode.
- Each episode represents a trajectory from a start state to a terminal state.

```
def qlearn(environment, alpha=0.001, gamma=0.9, epsilon=0.05):
    Q[TERMINAL,_] = 0 # policy
    for episode in range(max_episodes):
        s = s0
        while s not TERMINAL: # perform steps of one full
            episode
            a = epsilongreedy(Q[s], epsilon)
            (r, sp) = environment(s, a)
            Q[s,a] = Q[s,a] + alpha*(r+gamma*max(Q[sp])-Q[s,a])
            s = sp
     return Q
```

[3] Christopher JCH Watkins. 'Learning from Delayed Rewards'. PhD thesis. King's College, Cambridge, 1989.

Representation and Convergence

- Q-values are stored in a **Python array** indexed by (s, a) pairs:

$$Q[s, a]$$

- Q-function represents the expected return for taking action a in state s.
- Convergence is assumed to occur when enough episodes have been sampled.
- The update rule is **bootstrapped** from prior estimates:

$$Q(s, a) \leftarrow Q(s, a) + \alpha \left[r + \gamma \max_{a'} Q(s', a') - Q(s, a) \right]$$

Off-Policy Learning in Q-Learning

- Q-learning is an **off-policy** method.
- The update target uses the **maximum future Q-value**, not the value of the action taken by the current policy.
- This enables learning the optimal policy while following an exploratory behavior policy (e.g., ϵ-greedy).
- Hence, even though behavior is stochastic, the learned Q-values reflect an optimal deterministic policy.

Differences from Supervised Learning

- In Q-learning:
  - Samples are **not independent**.
  - Each next action **depends** on the current policy.
  - Successive states are **highly correlated** in a trajectory.
- Example:
  - If the agent samples a state where a ball is in the upper left corner,
  - The next state will likely also be near the upper left corner.
- This temporal correlation violates the i.i.d. assumption of supervised learning.

Consequences of Sample Dependence

- Correlated samples can cause:
  - **Slow learning** due to redundant experiences.
  - **Instability** or divergence in training.
  - The network may overfit to local regions of the state space.
- To mitigate this, RL uses:
  - **Exploration strategies** (ϵ-greedy, softmax, etc.).
  - **Experience replay** to decorrelate samples.

Need for Exploration

- Without sufficient exploration:
  - The agent may become trapped in local optima.
  - It may fail to discover high-reward states.
- Exploration ensures coverage of diverse states, improving Q-value estimation.
- Common strategies include:
  - ϵ-greedy policy: random action with probability ϵ.
  - Decaying ϵ: reduces randomness over time.

Summary of Bootstrapping in Q-Learning

- Q-learning updates are based on **bootstrapping previous estimates**.
- The process is **dynamic**: training samples and targets change during learning.
- Q-learning differs from supervised learning because:
  - Samples are temporally correlated.
  - Targets depend on current estimates (no static ground truth).
  - Learning is off-policy and depends on exploration.
- These factors make convergence difficult, especially for large problems.

Deep Reinforcement Learning Target-Error

- Deep learning and Q-learning share a striking structural similarity.
- Both algorithms consist of a **double loop**:
  - An **outer loop** over epochs or episodes.
  - An **inner loop** over samples or steps.
- Each iteration minimizes an error or difference between a prediction and a target.
- This similarity raises the question: **Can bootstrapping be combined with loss-function minimization?**

Combining Bootstrapping and Gradient Descent

- Mnih et al.[4] demonstrated that the two processes **can indeed be combined**.
- The result is **Deep Q-Learning (DQN)** — a method that merges:
  - Bootstrapping from Q-learning, and
  - Gradient-based parameter optimization from deep learning.
- The key idea: train a **Q-network** that approximates $Q_\theta(s, a)$ using backpropagation.

[4] Volodymyr Mnih et al. 'Playing Atari with Deep Reinforcement Learning'. In: (2013). cite arxiv:1312.5602Comment: NIPS Deep Learning Workshop 2013. URL: http://arxiv.org/abs/1312.5602.

Naive Deep Learning Version of Q-Learning

- The structure is still a double loop:
  1. Outer loop: controls episodes or training iterations.
  2. Inner loop: bootstraps Q-values by minimizing a loss function.
- The parameters θ of the Q-network are updated via **stochastic gradient descent**.

Naive Deep Learning Version of Q-Learning

```
def train_qlearn(environment, Qnet, alpha=0.001, gamma=0.0,
    epsilon=0.05
    s = s0                # initialize start state
    for epoch in range(max_epochs): # an epoch is one pass
        sum_sq = 0  # reset to zero for each pass
        while s not TERMINAL: # perform steps of one full
            episode
            a = epsilongreedy(Qnet(s,a)) # net: Q[s,a]-values
            (r, sp) = environment(a)
            output = Qnet.forward_pass(s, a)
            target = r + gamma * max(Qnet(sp))
            sum_sq += (target - output)**2
            s = sp
        grad = Qnet.gradient(sum_sq)
        Qnet.backward_pass(grad, alpha)
    return Qnet     # Q-values
```

The Deep Q-Learning Loss Function

- Deep Q-learning minimizes a loss based directly on the Q-learning update rule.
- The loss at iteration t is:

$$\mathcal{L}(\theta_t) = \mathbb{E}_{s,a,r,s'}\left[\left(r + \gamma \max_{a'} Q_{\theta_{t-1}}(s', a') - Q_{\theta_t}(s, a)\right)^2\right]$$

- This is the squared difference between:
  - The new Q-value $Q_{\theta_t}(s, a)$ (forward pass), and
  - The old bootstrapped target $r + \gamma \max_{a'} Q_{\theta_{t-1}}(s', a')$.

Gradient of the Deep Q-Learning Loss

- The gradient for the parameter update is given by:

$$\nabla_{\theta_i}\mathcal{L}_i(\theta_i) = \mathbb{E}_{s,a\sim\rho(\cdot);s'\sim\mathcal{E}}\left[\left(r + \gamma \max_{a'} Q_{\theta_{i-\mathbf{1}}}(s', a') - Q_{\theta_i}(s, a)\right)\nabla_{\theta_i} Q_{\theta_i}(s, a)\right]$$

- Here:
  - ρ: behavior distribution (policy used for exploration)
  - $\mathcal{E}$: environment dynamics (e.g., Atari emulator)
- This defines a **fixed-point iteration** process[5].

[5] Francisco S Melo and M Isabel Ribeiro. 'Convergence of Q-learning with linear function approximation'. In: *2007 European Control Conference (ECC)*. IEEE. 2007, pp. 2671–2678.

Moving Targets and Instability

- A crucial distinction from supervised learning:
  - In supervised learning, targets are **fixed**.
  - In deep reinforcement learning, targets are **moving**.
- The target values depend on the previous parameters θ_{t-1}:

$$y_t = r + \gamma \max_{a'} Q_{\theta_{t-1}}(s', a')$$

- Since both prediction and target evolve as learning progresses, **the optimization target moves during training**.

Implications of Moving Targets

- Moving targets can lead to:
  - **Instability**: network weights chase a shifting objective.
  - **Divergence**: updates may amplify errors instead of reducing them.
  - **Non-stationary training signals**.
- To mitigate these problems, DQN introduced:
  - **Target networks** — to stabilize the bootstrapped targets.
  - **Experience replay** — to decorrelate samples.
- These innovations made deep reinforcement learning feasible for large-scale tasks such as **Atari games**.

Summary: Deep RL Target-Error Concept

- Deep RL integrates:
  1. **Bootstrapping** from temporal-difference learning.
  2. **Loss minimization** through gradient descent.
- The target depends on older network weights, making it a **moving target**.
- Despite this challenge, stability can be achieved with architectural innovations (target networks, replay buffers).
- Deep Q-learning thus bridges the gap between tabular Q-learning and deep neural function approximation.

Three Core Challenges

- Our naive deep Q-learner faces three fundamental problems:
  1. **Coverage:** The state space is too large to sample fully.
  2. **Correlation:** Subsequent samples are highly correlated.
  3. **Convergence:** The optimization target moves during learning.
- These issues threaten convergence, stability, and generalization of deep RL agents.

Challenge 1: Coverage

- Proofs of Q-learning's convergence rely on a key assumption:

  All state-action pairs (s, a) must eventually be sampled.

- This ensures that $Q(s, a)$ converges to the optimal $Q^*(s, a)$.
- However, in large or continuous environments:
  - Full state coverage is **impossible**.
  - Many states may never be visited.
- $\Rightarrow$ No theoretical guarantee of convergence to the optimal policy.

Coverage in Practice

- Example: Atari game with millions of unique screen states.
- Even after millions of steps, the agent may have visited only a fraction.
- Consequently:
  - Q-values for unseen states remain inaccurate.
  - Policy may fail catastrophically in novel or rare situations.
- This is a form of **out-of-distribution generalization** failure.

Challenge 2: Correlation

- In reinforcement learning, samples are **not independent**.
- Each state s_{t+1} is generated from s_t by one action:

$$s_{t+1} = f(s_t, a_t)$$

- Hence, consecutive samples (s_t, a_t, r_t, s_{t+1}) are **highly correlated**.
- This violates the i.i.d. assumption of stochastic gradient descent.

Consequences of Sample Correlation

- Correlated samples can cause:
  - **Biased training**: updates reflect a narrow part of the state space.
  - **Local minima**: the policy becomes specialized to a small region.
  - **Feedback loops**: policy reinforces its own biases.
- Example:
  - A chess agent always plays one opening.
  - It learns strong Q-values only for that opening.
  - When the opponent plays a different opening, performance collapses.

The Specialization Trap

- When exploitation dominates exploration:
  - The agent repeatedly selects the same actions.
  - State trajectories become repetitive.
  - The agent gets stuck in a "specialization trap."
- This worsens both:
  - **Coverage**: fewer distinct states sampled.
  - **Convergence**: biased gradients lead to overfitting.
- The result: poor generalization and unstable learning.

Challenge 3: Convergence

- In supervised learning:
  - Targets y are **fixed**.
  - Loss $\mathcal{L}(\theta) = (y - f_\theta(x))^2$ minimizes toward a stable solution.
- In deep reinforcement learning:
  - Targets **move** because they depend on θ_{t-1}.
  - Bootstrapped target:

$$y_t = r + \gamma \max_{a'} Q_{\theta_{t-\mathbf{1}}}(s', a')$$

Moving Targets and Instability

- The loss at time t is:

$$\mathcal{L}(\theta_t) = \left(r + \gamma \max_{a'} Q_{\theta_{t-1}}(s', a') - Q_{\theta_t}(s, a) \right)^2$$

- Both prediction and target depend on parameters being optimized.
- $\Rightarrow$ Risk of:
  - **Overshooting** the target.
  - **Oscillation** or even **divergence**.
- Gradient descent "chases" a target that moves with every update.

Why Convergence is Difficult

- Reinforcement learning optimizes a function that depends on itself:

$$Q_\theta(s, a) \approx r + \gamma \max_{a'} Q_\theta(s', a')$$

- This circular dependency causes:
  - **Non-stationary targets**
  - **Instability** in gradient-based updates
- Considerable research effort has gone into finding algorithms that:
  - Break this circular dependency,
  - And stabilize learning despite moving targets.

Summary: The Three Challenges

1. Coverage

Large state spaces prevent full sampling $\Rightarrow$ incomplete Q-values.

2. Correlation

Sequential samples are correlated $\Rightarrow$ biased updates and specialization traps.

3. Convergence

Targets move with parameters $\Rightarrow$ instability and potential divergence.

- Overcoming these challenges led to key innovations: **Experience Replay** and **Target Networks**.

The Deadly Triad: Overview

- Combining **off-policy learning** with **nonlinear function approximation** can cause Q-values to diverge.[6,7,8]
- Three interacting elements make reinforcement learning unstable:
  1. Function approximation
  2. Bootstrapping
  3. Off-policy learning
- Together, they form the **Deadly Triad**[9].

[6] Leemon Baird. 'Residual algorithms: Reinforcement learning with function approximation'. In: *Machine Learning Proceedings 1995*. Elsevier, 1995, pp. 30–37.

[7] Geoffrey J Gordon. *Approximate solutions to Markov decision processes*. Carnegie Mellon University, 1999.

[8] John N Tsitsiklis and Benjamin Van Roy. 'Analysis of temporal-diffference learning with function approximation'. In: *Advances in Neural Information Processing Systems*. 1997, pp. 1075–1081.

[9] Richard S Sutton and Andrew G Barto. *Reinforcement learning, An Introduction, Second Edition*. MIT Press, 2018.

Function Approximation

- Function approximators (e.g., neural networks) estimate $Q(s, a)$ using **shared features** between states.
- Unlike exact tabular methods, deep networks generalize over state features:

$$Q(s, a) \approx f_\theta(\phi(s), a)$$

- Errors in shared features can cause **misidentification of states**.
- Reward values or Q-values can then be attributed incorrectly to unrelated states.

Implication

Misassigned values can cause **instability or divergence** during learning.

Bootstrapping

- In temporal-difference and Q-learning, current estimates depend on previous estimates:

$$Q(s,a) \leftarrow Q(s,a) + \alpha\left[r + \gamma \max_{a'} Q(s',a') - Q(s,a)\right]$$

- Bootstrapping speeds up training since values need not be computed from scratch.
- However, errors in early estimates can **propagate and amplify**.
- With function approximation, these errors can affect multiple states that share features.

Key Issue

Bootstrapping + Function Approximation $\Rightarrow$ Persistent and spreading errors.

Off-Policy Learning

- Off-policy methods (e.g., Q-learning) learn from a **behavior policy** π_b that differs from the **target policy** π.
- The learning update uses:

$$Q^{\pi}(s,a) = \mathbb{E}\left[r + \gamma \max_{a'} Q^{\pi}(s',a')\right]$$

- The policy used for exploration may not generate data representative of the optimal policy's state distribution.
- This can cause poor convergence or divergence, especially when combined with function approximation.

Observation

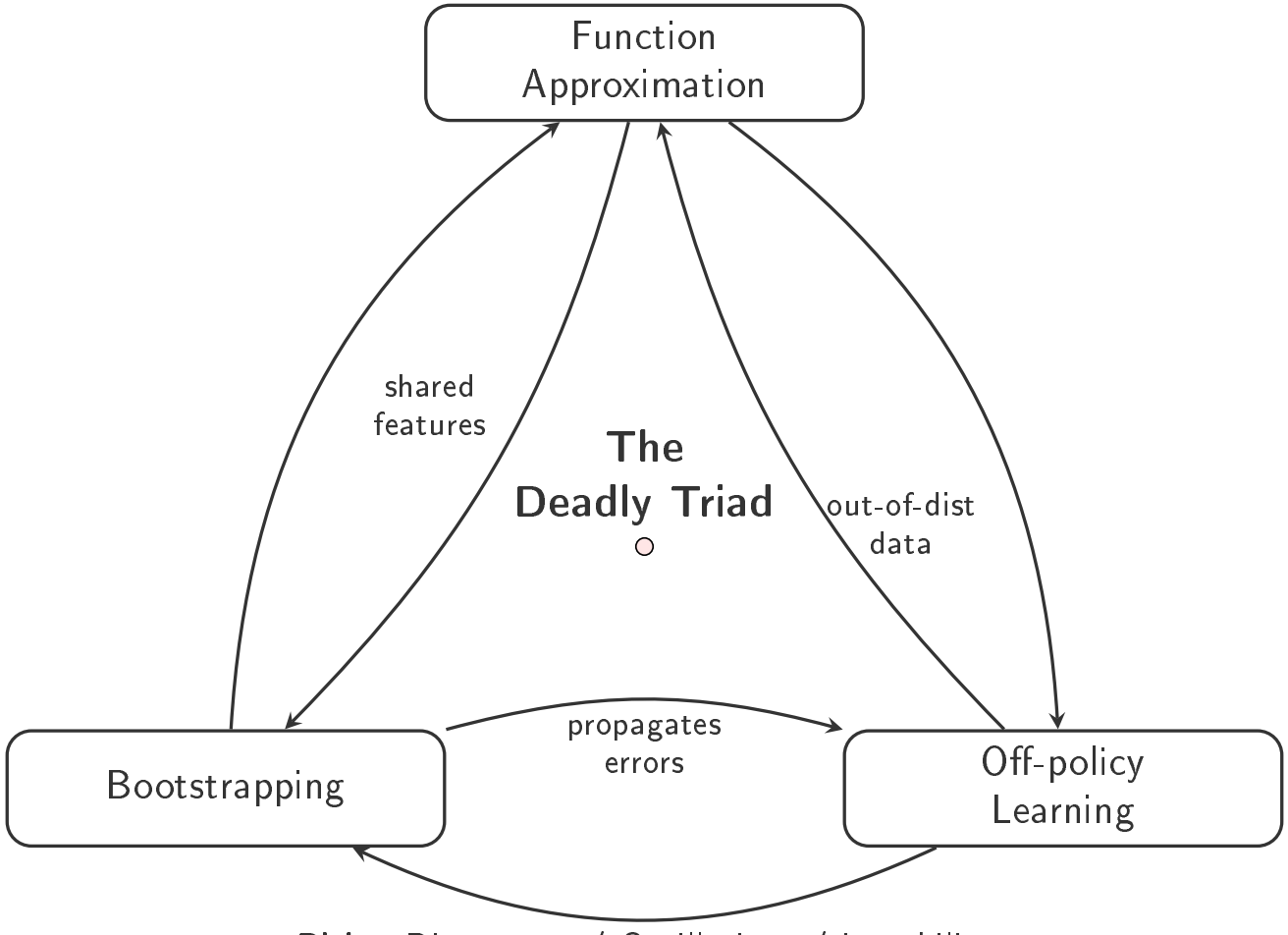
Off-policy learning is less stable than on-policy learning, and stability worsens with nonlinear function approximators.

Interaction of the Triad

- Each element of the triad alone can cause instability.
- Together, they can result in:
  - Divergent Q-values
  - Oscillatory learning
  - Poor convergence
- Example:

  function approx.+bootstrapping+off-policy data $\Rightarrow$ divergence

Illustration of the deadly triad interaction.



Risks: Divergence / Oscillations / Instability

Mitigations: Experience Replay, Target Networks, Double Q, On-policy methods

Avoiding the Deadly Triad

- Several techniques have been developed to mitigate instability:
  - Experience Replay (reduces correlation)
  - Target Networks (stabilize bootstrapping)
  - On-policy algorithms (e.g., SARSA, A3C)
  - Double Q-learning (reduces overestimation bias)
- Stable deep RL became possible with these methods[10].

Key Idea

Breaking at least one link in the triad (approximation, bootstrapping, or off-policy) helps achieve convergence.

[10] Volodymyr Mnih et al. 'Human-level control through deep reinforcement learning'. In: *Nature* 518.7540 (2015), pp. 529–533.