Deep Reinforcement Learning

Overview of main articles
Part 1. Value-based algorithms

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MSU

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Reinforcement Learning [reminder]

MDP

MDP is $\{\mathbb{S}, \mathbb{A}, \mathbb{T}, r\}$:

$\mathbb{S}$ — set of states

$\mathbb{A}$ — set of actions

$\mathbb{T}$ — probability $p(s' \mid s, a)$, where $s, s' \in \mathbb{S}, a \in \mathbb{A}$

r — function $\mathbb{S} \to \mathbb{R}$

RL Goal

We search for policy $\pi : \mathbb{S} \to \mathbb{A}$ which maximizes[1]

$$\mathbb{E} \sum_t r(s_t)$$

[1] over what probability distributions is this expectation?

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This goal does not suit infinite horizon case, so for generalization purposes goal is substituted with

$$\mathbb{E} \sum_t \gamma^t r(s_t)$$

for $\gamma \in (0, 1)$ and is referred as *discounted reward*.

[1] over what probability distributions is this expectation?

Definitions

For convenience[2]:

$$R = \sum_t \gamma^t r(s_t)$$

[2] *What does this random variable depend on?*

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For given policy π:

$$V^\pi(s) = \mathbb{E} R \mid s_0 = s$$

$$Q^\pi(s, a) = \mathbb{E} V(s') \mid s, a$$

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Let π^* be optimal policy.

[2] *What does this random variable depend on?*

Bellman Equation

For every π it's true:

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

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For finite-state case Q^{π^*} is finite vector of unknown values.
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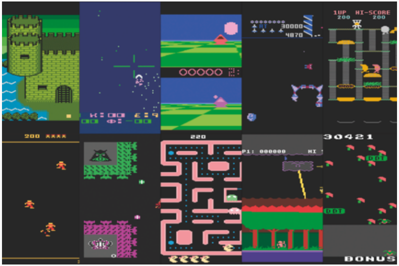
✓ Is a *contraction mapping* $\Rightarrow$ converges.

Deep Q-learning (2014)

Atari

* No prepared features for each game.
* Screen image as input.
* Finite-state case... not quite finite.



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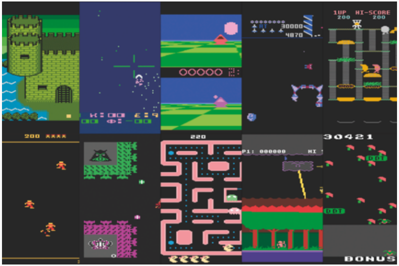
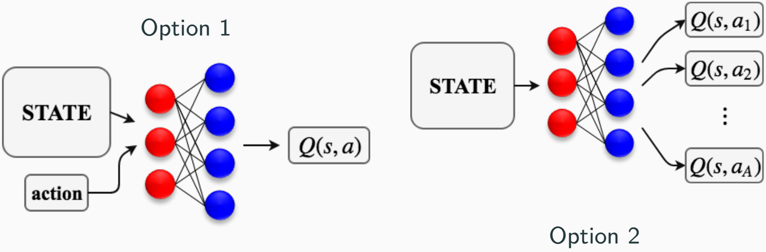


Atari games

We want to approximate $Q(s, a)$ with neural net.

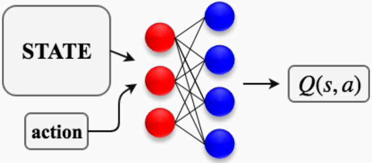
Q-network

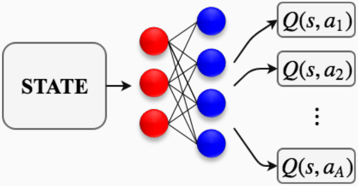


Q-network

Option 1

Requires forward pass for each action[1]





Option 2

Number of actions must be adequate

[1] Is there a case when option 1 might be better?

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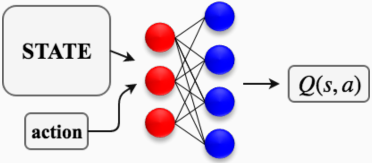

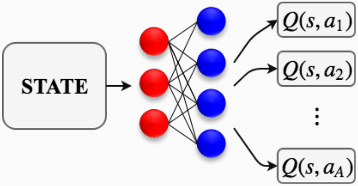

Option 2

Number of actions must be adequate

Atari: up to 18 discrete actions. Use option 2.

[1] Is there a case when option 1 might be better?

TD-learning to gradient descent

TD-learning is «similar» to gradient descent.

$$Q_{t+1}(s, a) = \alpha Q_t(s, a) + (1 - \alpha) \left[r(s') + \max_a Q_t(s', a) \right]$$

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Let $y = r(s') + \max_a Q_t(s',a)$.
If dependence of y from Q is ignored:

$$L = (Q_t(s,a) - y)^2$$

Q-learning

With $Q(s, a)$ as neural net, its parameters θ determine function.

$$Q_{t+1}(s, a, \theta) = Q_t(s, a, \theta) - \eta \nabla_Q L$$

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Let's "translate" gradient descent from space of Q functions to θ!

$$\theta_{t+1} = \theta_t - \beta \nabla_\theta L$$

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Problems:

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- × Target y changes after each step.
- × All theoretical guarantees are lost.

Experience Replay

Utilize all experienced transitions $(s, a, s', r, done)$ for generating a batch for stochastic optimization step.

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Batch of transitions is sampled uniformly from memory.

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Batch of transitions is sampled uniformly from memory.

✓ Decorellates samples.

* Target y can be calculated only for sampled batch.
* Only last N observed transitions may be stored

ε-greedy exploration

Problem: at the very beginning trajectories generated by $\pi(s) = \underset{a}{argmax}\ Q(s, a, \theta)$ are very similar.

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Atari: $\varepsilon(i) = 0.01 + 0.99\, exp\{-\frac{i}{30000}\}$ where i is frames counter. 

Details

- Gray-scale frames were downsampled and cropped to 84x84.
- Last 4 frames[3] were considered as state to satisfy MDP Markov's property.
- Same NN architecture was used for all games: 3 convolutional[4] and 2 feedforward layers.

[3] 3 for Space Invaders cause of laser blinking period
[4] why no max pooling here?

More details

Playing Atari with Deep Reinforcement Learning (2014)

- Reward was restricted to $\{+1, 0, -1\}$. Allowed to use same learning rate for all games.

:(50 hours per game / 10 000 000 frames per game.

:} Bought by Google after 7 games.

Stabilizing Q-learning

Unstability

Recall our target on each step:

$$y(s', r) = r + \max_{a'} Q(s', a', \theta)$$

- Changes each frame
- Formally depends on θ
- "Correlates" with actions chosen during playing
- Tends to overestimate true $V(s')$

$\Rightarrow$ loss is completely unstable and can even diverge.

Target network (2015)

Change the target not every step, but each K-th step.

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For this purpose:

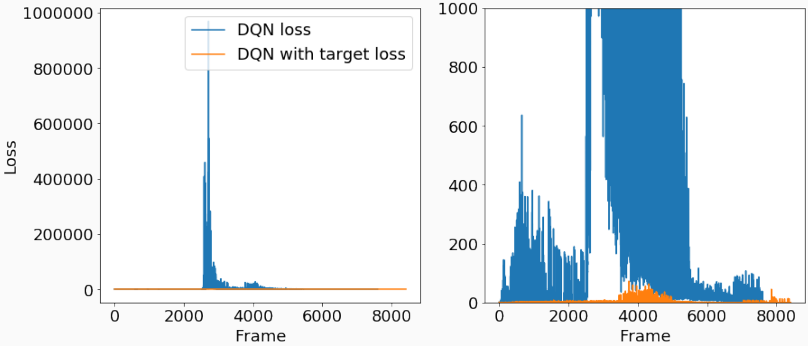
- Make a copy of Q-network, *target network* Q^{target}
- Use it on every step to calculate

$$y(s', r) = r + \max_{a'} Q^{\text{target}}(s', a')$$

- Each K-th step update Q^{target}'s parameters with current Q-network's weights.

Can be seen on loss

✓ Loss really stabilized!



Value overestimation

Recall our target is proxy of $V^{\pi^*}(s', a')$

$$y(s', r) = r + \max_{a'} Q(s', a')$$

Practice: this proxy overestimates true value of states.

Intuition: this max operator will prefer actions, for which $Q(s', a')$ is overestimating true value due to approximation error or luck.

Action Selection vs Evaluation

Recall Bellman Equation derivation and untangle our target:

$$y(s', r) = r + \max_{a'} Q(s', a') = r + Q(s', \underset{a'}{argmax}\, Q(s', a'))$$

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General idea:

> Use different approximations of Q for evaluation and for selection to avoid *max*.

Two Q-learnings

Basic way to do this:
run two Q-learning algorithms with two approximations of Q^{π^*}: $Q_1(s, a)$ and $Q_2(s, a)$.

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Targets for Q-learnings:

$$y_1 = r + Q_2\left(s', \underset{a'}{argmax}\, Q_1(s', a')\right)$$

$$y_2 = r + Q_1\left(s', \underset{a'}{argmax}\, Q_2(s', a')\right)$$

Double DQN (2015)

Deep Reinforcement Learning with Double Q-learning (2015)

- more convenient way to do this:

Use target network as one of two approximations.

[5] how many backwards?

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- **more convenient way to do this:**

Use target network as one of two approximations.

$$y = r + Q^{\text{target}}(s', \underset{a'}{argmax}\, Q(s', a'))$$

* Keep ignoring dependence of y from θ.
* Requires three forward passes on each step[5].

[5] how many backwards?

Comparing DQNs

Table 1: DQN targets

DQN	target y
Classic Deep Q-learning	$r + Q(s', \underset{a'}{argmax}\, Q(s', a'))$
With target-network	$r + Q^{\text{target}}(s', \underset{a'}{argmax}\, Q^{\text{target}}(s', a'))$
Double Deep Q-learning	$r + Q^{\text{target}}(s', \underset{a'}{argmax}\, Q(s', a'))$

Dueling DQN: Motivation

Note:

* In most states our choice of action does not affect the return.
* After finding $Q(s, a)$ Q-learning still gains no information about $Q(s, a')$ for $a' \neq a$.

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Learning $Q(s,a)$ should lead to learning $V(s)$

Advantage function

Define *advantage* function:

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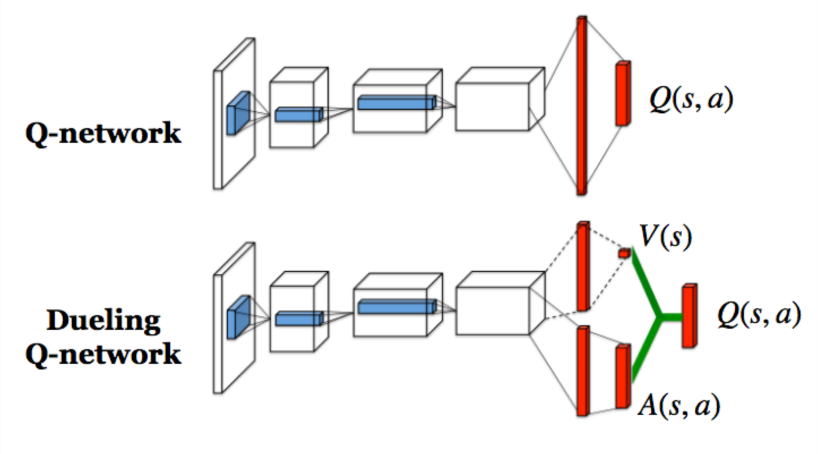
Rewrite Q-function in terms of value of state:

$$Q^\pi(s,a) = V^\pi(s) + A^\pi(s,a)$$

Dueling DQN (2016)

Dueling Network Architectures for Deep Reinforcement Learning (2016)



Dueling Q-network architecture

Struggling with identifiability

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Proposition:

$$Q(s,a) = V(s) + A(s,a) - \max_a A(s,a)$$

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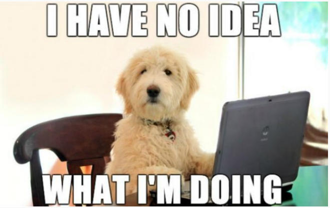

$$Q(s, a) = V(s) + A(s, a) - \underset{a}{mean}\, A(s, a)$$

suddenly worked better.

Dueling DQN: Results

✓ Learning $Q(s, a)$ leads to correcting $V(s)$.

* Only network architecture is changed.
* Double DQN still works for dueling architecture.

Prioritized replay memory (2015)

Motivation

In standard DQN we sample batch of transitions from replay memory uniformly.

- × Some transitions are more important than others
- × Replay memory is full of almost useless transitions

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$\delta = |y(s', r, done) - Q(s, a)|$ is
a good proxy of transition importance

Prioritized Replay Memory (2015)

Prioritized Experience Replay (2015):

$$p(\mathcal{T}) \propto \delta(\mathcal{T})^{\alpha}$$

Authors found $\alpha \approx 0.6$ is a good universal value. 

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Problems:

- × On each step this probability changes for all the replay memory [6]

[6] which capacity is on the order of 1M transitions

Prioritized Replay Memory (2015)

Prioritized Experience Replay (2015):

$$p(\mathcal{T}) \propto \delta(\mathcal{T})^{\alpha}$$

Authors found $\alpha \approx 0.6$ is a good universal value. 

Problems:

- $\times$ On each step this probability changes for all the replay memory [6]
  - $\approx$ on each step update δ only for the currently sampled batch

[6] which capacity is on the order of 1M transitions

Prioritized Replay Memory (2015)

Prioritized Experience Replay (2015):

$$p(\mathcal{T}) \propto \delta(\mathcal{T})^{\alpha}$$

Authors found $\alpha \approx 0.6$ is a good universal value. 

Problems:

- $\times$ On each step this probability changes for all the replay memory [6]
  - $\approx$ on each step update δ only for the currently sampled batch
- $\times$ Introduces bias (transitions are now sampled from hell knows what distribution).

[6] which capacity is on the order of 1M transitions

Background: Importance Sampling

For arbitrary distribution $q(x)$:

$$\begin{aligned}\mathbb{E}_{p(x)} f(x) = \int p(x) f(x) dx = \int \frac{q(x)}{q(x)} p(x) f(x) dx = \\ = \int q(x) \frac{p(x)}{q(x)} f(x) dx = \mathbb{E}_{q(x)} \frac{p(x)}{q(x)} f(x)\end{aligned}$$

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Applying Importance Sampling

If N is replay memory capacity:

$$L = \mathbb{E}_{\mathcal{T} \sim uniform}(y - Q(s,a))^2 = \mathbb{E}_{\mathcal{T} \sim prioritized} \frac{1}{Np(\mathcal{T})}(y - Q(s,a))^2$$

IS just adds weights to our batch:

$$w_i = \frac{1}{Np(\mathcal{T}_i)}$$

Annealing weights

Problem: at the beginning these weights might not be that relevant, yet slowing down learning.

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Let's smooth them at the beginning of learning:

$$L = \mathbb{E}_{\mathcal{T} \sim prioritized} \left(\frac{1}{Np(\mathcal{T})} \right)^{\beta} (y - Q(s, a))^2,$$

where β changes from 0.4 to 1 linearly during first 100 000 frames. 

Hints

* Weights significantly vary scale of loss function. Constant learning rate might be inappropriate.

  Hint:[7] normalize weights by dividing on $\max_i w_i$.

[7] max taken over all replay memory. Yet in some implementations it is taken over current batch

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* new transitions are stored with maximum priority.

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Noisy networks for exploration (2017)

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Noisy Nets for Exploration (2017):

$$w_i = \mu_i + \sigma_i \varepsilon_i, \quad \varepsilon \sim \mathcal{N}(0, 1)$$

* μ_i, σ_i are both learnable parameters.
* all weights are independent random variables
* use policy $\pi(s) = \underset{a}{argmax}\, Q(s, a, \mu, \sigma, \varepsilon)$

Optimized Loss

Formally, our loss[8] is now:

$$\mathbb{E}_{\varepsilon}\mathbb{E}_{\mathcal{T}}(Q(s, a, \theta, \varepsilon) - y(\mathcal{T}))^2$$

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* use different noise samples for it:

$$y = r + Q(s', \underset{a'}{argmax}\, Q(s', a', \varepsilon''), \varepsilon')$$

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Noise generation optimization

Problem: noise generation turns to be a bottleneck in terms of wall-clock time.

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  * for whole batch![10]

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[10] is this theoretically coherent?

Application tips

- ✓ No hyperparameters
  - * Except where to put noise in the network... Convolution layers better leave deterministic[11].

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  * yet ε-greedy strategy may also be used

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Categorical DQN (2017)

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Consider a state where you get 1000 or -1000 with probabilities 0.5.

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Learn a distribution over future reward instead of it's expectation.

Value Distribution

Recall

$$Q^\pi(s, a) = \mathbb{E} \sum_t r(s_t) \mid s, a$$

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For fixed policy π let's define *value distribution*:

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! It's a random variable!

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Value distribution satisfies a *recursive distributional equation*:

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✓ yes, for $d(Z_1, Z_2) = \sup\limits_{s,a} \mathcal{W}(Z_1(s,a), Z_2(s,a))$, where $\mathcal{W}$ is Wasserstein distance between two random variables.

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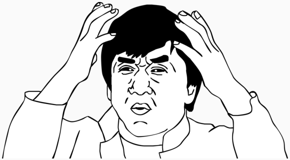

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Let's do point iteration anyway! Our wish:

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Loss

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* KL requires Z_{t+1} and Z_θ share domain.

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Options:

- Gaussian mixture
- Discrete

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Let's $\mathcal{P}$ be a family of categorical distribution on the grid from $V_{\min}$ to $V_{\max}$ with N atoms (outcomes).

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Let's $\mathcal{P}$ be a family of categorical distribution on the grid from $V_{\min}$ to $V_{\max}$ with N atoms (outcomes).

Parametrization:
For each action our neural network $Z(s, a)$ outputs N numbers, summing into 1

Calculating target

Suppose you have transition $(s, a, r, s', done)$, $Z(s, a) \in \mathcal{P}$. Then:

$$y(s') = r + \gamma Z(s', \max_{a'} \mathbb{E} Z(s', a'))$$

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Suppose you have transition $(s, a, r, s', done)$, $Z(s, a) \in \mathcal{P}$. Then:

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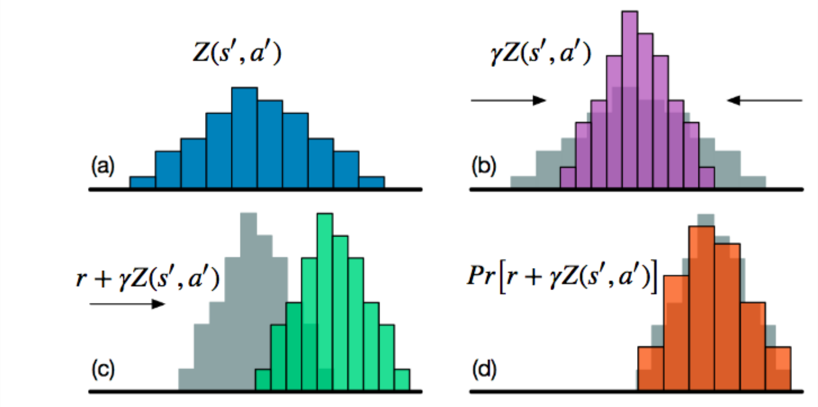

How it looks like

Failed to insert video into beamer ;o)

Rainbow DQN (2018)

Blend them all!

Multistep DQN: Motivation

Recall our target in classic DQN:

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

If we have nonzero reward at the end of M-step game, we need at least M iterations of Q-learning to «propagate» this reward to all visited states.

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Look more than one step ahead!

Multistep DQN: Realisation

- work with transitions $(s, a, r, r', r'', \ldots, r^{(M-1)}, s^{(M)}, done)$

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$\times$ formally can be used only with on-policy algorithms [14]

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$\times$ formally can be used only with on-policy algorithms [14]

$\times$ the further we look the worser y approximates $Q^{\pi^*}(s, a)$

$\Rightarrow$ number of steps should be chosen carefully.

[14] why?

Multistep Categorical DQN

Recall categorical DQN target:

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Loss stays the same:

$$L = \mathrm{KL}(p(y) \parallel p(Z))$$

Dueling Categorical DQN

Recall dueling DQN:

$$Q(s, a) = V(s) + A(s, a) - \underset{a}{mean}\, A(s, a)$$

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where $V_N(s)$ and $A_N(s,a)$ are categorical N-atomed distributions. 

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$$Z(s, a) = softmax(V_N(s) + A_N(s, a) - \underset{a}{mean}\, A_N(s, a))$$

where $V_N(s)$ and $A_N(s, a)$ are arbitrary N numbers[15]

[15] why couldn't we only add softmax?

Double dueling multi-step noised categorical DQN with prioritized replay AKA Rainbow

Rainbow: Combining Improvements in Deep Reinforcement Learning (2018):

Dueling + Multistep + Categorical + DQN +

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$$y = R + \gamma^N Z^{\text{target}}(s^{(N)}, \underset{a^{(N)}}{argmax}\, Z(s^{(N)}, a^{(N)}))$$

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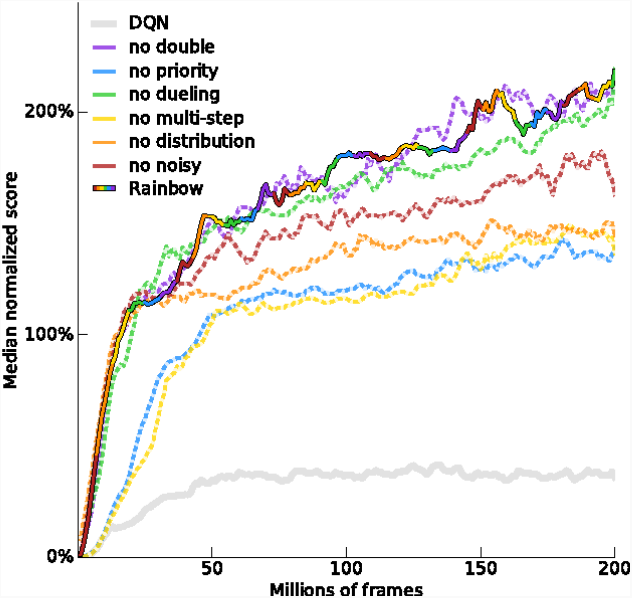
- **Noisy:** add noise to all fully connected layers
- **Prioritized Replay:** just use it[16]

[16] guess proxy of transition priority

Do we really need all this?



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Rainbow: resume

- * all improvements are important as they address different problems
- $\times$ a lot of hyperparameters
- ? Allegedly 10 hours for 7M frames on single GPU
  - :(I can't reproduce [17]

[17] 10 hours for 3M. Noise generation seems to be a problem!

Quantile Regression (2017)

Motivation

Categorical DQN was an obviously reconnaissance step into the field of *distributional RL*.

- $\times$ Proposed optimization step ignores Wasserstein's metric, for which some theoretical guarantees of converges persist.
- $\times$ KL-divergence can't be used for distributions with disjoint support, which limits $Z_\theta(s, a)$ to artificial boundaries.

Background: Wasserstein Metric

Let $F_Y(w), F_U(w)$ be cumulative distribution functions (CDF), i.e.

$$F_Y(x) = P(Y < x)$$
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$$F_Y^{-1}(\tau) = inf\{x \in \mathbb{R} \mid \tau \leq F_Y(x)\}$$
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p-Wasserstein Metric

$$W_p(Y, U) = \left(\int_0^1 |F_Y^{-1}(\tau) - F_U^{-1}(\tau)|^p d\tau \right)^{\frac{1}{p}}$$

Convergence properties

Recall distributional Bellman equation for given policy π:

$$Z^{\pi}(s, a) \overset{\mathrm{D}}{=} r + \gamma Z^{\pi}(s', a'), \quad a' \sim \pi(s') \tag{3}$$

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Let introduce the following metric in the space $\mathbb{Z} : \mathbb{S} \times \mathbb{A} \to \mathcal{P}(\mathbb{R})$:

$$D_p(Z_1, Z_2) = \sup_{s,a} \left[W_p(Z_1(s,a), Z_2(s,a)) \right] \tag{4}$$

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Theorem

Policy iteration update for 3 in $\mathbb{Z}$ is a contraction mapping for metric 4

QR-DQN Key Idea

Categorical DQN:

* fixed support (i.e. -10, -9.5 . . . 9.5, 10)
* variable probabilities (output of neural net)
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Distributional Reinforcement Learning with Quantile Regression (2017):

* variable support (output of neural net)
* fixed probabilities (i.e. 0, 0.1 . . . 0.9, 1)
* Wasserstein minimized

Optimization step goal

Let Z_θ be a family of *uniform* categorical distributions on the support $\{\theta_1 \ldots \theta_N\}$ for some fixed number of atoms N.

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$$y(\mathcal{T}) = p\left(r + (1 - \text{done})\gamma Z\left(s', \underset{a'}{argmax}\, \mathbb{E} Z(s', a')\right)\right)$$

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Note that if $\forall s, a\colon p\left(Z(s, a)\right)) \in Z_\theta$, then $y \in Z_\theta$!

✓ projection step is no longer required!

$$\text{Loss}(\mathcal{T}) \quad = \quad W_p(y(\mathcal{T}), Z(s, a))$$

The ambush!

Recall that $y(\mathcal{T})$ is also a random variable, sampled from environment dynamics...

Theorem

Let $Y(s,a)$ denote $y(s')$, where $s' \sim p(s' \mid s,a)$ and not taken fixed from experience replay. Then in general:

$$\underset{Z}{argmin}\, \mathbb{E} W_p(y(\mathcal{T}), Z(s,a)) \neq \underset{Z}{argmin}\, W_p(Y(s,a), Z(s,a))$$

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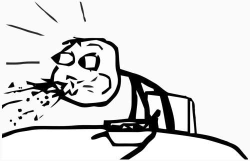

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We want to minimize the following distance:

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Quantiles direct optimization

Proposition

$$\min_{\theta_i} \int_{\frac{i-1}{N}}^{\frac{i}{N}} |F_Y^{-1}(\tau) - \theta_i| d\tau = \left\{ \theta \mid F_Y(\theta) = \frac{\frac{i-1}{N} + \frac{i}{N}}{2} \right\}$$

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Let's denote $\hat{\tau}_i = \frac{\frac{i-1}{N} + \frac{i}{N}}{2}$

Maybe we can directly optimize θ_i
with unbiased estimation of $F_Y^{-1}(\hat{\tau}_i)$

Background: Quantile Regression

Quantile Regression

For any random variable Y and $\tau \in [0, 1]$:

$$F_Y^{-1}(\tau) = \underset{x}{argmin}\, \mathbb{E}_Y (Y - x)\, (\tau - \mathbb{I}[Y < x])$$

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Proof.

$$\nabla_x \mathbb{E}_Y (Y - x)\,(\tau - \mathbb{I}[Y < x]) = \mathbb{E}_Y\,(\mathbb{I}[Y < x] - \tau) = 0$$

$$\int_{-\infty}^{x} dF_Y(Y) = \tau$$

$$F_Y(x) = \tau$$

$$x = F_Y^{-1}(\tau)$$

Quantile Regression Loss

For every quantile θ_i our loss is defined as:

$$\text{Loss}_{QR}(\theta_i) = \mathbb{E}_Y (Y - \theta_i)\left(\hat{\tau}_i - \mathbb{I}[Y < \theta_i]\right)$$

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&\approx \mathbb{E}_{y(s')} \nabla (y(s') - \theta_i)\left(\hat{\tau}_i - \mathbb{I}[y(s') < \theta_i]\right) \quad s' \sim p(s' \mid s, a)
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✓ this is an unbiased estimation of true quantiles!

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  - ✓ this expectation can be calculated.

Theoretical guarantees

For table-case instead of gradient optimization of NN weights we perform the following table update step:

$$\theta(s, a)_i = \underset{\theta_i}{argmin}\, \mathbb{E}_y (y - \theta_i)\left(\hat{\tau}_i - \mathbb{I}[y < \theta_i]\right) \tag{5}$$

Theoretical guarantees

For table-case instead of gradient optimization of NN weights we perform the following table update step:

$$\theta(s, a)_i = \underset{\theta_i}{argmin}\, \mathbb{E}_y (y - \theta_i)\left(\hat{\tau}_i - \mathbb{I}[y < \theta_i]\right) \tag{5}$$

Theorem

Point iteration method, applied for (5), converges for metric

$$D_p(Z_1, Z_2) = \sup_{s,a}\left[W_p(Z_1(s, a), Z_2(s, a))\right]$$

for $p \in [1, \infty]$. Moreover, for $p = +\infty$ update step is a contraction mapping, for $p < +\infty$ it may be not.

QR-DQN: Results

Convergence guarantees

	table-case	deep
DQN	✓	×
Categorical DQN	×	×
QR-DQN	✓ 	×

QR-DQN: Results

Convergence guarantees

	table-case	deep
DQN	✓	×
Categorical DQN	×	×
QR-DQN	✓ 	×

- ✓ allows arbitrary support; we do not need to bound the range of $Z(s, a)$ like we did in Categorical DQN.
- ✓ same computational cost as Categorical DQN.
- ! Rainbow QR-DQN is yet in the making ;o)

NEXT: see pt.2 for Policy Gradient algorithms