A distributional perspective on RL

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From “A Distributional Perspective on Reinforcement Learning”, Marc G. Bellemare, Will Dabney, Remi Munos. ICML (2017)

Classic perspective

- Transition operator

$$P^\pi : \mathbb{R}^{|\mathcal{S}|\times|\mathcal{A}|} \to \mathbb{R}^{|\mathcal{S}|\times|\mathcal{A}|}$$

$$P^\pi Q(s,a) := \mathbb{E}_{s'|s,a}\mathbb{E}_{a'|s'}Q(s',a')$$

- Bellman operator

$$\mathcal{T}^\pi : \mathbb{R}^{|\mathcal{S}|\times|\mathcal{A}|} \to \mathbb{R}^{|\mathcal{S}|\times|\mathcal{A}|}$$

$$\mathcal{T}^\pi Q(s,a) := R(s,a) + \gamma P^\pi Q(s,a)$$

- Bellman equation

$$Q(s,a) = \mathcal{T}^\pi Q(s,a)$$

Distributional perspective

- Probability distribution

  $Z(s, a) \sim q(z|s, a)$

- Value distribution

  $$Q(s, a) = \mathbb{E}_{z|s,a} Z(s, a) = \sum_z z q(z|s, a)$$

- Set of value distributions $\mathcal{Z}$

Distributional perspective

- Distributional transition operator

  $P_D^\pi : \mathcal{Z} \to \mathcal{Z}$

  $P_D^\pi Z(s,a) := \mathbb{E}_{s'|s,a} \mathbb{E}_{a'|s'} Z(s',a')$

- Distributional Bellman operator

  $\mathcal{T}_D^\pi : \mathcal{Z} \to \mathcal{Z}$

  $\mathcal{T}_D^\pi Z(s,a) := R(s,a) + \gamma P_D^\pi Z(s,a)$

- Distributional Bellman equation

  $Z(s,a) \overset{D}{=} \mathcal{T}_D^\pi Z(s,a)$

Distributional —> Classic

- Distributional Bellman equation

$$Z(s,a) \overset{D}{=} \mathcal{T}_D^\pi Z(s,a)$$

$$\mathbb{E}_{z|s,a} Z(s,a) = \mathbb{E}_{z|s,a} \mathcal{T}_D^\pi Z(s,a)$$

$$Q(s,a) = \mathbb{E}_{z|s,a} R(s,a) + \gamma \mathbb{E}_{z|s,a} \mathbb{E}_{s'|s,a} \mathbb{E}_{a'|s'} Z(s',a')$$

$$Q(s,a) = R(s,a) + \gamma \mathbb{E}_{s'|s,a} \mathbb{E}_{a'|s'} \mathbb{E}_{z|s',a'} Z(s',a')$$

- Classic Bellman equation

$$Q(s,a) = R(s,a) + \gamma P^\pi Q(s,a)$$

Probability distance

- Distributional Bellman equation

  $Z(s,a) \overset{D}{=} \mathcal{T}_D^{\pi} Z(s,a)$

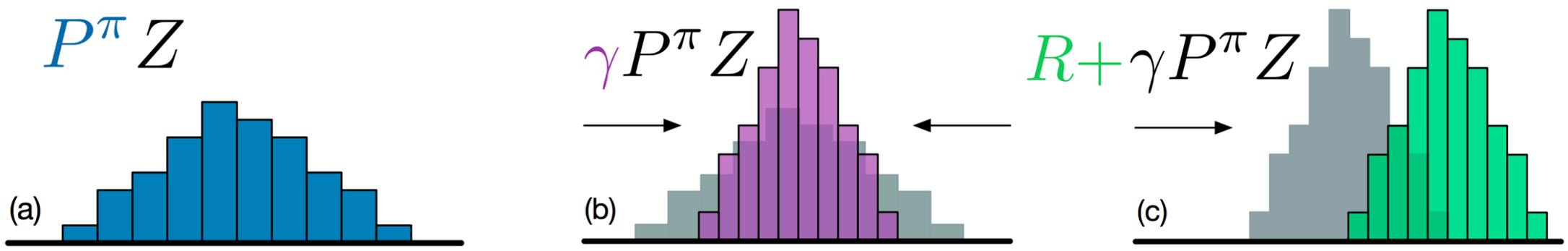
- How to define probability distance ?
  - Kullback-Leibler divergence
  - Total variation
  - Wasserstein metric

KL divergence

- Kullback-Leibler divergence

$$D_{\mathrm{KL}}(p\|q) = \mathbb{E}_p\left[\log \frac{p(z)}{q(z)}\right]$$

- Problem: goes to infinity if distributions have disjoint supports $D_{\mathrm{KL}}(p\|q) = \infty$

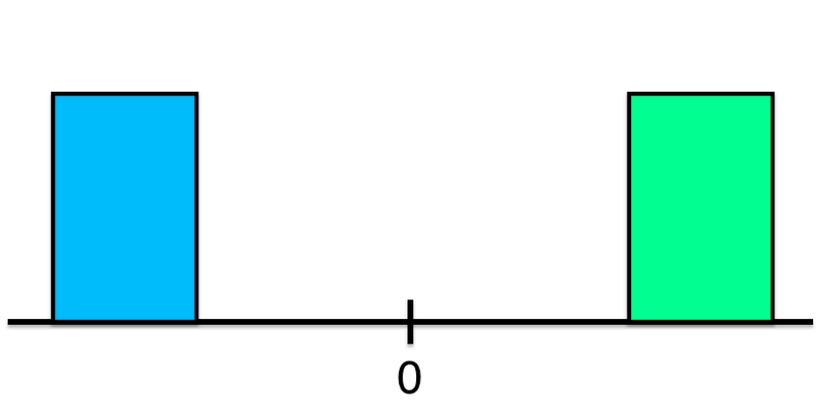


Total variation

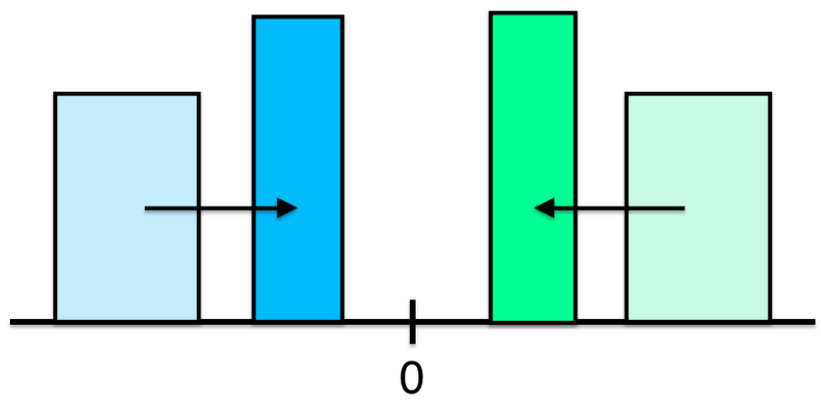
- Total variation

$$D_{\mathrm{TV}}(p\|q) = \sup_{A\in\mathcal{F}} |p(A) - q(A)|$$

- Problem: distance may remain the same after shift



$D_{\mathrm{TV}}(p\|q) = 1$

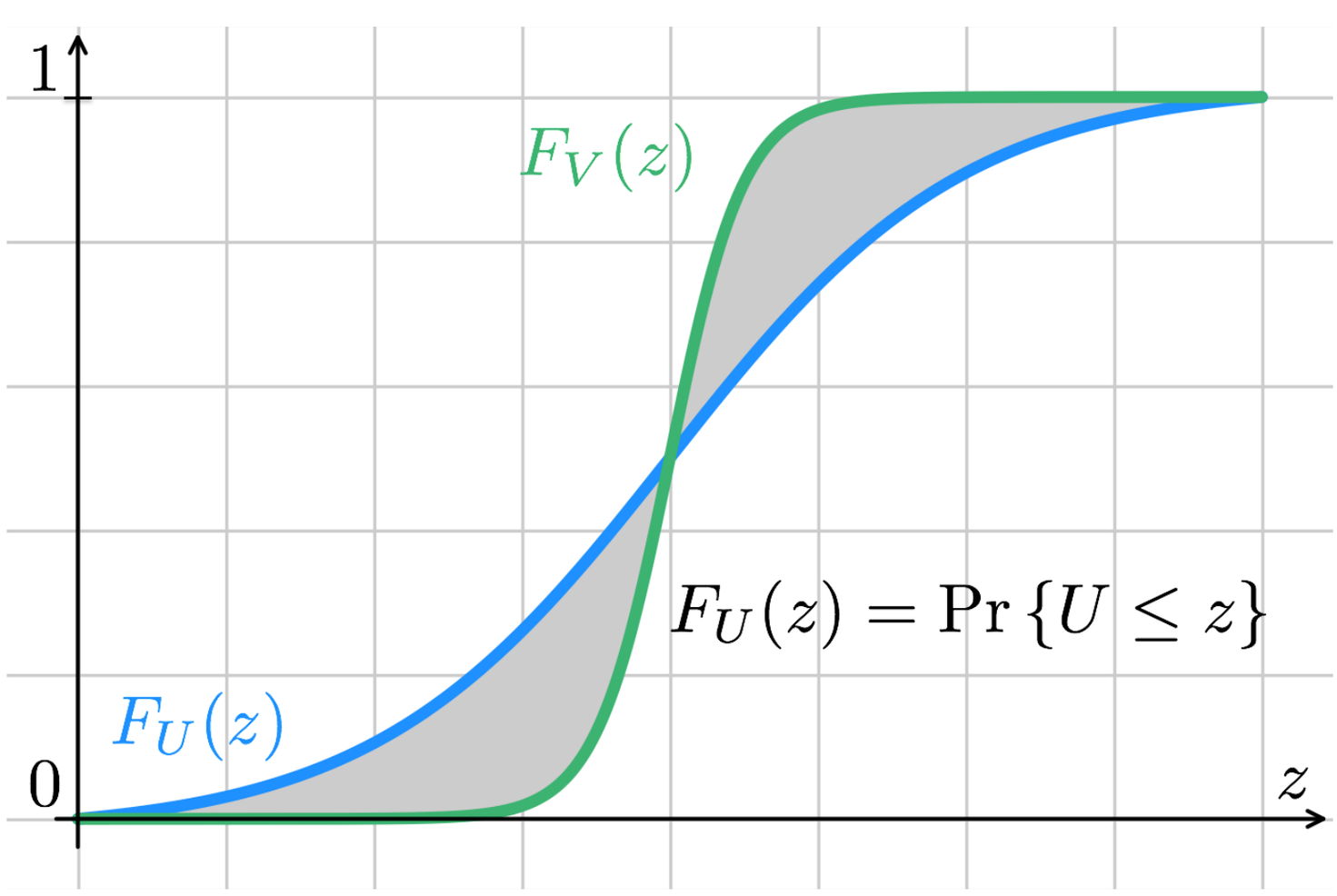


$D_{\mathrm{TV}}(p\|q) = 1$

Wasserstein metric

- Wasserstein metric

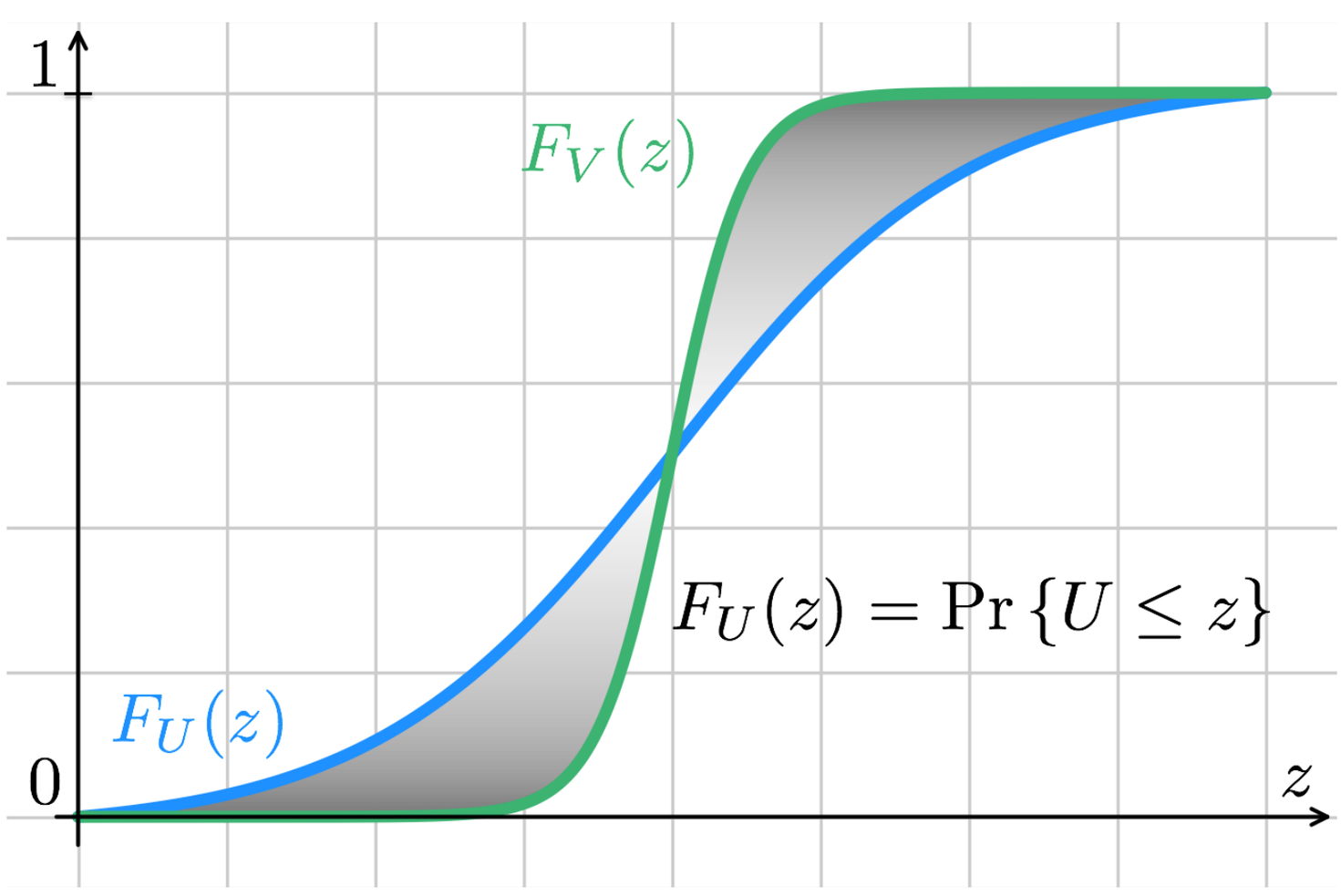
$$w_1(U,V) = \int_0^1 \left| F_U^{-1}(y) - F_V^{-1}(y) \right| dy$$



Wasserstein metric

- Wasserstein metric

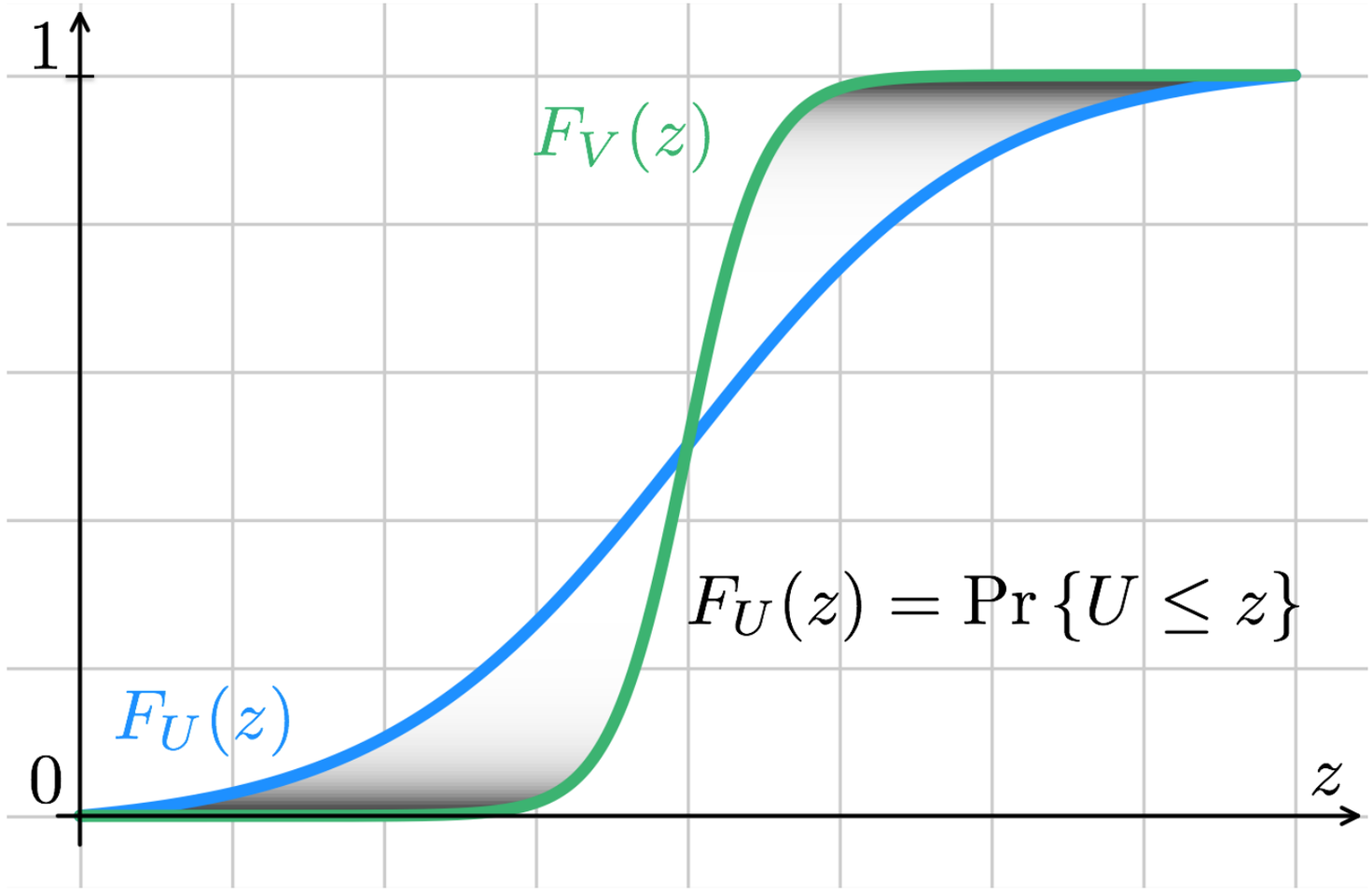
$$w_2(U,V) = \left(\int_0^1 \left| F_U^{-1}(y) - F_V^{-1}(y) \right|^2 dy \right)^{\frac{1}{2}}$$



Wasserstein metric

- Wasserstein metric

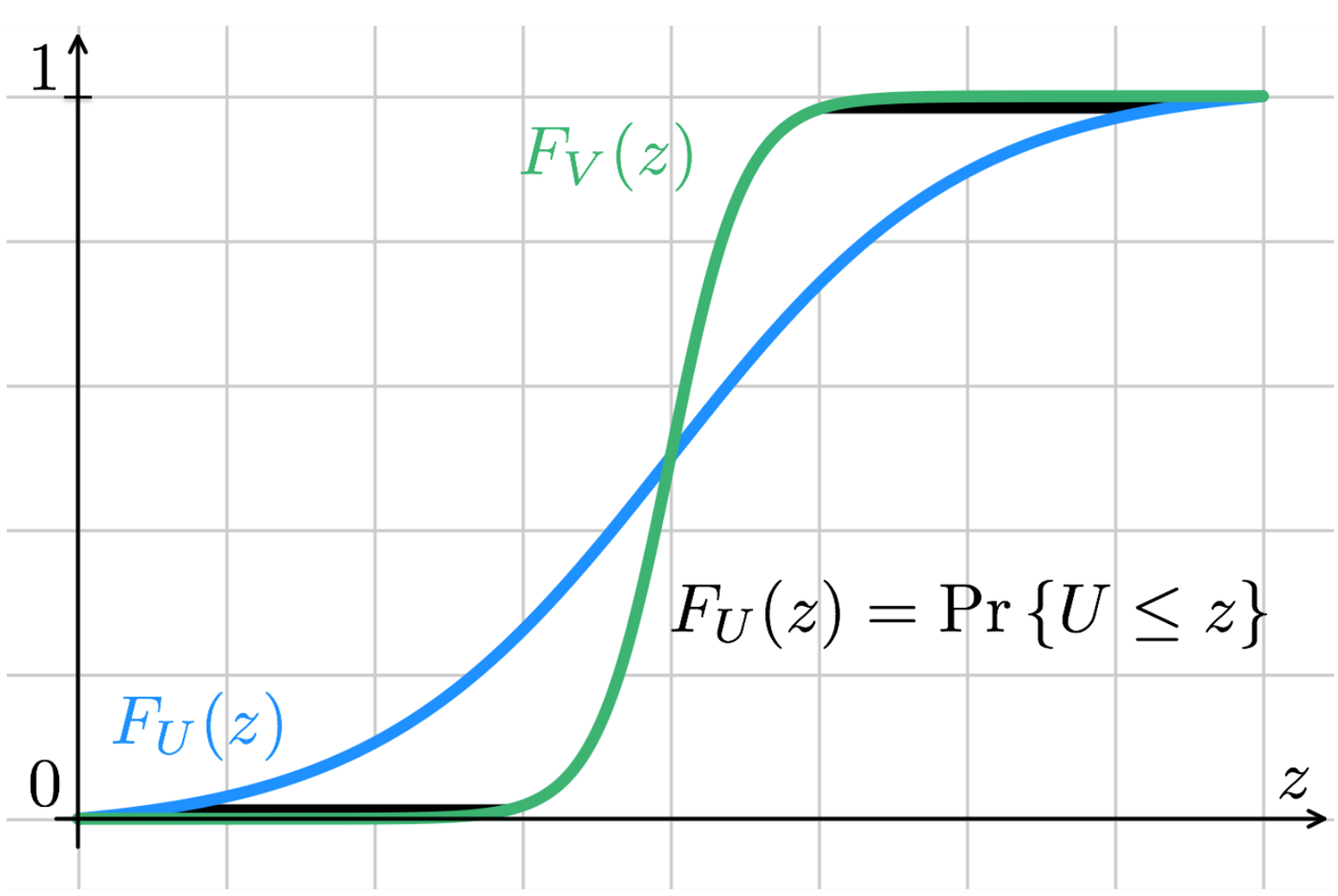
$$w_p(U,V) = \left(\int_0^1 \left| F_U^{-1}(y) - F_V^{-1}(y) \right|^p dy \right)^{\frac{1}{p}}$$



Wasserstein metric

- Wasserstein metric

$$w_\infty(U,V) = \sup_{0\le y\le 1} \left|F_U^{-1}(y) - F_V^{-1}(y)\right|$$



Metric properties

- Wasserstein metric properties

  $w_p(A+U, A+V) \leq w_p(U,V)$

  $w_p(aU, aV) \leq |a| w_p(U,V)$

  $w_p(AU, AV) \leq \|A\|_p w_p(U,V)$

- Maximal form of the Wasserstein metric

  $\bar{w}_p(Z_1, Z_2) := \sup_{s,a} w_p(Z_1(s,a), Z_2(s,a))$

Metric properties

- Wasserstein metric properties

  $w_p(A+U, A+V) \leq w_p(U,V)$

  $w_p(aU, aV) \leq |a| w_p(U,V)$

  $w_p(AU, AV) \leq \|A\|_p w_p(U,V)$

- Maximal form of the Wasserstein metric

  $\bar{w}_p(\mathcal{T}^\pi Z_1, \mathcal{T}^\pi Z_2) = \bar{w}_p(R + \gamma P^\pi Z_1, R + \gamma P^\pi Z_2)$

Metric properties

- Wasserstein metric properties

$$w_p(A+U, A+V) \leq w_p(U, V)$$

$$w_p(aU, aV) \leq |a| w_p(U, V)$$

$$w_p(AU, AV) \leq \|A\|_p w_p(U, V)$$

- Maximal form of the Wasserstein metric

$$\begin{aligned}\bar{w}_p(\mathcal{T}^\pi Z_1, \mathcal{T}^\pi Z_2) &= \bar{w}_p(R + \gamma P^\pi Z_1, R + \gamma P^\pi Z_2) \\ &\leq \bar{w}_p(\gamma P^\pi Z_1, \gamma P^\pi Z_2) \\ &\leq \gamma \bar{w}_p(P^\pi Z_1, P^\pi Z_2) \\ &\leq \gamma \bar{w}_p(Z_1, Z_2)\end{aligned}$$

Policy evaluation

- <u>Classic</u>

  The Bellman operator $\mathcal{T}^\pi : \mathbb{R}^{|\mathcal{S}|\times|\mathcal{A}|} \to \mathbb{R}^{|\mathcal{S}|\times|\mathcal{A}|}$

  $\mathcal{T}^\pi Q(s,a) := R(s,a) + \gamma P^\pi Q(s,a)$

  is a $\gamma-$contraction in l_∞.

- <u>Distributional</u>

  The Bellman operator $\mathcal{T}_D^\pi : \mathcal{Z} \to \mathcal{Z}$

  $\mathcal{T}_D^\pi Z(s,a) := R(s,a) + \gamma P_D^\pi Z(s,a)$

  is a $\gamma-$contraction in $\bar{w}_p,\ 1 \le p \le \infty$.

Control

- Definition. An optimal value distribution is the value distribution of an optimal policy. The set of optimal value distributions is $\mathcal{Z}^* := \left\{ Z^{\pi^*} : \pi^* \in \Pi^* \right\}$

- Definition. The set of greedy policies for $Z \in \mathcal{Z}$ is

$$\mathcal{G}_Z := \left\{ \pi : \sum_{a \in \mathcal{A}} \pi(a|s) \mathbb{E} Z(s,a) = \max_{a' \in \mathcal{A}} \mathbb{E} Z(s,a') \right\}.$$

- Definition. A distributional Bellman opt. operator $\mathcal{T}_D Z(s,a) := \mathcal{T}_D^\pi Z(s,a)$ for some $\pi \in \mathcal{G}_\pi$.

Control

- <u>Classic</u>

  The Bellman opt. operator $\mathcal{T} : \mathbb{R}^{|\mathcal{S}|\times|\mathcal{A}|} \to \mathbb{R}^{|\mathcal{S}|\times|\mathcal{A}|}$

  $$\mathcal{T}Q(s,a) := R(s,a) + \gamma \mathbb{E}_{s'|s,a} \max_{a' \in \mathcal{A}} Q(s,a')$$

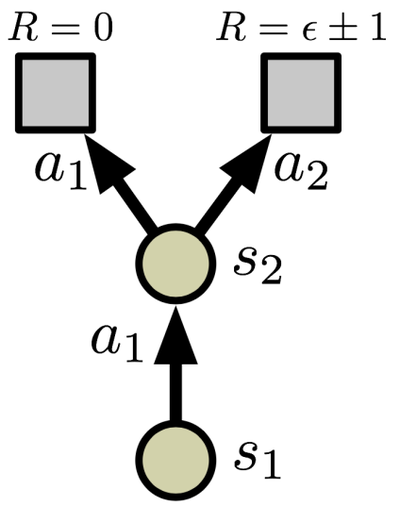
  is a $\gamma-$contraction in l_∞.

- <u>Distributional</u>

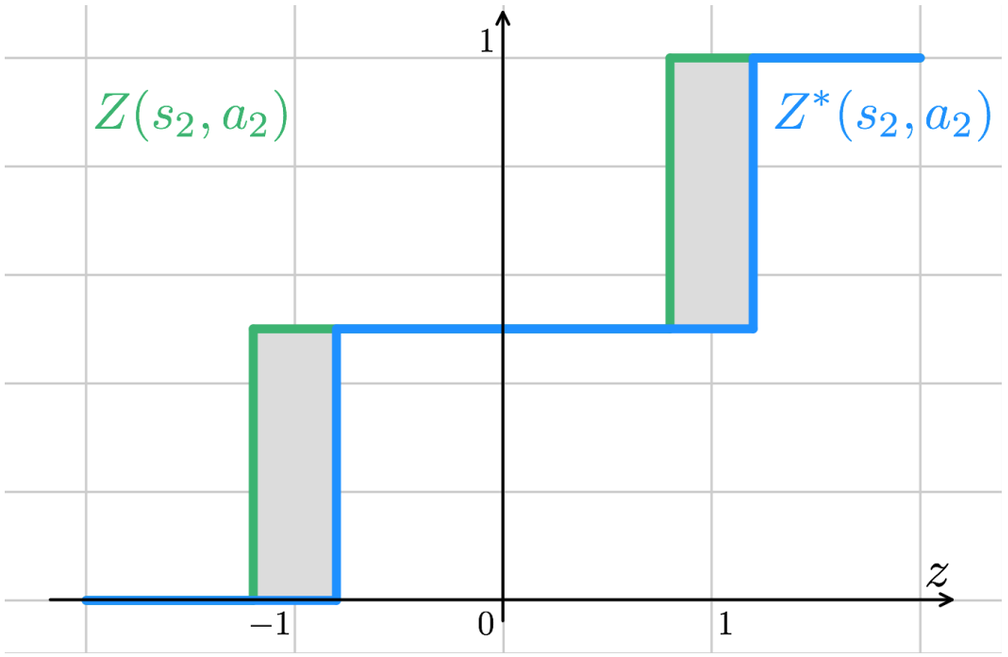
  The Bellman opt. operator $\mathcal{T}_D : \mathcal{Z} \to \mathcal{Z}$

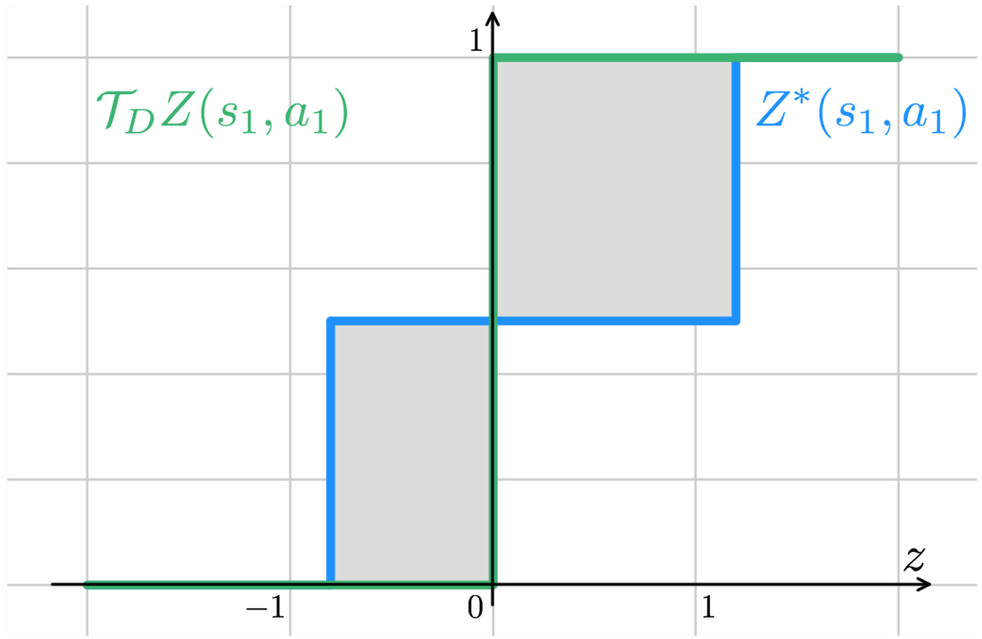
  is not a $\gamma-$contraction in $\bar{w}_p,\ 1 \leq p \leq \infty$.

Non-contraction example



	s_1, a_1	s_2, a_1	s_2, a_2
Z^*	$\epsilon \pm 1$	0	$\epsilon \pm 1$
Z	$\epsilon \pm 1$	0	$-\epsilon \pm 1$
$\mathcal{T}_D Z$	0	0	$\epsilon \pm 1$

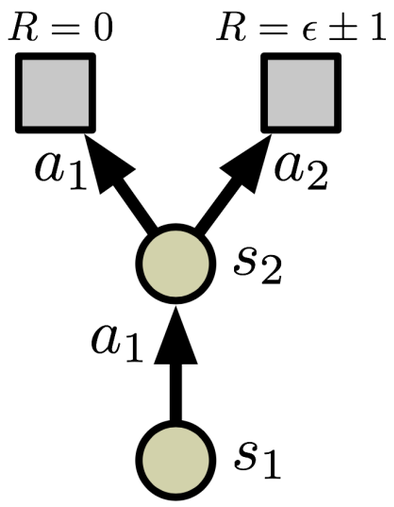




$$\bar{w}_1(Z, Z^*) = w_1(Z(s_2, a_2), Z^*(s_2, a_2)) = \frac{1}{2}2\epsilon + \frac{1}{2}2\epsilon = 2\epsilon$$

$$\bar{w}_1(\mathcal{T}_D Z, \mathcal{T}_D Z^*) = w_1(\mathcal{T}_D Z(s_1, a_1), Z^*(s_1, a_1)) = \frac{1}{2}(1-\epsilon) + \frac{1}{2}(1+\epsilon) = 1$$

Non-fixed point example



	s_1, a_1	s_2, a_1	s_2, a_2
Z^*	$\epsilon \pm 1$	0	$\epsilon \pm 1$
Z	$\epsilon \pm 1$	0	$-\epsilon \pm 1$
$\mathcal{T}_D Z$	0	0	$\epsilon \pm 1$

$$\mathcal{T}_D Z(s_1,a_1) = \begin{cases} Z(s_2,a_2), \ Z(s_1,a_1) = 0; \\ Z(s_2,a_1), \ Z(s_1,a_1) \neq 0. \end{cases}$$

$$(\mathcal{T}_D)^k Z^*(s_1,a_1) = \begin{cases} Z^*(s_2,a_1), \ k = 2l; \\ Z^*(s_2,a_2), \ k = 2l+1. \end{cases}$$

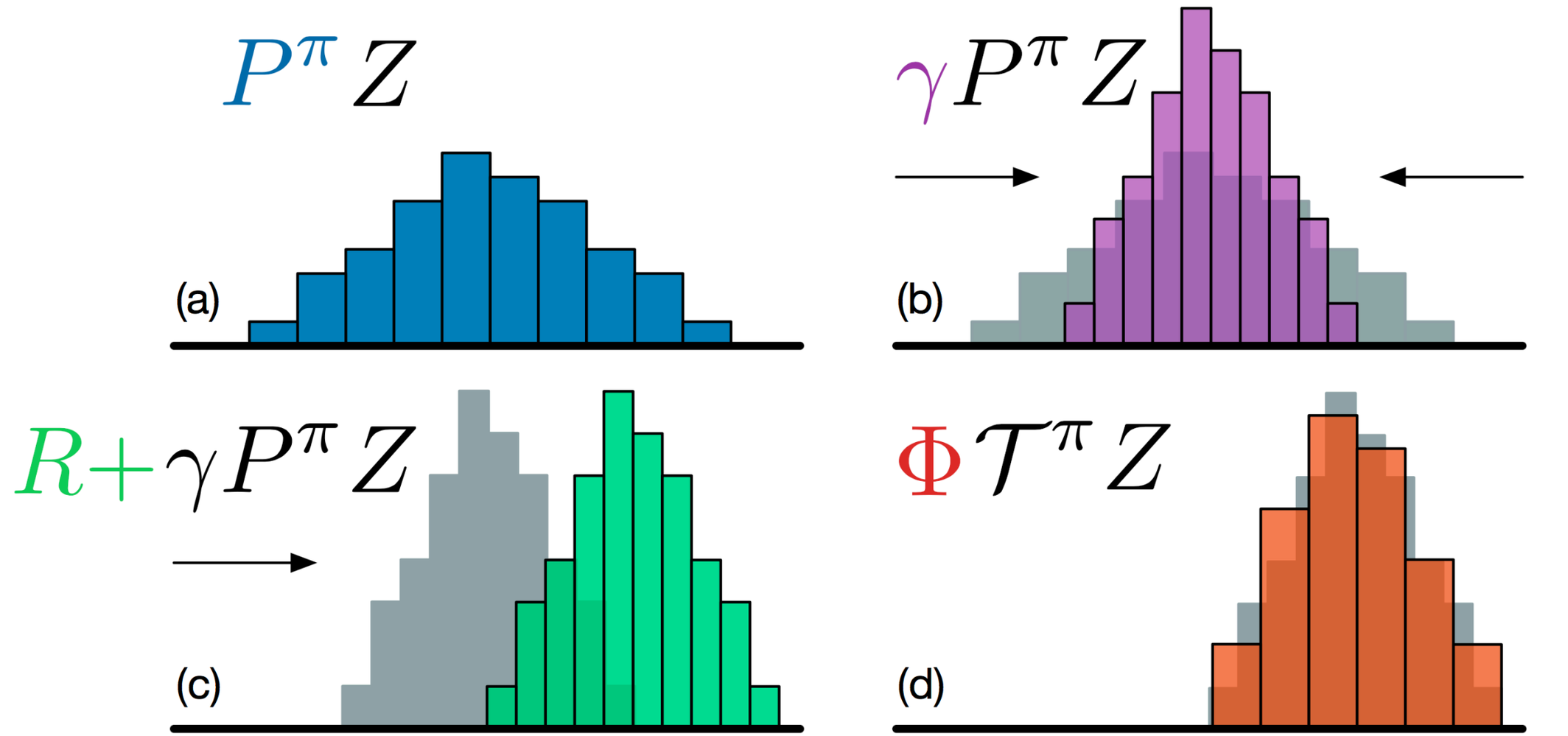
Control

- Lemma. Let $Z_1, Z_2 \in \mathcal{Z}$. Then

$$\|\mathbb{E}\mathcal{T}_D Z_1 - \mathbb{E}\mathcal{T}_D Z_2\|_\infty \leq \gamma \|\mathbb{E}Z_1 - \mathbb{E}Z_2\|_\infty$$

and in particular $\mathbb{E}Z_k \to Q^*$ exponentially quickly for the process $Z_{k+1} := \mathcal{T}_D Z_k,\ Z_0 \in \mathcal{Z}$.

From theory to practice



$$\mathcal{T}^\pi Z(s,a) \overset{D_{\mathrm{W}}}{=} Z(s,a)$$

Theory

$$\Phi \mathcal{T}^\pi Z(s,a) \overset{D_{\mathrm{KL}}}{=} Z(s,a)$$

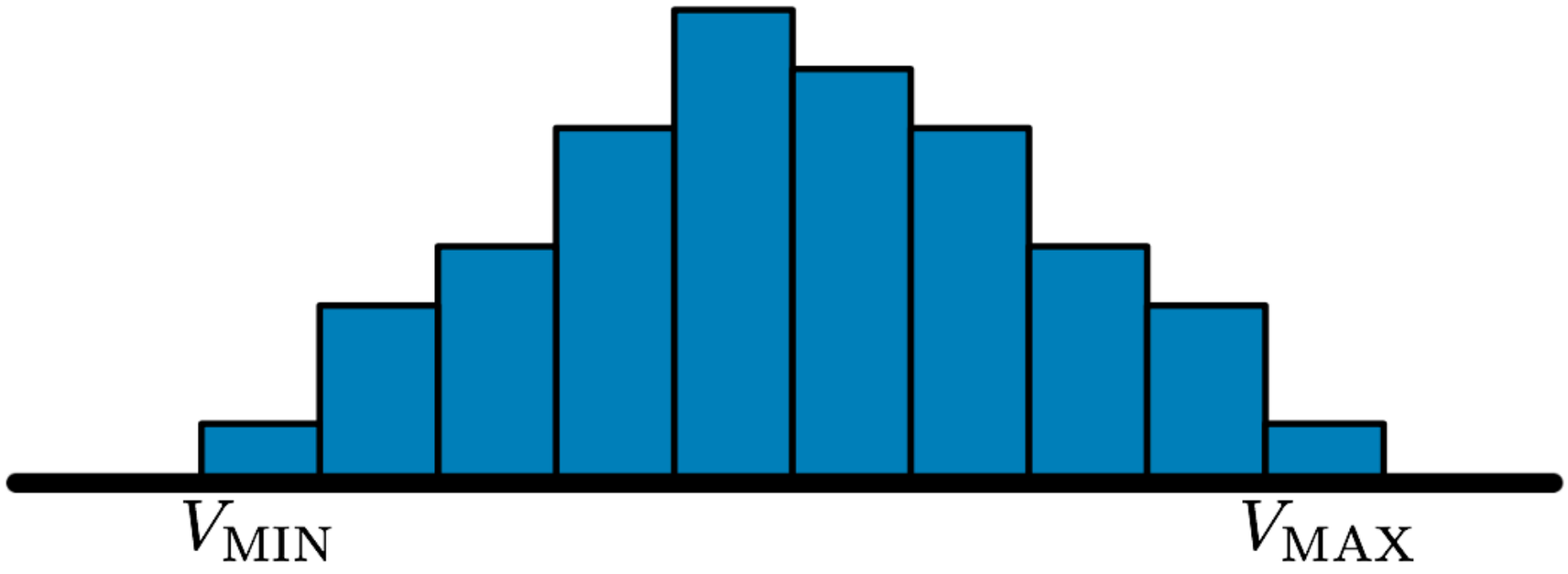
Practice

Categorical DQN

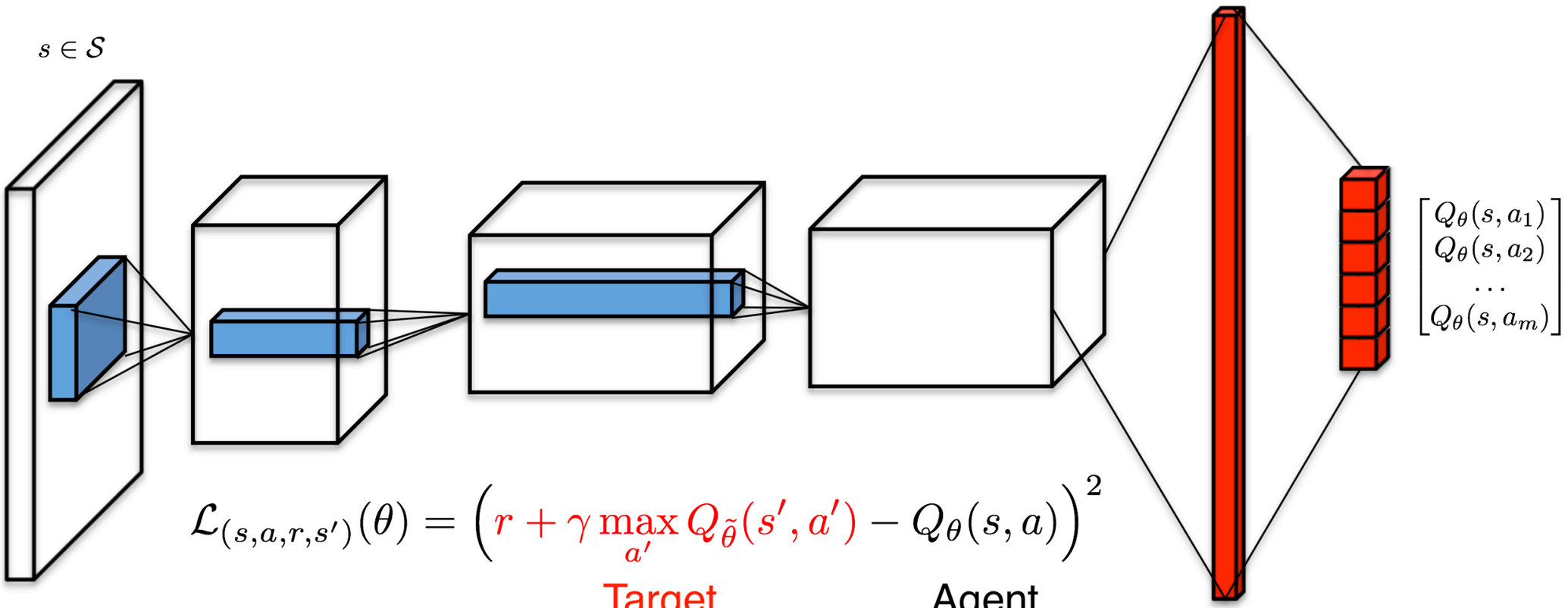
- Discrete probability distribution over $Z_\theta(s,a)$

$$Z_\theta(s,a) = z_i \;\; \text{w.p.} \;\; p_i(s,a;\theta) := \frac{e^{\theta_i(s,a)}}{\sum_{j=1}^{N} e^{\theta_j(s,a)}}$$

$$\{z_i = V_{\text{MIN}} + i\Delta z : 0 \le i < N\}, \; \Delta z := \frac{V_{\text{MAX}} - V_{\text{MIN}}}{N-1}$$



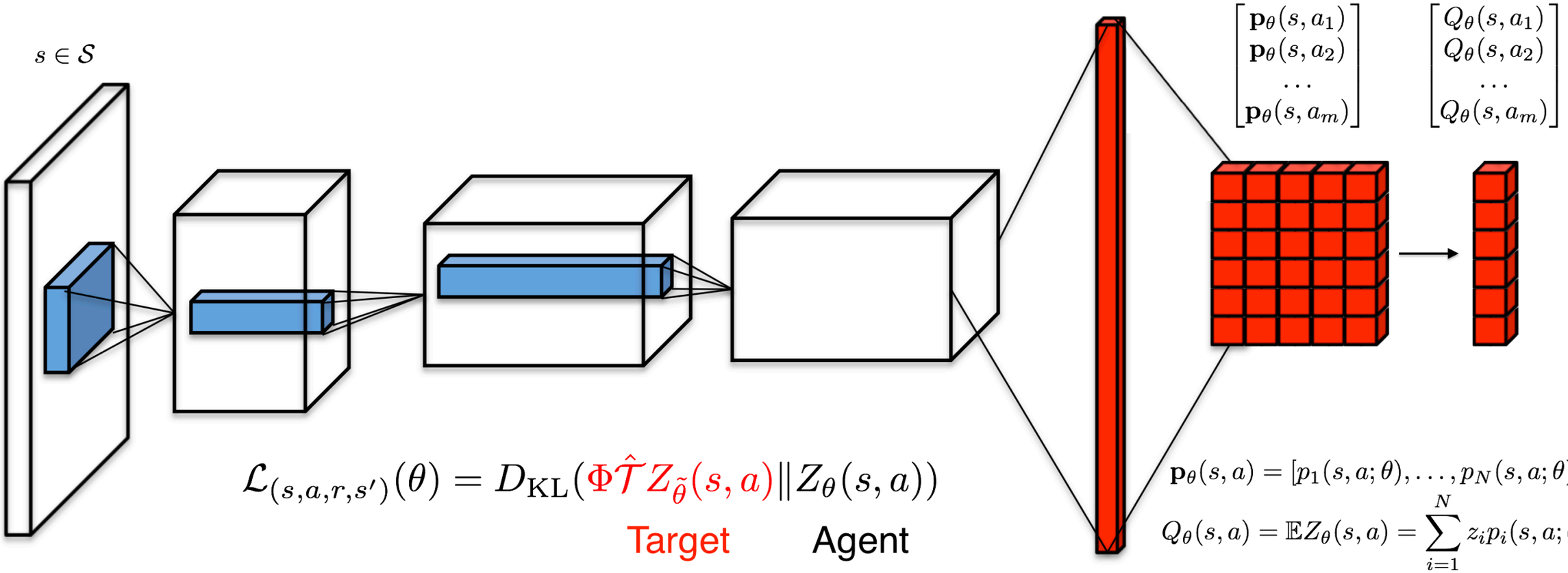
Classic DQN



$$\mathcal{L}_{(s,a,r,s')}(\theta) = \left(r + \gamma \max_{a'} Q_{\tilde{\theta}}(s', a') - Q_\theta(s, a)\right)^2$$

Target Agent

Categorical DQN



$$\mathcal{L}_{(s,a,r,s')}(\theta) = D_{\mathrm{KL}}(\Phi\hat{\mathcal{T}}Z_{\tilde{\theta}}(s,a) \| Z_\theta(s,a))$$

Target Agent

$$\mathbf{p}_\theta(s,a) = [p_1(s,a;\theta), \dots, p_N(s,a;\theta)]$$

$$Q_\theta(s,a) = \mathbb{E}Z_\theta(s,a) = \sum_{i=1}^{N} z_i p_i(s,a;\theta)$$

Categorical algorithm

Algorithm 1 Categorical Algorithm

input A transition $x_t, a_t, r_t, x_{t+1}, \gamma_t \in [0, 1]$

$Q(x_{t+1}, a) := \sum_i z_i p_i(x_{t+1}, a)$

$a^* \leftarrow \arg\max_a Q(x_{t+1}, a)$

$m_i = 0, \quad i \in 0, \ldots, N-1$

for $j \in 0, \ldots, N-1$ **do**

Compute the projection of $\hat{\mathcal{T}} z_j$ onto the support $\{z_i\}$

$\hat{\mathcal{T}} z_j \leftarrow [r_t + \gamma_t z_j]_{V_{\text{MIN}}}^{V_{\text{MAX}}}$

$b_j \leftarrow (\hat{\mathcal{T}} z_j - V_{\text{MIN}})/\Delta z \quad \# \, b_j \in [0, N-1]$

$l \leftarrow \lfloor b_j \rfloor, u \leftarrow \lceil b_j \rceil$

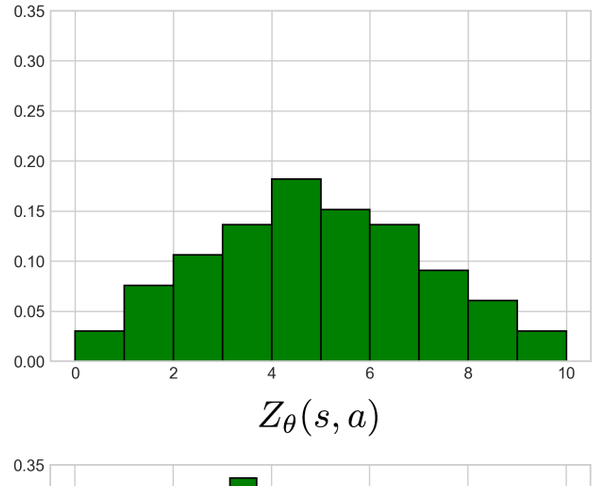
Distribute probability of $\hat{\mathcal{T}} z_j$

$m_l \leftarrow m_l + p_j(x_{t+1}, a^*)(u - b_j)$

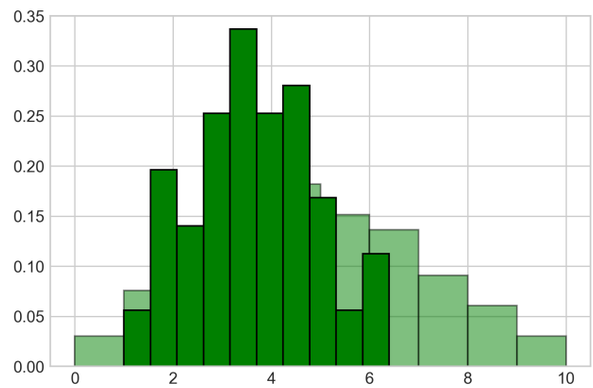
$m_u \leftarrow m_u + p_j(x_{t+1}, a^*)(b_j - l)$

end for

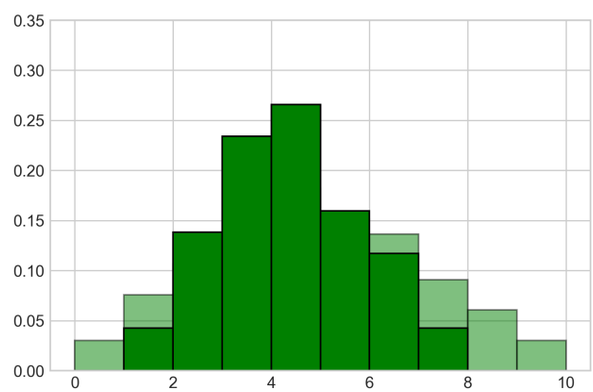
output $-\sum_i m_i \log p_i(x_t, a_t)$ # Cross-entropy loss



$Z_\theta(s, a)$

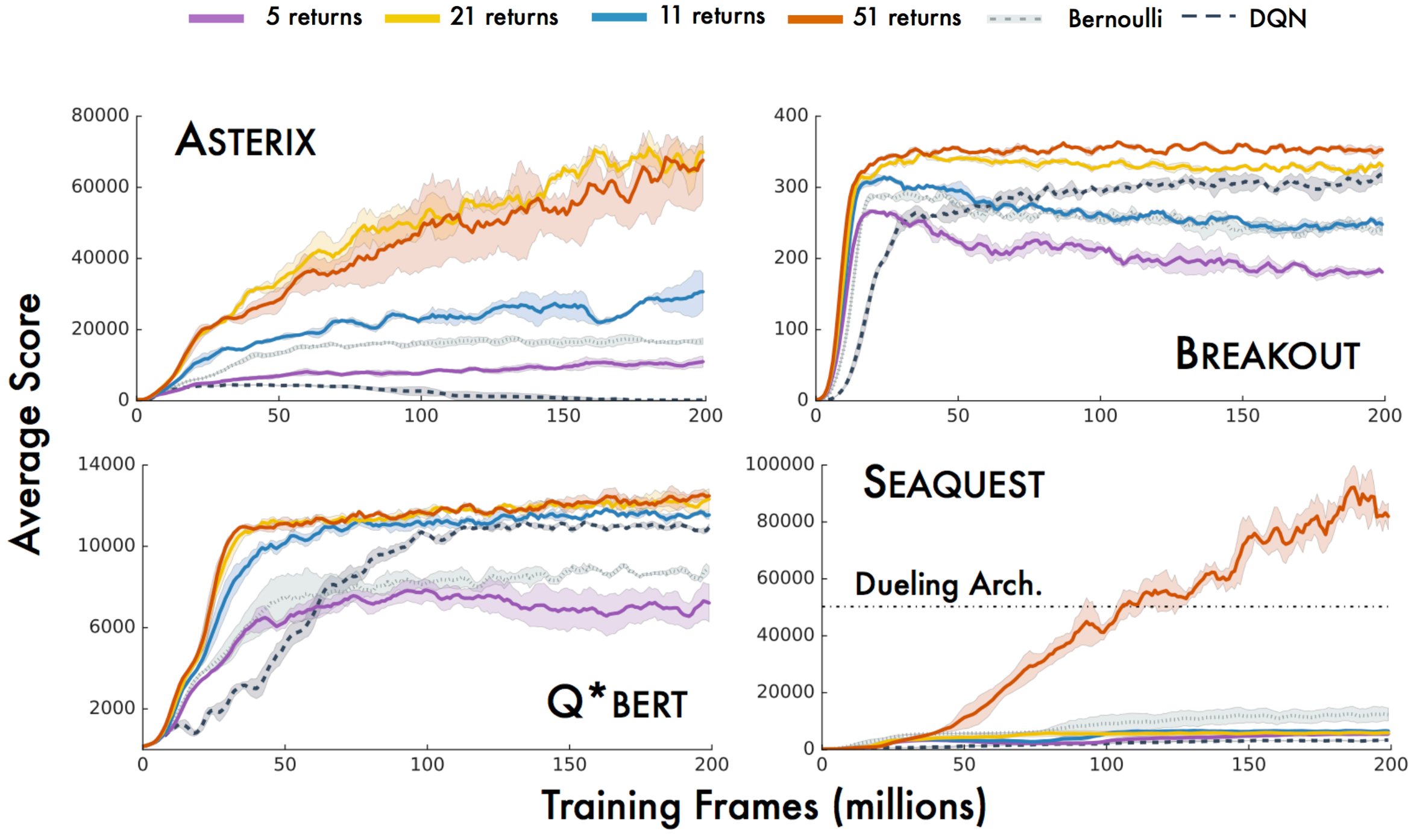


$\hat{\mathcal{T}} Z_\theta(s, a) = R(s, a) + \gamma Z_\theta(s', a')$



$\Phi \hat{\mathcal{T}} Z_\theta(s, a)$

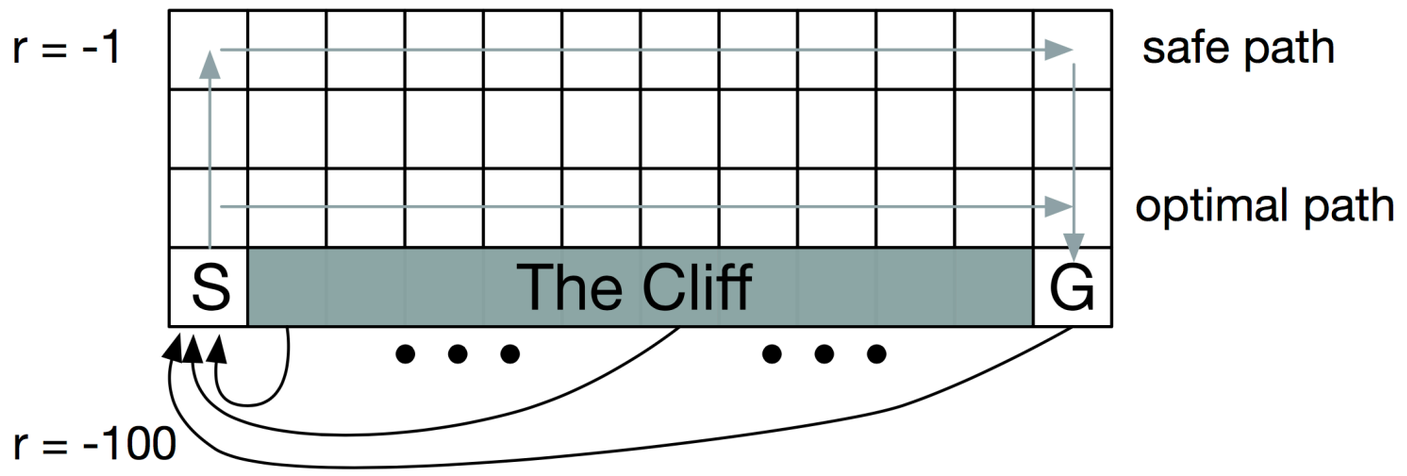
Results

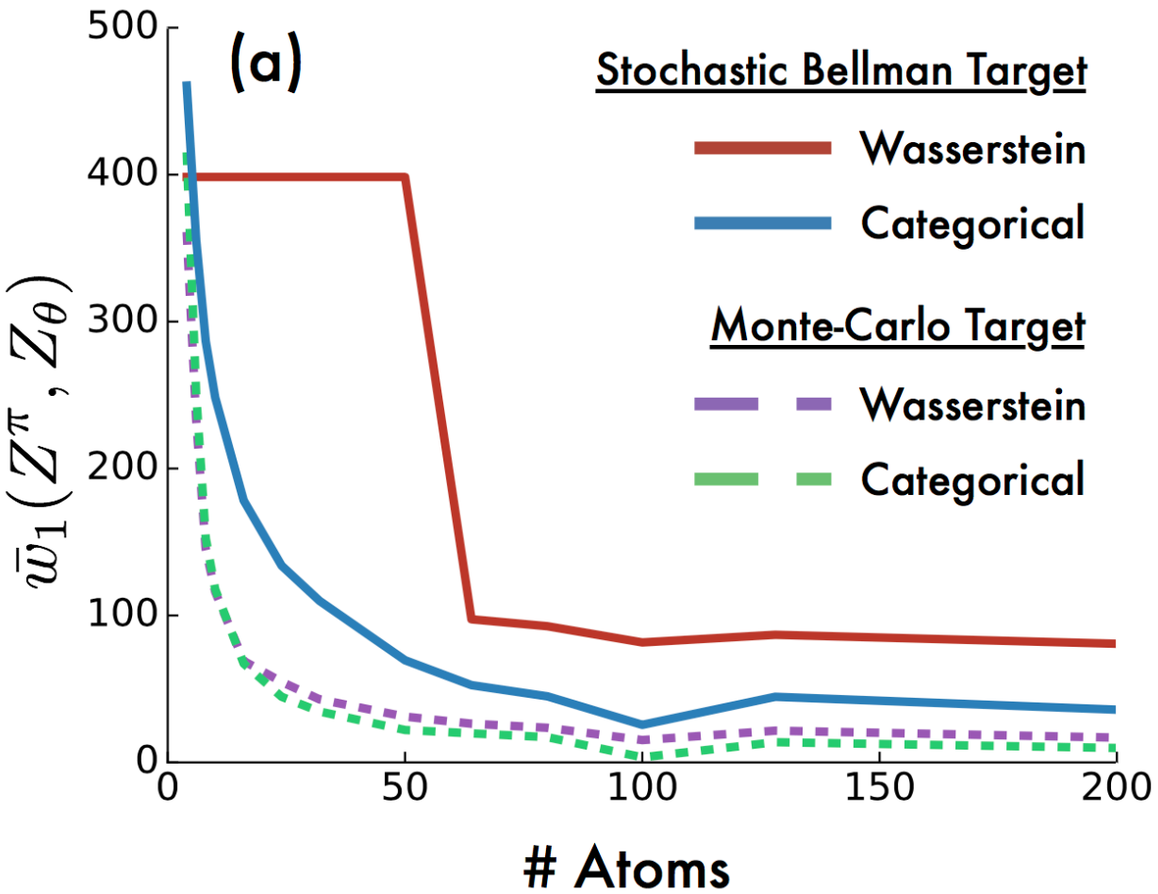

5 returns
21 returns
11 returns
51 returns
Bernoulli
DQN
Average Score
ASTERIX
BREAKOUT
Q*BERT
SEAQUEST
Dueling Arch.
Training Frames (millions)

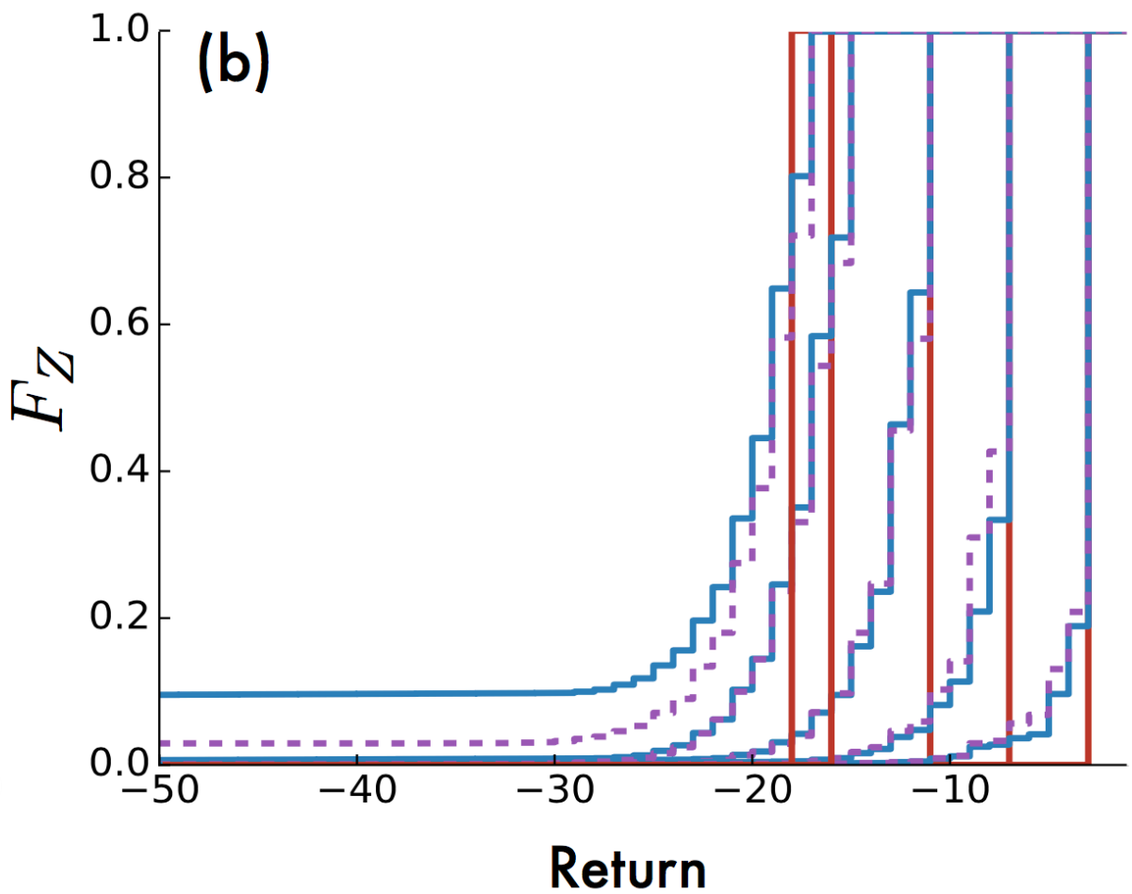
C51 Hyperparameters

- Adam optimizer: learning rate $\alpha = 2.5 \times 10^{-4}$
  batch size $L = 32$
  epsilon $\varepsilon_{\text{adam}} = 0.01/L$
- Distribution support $V_{\text{MIN}} = -10,\ V_{\text{MAX}} = 10$
- Number of atoms $N = 51$
- Implementation
  https://github.com/AlexGrinch/rl_algorithms

Wasserstein loss







Discussion

- Reduced chattering
- State aliasing
- A richer set of predictions
- Framework for inductive bias
- Well-behaved optimization