

# Learning Successor States and Reward-Free RL through the Forward-Backward Model

A Mathematical Viewpoint

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## Introduction

## Learning Successor States and Goal-Dependent Values: A Mathematical Viewpoint

Léonard Blier, Corentin Tallec, Yann Ollivier  ${\rm January}\ 19,\ 2021$ 

#### Abstract

In reinforcement learning, temporal difference-based algorithms can be sample-inefficient: for instance, with sparse rewards, no learning occurs until a reward is observed. This can be remedied by learning richer objects, such as a model of the environment, or successor states. Successor states model the expected future state occupancy from any given state [Dayan, 1993, Kulkarni et al., 2016], and summarize all paths in the environment for a given policy. They are related to goal-dependent value functions, which learn how to reach arbitrary states.

#### Motivation

Today we will talk about...

- 1. Successor states in tabular domains
- 2. Successor states in continuous domains
  - ▶ i.e., how to learn sparse rewards in continuous environments
- 3. The forward-backward model  $\Rightarrow$  very important for extending Reward-Free RL to Deep RL!

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- 2 Forward TD for Successor States: Tabular Case
- 3 Forward TD for Successor States: Continuous Case
- 4 Matrix Factorization: The Forward-Backward Representation
- **5** Deep Reward-Free RL
- **6** Conclusion

#### Introduction

- ► Successor states capture the expected future occupancy of each state, starting from a given state, under a fixed policy.
- ► They generalize the notion of *value functions* to goal-reaching problems: each potentia *goal state* is treated as providing a reward upon arrival.
- ► Learning successor states can be more efficient than learning separate value functions for each goal, especially in environments with sparse rewards.

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## **Markov Process and Successor States**

We consider a **Markov reward process** with state space S (possibly infinite or continuous), **transition operator**  $P^{\pi}$  (for some policy  $\pi$ ), and discount factor  $\gamma$ .

## Successor state operator M

For a fixed policy  $\pi$ , the successor state operator M maps any starting state s to a measure over future states, defined by:

$$M(s,A) = \sum_{t=1}^{\infty} \gamma^{t-1} \mathbb{P}(s_t \in A \mid s_0 = s, \pi)$$

for any measurable set of states A.

In a finite state space, M can be viewed as a matrix in  $\mathbb{R}^{|S| \times |S|}$  given by

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

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 $M_{s,s^\prime}$  is the discounted expected number of visits to state  $s^\prime$  starting from s

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 $M_{s,s'}$  is the discounted expected number of visits to state s' starting from s.

## Markov Process and Successor States: Feature Maps

## Successor state operator M

$$M(s, A) = \sum_{t=1}^{\infty} \gamma^{t-1} \mathbb{P}(s_t \in A \mid s_0 = s, \pi),$$

For any feature map  $\phi:S\to\mathbb{R}^d$  we can define the expected discounted sum of future state features

$$\psi(s) = \mathbb{E}\left[\sum_{t\geq 1} \gamma^{t-1} \phi(s_{t+1}) | s_1 = s\right].$$

Hence<sup>1</sup>

$$\psi(s) = \int_{S} \phi(s') M(s, \mathrm{d}s')$$

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<sup>&</sup>lt;sup>1</sup>For tabular domains we instead have  $\psi(s) = \sum_{s'} (I - \gamma P^{\pi})_s^{-1} \phi(s')$ 

## Markov Process and Successor States: how to learn this object?

#### Successor state operator M

$$M(s, A) = \sum_{t=1}^{\infty} \gamma^{t-1} \mathbb{P}(s_t \in A \mid s_0 = s, \pi),$$

- $\blacktriangleright$  How do we learn M?
- ► For continuous domains the question is tricky. We need to learn a density!
- $\blacktriangleright$  Consider a dominating measure  $\rho$  over  $S^{-2}$ . We define the density as

$$m(s, s') = \frac{M(s, ds')}{\rho(ds')}$$

You can think of  $\rho$  as the data distribution induced by  $\pi$ .

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<sup>&</sup>lt;sup>2</sup>E.g., Lebesgue, Gaussian. See also Radon-Nykodim derivative

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## The Forward Bellman Equation

## Theorem (Bellman Equation for Successor States)

The successor state operator M is the unique operator satisfying

$$M = I + \gamma P^{\pi} M,$$

on the state space (M is a fixed point of the Bellman operator  $\mathcal{T}M := I + \gamma P^{\pi}M$ )

#### Proof Sketch

Rearranging  $M=I+\gamma P^{\pi}M$  gives  $(I-\gamma P^{\pi})M=I$ . Thus M is a right-inverse of  $(I-\gamma P^{\pi})$ . By standard results (e.g. Neumann series),  $I-\gamma P^{\pi}$  is invertible for  $0\leq \gamma < 1$ , with inverse  $(I-\gamma P^{\pi})^{-1}$ . Therefore  $M=(I-\gamma P^{\pi})^{-1}$  is the unique solution.

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## **Bellman Operator Contractivity**

## Proposition (Contraction of Bellman Operator on M)

Equip the space of bounded operators on S with the sup-norm  $\|\cdot\|_{\infty}$ . The Bellman update  $\mathcal{T}M=I+\gamma P^{\pi}M$  is a  $\gamma$ -contraction in this norm<sup>3</sup>.

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For any two operators  $M_1, M_2$ :

$$\|\mathcal{T}M_1 - \mathcal{T}(M_2)\|_{\infty} = \|\gamma P^{\pi}(M_1 - M_2)\|_{\infty} \le \gamma \|M_1 - M_2\|_{\infty}.$$

For a learning rate  $\eta \leq 1$ , repeated updates  $M_{n+1} \leftarrow (1-\eta)M_n + \eta(I+\gamma P^{\pi}M_n)$  will converge to M.

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The Bellman equation  $M = I + \gamma P^{\pi}M$  suggests a TD-style iteration to learn M.

## Definition (Tabular TD Update for M)

In a finite state space, maintain an estimate M as an  $|S| \times |S|$  matrix. Upon observing a transition  $s \to s'$  in the Markov process, update for all  $s_2 \in S$ :

$$M_{s,s_2} \leftarrow M_{s,s_2} + \eta \, \delta M_{s,s_2}, \text{ where } \delta M_{s,s_2} \coloneqq \mathbf{1}_{\{s=s_2\}} + \gamma \, M_{s',s_2} - M_{s,s_2},$$

and  $\eta$  is the learning rate

- lacktriangle Here  $\mathbf{1}_{\{s=s_2\}}$  serves as a "reward" signal indicating if we have reached the target state  $s_2$ .
- ightharpoonup This update is equivalent to performing one-step TD for each possible goal  $s_2$  simultaneously.

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## **Interpretation: State-Goal Process**

The tabular TD update for M is equivalent to ordinary TD learning on an augmented state-goal MDP.

## Equivalence with goal-conditioned value functions

- $\blacktriangleright$  In this interpretation, we consider a process on pairs (s,g) where g is a fixed "goal" state:
  - ► Transition:  $(s,g) \to (s',g)$  with  $s' \sim P^{\pi}(\cdot|s)$ .
  - ▶ Reward:  $R^{\pi}(s,g) = 1$  if s = g (and 0 otherwise).
- Let Q(s,q) be the value (expected return) for this process.
  - ▶ Then the tabular successor representation  $M_{s,g}$  learned using the TD-style approach is exactly Q(s,g).
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Tabular TD Algorithm 12/38

## Forward TD for Successor States: Continuous Case

## Representing M in continuous state spaces

In continuous or large state spaces, storing M as a full matrix is infeasible.

▶ Instead, the idea is to represent M with a parameterized function  $M_{\theta}(s,g)$ . For example, assume:

$$m_{\theta}(s, s') \approx \frac{M(s, \mathrm{d}s')}{\rho(\mathrm{d}s')}$$

where  $m_{\theta}$  is a parametric function (e.g. a neural network) approximating the density of reaching s' from s.

In continuous spaces, M has a singular part due to the term I ( $M = I + \cdots$ ): for each s, the measure  $M(s, \cdot)$  comprises a Dirac mass at s.

The Continuous Case 13/38

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#### Goal

Find  $\theta$  such that  $M_{\theta}$  (parameterized by  $m_{\theta}$ ) satisfies the Bellman equation  $M_{\theta} = I + \gamma P^{\pi} M_{\theta}$ .

- ▶ We need some notion of distance. Define the norm  $\|M\|_{\rho}^2 = \mathbb{E}_{s,s'\sim\rho}[f(s,s')]$  with  $f(s,s') \coloneqq M(s,\mathrm{d}s')/\rho(\mathrm{d}s')$ .
- ▶ We can do this by minimizing the Bellman error

$$J(\theta) \coloneqq \frac{1}{2} \|M_{\theta} - (I + \gamma P^{\pi} M_{\theta})\|_{\rho}^{2}$$

and performing gradient descent on  $J(\theta)$ 

► However, we know from DQN that it's better to use a semi-stationary target. Therefore, we instead consider

$$J(\theta) \coloneqq \frac{1}{2} \|M_{\theta} - M^{\text{tar}}\|_{\theta}^{2}$$

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## Infinitely Sparse Rewards: A Cautionary Tale

- ▶ In a continuous state space, the reward  $\mathbf{1}_{\{s=g\}}$  becomes a Dirac delta, which is zero with probability 1 for any given g.
- **Key insight:** do *not* rely on sampling this rare event directly. when we are at state s, we know that the goal g = s was just achieved (for that particular g). Thus every transition provides some learning signal.
- We should be able to exploit this fact to compute a gradient. Expect  $\partial_{\theta} m_{\theta}(s,s)$  to appear in the gradient update: it captures the self-transition (s to itself) which ensures the sparse Dirac reward still contributes.

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## Forward TD with Function Approximation

#### Theorem (TD Update for Successor States with Approximation)

Consider the model  $M_{\theta}(s, ds') = m_{\theta}(s, s') \rho(ds')$ . For the loss  $J(\theta) \coloneqq \frac{1}{2} \|M_{\theta} - M^{\text{tar}}\|_{\rho}^2$ , the gradient of  $J(\theta)$  is

$$-\partial_{\theta}J(\theta) = \mathbb{E}_{s,s_{2} \sim \rho,s' \sim P^{\pi}(s,\mathrm{d}s')} \left[ \underbrace{\frac{\partial_{\theta}m_{\theta}(s,s)}{\partial_{\theta}m_{\theta}(s,s)} + \underbrace{\partial_{\theta}m_{\theta}(s,s_{2})(\gamma m_{\bar{\theta}}(s',s_{2}) - m_{\theta}(s,s_{2}))}_{\text{Nxt step error}} \right]$$

where  $\rho$  is a sampling distribution over states (e.g. stationary distribution, stationary buffer).

- ▶ This means we update  $\theta$  by sampling a transition  $s \to s'$  and an independent random state  $s_2$ , and then computing the above gradient term.
- ► This algorithm has the *same expected update* as naive parallel TD, but avoids the problem of getting zero reward in continuous state spaces.

We now look at the proof of the theorem. Recall that  $\|M\|_{\rho}^2 = \mathbb{E}_{s,s'\sim\rho}[f(s,s')^2]$  with  $f(s,s') \coloneqq M(s,\mathrm{d}s')/\rho(\mathrm{d}s')$ . Also let  $\langle M_1,M_2\rangle_{\rho} = \mathbb{E}_{s,s'\sim\rho}[f_1(s,s')f_2(s,s')]$ .

► Recall that

$$J(\theta) := \frac{1}{2} \|M_\theta - M^{\mathrm{tar}}\|_\rho^2 \quad \text{ and } \quad M^{\mathrm{tar}} = I + \gamma P^\pi M_{\tilde{\theta}}$$

for some fixed  $\bar{\theta}$ .

- $ightharpoonup M_{\theta}$  is absolutely continuous with respect to  $\rho$  while  $M_{\bar{\theta}}$ , is not, due to the I term. This makes the norm infinite, but the gradient is still well defined.
- ► To see this, note that

$$J(\theta) = \frac{1}{2} ||M_{\theta}||_{\rho}^{2} - \langle M_{\theta}, M^{\text{tar}} \rangle_{\rho} + \frac{1}{2} ||M^{\text{tar}}||_{\rho}^{2}$$

 $J(\theta)$  has the same minima as  $J'(\theta) = \frac{1}{2} \|M_{\theta}\|_{\rho}^2 - \langle M_{\theta}, M^{\text{tar}} \rangle_{\rho}!$  Namely, they differ by an "infinite" constant

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## Forward TD with Function Approximation

#### Theorem (TD Update for Successor States with Approximation)

Consider the model  $M_{\theta}(s, ds') = m_{\theta}(s, s')\rho(ds')$ . For the loss  $J(\theta) \coloneqq \frac{1}{2}\|M_{\theta} - M^{\mathrm{tar}}\|_{\rho}^2$ , the gradient of  $J(\theta)$  is

$$-\partial_{\theta}J(\theta) = \mathbb{E}_{s,s_2 \sim \rho,s' \sim P^{\pi}(s,\mathrm{d}s')} \left[ \underbrace{\frac{\partial_{\theta} m_{\theta}(s,s)}{\mathit{Singular term}}}_{\mathit{Singular term}} + \underbrace{\partial_{\theta} m_{\theta}(s,s_2)(\gamma m_{\bar{\theta}}(s',s_2) - m_{\theta}(s,s_2))}_{\mathit{Nxt step error}} \right]$$

where  $\rho$  is a sampling distribution over states (e.g. stationary distribution, stationary buffer).

Matrix Factorization: The

Forward-Backward

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## Matrix Factorization: Forward-Backward (FB) Representation

Even with function approximation, learning  $m_{\theta}(s, s')$  for all pairs can be challenging. A useful approach is to restrict M to a low-rank form:

#### **Definition (Forward-Backward Factorization)**

We approximate the successor operator by a rank-r factorization:

$$M(s, \mathrm{d}s') = F(s)^{\top} B(s') \rho(\mathrm{d}s'),$$

where  $F:S\to\mathbb{R}^r$  and  $B:S\to\mathbb{R}^r$  are learnable feature vectors (with parameters  $\theta_F,\theta_B$ ). In matrix form,  $M\approx FB^{\top}$ . We call F(s) the forward representation of state s and B(s') the backward representation of state s'.

Intuitively, F(s) encodes the long-term dynamics starting from s, while B(s') encodes how reachable state s' is (acting like a representation of "goals").

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#### Why the matrix $M=(I-\gamma P^{\pi})^{-1}$ should be low rank?

- 1. Denote by  $s_t$  the state at time t. In many systems we have that  $s_{t+\Delta} \approx s_t$  for  $\Delta$  sufficiently small.
- 2. Example: dynamical systems

$$\frac{dx}{dt} = Ax(t) \Rightarrow x(t+\Delta) = e^{A\Delta}x(t) = (I + A\Delta + \dots)x(t)$$

- 3. For continuous-time operators associated with random diffusions,  $I-P^{\pi}$  has few small and many large eigenvalues.
- 4. For such property to hold we must have  $P \approx I + X^{-1}$ , where  $X^{-1}$  is like a second-order term ( $\approx$  low rank).
- Results that use P to be low rank usually do not work well in practice (they miss the identity term!)

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Is there some connection with **SVD**? Let  $M_{approx} = F^{\top} B \rho$ .

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We are looking for the d-rank best approximation of  $M/\rho$  (SVD in  $L^2(\rho)$ ). See Eckart–Young–Mirsky theorem.

Is there some connection with SVD? Let  $M_{\rm approx} = F^{\top} B \rho$ .

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## Advantages of the FB Representation

▶ Direct value estimation: F and B together allow immediate computation of the value for any reward function. For example, if R(s) is a reward function

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- ▶ Generalization across states: The low-rank assumption provides a form of regularization or prior: states that have similar long-term dynamics will learn similar F and B representations.
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Low-Rank Approximation of  $\,M\,$ 

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## Shortcomings of the FB Representation

- ▶ Limited capacity (rank-r approximation): By constraining M to rank r, we cannot perfectly represent the true M. Important dynamics corresponding to smaller singular values of M may be neglected.
- ▶ This means fine-grained or rapidly changing aspects of the reward structure (e.g. very localized rewards that vary quickly from state to state) might be smoothed out or underrepresented. The FB model tends to focus on the dominant, "long-range" structures in the state space.
- ▶ Mitigation: One can combine the low-rank SSR with a standard value function to capture the residual. For example, use  $V(s) = F(s)^{\top}B(R) + v_{\phi}(s)$ , where  $v_{\phi}(s)$  is a separate value function learned for the specific reward.

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Deep Reward-Free RL

#### Forward-Backward for Deep-RL

#### Starting point

$$M^{\pi}(s, a, \mathrm{d}s') = F(s, a)^{\top} B(s') \rho(\mathrm{d}s').$$

- lacktriangle Consider a family of policies  $\{\pi_z\}$  parameterized by a vector  $z\in\mathbb{R}^d$ .
- ightharpoonup Assume that for all z, we can find  $(F_z, B)$  (F is parameterized by z) such that

$$M^z(s, a, \mathrm{d}s') = F_z^{\top}(s, a)B(s')\rho(\mathrm{d}s')$$

▶ Then, if  $\pi_z$  induces a distribution  $\rho$ 

$$Q^{z}(s, a) = \mathbb{E}^{\pi_{z}} \left[ \sum_{t \ge 1} \gamma^{t-1} r_{t} | s_{1} = s, a_{1} = as \right],$$

$$= \left[ (I - \gamma P^{\pi_{z}})^{-1} r \right] (s, a),$$

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FB Method for Reward-Free Deep RL

$$Q^{z}(s,a) = \int_{s'} F_{z}^{\top}(s,a)B(s')r(s')\rho(\mathrm{d}s').$$

Let

$$z_r = \mathbb{E}_{s \sim \rho} [B(s)r(s)].$$

If we define  $\pi_z$  by

$$\pi_z(s) = \arg\max_a (F_z(s, a)^\top z)$$

then  $\pi_{z_r}$  is the optimal policy for reward r, since  $Q^{z_r} = F_{z_r}^\top(s,a)z_r$ 

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#### Let's slow down...

 $z_r = \mathbb{E}_{s \sim \rho}[B(s)r(s)]$  is like a representation.

- ▶ If we think of the reward function r as a vector in some Hilbert space, then we are simply projecting r onto the space spanned by B
- lacktriangle For the method to make sense we need to have  $\mathbb{E}_{s\sim \rho}[B(s)B(s)^{\top}]$  to be full rank

$$z = B^{\top} r \Rightarrow r = (BB^{\top})^{-1} B^r$$

▶ The eigenvectors of  $\mathbb{E}_{s \sim \rho}[B(s)B(s)^{\top}]$  define a basis in this space.

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### Goal

We need to learn  $F_z$ , B. How?

$$M^{z}(s, a, ds') = F_{z}(s, a)^{\top} B(s') \rho(ds').$$

- $lackbox{ Remember the norm } \|M\|_{
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  ho}[m(s,s')^2].$
- ▶ **Goal**: find  $(F_z, B)$  such that, for all z, we have

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and

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▶ How? TD-Learning on  $J(\theta) = \|M_{\theta}^z - (I + \gamma P^{\pi_z} M_{\tilde{\theta}}^z)\|_{\rho}^2$ .

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FB Method for Reward-Free Deep RL

# Forward-backward method: training

 $\blacktriangleright$  Parametrize  $F_z, B$  by  $\theta.$  Let  $m^z_\theta = (F^\theta_z)^\top\,B^\theta_z$ , thus

$$M^z_\theta(s,a,\mathrm{d} s') = m^z_\theta(s,a,s') \rho(\mathrm{d} s').$$

▶ For  $(\theta, \bar{\theta})$ , define the learning objective:

$$J'(z;\theta) = \frac{1}{2} \|M_{\theta}^z\|_{\rho}^2 - \langle M_{\theta}^z, M^{\text{tar}} \rangle_{\rho}$$

where  $M^{\mathrm{tar}} = I + \gamma P^{\pi_z} M_{\bar{\theta}}^z$ .

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# Gradient with replay buffer

#### **Gradient step**

We know very well that  $\partial_{\theta}J'(\theta)=\partial_{\theta}J(\theta)$ , therefore

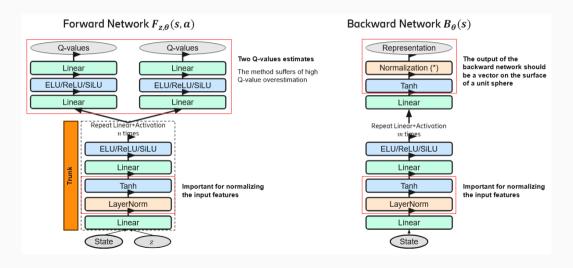
$$-\partial_{\theta}J(\theta) = \mathbb{E}_{(s,a,s')\sim D,(s_2,a_2)\sim D}\left[\partial_{\theta}m_{\theta}(s,a,s) + \partial_{\theta}m_{\theta}(s,a,s')(\gamma m_{\bar{\theta}}(s_2,a_2,s') - m_{\theta}(s,a,s'))\right]$$

where D is the data distribution induced by the policy and  $m_{\theta}^z(s,a,s') = F_z^{\theta}(s,a)^{\top}B_z^{\theta}(s')$ 

- ightharpoonup Practically speaking, D is the replay buffer. At every training step we sample two random independent samples from the replay buffer D.
- ightharpoonup One contributes due to visiting s' from s.
- Another from a different random state s".

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### Training procedure: networks



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# **Training**

### **Algorithm 1** Off-policy Training Procedure

- 1: Initialize  $\theta, \bar{\theta}$
- 2: while not converged do
- 3: Sample  $z \sim S^{d-1}$

▷ from the surface of a unit sphere

- 4: Collect data using policy  $\pi_z$  and add to replay buffer D
- 5: Sample batches  $(B, B') \sim D$  and compute gradient:

$$-\partial_{\theta}J(\theta) \approx \hat{\mathbb{E}}_{(s,a,s')\sim B,(s_2,a_2)\sim B'} \left[ \partial_{\theta}m_{\theta}(s,a,s') + \partial_{\theta}m_{\theta}(s,a,s') \left( \gamma m_{\theta}(s_2,a_2,s') - m_{\theta}(s,a,s') \right) \right]$$

- 6: where  $m^z_{\theta}(s,a,s') = F^z_{\theta}(s,a)^{\top} B^z_{\theta}(s')$
- 7: Update parameters  $\theta \leftarrow \theta \eta \partial_{\theta} J(\theta)$  using the computed gradient
- 8: **if** every N steps **then**
- 9: Set  $\bar{\theta} \leftarrow \theta$ .
- 10: end if
- 11: end while

### Other tricks and technicalities

- $lackbox{ We add a regularization term } \left\| E(B^{\top}B) I \right\|_{\rho}^{2}$  to ensure  $\operatorname{cov}(B) = I$ .
- ▶ The computation of the target value can be numerically unstable (large gradients).
- One way to solve the issue: replace the greedy  $\pi_z = \arg \max_a F_z(s,a)^\top z$  with a regularized version

$$\pi_z = \operatorname{softmax}(F_z(s, a)^\top z / \tau).$$

lacktriangle Use a combination of linear + layer normalization + tanh layers to extract features.

FB Method for Reward-Free Deep RL

### Test time

How does the method work at test time?

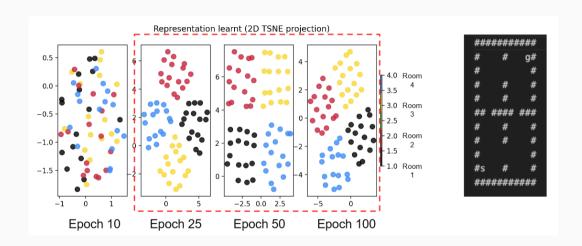
- ightharpoonup For a specific reward r we need to compute z.
- ▶ Recall  $z = \mathbb{E}_{s \sim \rho}[B(s)r(s)].$
- ▶ Sample a batch D from the buffer, and compute  $z_r = \frac{1}{|D|} \sum_{s \in D} B(s) r(s)$ .

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▶ Obtain the policy  $\pi_{z_r}(s) = \arg \max_a F_{z_r}(s)^{\top} z_r$ .

FB Method for Reward-Free Deep RL

# **4-Rooms Example**



Random initial state/goal at every episode.

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### Conclusions

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#### References i

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