Self-Predictive Representations for Combinatorial Generalization in Behavioral Cloning

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Keywords: Sequential Decision Making, Combinatorial Generalization, Representation Learning.

Summary

Behavioral cloning (BC) methods trained with supervised learning (SL) are an effective way to learn policies from human demonstrations in domains like robotics. Goal-conditioning these policies enables a single generalist policy to capture diverse behaviors contained within an offline dataset. While goal-conditioned behavior cloning (GCBC) methods can perform well on in-distribution training tasks, they do not necessarily generalize zero-shot to tasks that require conditioning on novel state-goal pairs, i.e. *combinatorial generalization*. In part, this limitation can be attributed to a lack of temporal consistency in the state representation learned by BC; if temporally related states are encoded to similar latent representations, then the out-of-distribution gap for novel state-goal pairs would be reduced. Hence, encouraging this temporal consistency in the representation space should facilitate combinatorial generalization. Successor representations, which encode the distribution of future states visited from the current state, nicely encapsulate this property. However, previous methods for learning successor representations have relied on contrastive samples, temporal-difference (TD) learning, or both. In this work, we propose a simple yet effective representation learning objective, BYOL-γ augmented GCBC.

Contribution(s)

1. We propose BYOL-γ, a novel representation learning objective that relates to the successor measure, which we prove in the finite MDP setting.
   Context: While prior theory supports this objective (Tang et al., 2023; Khetarpal et al., 2025), to our knowledge, we are the first to directly relate a BYOL-based objective to the successor measure and to use it in practice for representation learning.
2. Empirically, we demonstrate that such a BYOL objective can be used as auxiliary objective augmenting the capabilities of Behavior Cloning, and we find that BYOL-γ obtains competitive results on navigation tasks in OGBench compared to existing methods. Qualitatively, we show that the BYOL-γ objective learns similar representation structures to contrastive learning, encoding temporal distance between states.
   Context: We build on the setting of using auxiliary representation learning objectives for BC from Myers et al. (2025b), however we further illustrate the relationship between generalization and approximations to the succesor measure, and demonstrate that alternative representation learning can obtain competitive or better performance for achieving combinatorial generalization.

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Abstract

Behavioral cloning (BC) methods trained with supervised learning (SL) are an effective way to learn policies from human demonstrations in domains like robotics. Goal-conditioning these policies enables a single generalist policy to capture diverse behaviors contained within an offline dataset. While goal-conditioned behavior cloning (GCBC) methods can perform well on in-distribution training tasks, they do not necessarily generalize zero-shot to tasks that require conditioning on novel state-goal pairs, i.e. *combinatorial generalization*. In part, this limitation can be attributed to a lack of temporal consistency in the state representation learned by BC; if temporally related states are encoded to similar latent representations, then the out-of-distribution gap for novel state-goal pairs would be reduced. Hence, encouraging this temporal consistency in the representation space should facilitate combinatorial generalization. Successor representations, which encode the distribution of future states visited from the current state, nicely encapsulate this property. However, previous methods for learning successor representations have relied on contrastive samples, temporal-difference (TD) learning, or both. In this work, we propose a simple yet effective representation learning objective, BYOL-γ augmented GCBC, which is not only able to theoretically approximate the successor representation in the finite MDP case without contrastive samples or TD learning, but also, results in competitive empirical performance across a suite of challenging tasks requiring combinatorial generalization.

1 Introduction

Generalization has been a long-standing goal in machine learning and robotics. Recently, large-scale supervised models for language and vision have demonstrated impressive generalization when trained over vast amounts of data. In the robotics domain, this has motivated the development of large-scale supervised behavior cloning (BC) models trained on offline datasets of diverse demonstrations (Ghosh et al., 2024; Kim et al., 2024). However, these models still suffer from a lack of generalization. In particular, while BC methods can perform well on tasks directly observed in the dataset, they often fail to perform zero-shot transfer to tasks requiring novel combinations of in-distribution behavior, known as *combinatorial generalization*. In the robotics domain, where demonstration data is time-intensive and costly to produce, simply scaling the dataset is often not possible. Hence, achieving this type of generalization algorithmically will be critical to unlocking the potential for large-scale supervised policy training.

The property of combinatorial generalization has been previously formalized as the ability to "stitch" (Ghugare et al., 2024). Specifically, stitching refers to the ability of a policy to reach a goal state from a start state when trained on a dataset of trajectories which, provides sufficient coverage of the path to the goal, but which does not contain a single complete trajectory of the path. The lack of stitching observed in goal-conditioned behavioral cloning (GCBC) and, more generally, supervised learning, can be understood through the inductive biases of the model. By construction, BC methods

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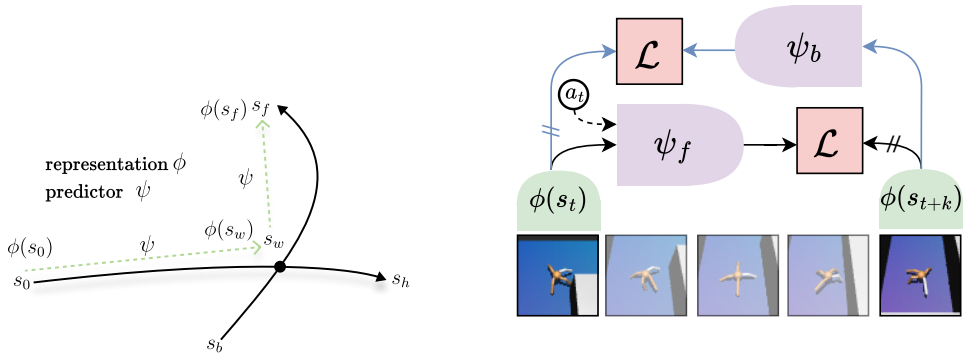

(a) (b)

Figure 1: **(a) Self-predictive Representations.** Example training trajectories, $s_0 \to s_h$ and $s_b \to s_f$, which intersect at w. After training on these trajectories, we evaluate on a task like $s_0 \to s_f$, requiring combinatorial generalization. To learn better representations for generalization, a self-predictive representation predicts a future state $\phi(w)$ from an earlier state $\phi(e)$ via $\psi(\phi(e))$. **(b) Representation learning with BYOL-γ.** We predict future state representations $\phi(s_{t+k})$ via $\psi_f(\phi(s_t), a)$, and also predict backwards with $\psi_b(\phi(s_{t+k}))$. The target offset is sampled geometrically: $k \sim \text{geom}(1-\gamma)$. Stop-gradients are denoted by //. We provide more details on the loss $\mathcal{L}$ in Section 4.2.

do not encode the inductive bias that the observed data are generated from a Markov decision process (MDP). In contrast, reinforcement learning (RL) policies that are trained via temporal difference (TD) learning directly utilize the structure of the MDP, and pass information through time using dynamic programming. Offline RL (Levine et al., 2020) has been proposed as a method for achieving stitching in policies trained on offline datasets. However, these methods are challenging to scale due to the instability of bootstrapping in TD learning when combined with fully offline training. Scaling has been more successful with supervised methods, such as in robotics, where training robot foundation models with BC (Ghosh et al., 2024; Kim et al., 2024) on large-scale datasets (O'Neill et al., 2024; Khazatsky et al., 2024) can lead to more general-purpose policies.

Various methods have attempted to imbue GCBC models with the ability to stitch by augmenting the training data using the Markovian assumption (Yamagata et al., 2023; Ghugare et al., 2024). However, these methods ultimately rely on similar training procedures as offline RL or otherwise require a distance metric already aligned with temporal distance in the MDP. Another approach frames stitching as a representation learning problem (Myers et al., 2025b). In this context, the objective is to learn a latent representation of states that reflects temporal proximity in the underlying MDP to facilitate generalization to unseen state-goal pairs. In particular, Myers et al. (2025b) train a representation that approximates the successor measure (SM) (Blier et al., 2021) through contrastive learning (CL) (van den Oord et al., 2019) as an auxiliary loss in GCBC, demonstrating enhanced combinatorial generalization. This is a promising step towards achieving combinatorial generalization in GCBC methods. In this work, we expand on this connection between the successor measure and combinatorial generalization, proposing an alternative objective that captures similar properties with a simpler learning procedure and achieves as good or better generalization performance.

In particular, in other domains, like vision, it has been found that contrastive learning can often be substituted with self-predictive representations (Grill et al., 2020), which have also been found to be useful as auxiliary losses for model-free RL (Schwarzer et al., 2020). Adapting the *Bootstrap Your Own Latent* (BYOL) framework (Grill et al., 2020) to the RL setting, representations can be trained by predicting the latent representation of the next state from the current latent state representation. These BYOL objectives have appealing properties, such as neither relying on negative examples nor reconstruction.

As motivation, we foremost evaluate the BYOL objective as an auxiliary loss for GCBC; however, we find that there exists an empirical and theoretical gap compared to contrastive methods. This

leads us to propose a novel objective, **BYOL-γ**, which removes the gap between self-predictive and contrastive objectives. Concretely, BYOL-γ predicts latent representations of states sampled from a γ-discounted future state distribution. While the standard BYOL objective has been shown to learn representations capturing spectral information about the one-step transition dynamics (Khetarpal et al., 2025), we show that the representations learned by BYOL-γ capture spectral information related to the successor measure. In the finite MDP case, we show that, in fact, BYOL-γ approximates the successor representation. Empirically, we demonstrate on the challenging OGBench dataset (Park et al., 2025) that BYOL-γ augmented GCBC is competitive with contrastive methods in improving combinatorial generalization. **Key contributions of our work** are as follows:

- We propose BYOL-γ, a novel representation learning objective that relates to the successor measure, which we prove in the finite MDP setting.
- Empirically, we demonstrate that such a BYOL objective can be used as auxiliary objective augmenting the capabilities of Behavior Cloning, and we find that BYOL-γ obtains competitive results on navigation tasks in OGBench compared to existing methods.
- Qualitatively, we show that the BYOL-γ objective learns similar representation structures to CL, encoding temporal distance between states.

2 Related Work

Stitching in Supervised Methods. Outcome (goals or return)-conditioned behavioral cloning (OCBC) methods (Schmidhuber, 2020; Chen et al., 2021; Emmons et al., 2022) provide a simple and scalable alternative to traditional offline RL (Levine et al., 2020) methods. However, these methods do not properly "stitch" and generalize to unseen outcomes Brandfonbrener et al. (2022); Ghugare et al. (2024). To reduce this problem, various works have proposed augmenting training data used by BC methods. Some work incorporates methodlogy from offline RL to label returns or goals for downstream SL (Char et al., 2022; Yamagata et al., 2023). Other work has considered relabeling goals through clustering states (Ghugare et al., 2024), which relies on a good distance metric in state-space and is limited to short trajectory stitches. Other work has utilized planing Zhou et al. (2024) for goal relabeling, or generative models to synthesize new trajectories (Lu et al., 2023; Lee et al., 2024). Rather than using models to generate data for BC, other work directly evaluates the combinatorial generalization achieved by planning with generative models (Luo et al., 2025). In this work, we neither require combining SL with explicit Q-learning, utilize generative models, or perform explicit planning.

Visual Representation Learning. Instead of auxiliary representation learning, prior work has considered using pretrained visual representations for BC. Utilizing pretrained BC has been a reliable method to efficiently learn policies and improve generalization (Radosavovic et al., 2022; Majumdar et al., 2023; Nair et al., 2022). Instead of pretraining representations out-of-domain, such as on large image datasets, DynaMo (Cui et al., 2024) evaluates pretraining representations in-domain on specific robotics datasets, and then performs a separate BC finetuning stage. However, we focus on representation learning as an auxiliary objective. For enhancing combinatorial generalization, this can be advantageous, as training as an auxiliary task maintains the structure of the representation space, and prevents overfitting the BC objective.

Representation learning in RL. Our objective is most closely related to approaches using auxiliary **BYOL objectives in online RL** (Gelada et al., 2019; Schwarzer et al., 2020; Ni et al., 2024; Voelcker et al., 2024). These objectives can help with sample-efficiency, such as in challenging, partially observed environments with sparse rewards, or with noisy states. Additionally, self-predictive dynamics models are used in planning and model-based RL (François-Lavet et al., 2019; Ye et al., 2021; Hansen et al., 2022). Various works have also characterized the dynamics of BYOL objectives in the RL setting, showing that BYOL objectives capture spectral information about the policy's transitions (Tang et al., 2023; Khetarpal et al., 2025). In the offline setting, how well Joint Embedding Predictive Architecture (JEPA) world models generalize when used for explicit planning has been studied Sobal et al. (2025), however not for combinatorial generalization. Additionally, certain representation structures for value functions, namely quasimetrics (Liu et al., 2023; Wang et al.,

2023; Wang and Isola, 2022; Myers et al., 2024) can also lead to policies that better generalize to longer horizons (Myers et al., 2025a). Quantities related to the **Successor Representation** (SR) (Dayan, 1993) , such as successor features (SF) (Barreto et al., 2017), and the successor measure (SM) (Blier et al., 2021) have been widely used for generalization and transfer in reinforcement learning (Carvalho et al., 2024). Similarly to BYOL, these objectives have been used for representation learning in RL (Lan et al., 2022; Farebrother et al., 2023). While prior BYOL methods either perform 1-step, or relatively short fixed n-step prediction, neither of these choices directly approximate the successor measure. Our setup is most related to temporal representation alignment (TRA) (Myers et al., 2025b), which recently proposed using contrastive learning as an auxiliary objective for BC to improve combinatorial generalization. In this work, we further build on the relationship between the SM and combinatorial generalization, and propose new representation learning objectives which can lead to better performance.

3 Background

Controlled Markov Process. We consider goal-conditioned decision-making problems, with state space $\mathcal{S}$, goals $g \in S$, action space $\mathcal{A}$, initial state distribution $p_0(s)$, dynamics $p(s_{t+1} \mid s_t, a)$, and with policies $\pi(a|s, g)$.

Successor Representation (SR) and Successor Measure (SM). In a finite MDP, the *successor representation* (SR) (Dayan, 1993) of a policy is:

$$M^\pi(s, s') := \mathbb{E}\left[\sum_{t\geq 0} \gamma^t \mathbb{1}_{(s_{t+1}=s')} \mid s_0 = s, \pi\right] \tag{1}$$

We use the convention of counting from s_{t+1}, writing in matrix form $M^\pi = \sum_{t\geq 0} \gamma^t (P^\pi)^{t+1}$. The transition matrix transition for policy π is P^π, with $P^\pi_{i,j} = \sum_a \pi(a|s = i) P_{i,a,j}$, where $P_{i,a,j} = p(s_{t+1} = j \mid s_t = i, a)$. The successor representation also satisfies the bellman equation, $M^\pi = P^\pi + \gamma P^\pi M^\pi = P^\pi (I - \gamma P^\pi)^{-1}$. For a fixed policy, the successor representation describes a type of temporal distance between states. The *successor measure* (SM) (Blier et al., 2021) extends SR to continuous spaces S: $M^\pi(s, X) := \sum_{t\geq 0} \gamma^t P(s_{t+1} \in X \mid s)\ \forall X \subset S$. We also define the *normalized* successor representation, or measure $\bar{M}^\pi = (1-\gamma) M^\pi$. In the finite case, the normalized successor representation $\tilde{M}^\pi$ has rows that sum to one like transitions P^π. Another quantity *successor features* (SF) (Barreto et al., 2017) are the expected discounted sum of future features $\phi(s) \in \mathbb{R}^d$: $\psi^\pi(s) = \mathbb{E}\left[\sum_{t\geq 0} \gamma^t \phi(s_{t+1}) \mid s_0 = s, \pi\right]$. We can relate SFs to the SM with $\psi^\pi(s) = \int_{s'} M^\pi(s, s')\phi(s')$. Each of these quantities can also be defined with conditioning on the first action and then following the policy, e.g. $M^\pi(s, a, s')$.

3.1 Representation Learning

We begin with two representation learning methods that approximate the density of the SM.

Forward-Backward. We consider a simplified version of the Forward-Backward loss that approximates the successor measure for a fixed policy π, discussed by Touati et al. (2023).

$$\min_{\phi,\psi} \mathbb{E}_{\substack{s_t\sim p(s), s'\sim p(s) \\ s_{t+1}\sim p^\pi(s_{t+1}|s_t)}} \left[(\psi(s_t)^T \phi(s') - \gamma \bar{\psi}(s_{t+1})^T \bar{\phi}(s'))^2\right] - 2\mathbb{E}_{\substack{s_t\sim p(s) \\ s_{t+1}\sim p^\pi(s_{t+1}|s_t)}} \left[\psi(s_t)^T \phi(s_{t+1})\right] \tag{2}$$

FB learns an approximation of the successor measure with factorization $M^\pi(s, s_+) \approx \psi(s_t)\phi(s_+)p(s_+)$ using TD learning. Given transitions (s_t, s_{t+1}) sampled by a policy π, the second term relates to fitting $M^\pi(s_t, s_{t+1})$. Given an independently sampled state s', the first term bootstraps an estimate of $M^\pi(s_t, s')$ from $\bar{M}^\pi(s_{t+1}, s')$, where $\bar{\phi}, \bar{\psi}$ denote stop-gradient operations.

Contrastive Learning. Temporal contrastive learning used in MDPs (Eysenbach et al., 2022) is related to a Monte Carlo (MC) approximation of the (discounted) successor measure. This can be

implemented with a InfoNCE (van den Oord et al., 2019) loss that maximizes the similarity of a positive pair between a state s_t and a future state from the same trajectory s_+, and minimizing the similarity of s_t and random states s_-:

$$\max_{\phi,\psi} \mathbb{E}_{\substack{s_t \sim p(s) \\ k \sim \text{geom}(1-\gamma) \\ s_+ = s_{t+k}, s_-^{2:N} \sim p(s)}} \left[\log \frac{e^{f(\psi(s_t), \phi(s_+))}}{\sum_{i=2}^{N} e^{f(\psi(s_t), \phi(s_-^i))}} \right] \tag{3}$$

A common choice for the energy function f is the inner product $f(\psi(s)\phi(s_+)) = \psi(s)^T \phi(s_+)$. A key aspect to note is that the positive sample s_+ comes from an MC sample from $s_+ \sim M^\pi(s_t, s_+)$. The optimal solution to (3) gives $\tilde{M}^\pi(s, s_+) \approx C \exp(\psi(s_t)^T \phi(s_+)) \cdot p(s)$. However in-practice, we only have dataset of MC samples from π, i.e. fixed-length trajectories, which means we do not actually estimate the SM of π. In Appendix C, we further elaborate on the relationship between the FB loss, and CL. Particularly, in the limit, an n-step version of FB is related to CL.

BYOL. We now look at an objective that captures information about single-step transition instead of the successor measure. In the context of RL, self-predictive models jointly learn a latent space and a dynamics model through predicting future latent representations. Self-predictive models rely on latent bootstrapped targets (BYOL) (Grill et al., 2020), avoiding reconstruction (generative models), or negative samples (contrastive learning). Self-predictive models are also a type of joint-embedding predictive architectures (JEPAs) (LeCun, 2022; Garrido et al., 2024).

Given an encoder which produces a representation $z_t = \phi(s_t)$, and dynamics $\psi(z_{t+1}|z_t)$ for a fixed policy π, we minimize the difference between our prediction and target representation in latent-space:

$$\min_{\phi,\psi} \mathbb{E}_{s_t \sim\, p(s), s_{t+1} \sim p^\pi(s_{t+1}|s_t),} \left[f(\psi(\phi(s_t)), \bar{\phi}(s_{t+1})) \right] \tag{4}$$

Where f is a convex function such as the squared l_2 norm, and $\bar{\phi}$ refers to an EMA target, or stop-gradient. Variants of this BYOL objective have been widely used to learn state abstractions, and work as an auxiliary loss when approximating the value function in deep RL (Gelada et al., 2019; Schwarzer et al., 2020; Ni et al., 2024). In the finite MDP, this objective captures spectral information about the policy's transition matrix P^π (Tang et al., 2023; Khetarpal et al., 2025) which we discuss in Appendix D.1.

3.2 Combinatorial Generalization from Offline Data

We now shift focus on how we can learn policies from offline data using behavioral cloning, and then introduce a combinatorial generalization gap that arises in this setting.

We consider a **dataset** $\mathcal{D} = \{(s_0^i, a_0^i, \cdots, s_T^i, a_T^i)\}_{i=1}^N$, composed of trajectories generated by a set of unknown policies $\{\beta_j(a|s)\}$. **Goal Conditioned Behavioral Cloning (GCBC)** trains a policy with maximum likelihood to reproduce the behaviors from the dataset. After sampling a current state, a goal is sampled as a future state from the same trajectory:

$$\max_\pi \mathcal{L}_{\text{BC}}(\pi) = \max_\pi \mathbb{E}_{\substack{\beta_j \sim p(\beta_j),\ s \sim p(s|\beta_j) \\ a \sim \beta_j(a \mid s),\ s_+ \sim M^{\beta_j}(s, s_+)}} \left[\log \pi(a|s, g = s_+) \right] \tag{5}$$

Generalization gap. While this policy can perform well in-distribution, the behavior cloning policy struggles to generalize to reach goals from states that are not in matching training trajectories. We now review a more formal definition of this type of generalization gap.

We consider Lemma 3.1 from Ghugare et al. (2024), which says there exists a single Markovian policy $\beta(a|s)$ that has the same occupancy as the mixture of j policies:

$$M^\beta(s) = \mathbb{E}_{p(\beta_j)} \left[M^{\beta_j}(s) \right] \tag{6}$$

This policy also has construction: $\beta(a \mid s) := \sum_j \beta_j(a \mid s) p(\beta_j \mid s)$, where $p(\beta_j \mid s)$ is the distribution over policies in s as reflected by the dataset.

Using the successor measure of the individual policies, and the mixture policy, we can quantify a gap between accomplishing out-of-distribution tasks versus in-distribution training tasks (Ghugare et al., 2024):

$$\underbrace{\mathbb{E}_{\substack{s_0 \sim M^{\beta}(s_0) \\ s_g \sim M^{\beta}(s_0, s_g)}} \left[u^{\pi}(s_0, s_g) \right]}_{\text{tasks requiring combinatorial generalization}} - \underbrace{\mathbb{E}_{\substack{\beta_j \sim p(\beta_j),\, s_0 \sim M^{\beta_j}(s_0) \\ s_g \sim M^{\beta_j}(s_0, s_g)}} \left[u^{\pi}(s_0, s_g) \right]}_{\text{in-distribution training tasks}} \tag{7}$$

Here, u is a performance metric of the policy π such as the success rate to reach s_g from s_0. As we perform well on in-distribution tasks due to a correspondence to Equation (5), the BC policy has no guarantees for the first term. This is because after sampling a state, the goal is sampled from the successor measure of the mixture policy.

4 Closing the Generalization Gap with Representations

In this section, we aim to close the aforementioned generalization gap. We consider a policy trained with the BC objective π to be made more robust to the tasks requiring combinatorial generalization through representation learning. We begin with a setup similar to Equation (7), but with a shared initial state s_0 for both the in-distribution and out-of-distribution task. For the in-distribution task, we sample a goal as before, labeled as s_w. However, for the out-of-distribution task, we sample a goal s_f to be a state that can be reached by the mixture policy β after s_w. (8):

$$\mathbb{E}_{\substack{\beta_j \sim p(\beta_j), s_0 \sim M^{\beta_j}(s) \\ s_w \sim M^{\beta_j}(s_0, s_w)}} \left[\underbrace{\mathbb{E}_{s_f \sim M^{\beta}(s_w, s_f)} \left[u^{\pi}(s_0, s_f)) \right]}_{\text{extended task requiring generalization}} - \underbrace{u^{\pi}(s_0, s_w)}_{\text{in-distribution task}} \right] \tag{8}$$

$$= \mathbb{E}_{\substack{\beta_j \sim p(\beta_j), s_0 \sim M^{\beta_j}(s) \\ s_w \sim M^{\beta_j}(s_0, s_w)}} \left[\underbrace{\mathbb{E}_{s_f \sim M^{\beta}(s_w, s_f)} \left[u^{\pi}(s_0, \phi(s_f)) \right]}_{\text{want invariance with respect to future goals through } \phi} - u^{\pi}(s_0, \phi(s_w)) \right] \tag{9}$$

Then, in Equation (9) we add a goal representation ϕ that processes the goal before going to policy π. Intuitively, a policy could achieve the out-of-distribution task by first going from s_0 to s_w (in-distribution), and then completing the remaining task s_w to s_f. In essence, we want that when conditioning on $\phi(s_f)$, the policy should first go to s_w, which can be achieved by learning ϕ, where $\phi(s_w)$ is similar to $\phi(s_f)$ (Myers et al., 2025b). More formally, for $s_f \sim M^{\beta}(s_w, s_f)$ we want an invariance $\phi(s_f) \approx \phi(s_w)$.

From this observation, we can understand that approximating the successor measure of the mixture policy β, when parameterized by ϕ, will build the desired representation. One choice for the representation learning objective can be the FB algorithm, which obtains a factorization $M^{\beta}(s, s_+) \approx \psi(s_t)\phi(s_+)p(s_+)$ (Touati et al., 2023). FB utilizes TD-learning to learn the same representations given transitions (s_t, s_{t+1}), regardless of how these transitions are divided between trajectories. However, FB may not scale as well to large datasets and high-dimensional state spaces. This may lead us to prefer an MC approximation of the SM, using CL. A key point here is that we do not have MC samples from β, only the individual policies β_j, so CL does not directly approximate M^{β}. However, in practice, CL can still build a representation space with a compositional structure (Myers et al., 2025b), and may be a more scalable option than FB.

4.1 BYOL-γ: Connecting self-predictive objectives to the successor representation

To build representations that lead to generalization, we propose a predictive objective, relying on neither TD learning nor negative samples. Specifically, we propose BYOL-γ which allows us to use the BYOL framework to capture information related to *successor representations* and its generalizations. Given a state s_t, a BYOL objective would normally sample a prediction target from

a one-step transition s_{t+1} as in Equation (4). However, we make a modification to predict empirical samples from the normalized successor measure:

$$\mathcal{L}_{\text{BYOL-}\gamma}(\phi, \psi) = \mathbb{E}_{\substack{s_t \sim p(s), k \sim \text{geom}(1-\gamma) \\ s_{t+k} \sim p^{\pi}(s_{t+k}|s_t)}} \left[f(\psi(\phi(s_t)), \bar{\phi}(s_{t+k})) \right] \tag{10}$$

Where f refers to an energy function, ϕ refers to the encoder, and ψ the predictor. With $\gamma = 0$, we have $s_{t+k} = s_{t+1}$ corresponding to an approximation of the one-step transitions, recovering the base BYOL objective. Figure 1b depicts our overall representation learning objective. We can view this objective as iteratively minimizing an upper-bound on the error between $\psi(\phi((s))$ and the true successor features of the policy ψ^{π} with changing basis features $\bar{\phi}$. With convex f, by Jensen's inequality we have:

$$\begin{aligned}
\mathcal{L}_{\text{BYOL-}\gamma}(\phi, \psi) &= \mathbb{E}_{s_t \sim p(s), s_+ \sim \tilde{M}^{\pi}(s_t, s_+)} \left[f(\psi(\phi(s_t)), \bar{\phi}(s_+)) \right] && (11) \\
&\geq \mathbb{E}_{s_t \sim p(s),} \left[f(\psi(\phi(s_t)) \mathbb{E}_{s_+ \sim \tilde{M}^{\pi}(s_t, s_+)} \bar{\phi}(s_+)) \right] && (12) \\
&= \mathbb{E}_{s_t \sim p(s)} \left[f(\psi(\phi(s_t)), (1-\gamma)\psi^{\pi}_{\bar{\phi}}(s_t) \right] && (13)
\end{aligned}$$

Specifically, in the finite MDP, we can precisely describe the relationship of our objective to the SR with the following result:

Theorem 4.1. *Given a finite MDP with linear representations $\Phi \in \mathbb{R}^{|\mathcal{S}| \times d}$, and predictor $\Psi \in \mathbb{R}^{d \times d}$, under assumptions of orthogonal initialization for Φ (Ass. D.1), a uniform initial state distribution $p_0(s)$ (Ass. D.2), and symmetric transition dynamics (Ass. D.3), minimizing the self-predictive learning objective $\mathcal{L}_{\text{BYOL-}\gamma}(\phi, \psi)$ approximates a matrix decomposition of the successor representation $\tilde{M}^{\pi} \approx \Phi\Psi\Phi^T$, corresponding to successor features $(1-\gamma)\Psi^{\pi} \approx \Psi\Phi$.*

Proof is in Appendix D.2, where we show that existing theory (Khetarpal et al., 2025) also translates to the proposed BYOL-γ objective. Finally, we can see the relation between this objective and CL (3), with the most striking difference being the removal of the denominator involving negative samples. Surprisingly, we reveal that this simplified system still captures similar information and also can lead to empirical generalization in Section 5.1.

BYOL-γ Variants. We discuss a few variants on our base objective, namely, we find it beneficial to consider **bidirectional prediction** (Guo et al., 2020; Tang et al., 2023) where we add an additional backwards predictor ψ_b which predicts a past representation from the future:

$$\mathcal{L}_{\text{BYOL-}\gamma}(\phi, \psi) = \mathbb{E}_{s_t \sim p(s), s_+ \sim \tilde{M}^{\pi}(s_t, s_+)} \left[f(\psi_f(\phi(s_t)), \bar{\phi}(s_+)) + f(\bar{\phi}(s_t), \psi_b(\phi(s_+)) \right] \tag{14}$$

We utilize an **action-conditioned** variant of the forward predictor $\psi_f(\phi(s_t), a_t)$, which can be interpreted as a temporally extended latent dynamics model, or capturing information about $\tilde{M}^{\pi}(s, a, s_+)$.

4.2 Training a policy with auxiliary BYOL-γ

We consider BYOL-γ as an auxiliary loss for a BC policy $\pi_{\Theta}(a|s, g)$, $\Theta = (\theta, \phi, \psi)$, to better address generalization of a policy. The parameters of the encoder and predictor correspond to ϕ, ψ, and θ includes additional parameters such as a policy head which transforms representations to actions. With this policy, we train with the objective:

$$\begin{aligned}
&\mathcal{L}_{\text{BC}}(\Theta) + \alpha \mathcal{L}_{\text{BYOL-}\gamma}(\phi, \psi) && (15) \\
&\quad = \mathbb{E}_{(s_t, a_t, s_+) \sim \mathcal{D}} \left[-\log \pi_{\Theta}(a|\phi(s), g = \phi(s_+)) \right] \\
&\quad + \alpha \mathbb{E}_{(s_t, a_t, s_+) \sim \mathcal{D}} \left[f(\psi_f(\phi(s_t), a_t), \bar{\phi}(s_+)) + f(\bar{\phi}(s_t), \psi_b(\phi(s_+)) \right]
\end{aligned}$$

For f, we choose a cross-entropy loss between the (softmax) normalized representations of the prediction and the target, similar to DINO (Caron et al., 2021): $f_{\text{CE}}(a, b) = \text{softmax}(b) \cdot \log \text{softmax}(a)$. We also find a normalized l_2 loss, $f_{l_2} = \| \frac{a}{\|a\|} - \frac{b}{\|b\|} \|_2^2$, commonly used in BYOL setups (Grill et al., 2020; Schwarzer et al., 2020) also works, which we ablate in Section 5.4. We describe additional training details in Appendix A.1.

5 Experiments

We have shown the theoretical basis for BYOL-γ as an appropriate choice of representation learning objective for combinatorial generalization. Next, we demonstrate its performance empirically. Namely, we compare our proposed method BYOL-γ to alternative representation learning methods. We compare representation learning algorithms across three axes: (1) First, we compare qualitatively whether the representations appear to capture temporal relationships (2) Second, we assess representations quantitatively by measuring zero-shot generalization performance on unseen tasks that require combinatorial generalization (3) Third, we assess generalization performance over an increasing generalization horizon. Finally, we perform ablations on the various components of our proposed method to demonstrate the relative importance of each algorithmic choice.

Environments We empirically evaluate how well our approach can help with combinatorial generalization on offline goal-reaching tasks on OGBench (Park et al., 2025), which contains both navigation and manipulation tasks, across both low-dimensional and visual observations. We focus on navigation environments, where OGBench provides `stitch` datasets, that assess combinatorial generalization by training on trajectories that span at most 4 maze cells, while evaluating on tasks that are longer, requiring combining information from multiple smaller trajectories.

Baselines We benchmark against non-hierarchical methods, that perform end-to-end control from state to low-level actions (e.g. joint-control). In addition to BYOL-γ used as an auxiliary loss for BC, we evaluate several baselines: **GCBC** is the standard behavioral cloning baseline, which we aim to improve upon with representation learning objectives. **Offline RL** from OGBench, including implicit {V,Q}-learning (**IVL, IQL**) (Kostrikov et al., 2022), Quasimetric RL (**QRL**)(Wang et al., 2023), and Contrastive RL (**CRL**) (Eysenbach et al., 2022). **BYOL** is a minimal version of our BYOL-γ setup with 1-step prediction ($\gamma = 0$), only forwards prediction (ψ_f) without action-conditioning ($\psi_f(\phi(s_t))$), and loss f_{l_2}. **TRA** (Myers et al., 2025b) is an auxiliary representation objective using contrastive learning related to an MC approximation of the successor measure **FB**, an on-policy version of forward-backward representation described in Equation (2) used as an auxiliary objective, and is related to TD approximation of the successor measure. We also compare to an n-step version of the BYOL objective in Appendix B.2.

Experimental Setup We match the training details of OGBench, and consider a similar representation learning setup to TRA. For TRA and FB, we utilize a similar setup described in Section 4.2. We found it was beneficial to add action conditioning to FB, but did not see an overall improvement for TRA, so we use the original setup without action-conditioning. We provide a full comparison for action-conditioning in Appendix B.1. We note that when we perform action-conditioning, we change the representation of the policy from $\pi(\phi(s), \psi(g))$ to $\pi(\phi(s), \phi(g))$. In Table 1, we utilize superscript a to denote methods with action-conditioning. Notably, we find that the weight of the auxiliary representation learning objectives (α) can be sensitive to both the embodiment, and size of environment (`medium` vs `large`). For each method, we perform a hyperparameter sweep over 4 α values, and report the best result for each environment in Table 1. We hold other hyperparameters constant across experiments, except with variation between non-visual and visual environments noted in Appendix A.

5.1 Qualitative analysis of representations

In Figure 2, we display a qualitative analysis of the representations. We visualize the similarity between the future prediction ψ for each state to $\phi(g)$ for a fixed goal g. We can see that **BYOL-γ** seems to learn a representation that encodes reachability between states, and has a similar structure to **FB**, which is known to approximate the successor measure. **TRA** and base **BYOL** seem to both capture similar structure and learn a less well-defined latent space. However, BYOL-γ and FB have more distinct similarity, and have visible "paths" of similar states. **BYOL-γ** also appears to capture the most similarity among more distant pairs of states. Compared to **TRA**, our hypothesis here is that

we have more optimistic similarity between distant states due to the lack of a negative term in the loss, which pushes representations apart.

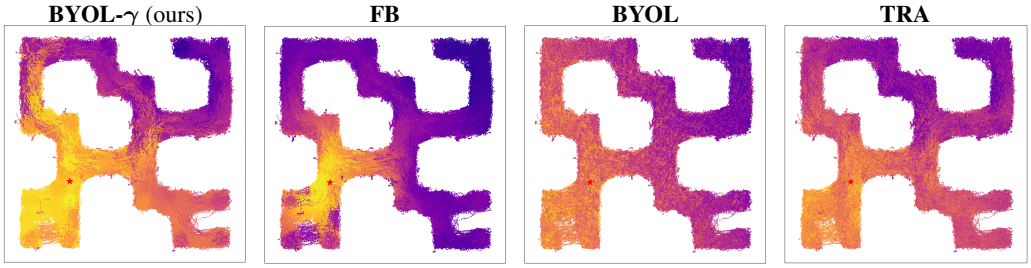

Figure 2: **Visualization of the Learned Representation: depicts the similarity between the prediction of the current state representation to the goal representation.** For **BYOL-γ** and **FB**, we visualize the cosine similarity between $\psi(\phi(s,a)), \phi(g)\ \forall s \in D$ for a fixed goal g which is indicated by the star marked in red. For **TRA**, we compare $\psi(s), \phi(g)$. **BYOL-γ** captures similar temporal relationships as the baseline methods.

5.2 Zero-shot performance on combinatorial generalization tasks

In Table 1, we provide the performance results across all methods. Overall, our proposed method **BYOL-γ**, shows improved performance vs. **GCBC** across most environments, and is either competitive with or outperforms **FB** and **TRA**. Importantly, we find that a minimal **BYOL** setup does not confer significant benefit over the base **GCBC** except in non-visual `antmaze` environments. Generally, auxiliary representation learning with **GCBC** outperforms existing offline RL methods.

Within the auxillary loss methods, we find that **FB** and **BYOL-γ** tend to outperform **TRA** on most environments. While we find that **FB** outperforms **BYOL-γ** on environments with smaller state spaces (`antmaze-{medium,large}`), we find that **BYOL-γ**'s simpler training procedure is beneficial in environments with larger state spaces (`humanoidmaze-{medium,large}`, `visual-antmaze-medium` and `visual-scene-play`).

Dataset	BYOL-γ^a	BYOL	TRA	FB^a	GCBC	GCIVL	GCIQL	QRL	CRL
antmaze-medium-stitch	58 ± 5	59 ± 4	54 ± 6	64 ± 6	45 ± 11	44 ± 6	29 ± 6	59 ± 7	53 ± 6
antmaze-large-stitch	19 ± 7	17 ± 6	11 ± 8	23 ± 4	3 ± 3	18 ± 2	7 ± 2	18 ± 2	11 ± 2
humanoidmaze-medium-stitch	51 ± 6	23 ± 3	45 ± 8	42 ± 4	29 ± 5	12 ± 2	12 ± 3	18 ± 2	36 ± 2
humanoidmaze-large-stitch	13 ± 3	3 ± 1	5 ± 4	11 ± 3	6 ± 3	1 ± 1	0 ± 0	3 ± 1	4 ± 1
antsoccer-arena-stitch	25 ± 5	12 ± 7	14 ± 4	22 ± 10	24 ± 8	21 ± 3	2 ± 0	1 ± 1	1 ± 0
visual-antmaze-medium-stitch	68 ± 4	57 ± 8	52 ± 3	49 ± 2	67 ± 4	6 ± 2	2 ± 0	0 ± 0	69 ± 2
visual-antmaze-large-stitch	26 ± 5	26 ± 5	17 ± 1	29 ± 2	24 ± 3	1 ± 1	0 ± 0	1 ± 1	11 ± 3
visual-scene-play	17 ± 1	13 ± 3	16 ± 3	14 ± 1	12 ± 2	25 ± 3	12 ± 2	10 ± 1	11 ± 2
average	35	26	27	32	26	16	8	14	25

Table 1: **OGBench: We find that BYOL-γ performs better overall compared to prior methods**. We report mean and standard deviation over 10 training seeds in non-visual environments, and 4 seeds in visual environments. We match the OGBench evaluation setup of 5 evaluation (state,goal) tasks, and 50 episodes per task. The success rate is then averaged over the last 3 checkpoints. We color the best non-RL method, and **bold** values within 95% of its value in the same row. We use superscript a to denote methods utilizing action-conditioning.

Interestingly, in `visual-antmaze` **TRA** and **FB** actually seem to hurt performance in comparison to base **GCBC**. On the other hand, with **BYOL-γ** we see no performance degradation over **GCBC** on the visual environments, a considerable improvement over other methods.

5.3 Evaluating generalization with increasing horizon

We conduct experiments to understand how success rate changes as an agent has to reach more challenging goals further away from its starting position. For each `maze` environment, we consider

Dataset	BYOL-γ^a	$-a$	f_{l_2}	$-\psi_b$	$\gamma = 0$
antmaze-medium-stitch	61 ± 6	63 ± 9	56 ± 4	67 ± 2	59 ± 5
antmaze-large-stitch	21 ± 5	27 ± 7	24 ± 6	19 ± 7	8 ± 4
humanoidmaze-medium-stitch	54 ± 5	48 ± 5	49 ± 6	$\mathbf{52} \pm 5$	18 ± 2
humanoidmaze-large-stitch	$\mathbf{14} \pm 2$	12 ± 6	15 ± 7	13 ± 2	3 ± 1
antsoccer-arena-stitch	21 ± 4	20 ± 5	11 ± 5	27 ± 7	$\mathbf{25} \pm 7$
visual-antmaze-medium-stitch	68 ± 4	$\mathbf{65} \pm 3$	63 ± 5	61 ± 4	54 ± 9
visual-antmaze-large-stitch	26 ± 5	25 ± 8	$\mathbf{27} \pm 7$	28 ± 2	$\mathbf{28} \pm 1$
average	33	33	31	33	24

Table 2: **BYOL-γ ablations.** We ablate components of our representation learning objective. For each ablation, we perform a hyperparameter sweep over α, and report the best result per-environment. For all environments, we report results over 4 seeds (for **BYOL-γ**, we use the first 4 of the 10 reported in Table 1). We color the best method, and **bold** values within 95% of its value in the same row.

the same base 5 evaluation tasks used in Table 1, but construct intermediate waypoints along the shortest path to the final goal determined by Breadth First Search. We also include an additional `maze` environment, `giant` on which all methods have zero success rates to reach distant goals. This gives a more holistic view on an agent's performance.

We display results in Figure 3 and Appendix E, where we can see how performance drops off for all methods after a generalization threshold denoted by the red bar. While all methods cannot fully reach distant goals on `giant`, we see that **BYOL-γ** has the slowest drop-off in performance. We note that this is a challenging task, that requires stitching up to approximately 8 different trajectories.

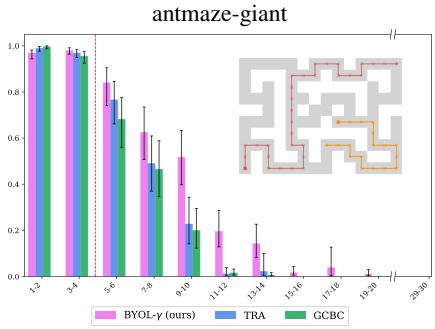

Figure 3: **Evaluating Generalization with Increasing Horizons**: shows that **BYOL-γ** not only performs well on goals in the near horizon, but also, generalizes well to goals that requiring stitching occurring after the red bar (> 4).

5.4 Components affecting generalization for representation learning

We ablate key components of the **BYOL-γ** objective in Table 2. This includes removing action conditioning for forward predictor ψ_f ($-a$), swapping the loss from cross-entropy to normalized squared l_2 norm (f_{l_2}), removing backwards predictor ψ_b, and predicting the representation of the adjacent state ($\gamma = 0$). Both removing action-conditioning, and backwards prediction overall lead to similar results, but variability per-environment. For f_{l2}, we obtain slightly worse average performance, and for $\gamma = 0$, we see the largest drop-off, especially on `humanoidmaze` environments.

6 Discussion

Limitations. While we demonstrate that BYOL-γ and other representation learning objectives offer a promising recipe for obtaining combinatorial generalization, we find that there still exists a generalization gap, especially on challenging navigation environments e.g. `giant`. We find a less significant improvement over BC on visual environments, which may motivate additional investigation. Additionally, we may anticipate more benefit from representation learning when applied to larger visual datasets, which has been fruitful in other domains.

Conclusion. In this work, we provide a stronger understanding of the relationship between quantities related to successor representations and the generalization of policies trained with behavioral cloning. We propose a new self-predictive representation learning objective, BYOL-γ, and show that it captures information related to the successor measure, resulting in a competitive choice of an auxiliary loss for better generalization. We demonstrate that augmenting behavior cloning with meaningful representations results in new capabilities such as improved combinatorial generalization, especially in larger and more complex environments.

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A Experimental Setup

Table 3: Hyperparameters for BYOL-γ

Hyperparameter	**Shared**
actor head	MLP (512,512,512)
representation encoder (ϕ)	MLP (64,64,64)
predictor (ψ)	MLP (64,64,64)
encoder ensemble	2
learning rate	3×10^{-4}
optimizer	Adam

	Non-visual	**Visual**
Gradient steps	1000k	500k
Batch size	1024	256
τ (EMA)	1.0	0.99
γ	0.99	{0.66, 0.99}
α (alignment)	{1,6,40,100}	{1,6,10,20}
additional encoder	n/a	impala_small
encoder output dimension	$\|s\|$	64

A.1 Implementation Details

In this section we provide more training details for BYOL-γ, and representation learning baselines. We match the training details of OGBench, including gradient steps, batch size, learning rate.

Network Architecture. We follow the same network architecture setup as TRA, where we utilize MLP-based encoders, and action head. For the output dimension of the encoder, we use the state dimension for non-visual experiments, and 64 for visual experiments. For the predictor ψ, we utilize an MLP of the same architecture as the encoder. For image-based tasks, there is an additional CNN, which then passes output to the MLP encoder.

Representation Ensemble. We follow the setup of TRA which utilizes representation ensembling, such that two copies of the encoder ϕ_1, ϕ_2 are in parallel. We also have two distinct predictors ψ_1, ψ_2 for each ensemble. As input to the policy head, we average the representations, $\bar{z} = \frac{\phi_1(s_t)+\phi_2(s_2)}{2}$. Each representation is trained independently for the BYOL loss, but the BC loss differentiates through both ϕs.

Alignment. We find that the choice of weight of the auxiliary loss for the representation learning objective is sensitive to both the robot embodiment and the environment size. For comparison, we perform a hyperparameter search over four alignment values for BYOL-γ, TRA, and FB, and then report the best value for each environment in Table 1.

Discount. For sampling the next-state, we utilize a discount factor of $\gamma = 0.99$ for all non-visual environments. For visual environments, we perform a hyperparameter search over $\{0.66, 0.99\}$, however all representation learning methods performed better at $\gamma = 0.66$.

A.2 BYOL-γ

Target network. For BYOL, we find that exponential moving average (EMA) target networks for the encoder ϕ are not necessary for non-visual environments ($\tau = 1$), but for visual environments,

we find that a fast target stabilizes training ($\tau = 0.99$):

$$\phi_{\text{target}} = \tau\phi_{\text{online}} + (1-\tau)\phi_{\text{target}}$$

A.3 TRA

In practice, TRA uses a symmetric version (Radford et al., 2021) of the InfoNCE objective discussed in Equation 3. We write this in batch form, $\mathcal{B} = \{(s_i, s_{+,i})\}_{i=1}^{|\mathcal{B}|}$ rather than in expectation:

$$\mathcal{L}_{\text{TRA}} = \mathbb{E}_{\mathcal{B}}\left[-\frac{1}{B}\sum_{i=1}^{|\mathcal{B}|}\log\frac{e^{f(\psi(s_i),\phi(s_{+,i}))}}{\sum_{j=1}^{|\mathcal{B}|}e^{f(\psi(s_i),\phi(s_{+,j})}} - \frac{1}{B}\sum_{i=1}^{|\mathcal{B}|}\log\frac{e^{f(\psi(s_i),\phi(s_{+,i}))}}{\sum_{j=1}^{|\mathcal{B}|}e^{f(\psi(s_j),\phi(s_{+,i})}}\right] \tag{16}$$

Additionally, TRA minimizes the squared norm of representations $\min_{\phi,\psi}\lambda\mathbb{E}_s[\frac{\|\phi(s)\|^2}{d} + \frac{\|\psi(s)\|^2}{d}]$ with $\lambda = 10^{-6}$. For TRA, we search over $\alpha = \{10, 40, 60, 100\}$.

A.4 FB

Prior work which trains FB for zero-shot policy optimization (Touati et al., 2023) typically normalizes ϕ with an additional loss term so that $\mathbb{E}\left[\phi\phi^T\right] \approx I_d$. However, we found that adding this loss term was not beneficial to performance in our setting and hence do not include it.

FB uses an EMA target network as described in A.2 with $\tau = 0.005$. For FB, we search over $\alpha = \{0.01, 0.05, 0.001, 0.005\}$.

A.5 Code.

We utilize the OGBench (Park et al., 2025) codebase and benchmark, and its extensions in the TRA codebase (Myers et al., 2025b) for equal comparison.

A.6 Compute Requirements

We perform all experiments utilizing single GPUs, predominately NVIDIA RTXA8000 and L40S. We utilize 6 CPU cores, 24G of RAM for non-visual environments, and 64G for visual experiments. Experiments take 2 to 4 hours for non-visual and 6 to 12 hours for visual environments.

B Ablations.

B.1 Action-conditioning

In this section, we ablate the component of performing action-conditioning for the predictor $\psi(s_t)$ vs $\psi(s_t, a_t)$ for TRA and FB. We consider a similar comparison for BYOL-γ in Table 2. For this comparison, when we perform action-conditioning, we utilize a policy representation $\pi(s = \phi(s), g = \phi(g))$, and otherwise $\pi(s = \psi(s), g = \phi(g))$. We find that results can be environment specific. On average, results are not improved for TRA, but we find an improvement for FB, hence in our main Table 1 we include the action-conditioned results for FB and the action-free results for TRA.

B.2 N-step BYOL

We provide an additional BYOL-based baseline that utilizes n-step next-representation recurrent prediction, while BYOL-γ uses non-recurrent prediction. We utilize the same BYOL-γ architecture with forward prediction, but with the following objective, computing loss with n terms, where ψ_f^n is shorthand for n recurrent calls:

$$\mathcal{L} = f(\psi_f(\phi(s_t, a_t), \bar{\phi}(s_{t+1})) + f(\psi_f(\psi_f(\phi(s_t, a_t), a_{t+1}), \bar{\phi}(s_{t+2})) + \cdots + f(\psi_f^n(\cdot), \bar{\phi}(s_{t+n}))$$

Dataset	TRA	TRA^a	FB	FB^a
antmaze-medium-stitch	54 ± 6	57 ± 12	$\mathbf{64} \pm 10$	$\mathbf{64} \pm 6$
antmaze-large-stitch	11 ± 8	7 ± 7	17 ± 6	$\mathbf{23} \pm 4$
humanoidmaze-medium-stitch	$\mathbf{45} \pm 8$	$\mathbf{45} \pm 5$	36 ± 3	$\mathbf{42} \pm 4$
humanoidmaze-large-stitch	5 ± 4	9 ± 4	6 ± 2	$\mathbf{11} \pm 3$
antsoccer-arena-stitch	14 ± 4	$\mathbf{25} \pm 8$	17 ± 5	22 ± 10
visual-antmaze-medium-stitch	$\mathbf{52} \pm 3$	33 ± 4	47 ± 5	$\mathbf{49} \pm 2$
visual-antmaze-large-stitch	17 ± 1	22 ± 5	$\mathbf{28} \pm 3$	$\mathbf{29} \pm 2$
visual-scene-play	16 ± 3	$\mathbf{18} \pm 2$	12 ± 2	14 ± 1
average	27	27	28	32

Table 4: **Action-conditioning ablations.** We ablate the choice to condition on the first action for predictor ψ for TRA and FB over 10 seeds for non-visual and 4 seeds for visual environments.

Dataset	BYOL-γ^a	$-\psi_b$	$\gamma = 0$	$-\psi_b, \gamma = 0$	BYOL$^a_{n=1}$	BYOL$^a_{n=3}$	BYOL$^a_{n=5}$
antmaze-medium-stitch	61 ± 6	$\mathbf{67} \pm 2$	59 ± 5	60 ± 5	60 ± 8	60 ± 7	58 ± 7
antmaze-large-stitch	$\mathbf{21} \pm 5$	19 ± 7	8 ± 4	13 ± 5	19 ± 4	8 ± 4	3 ± 3
humanoidmaze-medium-stitch	$\mathbf{54} \pm 5$	$\mathbf{52} \pm 5$	18 ± 2	27 ± 7	33 ± 4	32 ± 2	20 ± 1
humanoidmaze-large-stitch	$\mathbf{14} \pm 2$	$\mathbf{13} \pm 2$	3 ± 1	5 ± 2	3 ± 2	3 ± 1	5 ± 2
antsoccer-arena-stitch	21 ± 4	$\mathbf{27} \pm 7$	25 ± 7	23 ± 6	25 ± 12	11 ± 7	13 ± 9
average	34	36	23	26	28	23	20

Table 5: **N-step BYOL ablations**. We ablate the BYOL-γ to an n-step BYOL baseline, where we report results over 4 seeds. We color the best method, and **bold** values within 95% of its value in the same row.

Theoretically, in a finite MDP, we can interpret this objective of capturing information up to n-step transitions (Tang et al., 2023), i.e. information related to $\{P_a, P_a^2, \cdots, P_a^n\}$ is captured by loss terms $\{\psi_f, \psi_f^2, \cdots, \psi_f^n\}$ respectively. As BYOL-γ captures information related to $\tilde{M}^\pi = (1-\gamma)\sum_{t\geq 0} \gamma^t P_\pi^t$, these two objectives match in theory at $\gamma = 0$. In practice, as n-step operates recurrently, we are constrained to a shorter n which limits the ability for learning long-horizon information.

Empirically, we report comparison of n-step with $n = \{1, 3, 5\}$ to BYOL-γ in Table 5. We validate our n-step implementation in the base case ($n = 1$) with the ablation $\{-\psi_b, \gamma = 0\}$ to BYOL-γ making them equivalent. With increased multi-step prediction (as we increase n), we find worse performance on average.

C CL to FB

Here, illustrate that connection between CL and FB, showing that in the limit an n-step version of FB becomes similar to CL.

We can rewrite Equation (3) to see the connection between FB (TD) and CL (MC). Under assumptions that ϕ, ψ are centered ($\mathbb{E}[\phi] = \mathbb{E}[\psi] = 0$), and unit normalized $\|\phi\|_2, \|\psi\|_2 = 1$, if we apply a second-order Taylor expansion to the denominator of the CL loss (Touati et al., 2023) we have:

$$\text{CL}_{\text{InfoNCE}} \approx \frac{1}{2}\mathbb{E}_{s\sim p_0(s), s'\sim p_0(s')}\left[(\psi(s)^T\phi(s'))^2\right] - 2\mathbb{E}_{\substack{k\sim\text{geom}(1-\gamma)\\ s_t\sim p_0, s_{t+k}\sim p^\pi(s_{t+k}|s_t)}}\left[\psi(s_t)^T\phi(s_{t+k})\right] \tag{17}$$

Next, we can consider an n-step variant of the FB loss (Blier et al., 2021) which we refer to as $\text{FB}(n)$:

$$\min_{\phi,\psi} \mathbb{E}_{\substack{s_t\sim p_0\\ s'\sim p_0}}\left[(\psi(s_t)^T\phi(s') \;-\; \gamma^n\bar{\psi}(s_{t+n})^T\bar{\phi}(s'))^2\right] - 2\sum_{i=1}^{n}\mathbb{E}_{s_t\sim p_0, s_{t+i}\sim p^\pi}\left[\gamma^i\psi(s_t)^T\phi(s_{t+i})\right] \tag{18}$$

We can make the full connection to CL with infinite horizon n:

$$\underset{n\to\infty}{\text{FB}(n)} = \mathbb{E}_{\substack{s_t\sim p_0\\ s'\sim p_0}}\left[(\psi(s_t)^T\phi(s'))^2\right] - 2\sum_{i=1}^{n}\mathbb{E}_{\substack{s_t\sim p_0\\ s_{t+i}\sim p^\pi(s_{t+i}s_0)}}\left[\gamma^i\psi(s_t)^T\phi(s_{t+i})\right] \tag{19}$$

$$= \mathbb{E}_{\substack{s_t\sim p_0\\ s'\sim p_0}}\left[(\psi(s_t)^T\phi(s'))^2\right] - \frac{2\gamma}{(1-\gamma)}\sum_{i=1}^{n}\mathbb{E}_{\substack{s_t\sim p_0\\ s_{t+i}\sim p^\pi(s_{t+i}s_0)}}\left[(1-\gamma)\gamma^{i-1}\psi(s_t)^T\phi(s_{t+i})\right] \tag{20}$$

$$= \mathbb{E}_{\substack{s_t\sim p_0\\ s'\sim p_0}}\left[(\psi(s_t)^T\phi(s'))^2\right] - \frac{2\gamma}{(1-\gamma)}\mathbb{E}_{\substack{k\sim\text{geom}(1-\gamma)\\ s_t\sim p_0, s_{t+k}\sim p^\pi(s_{t+k}|s_t)}}\left[\psi(s_t)^T\phi(s_{t+k})\right] \tag{21}$$

Thus, we can see that in the infinite horizon form of $\text{FB}(n)$, it is related to the form of $\text{CL}_{\text{InfoNCE}}$ in (3), but with the positive contrastive term weighted by factor $\frac{\gamma}{1-\gamma}$.

D Finite MDP

D.1 BYOL

BYOL as an Ordinary Differential Equation (ODE) In finite MDPs, we can characterize the BYOL objective which gives intuition about what information is captured in ϕ, ψ, and conditions that may be useful for stability (Tang et al., 2023; Khetarpal et al., 2025). Consider a finite MDP with transition P^π, linear d-dimensional encoder $\Phi \in \mathbb{R}^{|S|\times d}$, and linear action-free latent-dynamics $\Psi \in \mathbb{R}^{d\times d}$. In a finite MDP, Equation (4) becomes:

$$\min_{\Phi,\Psi}\text{BYOL}(\Phi,\Psi) := \min_{\Phi,\Psi}\mathbb{E}_{s_t\sim\, p(s), s_{t+1}\sim P^\pi,}\left[\|\psi^T\Phi^T s_t - \bar{\Phi}^T s_{t+1}\|_2^2\right] \tag{22}$$

A property to prevent this objective from collapsing is that Ψ is updated more quickly than Φ. In practice, this is commonly realized as the dynamics are generally a smaller network than the encoder. This system can be analyzed in an ideal setup, where we first find the optimal Ψ, each time before taking a gradient step for Φ, which leads to the ODE for representations Φ (Tang et al., 2023):

$$\Psi^* \in \arg\min_{\Psi}\text{BYOL}(\Phi,\Psi), \quad \dot{\Phi} = -\nabla_\Phi\text{BYOL}(\Phi,\Psi)|_{\Psi=\Psi^*} \tag{23}$$

We are able to analyze this ODE with the following assumptions (Tang et al., 2023):

Assumption D.1 (Orthogonal initialization)**.** $\Phi^\top\Phi = I$

Assumption D.2 (Uniform state distribution)**.** $p_0(s) = \frac{1}{|\mathcal{S}|}$
Assumption D.3 (Symmetric dynamics)**.** $P^\pi = (P^\pi)^\top$

Under these three assumptions, Khetarpal et al. (2025) prove that the BYOL ODE is equivalent to monotonically minimizing the surrogate objective:

$$\min_{\Psi} \|P^\pi - \Phi\Psi\Phi^T\|_F + C \tag{24}$$

Where $\|\cdot\|_F$ is the Frobenius matrix norm. Thus, we can understand that the BYOL objective as learning a d-rank decomposition of the underlying dynamics P^π. Additionally, the top d eigenvectors of P^π match those of $(I - \gamma P^\pi)^{-1} = M^\pi$ (Chandak et al., 2023). However, we will highlight that there are key differences when *learning* a low-rank decomposition between P^π and M^π. This is described by Touati et al. (2023), where we can consider that in a real-world problem with underlying continuous-time dynamics, actions have little effect, and P^π is close to the identity, i.e. close to full-rank. However, M^π, which takes powers of $(P^\pi)^t$, has a "sharpening effect" on the difference between eigenvalues, which gives a clearer learning signal. This is intuitive on a real-world problem like robotics, even with discrete-time dynamics, where $s_{t+1} \approx s_t$, but we have larger differences between s_t and s_{t+k}.

D.2 BYOL-γ

In the finite MDP, we now verify theorem 4.1 , where BYOL-γ approximates the successor representation with matrix decomposition $\tilde{M}^\pi \approx \Phi\Psi\Phi^T$.

We consider the same objective (22), where we need to update the expectation of the sampling distribution:

$$\min_{\Phi,\Psi} \text{BYOL-}\gamma(\Phi,\Psi) := \min_{\Phi,\Psi} \mathbb{E}_{s_t \sim\, p(s), s_+ \sim \tilde{M}^\pi}, \left[\|\psi^T \Phi^T s_t - \bar{\Phi}^T s_+\|_2^2\right] \tag{25}$$

Assuming that this objective is optimized under the ODE (23). We have that our objective monotonically minimizes:

$$\min_{\Psi} \|\tilde{M}^\pi - \Phi\Psi\Phi^T\|_F + C \tag{26}$$

This directly translates as we can consider $\tilde{M}^\pi = P^\pi$ as simply a valid transition matrix for a new, temporally abstract, version of the original MDP. We maintain the original assumptions D.1, D.2, and D.3. We do not need an additional assumption for $\tilde{M}^\pi$, as assumption D.3 for symmetric P^π implies a symmetric $\tilde{M}^\pi = (1-\gamma)\sum_{t\geq 0} \gamma^t P_\pi^t$,

Under this setup, we also have that $\Psi\Phi \in \mathbb{R}^{n\times d}$ relates to the successor feature matrix, where each row $(\Psi\Phi)_i$ contains the vector $(1-\gamma)\psi^\pi(s_i)$:

$$\begin{aligned}
(1-\gamma)\psi^\pi(s_i) &= \sum_j \tilde{M}^\pi(s_i, s_j)\phi(s_j) && (27)\\
&= (\tilde{M}^\pi \Phi)_i && (28)\\
&\approx (\Phi\Psi\Phi^T\Phi)_i && (29)\\
&= (\Phi\Psi)_i && (30)
\end{aligned}$$

In other words, in the restricted finite MDP, where we minimize (26), we are simultaneously learning successor features $\psi^\pi \approx \Psi\Phi$ and basis features Φ.

E Additional Results for Horizon Generalization

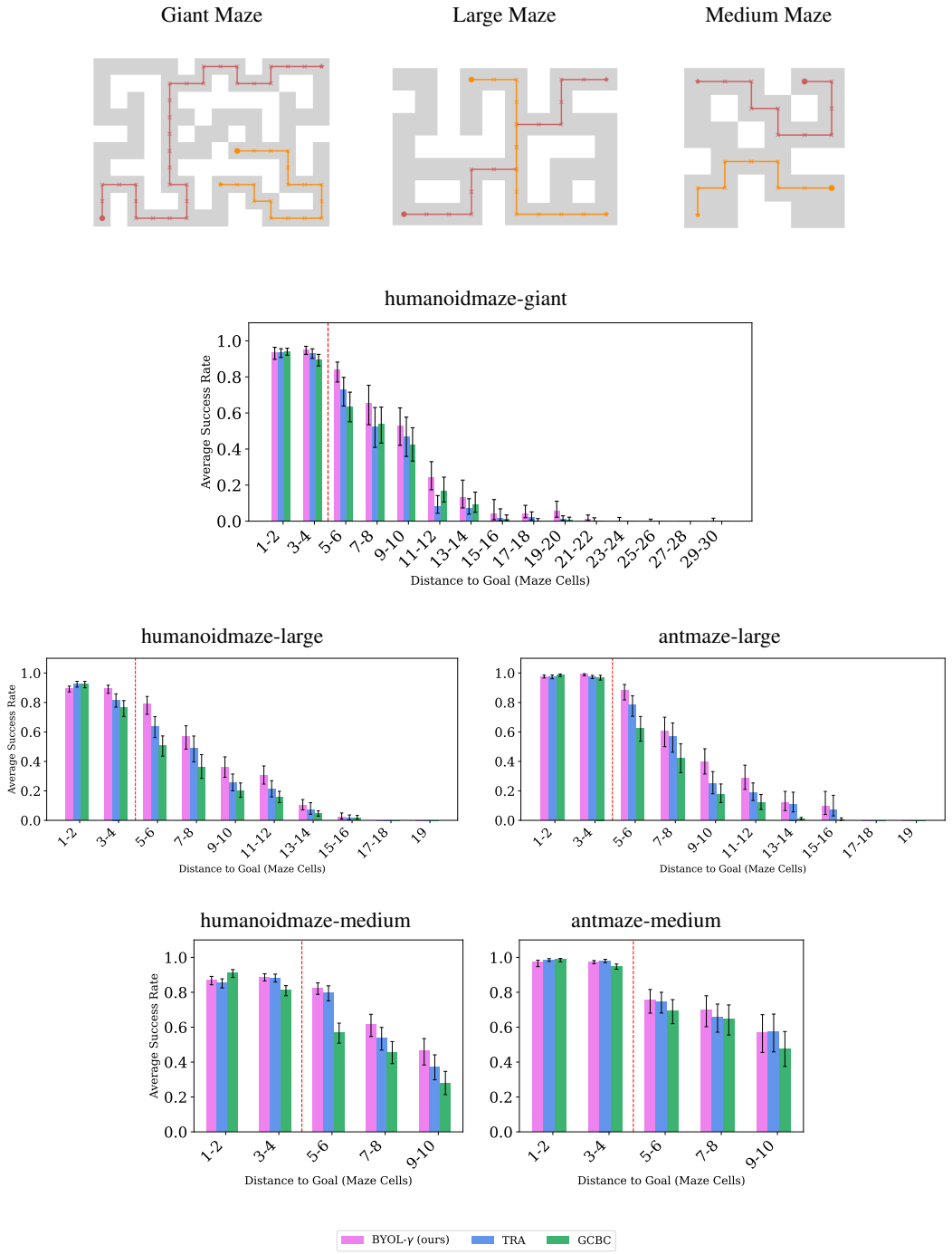

Figure 4: **Evaluating Generalization with Increasing Horizons:** The distances to the right of the red dotted line require combinatorial generalization. The maze maps show examples of how intermediate goals are selected along the optimal path.

We include additional results matching the setup in Section 5.3, for `antmaze-medium`, and `{humanoidmaze}-{medium,large,giant}` in Figure 4. We can observe that BYOL-γ leads in performance as the distance between the start and goal grows when compared to other methods.