
A Generalized Bisimulation Metric of State Similarity between Markov Decision Processes: From Theoretical Propositions to Applications

Zhenyu Tao, Wei Xu, Xiaohu You
Southeast University
Purple Mountain Laboratories
{zhenyu_tao, wxu, xhyu}@seu.edu.cn

Abstract

The bisimulation metric (BSM) is a powerful tool for computing state similarities within a Markov decision process (MDP), revealing that states closer in BSM have more similar optimal value functions. While BSM has been successfully utilized in reinforcement learning (RL) for tasks like state representation learning and policy exploration, its application to multiple-MDP scenarios, such as policy transfer, remains challenging. Prior work has attempted to generalize BSM to pairs of MDPs, but a lack of rigorous analysis of its mathematical properties has limited further theoretical progress. In this work, we formally establish a generalized bisimulation metric (GBSM) between pairs of MDPs, which is rigorously proven with the three fundamental properties: GBSM symmetry, inter-MDP triangle inequality, and the distance bound on identical state spaces. Leveraging these properties, we theoretically analyse policy transfer, state aggregation, and sampling-based estimation in MDPs, obtaining explicit bounds that are strictly tighter than those derived from the standard BSM. Additionally, GBSM provides a closed-form sample complexity for estimation, improving upon existing asymptotic results based on BSM. Numerical results validate our theoretical findings and demonstrate the effectiveness of GBSM in multi-MDP scenarios.

1 Introduction

Markov decision processes (MDPs) serve as a foundational framework for modeling decision-making problems in Reinforcement Learning (RL) [1]. To enable efficient analysis of MDPs, Ferns et al. [2] proposed the bisimulation metric (BSM) based on the Wasserstein distance, also known as the Kantorovich–Rubinstein metric, to quantify state similarity in a policy-independent manner. BSM provides theoretical guarantees that states closer under this metric exhibit more similar optimal value functions. Meanwhile, BSM is a pseudometric [3] satisfying: (1) Symmetry: $d(s, s') = d(s', s)$, (2) Triangle inequality: $d(s, s') \leq d(s, s'') + d(s'', s')$, and (3) Indiscernibility of identicals: $s = s' \Rightarrow d(s, s') = 0$. These three properties, combined with BSM’s measuring capability on optimal value functions, have driven its applications across diverse RL applications. It has been successfully employed in state aggregation [4, 5], representation learning [6, 7], policy exploration [8, 9], goal-conditioned RL [10], safe RL [11], etc.

However, since BSM is inherently defined over a single MDP, its application to theoretical analyses involving multiple MDPs faces notable obstacles. For instance, Phillips [12] applied BSM to policy transfer by constructing a disjoint union of the source and target MDPs’ state spaces. While this allows inter-MDP comparisons through BSM, the disjoint union enforces zero transition probabilities between states across the two MDPs. Consequently, this method fixes the total variation distance between their transition probabilities at one, hindering further simplifications and

analysis. It necessitates iterative calculation of distances across the entire state space, leading to prohibitive computational costs in deep RL tasks as noted in [13]. Also, in order to compute state similarities in continuous or large-space discrete MDPs, Ferns et al. [14] proposed a state similarity approximation method through state aggregation and sampling-based estimation. Although they proved the convergence of approximated state similarities to actual ones by leveraging properties of BSM and the Wasserstein distance, their approach only derived a fairly loose approximation error bound and failed to obtain an explicit sample complexity (i.e., the lower bound on the number of samples required to achieve the specified level of accuracy) for the estimation error. Specifically, the estimation error bound (see Eq. 7.1 in [14]) depends on the former aggregation process, resulting in an asymptotic sample complexity rather than a closed-form expression. In addition, for representation learning, Zhang et al. [6] and Kemertas and Aumentado-Armstrong [15] leveraged BSM to establish value function approximation bounds under optimal and non-optimal policies, respectively. However, BSM-based analysis between the original and aggregated MDPs results in loose bounds, particularly with large discount factors.

Several works have attempted to extend the definition of BSM for evaluating similarity between multiple MDPs [16–18]. Notably, when extended to multi-MDP scenarios, this modified version of BSM loses its pseudometric properties, as s and s' in $d(s, s')$ represent states in different MDPs. To the best of our knowledge, prior works have typically extended the single-MDP formulation to two MDPs, without rigorously retaining the metric properties. Specifically, Castro and Precup [16] utilized its evaluation capability on optimal value functions to analyze policy transfer. Due to the lack of metric properties, the derived theoretical performance bound is limited to transferring the optimal policy within the source MDP, as it can only reflect the effect of one-step action rather than the long-term impact of the transferred policy (see Theorem 5 in [16]). While Song et al. [17] successfully employed such a modified BSM in assessing MDP similarities and improving the long-term reward in policy transfer, their investigation focused on empirical validation rather than in-depth theoretical analysis. Furthermore, a comprehensive survey on various state similarity measures between MDPs [18], which highlighted the modified BSM as an effective approach, also emphasized the limited theoretical guarantees in current methodologies. This raises the following two questions:

Q1. Does the modified BSM possess any metric properties when computing state similarities between multiple MDPs, akin to the pseudometric properties of BSM within a single MDP?

Q2. If so, how can these properties facilitate the theoretical analysis involving multiple MDPs?

To answer Q1, we present a formal definition for the modified BSM in multi-MDP scenarios, which we refer to as generalized BSM (GBSM), and rigorously establish three metric properties that align with the pseudometric properties of BSM. These properties are summarized as (1) GBSM symmetry, (2) inter-MDP triangle inequality, and (3) the distance bound on identical state spaces. To answer Q2, we apply GBSM in the theoretical analyses of policy transfer, state aggregation, and sampling-based estimation of MDPs, yielding explicit bounds for policy transfer performance, aggregation error, and estimation error, respectively. Notably, when the compared MDPs are identical, the error bound of GBSM reduces to the error bound of BSM for a single MDP. We prove that the GBSM-derived bound is strictly tighter than the bound directly obtained from BSM, along with an explicit and closed-form sample complexity for approximation that advances beyond the asymptotic results of [14]. Numerical results corroborate our theoretical findings.

2 Background

Before describing the details of our contributions, we give a brief review of the required background in reinforcement learning and the bisimulation metric.

Reinforcement Learning We consider an MDP $\langle \mathcal{S}, \mathcal{A}, \mathbb{P}, R, \gamma \rangle$ defined by a finite state space \mathcal{S} , a finite action space \mathcal{A} , transition probability $\mathbb{P}(\tilde{s}|s, a)$ ($a \in \mathcal{A}$, $\{\tilde{s}, s\} \in \mathcal{S}$, and \tilde{s} denotes the next state), a reward function $R(s, a)$, and a discount factor γ . Policies $\pi(\cdot|s)$ are mappings from states to distributions over actions, inducing a value function recursively defined by $V^\pi(s) := \mathbb{E}_{a \sim \pi(\cdot|s)} [R(s, a) + \gamma \mathbb{E}_{\tilde{s} \sim \mathbb{P}(\cdot|s, a)} [V^\pi(\tilde{s})]]$. In RL, we are concerned with finding the optimal policy $\pi^* = \arg \max_\pi V^\pi$, which induces the optimal value function denoted by V^* .

Bisimulation Metric Different definitions of BSM exist in the literature [2, 4, 14]. In this paper, we adopt the formulation from [4], setting the weighting constant to its maximum value $c = \gamma$. The BSM is then defined as:

$$d^\sim(s, s') = \max_a \{ |R(s, a) - R(s', a)| + \gamma W_1(\mathbb{P}(\cdot|s, a), \mathbb{P}(\cdot|s', a); d^\sim) \}, \forall s, s' \in \mathcal{S}. \quad (1)$$

Here, W_1 is the 1-Wasserstein distance, measuring the minimal transportation cost between distributions $\mathbb{P}(\cdot|s, a)$ to $\mathbb{P}(\cdot|s', a)$, with d^\sim as the cost function. Ferns et al. [2] showed that this metric consistently bounds differences in the optimal value function, i.e., $|V^*(s) - V^*(s')| \leq d^\sim(s, s')$.

3 Generalized Bisimulation Metric

We now present a formal definition of the proposed GBSM and derive its key metric properties.

Definition 3.1 (Generalized bisimulation metric). *Given two MDPs $\mathcal{M}_1 = \langle \mathcal{S}_1, \mathcal{A}, \mathbb{P}_1, R_1, \gamma \rangle$ and $\mathcal{M}_2 = \langle \mathcal{S}_2, \mathcal{A}, \mathbb{P}_2, R_2, \gamma \rangle$, the GBSM between any state $s \in \mathcal{S}_1$ and any state $s' \in \mathcal{S}_2$ is defined as:*

$$d((s, \mathcal{M}_1), (s', \mathcal{M}_2)) = \max_a \{ |R_1(s, a) - R_2(s', a)| + \gamma W_1(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s', a); d^{1-2}) \}. \quad (2)$$

For notational simplicity, we use $d^{1-2}(s, s')$ to denote $d((s, \mathcal{M}_1), (s', \mathcal{M}_2))$, where the superscript 1-2 indicates the direction of GBSM from \mathcal{M}_1 to \mathcal{M}_2 . Before proving the existence of GBSM, we first introduce the Wasserstein distance [19], which is defined through the following primal linear program (LP):

$$\begin{aligned} W_1(P, Q; d) &= \min_{\lambda} \sum_{i=1}^{|\mathcal{S}_1|} \sum_{j=1}^{|\mathcal{S}_2|} \lambda_{i,j} d(s_i, s_j), \\ \text{subject to } &\sum_{j=1}^{|\mathcal{S}_2|} \lambda_{i,j} = P(s_i), \forall i; \sum_{i=1}^{|\mathcal{S}_1|} \lambda_{i,j} = Q(s_j), \forall j; \lambda_{i,j} \geq 0, \forall i, j. \end{aligned} \quad (3)$$

Here, P and Q are distributions on \mathcal{S}_1 and \mathcal{S}_2 , respectively, and $s_i \in \mathcal{S}_1, s_j \in \mathcal{S}_2$. It represents the minimum transportation cost from P to Q under cost function $d: \mathcal{S}_1 \times \mathcal{S}_2 \rightarrow \mathbb{R}_+$, and is equivalent to the following dual LP according to the Kantorovich duality [20]:

$$\begin{aligned} W_1(P, Q; d) &= \max_{\mu, \nu} \sum_{i=1}^{|\mathcal{S}_1|} \mu_i P(s_i) - \sum_{j=1}^{|\mathcal{S}_2|} \nu_j Q(s_j), \\ \text{subject to } &\mu_i - \nu_j \leq d(s_i, s_j), \forall i, j. \end{aligned} \quad (4)$$

Then the existence of such a d^{1-2} satisfying Eq. 2 is established by the following theorem.

Theorem 3.2 (Existence and convergence of GBSM). *Let d_0^{1-2} be a constant zero function and define*

$$d_n^{1-2}(s, s') = \max_a \{ |R_1(s, a) - R_2(s', a)| + \gamma W_1(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s', a); d_{n-1}^{1-2}) \}, n \in \mathbb{N} \quad (5)$$

Then d_n^{1-2} converges to the fixed point d^{1-2} uniformly with $n \rightarrow \infty$. Let $\bar{R} = \max_{s, s', a} |R_1(s, a) - R_2(s', a)|$, and the convergence of d_n^{1-2} to d^{1-2} satisfies

$$d^{1-2}(s, s') - d_n^{1-2}(s, s') \leq \gamma^n \bar{R} / (1 - \gamma). \quad (6)$$

Proof Sketch. The existence of d^{1-2} is established through the fixed-point theorem [21] and the definition of the Wasserstein distance, similar to the proof of BSM in [2]. The convergence is proved via the LP in (3) and induction. (See Appendix A for the complete proof.) \square

Similar to BSM, which evaluates the state similarity through the optimal value function, GBSM naturally bounds differences in the optimal value function between two MDPs.

Theorem 3.3 (Optimal value difference bound between MDPs). *Let V_1^* and V_2^* denote the optimal value functions in \mathcal{M}_1 and \mathcal{M}_2 , respectively. Then the GBSM provides an upper bound for the difference between the optimal values for any state pair $(s, s') \in \mathcal{S}_1 \times \mathcal{S}_2$:*

$$|V_1^*(s) - V_2^*(s')| \leq d^{1-2}(s, s'). \quad (7)$$

Proof Sketch. We first construct a recursive form of the optimal value function by $V^{(n)}(s) = \max_a \{R(s, a) + \gamma \mathbb{E}_{\tilde{s} \sim \mathbb{P}(\cdot|s, a)} [V^{(n-1)}(\tilde{s})]\}$, with base case $V^{(0)}(s) = 0$ and $\lim_{n \rightarrow \infty} V^{(n)}(s) = V^*$. The proof proceeds by induction on n . The key insight is that $(V_1^{(n)}(s_k))_{k=1}^{|\mathcal{S}_1|}$ and $(V_2^{(n)}(s_k))_{k=1}^{|\mathcal{S}_2|}$ form a feasible, but not necessarily the optimal, solution to the dual LP in (4) for $W_1(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s', a); d_n^{1-2})$. (See Appendix B for the complete proof.) \square

Now, we start to establish the three fundamental metric properties of GBSM, which we term GBSM symmetry, inter-MDP triangle inequality, and the distance bound on identical state spaces. These properties are designed to align with pseudometric properties of BSM, including symmetry, triangle inequality, and indiscernibility of identical.

Theorem 3.4 (GBSM symmetry). *Let d^{1-2} be the GBSM from \mathcal{M}_1 to \mathcal{M}_2 , and d^{2-1} be the GBSM in the opposite direction, then we have*

$$d^{1-2}(s, s') = d^{2-1}(s', s), \forall (s, s') \in \mathcal{S}_1 \times \mathcal{S}_2. \quad (8)$$

Proof. This property can be readily proved through induction. We have $|R_1(s, a) - R_2(s', a)| = |R_2(s', a) - R_1(s, a)|$ for the base case. With the assumption of $d_n^{1-2}(s, s') = d_n^{2-1}(s', s)$, we have $W_1(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s', a); d_n^{1-2}) = W_1(\mathbb{P}_2(\cdot|s', a), \mathbb{P}_1(\cdot|s, a); d_n^{2-1})$, and from (5) we have $d_{n+1}^{1-2}(s, s') = d_{n+1}^{2-1}(s', s)$. It is therefore concluded that $d_n^{1-2}(s, s') = d_n^{2-1}(s', s)$ for all $n \in \mathbb{N}$ and $(s, s') \in \mathcal{S}_1 \times \mathcal{S}_2$. Taking $n \rightarrow \infty$ yields the desired result. \square

Theorem 3.5 (Inter-MDP triangle inequality of GBSM). *Given MDPs $\mathcal{M}_1 = \langle \mathcal{S}_1, \mathcal{A}, \mathbb{P}_1, R_1, \gamma \rangle$, $\mathcal{M}_2 = \langle \mathcal{S}_2, \mathcal{A}, \mathbb{P}_2, R_2, \gamma \rangle$, and $\mathcal{M}_3 = \langle \mathcal{S}_3, \mathcal{A}, \mathbb{P}_3, R_3, \gamma \rangle$, GBSMs between the three MDPs satisfy*

$$d^{1-2}(s, s') \leq d^{1-3}(s, s'') + d^{3-2}(s'', s'), \forall (s, s', s'') \in \mathcal{S}_1 \times \mathcal{S}_2 \times \mathcal{S}_3. \quad (9)$$

Here, the GBSM between any two MDPs can be arbitrarily reversed according to its symmetry.

Proof. First, we need to prove the transitive property of inequality on the Wasserstein distance, that is, the Wasserstein distance between the three distributions follows $W_1(\mathbb{P}^1, \mathbb{P}^2; d^{1-2}) \leq W_1(\mathbb{P}^1, \mathbb{P}^3; d^{1-3}) + W_1(\mathbb{P}^3, \mathbb{P}^2; d^{3-2})$ if (9) holds, where $\mathbb{P}^1, \mathbb{P}^2$, and \mathbb{P}^3 denote arbitrary distributions on $\mathcal{S}_1, \mathcal{S}_2$, and \mathcal{S}_3 .

Let $(s_i, s_j, s_k) \in \mathcal{S}_1 \times \mathcal{S}_2 \times \mathcal{S}_3$. Define $\lambda^{1,3}$ as the optimal transportation plan for $W_1(\mathbb{P}^1, \mathbb{P}^3; d^{1-3})$ in primal LP (3), with elements $\lambda_{i,k}^{1,3}$ satisfying $\sum_{k=1}^{|\mathcal{S}_3|} \lambda_{i,k}^{1,3} = \mathbb{P}^1(s_i)$ and $\sum_{i=1}^{|\mathcal{S}_1|} \lambda_{i,k}^{1,3} = \mathbb{P}^3(s_k)$. Similarly define $\lambda^{3,2}$ for $W_1(\mathbb{P}^3, \mathbb{P}^2; d^{3-2})$ with elements $\lambda_{k,j}^{3,2}$. Construct $\lambda^{1,3,2}$ with elements $\lambda_{i,k,j}^{1,3,2}$ satisfying $\sum_{j=1}^{|\mathcal{S}_2|} \lambda_{i,k,j}^{1,3,2} = \lambda_{i,k}^{1,3}$ and $\sum_{i=1}^{|\mathcal{S}_1|} \lambda_{i,k,j}^{1,3,2} = \lambda_{k,j}^{3,2}$. Such a $\lambda^{1,3,2}$ does exist according to the Gluing Lemma in [22]. Then, note that

$$\begin{aligned} \sum_{j=1}^{|\mathcal{S}_2|} \sum_{k=1}^{|\mathcal{S}_3|} \lambda_{i,k,j}^{1,3,2} &= \sum_{k=1}^{|\mathcal{S}_3|} \lambda_{i,k}^{1,3} = \mathbb{P}^1(s_i), \\ \sum_{i=1}^{|\mathcal{S}_1|} \sum_{k=1}^{|\mathcal{S}_3|} \lambda_{i,k,j}^{1,3,2} &= \sum_{k=1}^{|\mathcal{S}_3|} \lambda_{k,j}^{3,2} = \mathbb{P}^2(s_j), \end{aligned}$$

thus $\sum_{k=1}^{|\mathcal{S}_3|} \lambda^{1,3,2}$ is a feasible, but not necessarily the optimal, solution to the primal LP in (3) for $W_1(\mathbb{P}^1, \mathbb{P}^2; d^{1-2})$. Consequently, we have

$$\begin{aligned} W_1(\mathbb{P}^1, \mathbb{P}^2; d^{1-2}) &\leq \sum_{i=1}^{|\mathcal{S}_1|} \sum_{j=1}^{|\mathcal{S}_2|} \left(\sum_{k=1}^{|\mathcal{S}_3|} \lambda_{i,k,j}^{1,3,2} \right) d^{1-2}(s_i, s_j) \\ &\stackrel{(a)}{\leq} \sum_{i=1}^{|\mathcal{S}_1|} \sum_{j=1}^{|\mathcal{S}_2|} \left(\sum_{k=1}^{|\mathcal{S}_3|} \lambda_{i,k,j}^{1,3,2} \right) \left(d^{1-3}(s_i, s_k) + d^{3-2}(s_k, s_j) \right) \\ &= \sum_{i=1}^{|\mathcal{S}_1|} \sum_{k=1}^{|\mathcal{S}_3|} \lambda_{i,k}^{1,3} d^{1-3}(s_i, s_k) + \sum_{k=1}^{|\mathcal{S}_3|} \sum_{j=1}^{|\mathcal{S}_2|} \lambda_{k,j}^{3,2} d^{3-2}(s_k, s_j) \\ &= W_1(\mathbb{P}^1, \mathbb{P}^3; d^{1-3}) + W_1(\mathbb{P}^3, \mathbb{P}^2; d^{3-2}). \end{aligned} \quad (10)$$

Here, step (a) stems from the assumption on d . We have now established the transitivity of the inter-MDP triangle inequality on the Wasserstein distance.

Armed with (10), we are ready to prove the inter-MDP triangle inequality of the GBSM through induction. For the base case,

$$\begin{aligned} d_1^{1-2}(s, s') &\leq \max_a \{|R_1(s, a) - R_3(s'', a)| + |R_3(s'', a) - R_2(s', a)|\} \\ &\leq \max_a \{|R_1(s, a) - R_3(s'', a)|\} + \max_a \{|R_3(s'', a) - R_2(s', a)|\} \\ &= d_1^{1-3}(s, s'') + d_1^{3-2}(s'', s'), \quad \forall (s, s', s'') \in \mathcal{S}_1 \times \mathcal{S}_2 \times \mathcal{S}_3. \end{aligned}$$

By the induction hypothesis, we assume that for an arbitrary $n \in \mathbb{N}$,

$$d_n^{1-2}(s, s') \leq d_n^{1-3}(s, s'') + d_n^{3-2}(s'', s'), \quad \forall (s, s', s'') \in \mathcal{S}_1 \times \mathcal{S}_2 \times \mathcal{S}_3.$$

The induction follows

$$\begin{aligned} d_{n+1}^{1-2}(s, s') &\leq \max_a \{|R_1(s, a) - R_3(s'', a)| + |R_3(s'', a) - R_2(s', a)|\} \\ &\quad + \gamma W_1(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_3(\cdot|s'', a); d_n^{1-3}) + \gamma W_1(\mathbb{P}_3(\cdot|s'', a), \mathbb{P}_2(\cdot|s', a); d_n^{3-2}) \\ &\leq \max_a \{|R_1(s, a) - R_3(s'', a)| + \gamma W_1(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_3(\cdot|s'', a); d_n^{1-3})\} \\ &\quad + \max_a \{|R_3(s'', a) - R_2(s', a)| + \gamma W_1(\mathbb{P}_3(\cdot|s'', a), \mathbb{P}_2(\cdot|s', a); d_n^{3-2})\} \\ &= d_{n+1}^{1-3}(s, s'') + d_{n+1}^{3-2}(s'', s'), \quad \forall (s, s', s'') \in \mathcal{S}_1 \times \mathcal{S}_2 \times \mathcal{S}_3. \end{aligned}$$

Here, the first inequality follows from (10), i.e., the transitivity of the inequality. Now we have $d_n^{1-2}(s, s') \leq d_n^{1-3}(s, s'') + d_n^{3-2}(s'', s')$ for all $n \in \mathbb{N}$. Taking $n \rightarrow \infty$, we establish the inter-MDP triangle inequality of GBSM. \square

Since the identical states only exist within the same state space, we establish the distance bound only when \mathcal{M}_1 and \mathcal{M}_2 share the same state space \mathcal{S} . This property is formulated as follows:

Theorem 3.6 (Distance bound on identical state spaces). *When \mathcal{M}_1 and \mathcal{M}_2 share the same \mathcal{S} ,*

$$\max_s d^{1-2}(s, s) \leq \frac{1}{1-\gamma} \max_{s,a} \left\{ |R_1(s, a) - R_2(s, a)| + \frac{\gamma \bar{R}}{1-\gamma} \text{TV}(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s, a)) \right\}, \quad (11)$$

where TV represents the total variation distance defined by $\text{TV}(P, Q) = \frac{1}{2} \sum_{s \in \mathcal{S}} |P(s) - Q(s)|$.

Proof. Consider a special transportation plan between distributions P and Q . This plan preserves all mass shared between P and Q , defined as $\min\{P(s), Q(s)\}$ for all s . The remaining mass, where $P(s) > Q(s)$, is distributed to states where $P(s) < Q(s)$. Then the total mass to be transported is quantified by the total variation distance, where the transportation cost with the cost function d is bounded by $\max_{s,s'} d(s, s')$. The shared mass is given by $1 - \text{TV}(P, Q)$, with the cost bounded by $\max_s d(s, s)$. While this plan adheres to the definition of Wasserstein distance, it can hardly be optimal. Then we have

$$W_1(P, Q; d) \leq \text{TV}(P, Q) \max_{s,s'} d(s, s') + (1 - \text{TV}(P, Q)) \max_s d(s, s). \quad (12)$$

According to its recursive definition, GBSM is a mapping bounded by $[0, \bar{R}/(1-\gamma)]$, then

$$\begin{aligned} \max_s d^{1-2}(s, s) &\leq \max_{s,a} \{|R_1(s, a) - R_2(s, a)| + \gamma \text{TV}(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s, a)) \max_{s,s'} d^{1-2}(s, s')\} \\ &\quad + \gamma \max_{s,a} \{(1 - \text{TV}(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s, a))) \max_s d^{1-2}(s, s)\} \\ &\leq \max_{s,a} \left\{ |R_1(s, a) - R_2(s, a)| + \frac{\gamma \bar{R}}{1-\gamma} \text{TV}(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s, a)) \right\} + \gamma \max_s d^{1-2}(s, s). \end{aligned}$$

Rearranging the inequality yields the desired result. \square

A direct consequence of Theorem 3.6 is that if $\mathcal{M}_1 = \mathcal{M}_2$, where $R_1 = R_2$ and $\mathbb{P}_1 = \mathbb{P}_2$, the right-hand side of the inequality becomes zero. It indicates that

$$d^{1-1}(s, s) = d((s, \mathcal{M}_1), (s, \mathcal{M}_1)) = 0, \quad \forall s \in \mathcal{S}_1, \quad (13)$$

confirming the indiscernibility of identicals of GBSM when the compared objects (state-MDP pairs) are genuinely identical. We denote the maximization term $\max_a \{|R_1(s, a) - R_2(s, a)| + \frac{\gamma \bar{R}}{1-\gamma} \text{TV}(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s, a))\}$ in Theorem 3.6 as $d_{\text{TV}}^{1-2}(s, s)$ in the following.

We now have a formal definition of GBSM and have rigorously proved the metric properties. Notably, when all compared MDPs are identical, GBSM reduces to the standard BSM. In this case, the three fundamental properties of GBSM reduce to the corresponding pseudometric properties of BSM.

4 Applications of GBSM in Multi-MDP Analysis

To demonstrate the effectiveness of GBSM in multi-MDP scenarios, we apply it to theoretical analyses of policy transfer, state aggregation, and sampling-based estimation of MDPs.

4.1 Performance Bound of Policy Transfer Using GBSM

Using GBSM, we analyze policy transfer from a source MDP \mathcal{M}_1 to a target MDP \mathcal{M}_2 and derive a theoretical performance bound for the transferred policy. This bound takes the form of a regret (defined as the expected discounted reward loss incurred by following the transferred policy instead of the optimal one [23]). Specifically, it is a weighted sum of the GBSM between the two MDPs and the regret within the source MDP itself, formulated by the following.

Theorem 4.1 (Regret bound on policy transfer). *Consider transferring a policy π from \mathcal{M}_1 to \mathcal{M}_2 . The transferred policy acts as $\pi(\cdot|f(s'))$ for $s' \in \mathcal{S}_2$, where $f : \mathcal{S}_2 \rightarrow \mathcal{S}_1$ is a mapping from target states to source states. The regret of π in \mathcal{M}_2 is bounded by*

$$\max_{s' \in \mathcal{S}_2} |V_2^*(s') - V_2^\pi(s')| \leq \frac{2}{1-\gamma} \max_{s' \in \mathcal{S}_2} d^{1-2}(f(s'), s') + \frac{1+\gamma}{1-\gamma} \max_{s \in \mathcal{S}_1} |V_1^*(s) - V_1^\pi(s)|. \quad (14)$$

Proof Sketch. The proof of (14) is similar to the proof in [12] and is conducted by replacing the BSM by GBSM. (See Appendix C for the complete proof.) \square

Special cases of Theorem 4.1 yield the following refined bounds:

Corollary 4.2 (Optimal mapping for policy transfer). *When $f(s') = \arg \min_{s \in \mathcal{S}_1} d^{1-2}(s, s')$, $\forall s' \in \mathcal{S}_2$, the bound tightens to:*

$$\max_{s' \in \mathcal{S}_2} |V_2^*(s') - V_2^\pi(s')| \leq \frac{2}{1-\gamma} \max_{s' \in \mathcal{S}_2} \left\{ \min_{s \in \mathcal{S}_1} d^{1-2}(s, s') \right\} + \frac{1+\gamma}{1-\gamma} \max_{s \in \mathcal{S}_1} |V_1^*(s) - V_1^\pi(s)|. \quad (15)$$

Corollary 4.3 (Policy transfer with identical state space). *When \mathcal{M}_1 and \mathcal{M}_2 share the same state space \mathcal{S} and $f(s) = s$, we have*

$$\max_{s \in \mathcal{S}} |V_2^*(s) - V_2^\pi(s)| \leq \frac{2}{(1-\gamma)^2} \max_{s \in \mathcal{S}} d_{TV}^{1-2}(s, s) + \frac{1+\gamma}{1-\gamma} \max_{s \in \mathcal{S}} |V_1^*(s) - V_1^\pi(s)|. \quad (16)$$

Proof Sketch. This corollary utilizes the distance bound on identical state spaces in Theorem 3.6. \square

In contrast to the approach of [12], which constructs a disjoint union state space for analysis, we provide a similar theoretical bound by directly analyzing the relationship between the source and target MDPs. This method avoids a constant total variation distance, thereby enabling simplifications such as the bound based on d_{TV}^{1-2} , as well as the approximation method in the following section. Meanwhile, calculating BSM on the disjoint union of two MDPs renders a significant computational complexity scaling with $|\mathcal{S}_1 + \mathcal{S}_2|^2$. In contrast, our GBSM is directly computing between \mathcal{M}_1 and \mathcal{M}_2 , with a reduced complexity scaling with $|\mathcal{S}_1| \cdot |\mathcal{S}_2|$.

4.2 Approximation Methods and Corresponding Error Bounds

When the state space is extensive and actual transition probabilities are inaccessible, approximation methods are necessary for the efficient computation of state similarities. In the single MDP scenario, Ferns et al. [14] proposed a state similarity approximation (SSA) method based on state aggregation and sampling-based estimation. Let $\mathcal{U} \subseteq \mathcal{S}$ be a set of selected representative states, $[\cdot] : \mathcal{S} \rightarrow \mathcal{U}$ an aggregation mapping, $\tilde{\sigma} = \max_{s \in \mathcal{S}} \{d^\sim(s, [s])\}$ the maximum aggregation distance, and K the number of samples used to empirically estimate each transition probability. The SSA error satisfies

$$\max_{s, s'} |d^\sim(s, s') - d_{\tilde{\sigma}, K}^\sim([s], [s'])| \leq \frac{2\tilde{\sigma}(2+\gamma)}{1-\gamma} + \frac{2\gamma}{1-\gamma} \max_{a, s} W_1 \left([\hat{\mathbb{P}}](\cdot|[s], a), [\mathbb{P}](\cdot|[s], a); d^\sim \right). \quad (17)$$

Here, $d_{\tilde{\sigma}, K}^\sim$ denotes the BSM on the approximated MDP, $[\mathbb{P}]$ denotes the transition probability between aggregated states, and $[\hat{\mathbb{P}}]$ represents its empirical counterparts estimated from K samples.

However, the BSM-based aggregation error bound $2\tilde{\sigma}(2 + \gamma)/(1 - \gamma)$ is fairly loose, while the sample complexity for the estimation error is limited to asymptotic expressions.

Beyond approximating state similarities, it is crucial to quantify the difference between optimal value functions within the original MDPs and their approximated counterparts in aggregated MDPs. Using a BSM-based analysis, Zhang et al. [6] established a value function approximation (VFA) bound on this difference, given by $2\tilde{\sigma}/(1 - \gamma)$, but it also suffers from looseness when γ becomes large.

To address this, we apply the GBSM to directly compute state similarities between the original MDPs and their aggregated/estimated counterparts. Beyond extending the approach in [14] to the multi-MDP setting, our GBSM-based analysis yields significantly tighter approximation bounds for both SSA and VFA, and provides an explicit and closed-form expression for the sample complexity.

4.2.1 State Aggregation

Given the previously defined \mathcal{S} , \mathcal{U} , and $[\cdot]$, the aggregated state space $[\mathcal{S}]$ is defined such that the reward function and transition probability of each state are replaced by those of its representative state, given by $R(s, a) = R([\mathcal{s}], a)$ and $\mathbb{P}(\cdot|s, a) = \mathbb{P}(\cdot|[\mathcal{s}], a)$ for all $s \in \mathcal{S}$. The aggregated transition probability is defined as $[\mathbb{P}](s'|s, a) = \sum_{s'' \in \mathcal{S}, [s''] = s'} \mathbb{P}(s''|s, a)$. Note that $[\mathbb{P}](s'|s, a) = 0$ when $s' \notin \mathcal{U}$. With this construction, we define the aggregated MDP for \mathcal{M}_1 as $\mathcal{M}_{[1]} = \langle [\mathcal{S}_1], \mathcal{A}, [\mathbb{P}_1], R_1, \gamma \rangle$. First, we obtain the VFA bound directly from GBSM.

Theorem 4.4 (VFA error bound). *Given MDP \mathcal{M}_1 and its aggregated counterpart $\mathcal{M}_{[1]}$, the VFA bound is given by*

$$\max_{s \in \mathcal{S}_1} |V_1^*(s) - V_{[1]}^*(s)| \leq \sigma_1 \leq \tilde{\sigma}_1 / (1 - \gamma). \quad (18)$$

where $\sigma_1 = \max_{s \in \mathcal{S}_1} d^{1-[1]}(s, s)$ and $\tilde{\sigma}_1 = \max_{s \in \mathcal{S}_1} d^\sim(s, [s])$.

Proof. The first inequality is a direct consequence of Theorem 3.3. For the second one, We construct an intermediate MDP defined by $\mathcal{M}_{1_{[s]}} = \langle [\mathcal{S}_1], \mathcal{A}, \mathbb{P}_1, R_1, \gamma \rangle$ and prove $d^{1-1_{[s]}}(s, s) = d^{1-[1]}(s, s)$ for all $s \in \mathcal{S}_1$ through induction. For the base case, $d_1^{1_{[s]}}(s, s) = \max_a |R_1([\mathcal{s}], a) - R_1([\mathcal{s}], a)| = 0$. By the induction hypothesis, we assume that $d_n^{1_{[s]}}(s, s) = 0$ for any n , then

$$\begin{aligned} d_{n+1}^{1_{[s]}}(s, s) &= \max_a \{ |R_1([\mathcal{s}], a) - R_1([\mathcal{s}], a)| + \gamma W_1(\mathbb{P}(\cdot|[\mathcal{s}], a), [\mathbb{P}](\cdot|[\mathcal{s}], a); d_n^{1_{[s]}}) \} \\ &\leq \gamma \max_a \sum_{\tilde{s} \in \mathcal{S}_1} \mathbb{P}(\tilde{s}|\tilde{[s]}, a) d_n^{1_{[s]}}(\tilde{s}, [\tilde{s}]). \end{aligned}$$

The inequality here follows from a transportation plan that moves the mass from each \tilde{s} to its representative state $[\tilde{s}]$. Note that the reward function and transition probability of each state are the same as its representative states in $\mathcal{M}_{1_{[s]}}$, thus $d_n^{1_{[s]}}(\tilde{s}, [\tilde{s}]) = d_n^{1_{[s]}}([\tilde{s}], [\tilde{s}]) = 0$, and thereby we have $d_{n+1}^{1_{[s]}}(s, s) = 0$. Now we have established $d_n^{1_{[s]}}(s, s) = 0$ for all $n \in \mathbb{N}$ and $s \in \mathcal{S}_1$. Taking $n \rightarrow \infty$, we have $d^{1-1_{[s]}}(s, s) = 0, \forall s \in \mathcal{S}_1$. Using the inter-MDP triangle inequality in Theorem 3.5, we derive $d^{1-1_{[s]}}(s, s) = d^{1-[1]}(s, s)$ for all $s \in \mathcal{S}_1$.

Next, we prove the inequality between σ_1 and $\tilde{\sigma}_1$. For representative states $s_u \in \mathcal{U}_1 \subseteq \mathcal{S}_1$, we have

$$\begin{aligned} d^{1-1_{[s]}}(s_u, s_u) &= \max_a \{ |R_1(s_u, a) - R_1(s_u, a)| + \gamma W_1(\mathbb{P}(\cdot|s_u, a), \mathbb{P}(\cdot|s_u, a); d^{1-1_{[s]}}) \} \\ &= \gamma \max_a \{ W_1(\mathbb{P}(\cdot|s_u, a), \mathbb{P}(\cdot|s_u, a); d^{1-1_{[s]}}) \} \\ &\leq \gamma \max_a \left\{ \sum_{\tilde{s} \in \mathcal{S}} \mathbb{P}(\tilde{s}|s_u, a) d^{1-1_{[s]}}(\tilde{s}, \tilde{[s]}) \right\} \\ &\leq \gamma \max_s d^{1-1_{[s]}}(s, s) = \gamma \max_s d^{1-1_{[s]}}(s, [s]). \end{aligned}$$

Here, the first inequality follows from a straightforward transportation plan that keeps all the mass at its position. The last equality is because s and $[s]$ share the same reward function and transition probability in $\mathcal{M}_{1_{[s]}}$. Then, according to the inter-MDP triangle inequality in Theorem 3.5, we have

$$d^{1-1_{[s]}}(s, [s]) \leq d^{1-1}(s, [s]) + d^{1-1_{[s]}}([\mathcal{s}], [s]) \leq d^{1-1}(s, [s]) + \gamma \max_s d^{1-1_{[s]}}(s, [s])$$

Taking the maximum of both sides, rearranging the inequality, and combining the established $d^{1-1_{[s]}}(s, s) = d^{1-[1]}(s, s)$, we have

$$\begin{aligned} \sigma_1 &= \max_s d^{1-[1]}(s, s) = \max_s d^{1-1_{[s]}}(s, s) = \max_s d^{1-1_{[s]}}(s, [s]) \\ &\leq \max_s d^{1-1}(s, [s]) / (1 - \gamma) = \max_s d^\sim(s, [s]) / (1 - \gamma) = \tilde{\sigma}_1 / (1 - \gamma), \end{aligned}$$

demonstrating significant tightness compared to the BSM-based bound $2\tilde{\sigma}_1/(1-\gamma)$ in [6]. \square

Then the aggregation error bound for SSA is established as follows.

Theorem 4.5 (SSA aggregation error bound). *Given MDPs $\mathcal{M}_1, \mathcal{M}_2$ and their aggregated counterparts $\mathcal{M}_{[1]}, \mathcal{M}_{[2]}$, the SSA error bound is given by*

$$\max_{s,s'} |d^{1-2}(s, s') - d^{[1]-[2]}(s, s')| \leq \sigma_1 + \sigma_2 \leq (\tilde{\sigma}_1 + \tilde{\sigma}_2)/(1-\gamma). \quad (19)$$

Proof. This theorem is easily derived by combining Theorem 3.5 and Theorem 4.4. \square

When the compared MDPs are identical, i.e., $\mathcal{M}_2 = \mathcal{M}_1 = \langle \mathcal{S}, \mathcal{A}, \mathbb{P}, R, \gamma \rangle$, Theorem 4.5 reduces to the aggregation error bound in the single-MDP scenario as

$$\max_{s,s'} |d^{1-1}(s, s') - d^{[1]-[1]}(s, s')| \leq 2\sigma_1 \leq 2\tilde{\sigma}_1/(1-\gamma),$$

indicating significant tightness of the GBSM-based bound $2\sigma_1$ compared to the BSM-based one $2\tilde{\sigma}_1(2+\gamma)/(1-\gamma)$ [14].

4.2.2 Sampling-based Estimation

To estimate a probability distribution P through statistical sampling, we define the empirical distribution based on K samples as $\hat{P}(x) = \frac{1}{K} \sum_{i=1}^K \delta_{X_i}(x)$, where $\{X_1, X_2, \dots, X_K\}$ are K independent points sampled from P and δ denotes the Dirac measure at X_i such that $\delta_{X_i}(x) = 1$ if $x = X_i$ and 0 otherwise. Then the empirical MDP for \mathcal{M}_1 is constructed by sampling K points for each $\mathbb{P}_1(\cdot|s, a)$, defined by $\mathcal{M}_{\hat{1}} = \langle \mathcal{S}_1, \mathcal{A}, \hat{\mathbb{P}}_1, R_1, \gamma \rangle$. The estimation error bound is derived as follows.

Theorem 4.6 (SSA estimation error bound). *Given MDPs $\mathcal{M}_1, \mathcal{M}_2$ and their empirically estimated counterparts $\mathcal{M}_{\hat{1}}, \mathcal{M}_{\hat{2}}$, the SSA error bound is given by*

$$\max_{s,s'} |d^{1-2}(s, s') - d^{\hat{1}-\hat{2}}(s, s')| \leq \max_s d^{1-\hat{1}}(s, s) + \max_{s'} d^{2-\hat{2}}(s', s'). \quad (20)$$

To reach an error less than ϵ with a probability of $1 - \alpha$, the sample complexity is given by

$$K \geq -\ln(\alpha/2) \frac{\gamma^2 \bar{R}^2 |\mathcal{S}|^2}{2\epsilon^2(1-\gamma)^4}, \quad (21)$$

for each state-action pair in \mathcal{M}_1 (where $|\mathcal{S}| = |\mathcal{S}_1|$) and \mathcal{M}_2 (where $|\mathcal{S}| = |\mathcal{S}_2|$).

Proof. Inequality (20) is easily obtained from Theorem 3.5. In terms of the sample complexity, we derive the following using Theorem 3.6

$$\begin{aligned} & \max_{s,s'} |d^{1-2}(s, s') - d^{\hat{1}-\hat{2}}(s, s')| \\ & \leq \frac{\gamma \bar{R}}{(1-\gamma)^2} \left(\max_{s,a} \text{TV}(\mathbb{P}_1(\cdot|s, a), \hat{\mathbb{P}}_1(\cdot|s, a)) + \max_{s',a} \text{TV}(\mathbb{P}_2(\cdot|s', a), \hat{\mathbb{P}}_2(\cdot|s', a)) \right) \\ & = \frac{\gamma \bar{R}}{2(1-\gamma)^2} \left(\max_{s,a} \left\{ \sum_{\tilde{s} \in \mathcal{S}_1} |\mathbb{P}_1(\tilde{s}|s, a) - \hat{\mathbb{P}}_1(\tilde{s}|s, a)| \right\} + \max_{s',a} \left\{ \sum_{\tilde{s} \in \mathcal{S}_2} |\mathbb{P}_2(\tilde{s}|s', a) - \hat{\mathbb{P}}_2(\tilde{s}|s', a)| \right\} \right). \end{aligned}$$

To ensure the estimation error remains below ϵ , we require $|\mathbb{P}_1(\tilde{s}|s, a) - \hat{\mathbb{P}}_1(\tilde{s}|s, a)| \leq \frac{\epsilon(1-\gamma)^2}{\gamma \bar{R} |\mathcal{S}_1|}$ and $|\mathbb{P}_2(\tilde{s}|s', a) - \hat{\mathbb{P}}_2(\tilde{s}|s', a)| \leq \frac{\epsilon(1-\gamma)^2}{\gamma \bar{R} |\mathcal{S}_2|}$. Next, by applying the Hoeffding's inequality [24] that is defined by $\Pr\{|\hat{P}(s) - P(s)| \geq \epsilon\} \leq 2e^{-2K\epsilon^2}$, we derive the desired sample complexity. \square

When the compared MDPs are identical, the estimation SSA bound in Theorem 4.6 reduces to $2 \max_s d^{1-\hat{1}}(s, s)$ for BSM. We now prove the tightness of this new sampling error bound compared to the existing bound $\frac{2\gamma}{1-\gamma} \max_{a,s} W_1(\hat{\mathbb{P}}(\cdot|s, a), \mathbb{P}(\cdot|s, a); d^\sim)$ in [14]. According to the transitive property of inequality on the Wasserstein distance defined in (10), we have

$$\begin{aligned} d^{1-\hat{1}}(s, s) & = \gamma W_1(\mathbb{P}(\cdot|s, a), \hat{\mathbb{P}}(\cdot|s, a); d^{1-\hat{1}}) \\ & \leq \gamma W_1(\mathbb{P}(\cdot|s, a), \hat{\mathbb{P}}(\cdot|s, a); d^{1-1}) + \gamma W_1(\hat{\mathbb{P}}(\cdot|s, a), \hat{\mathbb{P}}(\cdot|s, a); d^{1-\hat{1}}) \\ & \leq \gamma W_1(\hat{\mathbb{P}}(\cdot|s, a), \mathbb{P}(\cdot|s, a); d^{1-1}) + \gamma \max_s d^{1-\hat{1}}(s, s). \end{aligned}$$

Taking the maximum of both sides and rearranging the inequality yields

$$2 \max_s d^{1-\hat{1}}(s, s) \leq 2\gamma \max_{a,s} W_1(\hat{\mathbb{P}}(\cdot|s, a), \mathbb{P}(\cdot|s, a); d^{1-\hat{1}})/(1 - \gamma).$$

Since $d^{1-\hat{1}} \triangleq d^\sim$, we have now proved the tightness of the new sampling error bound compared to the one derived from BSM in [14].

Furthermore, in case the approximation combines both state aggregation and sampling-based estimation, where the approximated MDP is defined as $\mathcal{M}_{[\hat{1}]} = \langle [\mathcal{S}_1], \mathcal{A}, [\hat{\mathbb{P}}_1], R_1, \gamma \rangle$, we have

$$\max_{s,s'} |d^{1-\hat{1}}(s, s') - d^{[\hat{1}]-[\hat{1}]}(s, s')| \leq 2 \max_s d^{1-\hat{1}}(s, s) \leq 2 \max_s d^{1-[\hat{1}]}(s, s) + 2 \max_s d^{[\hat{1}]-[\hat{1}]}(s, s)$$

via the inter-MDP triangle inequality. It enables a decoupled analysis of error, and thus results in an explicit and closed-formed sample complexity, i.e., $K \geq -\ln(\alpha/2) \frac{\gamma^2 \bar{R}^2 |\mathcal{U}|^2}{2\epsilon^2(1-\gamma)^4}$ for an error below ϵ with probability of $1 - \alpha$, where \mathcal{U} is the set of representative states.

5 Extensions to BSM variants

The proposed GBSM framework is readily extendable to numerous variants of BSM to enhance its applicability, such as lax BSM [25] and on-policy BSM [26].

Lax GBSM enables the computation of state similarities between MDPs with different action spaces. To relax GBSM to lax GBSM, we first adapt (2) to

$$\delta(d)((s, a), (s', a')) = |R_1(s, a) - R_2(s', a')| + \gamma W_1(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s', a'); d), \quad (22)$$

and define the lax function as $F_{\text{lax}}(d|s, s') = H(X_s, X_{s'}; \delta(d))$, where $X_s = \{(s, a) | a \in \mathcal{A}_1\}$, $X_{s'} = \{(s', a') | a' \in \mathcal{A}_2\}$, and H is the Hausdorff metric. Iterating from $d_{\text{lax},0}^{1-2}(s, s') = 0$ and $d_{\text{lax},n+1}^{1-2} = F_{\text{lax}}(d_{\text{lax},n}^{1-2}|s, s')$, $d_{\text{lax},n}^{1-2}$ converges to a similar fixed point d_{lax}^{1-2} that satisfies $|V_1^*(s) - V_2^*(s')| \leq d_{\text{lax}}^{1-2}(s, s')$ in Theorem 3.3. Next, the symmetry (Theorem 3.4) and triangle inequality (Theorem 3.5) can be readily established for d_{lax}^{1-2} . For MDPs sharing same \mathcal{S} and \mathcal{A} , we have $d_{\text{lax}}^{1-2} \leq d^{1-2} \leq d_{\text{TV}}^{1-2}/(1 - \gamma)$ (Theorem 3.6). Since these fundamental metric properties hold, the bounds for state aggregation (Theorem 4.5) and estimation (Theorem 4.6) also follow directly. For policy transfer, a similar regret bound (replacing d^{1-2} in Theorem 4.1 by d_{lax}^{1-2}) can be established by defining an additional action mapping $g: \mathcal{A}_1 \rightarrow \mathcal{A}_2$ for transfer. Due to the introduction of max-min term via Hausdorff metric, the lax GBSM-based transfer bound requires an assumption on this action mapping, i.e., $g(a) = \arg \min_{a'} \delta((f(s'), a), (s', a'); d_{\text{lax}}^{1-2})$ for each s' and a . See Appendix D for the proof.

On-policy GBSM computes state similarities between MDPs under non-optimal policies. To achieve this, we rewrite (2) to

$$d_\pi^{1-2}(s, s') = |R_1^\pi(s) - R_2^\pi(s')| + \gamma W_1(\mathbb{P}_1^\pi(\cdot|s), \mathbb{P}_2^\pi(\cdot|s'); d_\pi^{1-2}), \quad (23)$$

where $R_1^\pi(s) = \sum_a \pi(a|s) R_1(s, a)$ and $\mathbb{P}_1^\pi(\tilde{s}|s) = \sum_a \pi(a|s) \mathbb{P}_1(\tilde{s}|s, a)$, $\forall \tilde{s} \in \mathcal{S}_1$ represent the expected reward and transition probabilities for a non-optimal policy π in \mathcal{M}_1 , with corresponding terms R_2^π and \mathbb{P}_2^π defined similarly for \mathcal{M}_2 . Our theoretical properties are also preserved in this setting: the value difference bound in Theorem 3.3 now applies to the on-policy value function by $|V_1^\pi(s) - V_2^\pi(s')| \leq d_\pi^{1-2}(s, s')$. Then metric properties Theorem 3.4 and 3.5 follow directly, and $d_\pi^{1-2}(s, s')$ is bounded by an on-policy TV-based metric $d_{\text{TV},\pi}^{1-2}(s, s') = \{|R_1^\pi(s) - R_2^\pi(s')| + \frac{\gamma \bar{R}}{1-\gamma} \text{TV}(\mathbb{P}_1^\pi(\cdot|s), \mathbb{P}_2^\pi(\cdot|s'))\}$ as the Theorem 3.6 for on-policy GBSM. As a direct consequence, we have $\max_s |V_1^\pi(s) - V_{[\hat{1}]}^\pi(s)| \leq \max_s d_\pi^{1-[\hat{1}]}(s, s) \leq \max_s \tilde{d}_\pi(s, [s])/(1 - \gamma)$, a tighter bound for VFA with non-optimal policy compared with the existing result $2\tilde{d}_\pi(s, [s])/(1 - \gamma)$ in [15]. See Appendix E for the proof.

6 Numerical Results

In this section, we empirically validate the theoretical results derived from GBSM. To this end, we construct MDPs with randomly generated reward functions and transition probabilities, along with their aggregated and estimated counterparts. Specifically, we use random Garnet MDPs with

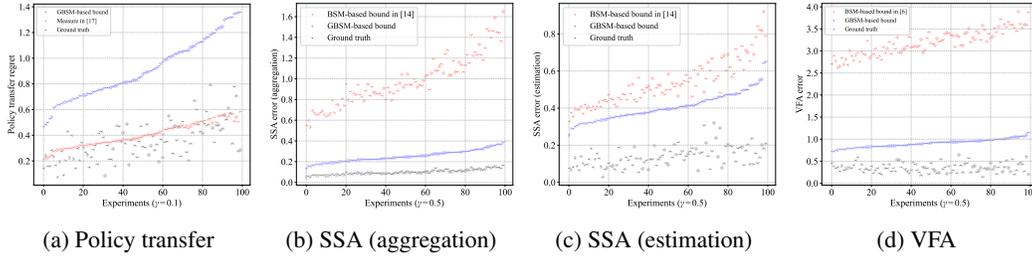


Figure 1: Experiments on random Garnet MDPs.

$|\mathcal{S}| = 20, |\mathcal{A}| = 5$, and a 50% branching factor. In the aggregated MDPs, the reward functions and transition probabilities for half of the states are replaced by those of their representative states, while the estimated MDPs are established by introducing a Gaussian noise with a standard deviation ranging from 0.1 to 0.3 to the transition probabilities.

To demonstrate the application of policy transfer between MDPs, we calculate the bound in Theorem 4.1 and the existing measure between MDPs in [17], and calculate the ground-truth regret by computing the precise value functions under a tabular Q-learning setting. Then, we calculate the aggregation and estimation SSA bounds using BSM and GBSM, respectively. The BSM-based SSA bounds are computed via (17). Since the estimation error bound in (17) depends on the aggregation process, we decouple the two for clearer analysis. Specifically, the BSM-based aggregation SSA bound is given by $2\tilde{\sigma}_1(2+\gamma)/(1-\gamma)$, and the estimation SSA bound is $\frac{2\gamma}{1-\gamma} \max_{a,s} W_1(\mathbb{P}(\cdot|s, a), \mathbb{P}(\cdot|s, a); d^\sim)$ [14]. The GBSM-based SSA bounds follow from Theorem 4.5 (aggregation) and Theorem 4.6 (estimation). For VFA bounds comparison, we employ the GBSM-based bound in Theorem 4.4 and compare with the BSM-based bound $2\tilde{\sigma}_1/(1-\gamma)$ in [6]. We also compare them with the ground-truth error values to assess their tightness.

We conduct 100 independent experiments for each $\gamma \in \{0.1, 0.2, \dots, 0.9\}$. The x-axis represents the experiment index of 100 independent trials, while the y-axis plots the values of ground-truth error and (G)BSM-based bounds in each trial. Figure 1a shows that the empirical metric in [17] fails to bound the transfer regret, while our GBSM-based bound is consistently effective. In terms of the SSA and VFA error, as depicted in Figure 1b, 1c, and 1d, the bounds based on GBSM are significantly tighter than those derived from BSM, which corroborates our theoretical findings and highlights the effectiveness of GBSM in multi-MDP analysis. Complete results are provided in Appendix F.

7 Conclusion

Application and limitation The first application is the sim-to-real policy transfer, where GBSM can be calculated between the simulated MDP and real-world MDP to predict transferred performance and serve as a metric for improving the simulation environment. Meanwhile, the approximation methods could be employed to address the inaccessibility of precise transition probabilities and reward functions in the real world. Another potential application is in multi-task RL, where GBSM can coordinate policy optimization across different MDPs, cluster similar tasks for efficient training, and mitigate gradient interference issues. The limitation mainly lies in the discounted reward formulation in GBSM. In real-world tasks, the goal is typically to maximize the long-term average reward. However, most of the theoretical results in this paper are divided by $1-\gamma$, and taking γ to 1 would yield an infinite result. Investigating metrics tailored for the average-reward MDP is an important and promising direction for future research.

Discussion In this paper, we have formally introduced GBSM and established its fundamental theoretical properties, including GBSM symmetry, inter-MDP triangle inequality, and distance bound on identical state spaces. Leveraging these properties, we provide tighter bounds for policy transfer, state aggregation, and sampling-based estimation of MDPs, compared to the ones derived from BSM. To our knowledge, this is the first rigorous theoretical investigation of GBSM beyond simple definitional adaptation. We believe this work introduces a valuable new tool for multi-MDP analysis.

References

- [1] Richard S Sutton, Andrew G Barto, et al. *Reinforcement learning: An introduction*. MIT press, Cambridge, MA, USA, 1998.
- [2] Norm Ferns, Prakash Panangaden, and Doina Precup. Metrics for finite markov decision processes. In *Proceedings of the 20th Conference on Uncertainty in Artificial Intelligence, UAI '04*, page 162–169, Arlington, Virginia, USA, 2004. AUAI Press. ISBN 0974903906.
- [3] Lothar Collatz. *Functional analysis and numerical mathematics*. Academic Press, 2014.
- [4] Norm Ferns, Pablo Samuel Castro, Doina Precup, and Prakash Panangaden. Methods for computing state similarity in markov decision processes. In *Proceedings of the Twenty-Second Conference on Uncertainty in Artificial Intelligence, UAI'06*, page 174–181, Arlington, Virginia, USA, 2006. AUAI Press. ISBN 0974903922.
- [5] Sherry Shanshan Ruan, Gheorghe Comanici, Prakash Panangaden, and Doina Precup. Representation discovery for mdps using bisimulation metrics. In *Proceedings of the Twenty-Ninth AAAI Conference on Artificial Intelligence, AAAI'15*, page 4202–4203. AAAI Press, 2015. ISBN 0262511290.
- [6] Amy Zhang, Rowan Thomas McAllister, Roberto Calandra, Yarín Gal, and Sergey Levine. Learning invariant representations for reinforcement learning without reconstruction. In *9th International Conference on Learning Representations, ICLR 2021, Virtual Event, Austria, May 3-7, 2021*. OpenReview.net, 2021. URL <https://openreview.net/forum?id=-2FCwDKRREu>.
- [7] Hongyu Zang, Xin Li, Leiji Zhang, Yang Liu, Baigui Sun, Riashat Islam, Rémi Tachet des Combes, and Romain Laroche. Understanding and addressing the pitfalls of bisimulation-based representations in offline reinforcement learning. In *Proceedings of the 37th International Conference on Neural Information Processing Systems, NIPS '23*, Red Hook, NY, USA, 2023. Curran Associates Inc.
- [8] Anirban Santara, Rishabh Madan, Pabitra Mitra, and Balaraman Ravindran. Extra: Transfer-guided exploration. In *Proceedings of the 19th International Conference on Autonomous Agents and MultiAgent Systems, AAMAS '20*, page 1987–1989, Richland, SC, 2020. International Foundation for Autonomous Agents and Multiagent Systems. ISBN 9781450375184.
- [9] Yiming Wang, Ming Yang, Renzhi Dong, Binbin Sun, Furui Liu, and Leong Hou U. Efficient potential-based exploration in reinforcement learning using inverse dynamic bisimulation metric. In *Proceedings of the 37th International Conference on Neural Information Processing Systems, NIPS '23*, Red Hook, NY, USA, 2023. Curran Associates Inc.
- [10] Philippe Hansen-Estruch, Amy Zhang, Ashvin Nair, Patrick Yin, and Sergey Levine. Bisimulation makes analogies in goal-conditioned reinforcement learning. In Kamalika Chaudhuri, Stefanie Jegelka, Le Song, Csaba Szepesvari, Gang Niu, and Sivan Sabato, editors, *Proceedings of the 39th International Conference on Machine Learning*, volume 162 of *Proceedings of Machine Learning Research*, pages 8407–8426, Baltimore, Maryland, USA, 17–23 Jul 2022. PMLR. URL <https://proceedings.mlr.press/v162/hansen-estruch22a.html>.
- [11] Rongrong Wang, Yuhu Cheng, and Xuesong Wang. Constrained visual representation learning with bisimulation metrics for safe reinforcement learning. *IEEE Transactions on Image Processing*, 34:379–393, 2025. doi: 10.1109/TIP.2024.3523798.
- [12] Caitlin Phillips. Knowledge transfer in markov decision processes. Technical report, Technical report, McGill University, School of Computer Science, 2006.
- [13] Matthew E Taylor and Peter Stone. Transfer learning for reinforcement learning domains: A survey. *Journal of Machine Learning Research*, 10(7), 2009.
- [14] Norm Ferns, Prakash Panangaden, and Doina Precup. Bisimulation metrics for continuous markov decision processes. *SIAM Journal on Computing*, 40(6):1662–1714, 2011.

- [15] Mete Kemertas and Tristan Aumentado-Armstrong. Towards robust bisimulation metric learning. In *Proceedings of the 35th International Conference on Neural Information Processing Systems, NIPS '21*, Red Hook, NY, USA, 2021. Curran Associates Inc. ISBN 9781713845393.
- [16] Pablo Castro and Doina Precup. Using bisimulation for policy transfer in mdps. In *Proceedings of the AAAI Conference on Artificial Intelligence, AAAI 2010*, pages 1065–1070, Atlanta, GA, Jul. 2010.
- [17] Jinhua Song, Yang Gao, Hao Wang, and Bo An. Measuring the distance between finite markov decision processes. In *Proceedings of the 2016 International Conference on Autonomous Agents & Multiagent Systems, AAMAS '16*, page 468–476, Richland, SC, 2016. International Foundation for Autonomous Agents and Multiagent Systems.
- [18] Javier García, Álvaro Visús, and Fernando Fernández. A taxonomy for similarity metrics between markov decision processes. *Machine Learning*, 111(11):4217–4247, 2022.
- [19] Cédric Villani. *Topics in Optimal Transportation*, volume 58. American Mathematical Soc., 2021.
- [20] Leonid Vasilevich Kantorovich and SG Rubinshtein. On a space of totally additive functions. *Vestnik of the St. Petersburg University: Mathematics*, 13(7):52–59, 1958.
- [21] Alfred Tarski. A lattice-theoretical fixpoint theorem and its applications. *Pacific Journal of Mathematics*, 5(2):285–309, June 1955.
- [22] Cédric Villani et al. *Optimal Transport: Old and New*, volume 338. Springer, 2009.
- [23] Leslie Pack Kaelbling, Michael L Littman, and Andrew W Moore. Reinforcement learning: A survey. *Journal of artificial intelligence research*, 4:237–285, 1996.
- [24] Wassily Hoeffding. Probability inequalities for sums of bounded random variables. *The collected works of Wassily Hoeffding*, pages 409–426, 1994.
- [25] Jonathan J. Taylor, Doina Precup, and Prakash Panangaden. Bounding performance loss in approximate mdp homomorphisms. In *Proceedings of the 22nd International Conference on Neural Information Processing Systems, NIPS'08*, page 1649–1656, Red Hook, NY, USA, 2008. Curran Associates Inc. ISBN 9781605609492.
- [26] Pablo Samuel Castro. Scalable methods for computing state similarity in deterministic markov decision processes. *Proceedings of the AAAI Conference on Artificial Intelligence*, 34(06): 10069–10076, Apr. 2020. doi: 10.1609/aaai.v34i06.6564. URL <https://ojs.aaai.org/index.php/AAAI/article/view/6564>.

NeurIPS Paper Checklist

1. Claims

Question: Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope?

Answer: [\[Yes\]](#)

Justification: Our paper contains everything that is covered in the abstract.

Guidelines:

- The answer NA means that the abstract and introduction do not include the claims made in the paper.
- The abstract and/or introduction should clearly state the claims made, including the contributions made in the paper and important assumptions and limitations. A No or NA answer to this question will not be perceived well by the reviewers.
- The claims made should match theoretical and experimental results, and reflect how much the results can be expected to generalize to other settings.
- It is fine to include aspirational goals as motivation as long as it is clear that these goals are not attained by the paper.

2. Limitations

Question: Does the paper discuss the limitations of the work performed by the authors?

Answer: [\[Yes\]](#)

Justification: We discuss the need to develop further theory, algorithms, and implementations for scenarios involving multiple MDPs in the conclusion.

Guidelines:

- The answer NA means that the paper has no limitation while the answer No means that the paper has limitations, but those are not discussed in the paper.
- The authors are encouraged to create a separate "Limitations" section in their paper.
- The paper should point out any strong assumptions and how robust the results are to violations of these assumptions (e.g., independence assumptions, noiseless settings, model well-specification, asymptotic approximations only holding locally). The authors should reflect on how these assumptions might be violated in practice and what the implications would be.
- The authors should reflect on the scope of the claims made, e.g., if the approach was only tested on a few datasets or with a few runs. In general, empirical results often depend on implicit assumptions, which should be articulated.
- The authors should reflect on the factors that influence the performance of the approach. For example, a facial recognition algorithm may perform poorly when image resolution is low or images are taken in low lighting. Or a speech-to-text system might not be used reliably to provide closed captions for online lectures because it fails to handle technical jargon.
- The authors should discuss the computational efficiency of the proposed algorithms and how they scale with dataset size.
- If applicable, the authors should discuss possible limitations of their approach to address problems of privacy and fairness.
- While the authors might fear that complete honesty about limitations might be used by reviewers as grounds for rejection, a worse outcome might be that reviewers discover limitations that aren't acknowledged in the paper. The authors should use their best judgment and recognize that individual actions in favor of transparency play an important role in developing norms that preserve the integrity of the community. Reviewers will be specifically instructed to not penalize honesty concerning limitations.

3. Theory assumptions and proofs

Question: For each theoretical result, does the paper provide the full set of assumptions and a complete (and correct) proof?

Answer: [\[Yes\]](#)

Justification: All the proofs for results are included in the main text and appendix.

Guidelines:

- The answer NA means that the paper does not include theoretical results.
- All the theorems, formulas, and proofs in the paper should be numbered and cross-referenced.
- All assumptions should be clearly stated or referenced in the statement of any theorems.
- The proofs can either appear in the main paper or the supplemental material, but if they appear in the supplemental material, the authors are encouraged to provide a short proof sketch to provide intuition.
- Inversely, any informal proof provided in the core of the paper should be complemented by formal proofs provided in appendix or supplemental material.
- Theorems and Lemmas that the proof relies upon should be properly referenced.

4. Experimental result reproducibility

Question: Does the paper fully disclose all the information needed to reproduce the main experimental results of the paper to the extent that it affects the main claims and/or conclusions of the paper (regardless of whether the code and data are provided or not)?

Answer: [NA]

Justification: This is a theory paper that only involves very simple numerical computations.

Guidelines:

- The answer NA means that the paper does not include experiments.
- If the paper includes experiments, a No answer to this question will not be perceived well by the reviewers: Making the paper reproducible is important, regardless of whether the code and data are provided or not.
- If the contribution is a dataset and/or model, the authors should describe the steps taken to make their results reproducible or verifiable.
- Depending on the contribution, reproducibility can be accomplished in various ways. For example, if the contribution is a novel architecture, describing the architecture fully might suffice, or if the contribution is a specific model and empirical evaluation, it may be necessary to either make it possible for others to replicate the model with the same dataset, or provide access to the model. In general, releasing code and data is often one good way to accomplish this, but reproducibility can also be provided via detailed instructions for how to replicate the results, access to a hosted model (e.g., in the case of a large language model), releasing of a model checkpoint, or other means that are appropriate to the research performed.
- While NeurIPS does not require releasing code, the conference does require all submissions to provide some reasonable avenue for reproducibility, which may depend on the nature of the contribution. For example
 - (a) If the contribution is primarily a new algorithm, the paper should make it clear how to reproduce that algorithm.
 - (b) If the contribution is primarily a new model architecture, the paper should describe the architecture clearly and fully.
 - (c) If the contribution is a new model (e.g., a large language model), then there should either be a way to access this model for reproducing the results or a way to reproduce the model (e.g., with an open-source dataset or instructions for how to construct the dataset).
 - (d) We recognize that reproducibility may be tricky in some cases, in which case authors are welcome to describe the particular way they provide for reproducibility. In the case of closed-source models, it may be that access to the model is limited in some way (e.g., to registered users), but it should be possible for other researchers to have some path to reproducing or verifying the results.

5. Open access to data and code

Question: Does the paper provide open access to the data and code, with sufficient instructions to faithfully reproduce the main experimental results, as described in supplemental material?

Answer: [NA]

Justification: This is a theory paper that only involves very simple numerical computations, and there is no training data or training/evaluation codes.

Guidelines:

- The answer NA means that paper does not include experiments requiring code.
- Please see the NeurIPS code and data submission guidelines (<https://nips.cc/public/guides/CodeSubmissionPolicy>) for more details.
- While we encourage the release of code and data, we understand that this might not be possible, so “No” is an acceptable answer. Papers cannot be rejected simply for not including code, unless this is central to the contribution (e.g., for a new open-source benchmark).
- The instructions should contain the exact command and environment needed to run to reproduce the results. See the NeurIPS code and data submission guidelines (<https://nips.cc/public/guides/CodeSubmissionPolicy>) for more details.
- The authors should provide instructions on data access and preparation, including how to access the raw data, preprocessed data, intermediate data, and generated data, etc.
- The authors should provide scripts to reproduce all experimental results for the new proposed method and baselines. If only a subset of experiments are reproducible, they should state which ones are omitted from the script and why.
- At submission time, to preserve anonymity, the authors should release anonymized versions (if applicable).
- Providing as much information as possible in supplemental material (appended to the paper) is recommended, but including URLs to data and code is permitted.

6. Experimental setting/details

Question: Does the paper specify all the training and test details (e.g., data splits, hyper-parameters, how they were chosen, type of optimizer, etc.) necessary to understand the results?

Answer:[NA]

Justification: There is no training or test in this paper.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The experimental setting should be presented in the core of the paper to a level of detail that is necessary to appreciate the results and make sense of them.
- The full details can be provided either with the code, in appendix, or as supplemental material.

7. Experiment statistical significance

Question: Does the paper report error bars suitably and correctly defined or other appropriate information about the statistical significance of the experiments?

Answer: [NA]

Justification: This is a theory paper that only involves very simple numerical computations.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The authors should answer "Yes" if the results are accompanied by error bars, confidence intervals, or statistical significance tests, at least for the experiments that support the main claims of the paper.
- The factors of variability that the error bars are capturing should be clearly stated (for example, train/test split, initialization, random drawing of some parameter, or overall run with given experimental conditions).
- The method for calculating the error bars should be explained (closed form formula, call to a library function, bootstrap, etc.)
- The assumptions made should be given (e.g., Normally distributed errors).

- It should be clear whether the error bar is the standard deviation or the standard error of the mean.
- It is OK to report 1-sigma error bars, but one should state it. The authors should preferably report a 2-sigma error bar than state that they have a 96% CI, if the hypothesis of Normality of errors is not verified.
- For asymmetric distributions, the authors should be careful not to show in tables or figures symmetric error bars that would yield results that are out of range (e.g. negative error rates).
- If error bars are reported in tables or plots, The authors should explain in the text how they were calculated and reference the corresponding figures or tables in the text.

8. Experiments compute resources

Question: For each experiment, does the paper provide sufficient information on the computer resources (type of compute workers, memory, time of execution) needed to reproduce the experiments?

Answer: [NA]

Justification: This is a theory paper that only involves very simple numerical computations.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The paper should indicate the type of compute workers CPU or GPU, internal cluster, or cloud provider, including relevant memory and storage.
- The paper should provide the amount of compute required for each of the individual experimental runs as well as estimate the total compute.
- The paper should disclose whether the full research project required more compute than the experiments reported in the paper (e.g., preliminary or failed experiments that didn't make it into the paper).

9. Code of ethics

Question: Does the research conducted in the paper conform, in every respect, with the NeurIPS Code of Ethics <https://neurips.cc/public/EthicsGuidelines>?

Answer: [Yes]

Justification: The research conducted in the paper conforms with the NeurIPS Code of Ethics.

Guidelines:

- The answer NA means that the authors have not reviewed the NeurIPS Code of Ethics.
- If the authors answer No, they should explain the special circumstances that require a deviation from the Code of Ethics.
- The authors should make sure to preserve anonymity (e.g., if there is a special consideration due to laws or regulations in their jurisdiction).

10. Broader impacts

Question: Does the paper discuss both potential positive societal impacts and negative societal impacts of the work performed?

Answer: [NA]

Justification: To our knowledge, this theory paper has no positive/negative social impact.

Guidelines:

- The answer NA means that there is no societal impact of the work performed.
- If the authors answer NA or No, they should explain why their work has no societal impact or why the paper does not address societal impact.
- Examples of negative societal impacts include potential malicious or unintended uses (e.g., disinformation, generating fake profiles, surveillance), fairness considerations (e.g., deployment of technologies that could make decisions that unfairly impact specific groups), privacy considerations, and security considerations.

- The conference expects that many papers will be foundational research and not tied to particular applications, let alone deployments. However, if there is a direct path to any negative applications, the authors should point it out. For example, it is legitimate to point out that an improvement in the quality of generative models could be used to generate deepfakes for disinformation. On the other hand, it is not needed to point out that a generic algorithm for optimizing neural networks could enable people to train models that generate Deepfakes faster.
- The authors should consider possible harms that could arise when the technology is being used as intended and functioning correctly, harms that could arise when the technology is being used as intended but gives incorrect results, and harms following from (intentional or unintentional) misuse of the technology.
- If there are negative societal impacts, the authors could also discuss possible mitigation strategies (e.g., gated release of models, providing defenses in addition to attacks, mechanisms for monitoring misuse, mechanisms to monitor how a system learns from feedback over time, improving the efficiency and accessibility of ML).

11. Safeguards

Question: Does the paper describe safeguards that have been put in place for responsible release of data or models that have a high risk for misuse (e.g., pretrained language models, image generators, or scraped datasets)?

Answer: [NA]

Justification: The paper poses no such risks.

Guidelines:

- The answer NA means that the paper poses no such risks.
- Released models that have a high risk for misuse or dual-use should be released with necessary safeguards to allow for controlled use of the model, for example by requiring that users adhere to usage guidelines or restrictions to access the model or implementing safety filters.
- Datasets that have been scraped from the Internet could pose safety risks. The authors should describe how they avoided releasing unsafe images.
- We recognize that providing effective safeguards is challenging, and many papers do not require this, but we encourage authors to take this into account and make a best faith effort.

12. Licenses for existing assets

Question: Are the creators or original owners of assets (e.g., code, data, models), used in the paper, properly credited and are the license and terms of use explicitly mentioned and properly respected?

Answer: [NA]

Justification: The paper does not use existing assets.

Guidelines:

- The answer NA means that the paper does not use existing assets.
- The authors should cite the original paper that produced the code package or dataset.
- The authors should state which version of the asset is used and, if possible, include a URL.
- The name of the license (e.g., CC-BY 4.0) should be included for each asset.
- For scraped data from a particular source (e.g., website), the copyright and terms of service of that source should be provided.
- If assets are released, the license, copyright information, and terms of use in the package should be provided. For popular datasets, paperswithcode.com/datasets has curated licenses for some datasets. Their licensing guide can help determine the license of a dataset.
- For existing datasets that are re-packaged, both the original license and the license of the derived asset (if it has changed) should be provided.

- If this information is not available online, the authors are encouraged to reach out to the asset’s creators.

13. **New assets**

Question: Are new assets introduced in the paper well documented and is the documentation provided alongside the assets?

Answer: [NA]

Justification: The paper does not release new assets

Guidelines:

- The answer NA means that the paper does not release new assets.
- Researchers should communicate the details of the dataset/code/model as part of their submissions via structured templates. This includes details about training, license, limitations, etc.
- The paper should discuss whether and how consent was obtained from people whose asset is used.
- At submission time, remember to anonymize your assets (if applicable). You can either create an anonymized URL or include an anonymized zip file.

14. **Crowdsourcing and research with human subjects**

Question: For crowdsourcing experiments and research with human subjects, does the paper include the full text of instructions given to participants and screenshots, if applicable, as well as details about compensation (if any)?

Answer: [NA]

Justification: The paper does not involve crowdsourcing nor research with human subjects.

Guidelines:

- The answer NA means that the paper does not involve crowdsourcing nor research with human subjects.
- Including this information in the supplemental material is fine, but if the main contribution of the paper involves human subjects, then as much detail as possible should be included in the main paper.
- According to the NeurIPS Code of Ethics, workers involved in data collection, curation, or other labor should be paid at least the minimum wage in the country of the data collector.

15. **Institutional review board (IRB) approvals or equivalent for research with human subjects**

Question: Does the paper describe potential risks incurred by study participants, whether such risks were disclosed to the subjects, and whether Institutional Review Board (IRB) approvals (or an equivalent approval/review based on the requirements of your country or institution) were obtained?

Answer: [NA]

Justification: The paper does not involve crowdsourcing nor research with human subjects.

Guidelines:

- The answer NA means that the paper does not involve crowdsourcing nor research with human subjects.
- Depending on the country in which research is conducted, IRB approval (or equivalent) may be required for any human subjects research. If you obtained IRB approval, you should clearly state this in the paper.
- We recognize that the procedures for this may vary significantly between institutions and locations, and we expect authors to adhere to the NeurIPS Code of Ethics and the guidelines for their institution.
- For initial submissions, do not include any information that would break anonymity (if applicable), such as the institution conducting the review.

16. **Declaration of LLM usage**

Question: Does the paper describe the usage of LLMs if it is an important, original, or non-standard component of the core methods in this research? Note that if the LLM is used only for writing, editing, or formatting purposes and does not impact the core methodology, scientific rigorousness, or originality of the research, declaration is not required.

Answer: [NA]

Justification: The core method development in this research does not involve LLMs as any important, original, or non-standard components.

Guidelines:

- The answer NA means that the core method development in this research does not involve LLMs as any important, original, or non-standard components.
- Please refer to our LLM policy (<https://neurips.cc/Conferences/2025/LLM>) for what should or should not be described.

A Proof of Theorem 3.2

This section provides a detailed proof of the existence and convergence of GBSM.

A.1 The Existence of d^{1-2}

To prove the existence of d^{1-2} , we introduce the Knaster-Tarski fixed-point theorem. Let (\mathcal{X}, \preceq) denote a partial order, which means certain pairs of elements within the set \mathcal{X} are comparable under the homogeneous relation \preceq [21]. If this partial order has least upper bounds and greatest lower bounds for its arbitrary subsets, it is called a complete lattice. The Knaster-Tarski fixed-point theorem asserts that for a continuous function on a complete lattice, the iterative application of this function to the least element of the lattice converges to a fixed point \bar{x} , which satisfies $\bar{x} = f(\bar{x})$. Formally, the theorem is stated as follows.

Lemma A.1 (Knaster-Tarski fixed-point theorem [21]). *If the partial order (\mathcal{X}, \preceq) is a complete lattice and $f: \mathcal{X} \rightarrow \mathcal{X}$ is a continuous function. Then, f has a least fixed point, given by*

$$\text{fix}(f) = \sqcup_{n \in \mathbb{N}} f^{(n)}(x_0), \quad (24)$$

where x_0 is the least element of \mathcal{X} , \sqcup denotes the least upper bound, $f^{(n)}(x_0) = f(f^{(n-1)}(x_0))$, and $f^{(1)}(x_0) = f(x_0)$. Here, the continuity of f is defined such that for any increasing sequence $\{x_n\}$ in \mathcal{X} , it satisfies

$$f(\sqcup_{n \in \mathbb{N}} \{x_n\}) = \sqcup_{n \in \mathbb{N}} \{f(x_n)\}. \quad (25)$$

Let \mathcal{D} denote the set of all cost functions, which are defined as maps that satisfy $\mathcal{S}_1 \times \mathcal{S}_2 \rightarrow [0, \frac{\bar{R}}{1-\gamma}]$. Equip \mathcal{D} with the usual pointwise ordering: Consider two cost function, say d and $d' \in \mathcal{D}$, denote $d \leq d'$ if and only if $d(s, s') \leq d'(s, s')$ for any $s \in \mathcal{S}_1$ and $s' \in \mathcal{S}_2$. Then \mathcal{D} forms a complete lattice with the least element d_0^{1-2} , i.e., the constant zero function. Given s and s' , we regard the recursive definition in (5) as a function of d and accordingly define $F: \mathcal{D} \rightarrow \mathcal{D}$ by

$$F(d | s, s') = \max_a \left\{ |R_1(s, a) - R_2(s', a)| + \gamma W_1(\mathbb{P}_1(\cdot | s, a), \mathbb{P}_2(\cdot | s', a); d) \right\}. \quad (26)$$

Utilizing the Knaster-Tarski fixed-point theorem, the existence of d^{1-2} is achieved if the continuity of F holds on \mathcal{D} .

We first prove the continuity of the second term in F . Define $F_{W_1}: \mathcal{D} \rightarrow \mathcal{D}$ by

$$F_{W_1}(d | s, s') = W_1(\mathbb{P}_1(\cdot | s, a), \mathbb{P}_2(\cdot | s', a); d). \quad (27)$$

Lemma A.2. *F_{W_1} is continuous on \mathcal{D} .*

Proof. We follow the definition of continuity defined in Lemma A.1. Let $s_i \in \mathcal{S}_1$ and $s_j \in \mathcal{S}_2$. Regard $F_{W_1}(s_i, s_j; d)$ as a function of d . Without loss of generality, we denote probability distributions $\{\mathbb{P}_1(\cdot | s_i, a), \mathbb{P}_2(\cdot | s_j, a)\}$ as $\{P, Q\}$ for brevity, and let $\rho \leq \rho'$, $\{\rho, \rho'\} \in \mathcal{D}$. Considering the optimal solution $\{\mu, \nu\}$ for $W_1(P, Q; \rho)$ in the dual LP in (4), we have

$$\mu_i - \nu_j \leq \rho(s_i, s_j) \leq \rho'(s_i, s_j), \quad \forall i, j, \quad (28)$$

which is derived from the pointwise ordering in \mathcal{D} . Here, for the other $W_1(P, Q; \rho')$, $\{\mu, \nu\}$ is a feasible, though not necessarily optimal, solution to the dual LP in (4). Thus, we have

$$\begin{aligned} W_1(P, Q; \rho) &= \sum_{i=1}^{|\mathcal{S}_1|} \mu_i P(s_i) - \sum_{j=1}^{|\mathcal{S}_2|} \nu_j Q(s_j) \\ &\leq W_1(P, Q; \rho'), \quad \forall \rho \leq \rho'. \end{aligned} \quad (29)$$

By such a monotonicity, we have $W_1(P, Q; \rho) \leq W_1(P, Q; \sqcup_{n \in \mathbb{N}} \{\rho_n\})$, $\forall \rho \in \{\rho_n\}$ for any increasing sequence $\{\rho_n\}$ on \mathcal{D} . This further implies that $\sqcup_{n \in \mathbb{N}} \{W_1(P, Q; \rho_n)\} \leq W_1(P, Q; \sqcup_{n \in \mathbb{N}} \{\rho_n\})$.

We use the primal LP for the other side. Let λ^n denote the optimal solution in (3) for $W_1(P, Q; \rho_n)$, which also satisfies the conditions for $W_1(P, Q; \sqcup_{n \in \mathbb{N}} \{\rho_n\})$. Define $\epsilon_{i,j}^n = \sqcup_{n \in \mathbb{N}} \{\rho_n\}(s_i, s_j) -$

$\rho_n(s_i, s_j)$, then $\epsilon_{i,j}^n \geq 0$ and $\lim_{n \rightarrow \infty} \epsilon_{i,j}^n = 0$ due to the monotonicity of the increasing sequence of $\{\rho_n\}$. Then, we have

$$\begin{aligned}
W_1(P, Q; \sqcup_{n \in \mathbb{N}} \{\rho_n\}) &\stackrel{(a)}{\leq} \sum_{i=1}^{|\mathcal{S}_1|} \sum_{j=1}^{|\mathcal{S}_2|} \lambda_{i,j}^n \cdot \sqcup_{n \in \mathbb{N}} \{\rho_n\}(s_i, s_j) \\
&= \sum_{i=1}^{|\mathcal{S}_1|} \sum_{j=1}^{|\mathcal{S}_2|} \lambda_{i,j}^n \rho_n(s_i, s_j) + \sum_{i=1}^{|\mathcal{S}_1|} \sum_{j=1}^{|\mathcal{S}_2|} \lambda_{i,j}^n \epsilon_{i,j}^n \\
&= W_1(P, Q; \rho_n) + \sum_{i,j=1}^{|\mathcal{S}|} \lambda_{i,j}^n \epsilon_{i,j}^n \\
&\leq \sqcup_{n \in \mathbb{N}} \{W_1(P, Q; \rho_n)\} + \max_{i,j} \{\epsilon_{i,j}^n\}.
\end{aligned} \tag{30}$$

Here, step (a) follows from the fact that λ^n is the optimal solution for $W_1(P, Q; \rho_n)$ rather than $W_1(P, Q; \sqcup_{n \in \mathbb{N}} \{\rho_n\})$. Taking $n \rightarrow \infty$, we have $\sqcup_{n \in \mathbb{N}} \{W_1(P, Q; \rho_n)\} \geq W_1(P, Q; \sqcup_{n \in \mathbb{N}} \{\rho_n\})$. Following from the above two inequalities from both directions, it is readily to get $\sqcup_{n \in \mathbb{N}} \{W_1(P, Q; \rho_n)\} = W_1(P, Q; \sqcup_{n \in \mathbb{N}} \{\rho_n\})$. Thus, for any i and j ,

$$\begin{aligned}
F_{W_1}(\sqcup_{n \in \mathbb{N}} \{\rho_n\} | s_i, s_j) &= W_1(\mathbb{P}_1(\cdot | s_i, a), \mathbb{P}_2(\cdot | s_j, a); \sqcup_{n \in \mathbb{N}} \{\rho_n\}) \\
&= \sqcup_{n \in \mathbb{N}} \{W_1(\mathbb{P}_1(\cdot | s_i, a), \mathbb{P}_2(\cdot | s_j, a); \rho_n)\} \\
&= \sqcup_{n \in \mathbb{N}} \{F_{W_1}(\rho_n | s_i, s_j)\}.
\end{aligned} \tag{31}$$

Now that the continuity of F_{W_1} in (27) on \mathcal{D} is established. \square

Armed with Lemma A.2, we are ready to establish the continuity of F as follows.

Lemma A.3. *F is continuous on \mathcal{D} .*

Proof. Considering an arbitrary increasing sequence $\{\rho_n\}$ on \mathcal{D} , for any i and j , we have

$$\begin{aligned}
&F(\sqcup_{n \in \mathbb{N}} \{\rho_n\} | s_i, s_j) \\
&= \max_a \{|R_1(s_i, a) - R_2(s_j, a)| + \gamma W_1(\mathbb{P}_1(\cdot | s_i, a), \mathbb{P}_2(\cdot | s_j, a); \sqcup_{n \in \mathbb{N}} \{\rho_n\})\} \\
&= \max_a \{|R_1(s_i, a) - R_2(s_j, a)| + \gamma \sqcup_{n \in \mathbb{N}} \{W_1(\mathbb{P}_1(\cdot | s_i, a), \mathbb{P}_2(\cdot | s_j, a); \rho_n)\}\} \\
&= \sqcup_{n \in \mathbb{N}} \left\{ \max_a \{|R_1(s_i, a) - R_2(s_j, a)| + \gamma W_1(\mathbb{P}_1(\cdot | s_i, a), \mathbb{P}_2(\cdot | s_j, a); \rho_n)\} \right\} \\
&= \sqcup_{n \in \mathbb{N}} \{F(\rho_n | s_i, s_j)\}.
\end{aligned} \tag{32}$$

\square

Now that the existence of d^{1-2} is established by using Lemma A.1 and Lemma A.3.

A.2 The Convergence of d_n^{1-2} to d^{1-2}

Due to the continuity of F and using the induction starting from $d_0^{1-2} \leq d_1^{1-2}$, $\{d_n^{1-2}\}$ forms an increasing sequence on \mathcal{D} . Given that $d^{1-2} = \sqcup_{n \in \mathbb{N}} F^{(n)}(d_0^{1-2})$, we have $d^{1-2} \geq d_n^{1-2}$ for any n . Also,

$$\begin{aligned}
d^{1-2}(s_i, s_j) &= \max_a \left\{ |R_1(s_i, a) - R_2(s_j, a)| + \gamma W_1(\mathbb{P}_1(\cdot | s_i, a), \mathbb{P}_2(\cdot | s_j, a); d^{1-2}) \right\} \\
&\leq \bar{R} + \gamma \max_{i,j} \{d^{1-2}(s_i, s_j)\} \\
\Rightarrow \max_{i,j} \{d^{1-2}(s_i, s_j)\} &\leq \bar{R}/(1 - \gamma), \quad \forall (s_i, s_j) \in \mathcal{S}_1 \times \mathcal{S}_2.
\end{aligned} \tag{33}$$

We begin with a simple inequality for the Wasserstein distance before proving the convergence of GBSM. Let λ^n denote the optimal solution for $W_1(P, Q; d_n^{1-2})$, then for any d_n^{1-2}

$$\begin{aligned}
W_1(P, Q; d^{1-2}) &\leq \sum_{i=1}^{|\mathcal{S}_1|} \sum_{j=1}^{|\mathcal{S}_2|} \lambda_{i,j}^n d^{1-2}(s_i, s_j) \\
&= \sum_{i=1}^{|\mathcal{S}_1|} \sum_{j=1}^{|\mathcal{S}_2|} \lambda_{i,j}^n (d^{1-2}(s_i, s_j) - d_n^{1-2}(s_i, s_j) + d_n^{1-2}(s_i, s_j)) \\
&\leq \max_{i,j} \{d^{1-2}(s_i, s_j) - d_n^{1-2}(s_i, s_j)\} + W_1(P, Q; d_n^{1-2}).
\end{aligned} \tag{34}$$

The first inequality follows from the fact that λ^n is the optimal solution for $W_1(P, Q; d_n^{1-2})$ rather than $W_1(P, Q; d^{1-2})$.

Now we employ the mathematical induction. For the base case, we have

$$\begin{aligned}
& d^{1-2}(s, s') - d_1^{1-2}(s, s') \\
&= \max_a \{ |R_1(s, a) - R_2(s', a)| + \gamma W_1(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s', a); d^{1-2}) \} \\
&\quad - \max_a \{ |R_1(s, a) - R_2(s', a)| \} \\
&\leq \max_a \{ |R_1(s, a) - R_2(s', a)| \} + \gamma \max_a \{ W_1(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s', a); d^{1-2}) \} \\
&\quad - \max_a \{ |R_1(s, a) - R_2(s', a)| \} \\
&= \gamma \max_a \{ W_1(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s', a); d^{1-2}) \} \\
&\leq \gamma \max_{s, s'} \{ d^{1-2}(s, s') \} = \gamma \bar{R}/(1 - \gamma), \quad \forall (s, s') \in \mathcal{S}_1 \times \mathcal{S}_2.
\end{aligned} \tag{35}$$

By the induction hypothesis, we assume that for an arbitrary n ,

$$d^{1-2}(s, s') - d_n^{1-2}(s, s') \leq \gamma^n \bar{R}/(1 - \gamma), \quad \forall (s, s') \in \mathcal{S}_1 \times \mathcal{S}_2. \tag{36}$$

Then we have

$$\begin{aligned}
& d^{1-2}(s, s') - d_{n+1}^{1-2}(s, s') \\
&= \max_a \{ |R_1(s, a) - R_2(s', a)| + \gamma W_1(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s', a); d^{1-2}) \} \\
&\quad - \max_a \{ |R_1(s, a) - R_2(s', a)| + \gamma W_1(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s', a); d_n^{1-2}) \} \\
&\leq \max_a \{ (|R_1(s, a) - R_2(s', a)| + \gamma W_1(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s', a); d^{1-2})) \\
&\quad - (|R_1(s, a) - R_2(s', a)| + \gamma W_1(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s', a); d_n^{1-2})) \} \\
&= \gamma \max_a \{ W_1(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s', a); d^{1-2}) - W_1(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s', a); d_n^{1-2}) \} \\
&\stackrel{(a)}{\leq} \gamma \max_a \{ \max_{s, s'} \{ d^{1-2}(s, s') - d_n^{1-2}(s, s') \} + W_1(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s', a); d_n^{1-2}) \\
&\quad - W_1(\mathbb{P}_1(\cdot|s, a), \mathbb{P}_2(\cdot|s', a); d_n^{1-2}) \} \\
&= \gamma \max_{s, s'} \{ d^{1-2}(s, s') - d_n^{1-2}(s, s') \} \leq \gamma^{n+1} \bar{R}/(1 - \gamma), \quad \forall (s, s') \in \mathcal{S}_1 \times \mathcal{S}_2.
\end{aligned} \tag{37}$$

Here, step (a) uses (34). Following from (35)-(37), $d^{1-2}(s, s') - d_n^{1-2}(s, s') \leq \gamma^n \bar{R}/(1 - \gamma)$ holds for all $n \in \mathbb{N}$.

B Proof of Theorem 3.3

This proves the optimal value difference bound between MDPs by induction. For the base case, we have

$$\begin{aligned}
|V_1^{(1)}(s_i) - V_2^{(1)}(s_j)| &= |\max_a R_1(s_i, a) - \max_a R_2(s_j, a)| \\
&\leq \max_a |R_1(s_i, a) - R_2(s_j, a)| \\
&= d_1^{1-2}(s_i, s_j), \quad \forall (s_i, s_j) \in \mathcal{S}_1 \times \mathcal{S}_2.
\end{aligned} \tag{38}$$

By the induction hypothesis, we assume that for an arbitrary n ,

$$\begin{aligned}
V_1^{(n)}(s_i) - V_2^{(n)}(s_j) &\leq |V_1^{(n)}(s_i) - V_2^{(n)}(s_j)| \\
&\leq d_n^{1-2}(s_i, s_j), \quad \forall (s_i, s_j) \in \mathcal{S}_1 \times \mathcal{S}_2.
\end{aligned} \tag{39}$$

Then the induction follows

$$\begin{aligned}
& \left| V_1^{(n+1)}(s_i) - V_2^{(n+1)}(s_j) \right| \\
&= \left| \max_a \left\{ R_1(s_i, a) + \gamma \sum_{k=1}^{|\mathcal{S}_1|} \mathbb{P}_1(s_k | s_i, a) V_1^{(n)}(s_k) \right\} \right. \\
&\quad \left. - \max_a \left\{ R_2(s_j, a) + \gamma \sum_{k=1}^{|\mathcal{S}_2|} \mathbb{P}_2(s_k | s_j, a) V_2^{(n)}(s_k) \right\} \right| \\
&\leq \max_a \left\{ \left| \left(R_1(s_i, a) + \gamma \sum_{k=1}^{|\mathcal{S}_1|} \mathbb{P}(s_k | s_i, a) V_1^{(n)}(s_k) \right) \right. \right. \\
&\quad \left. \left. - \left(R_2(s_j, a) + \gamma \sum_{k=1}^{|\mathcal{S}_2|} \mathbb{P}_2(s_k | s_j, a) V_2^{(n)}(s_k) \right) \right| \right\} \\
&\leq \max_a \left\{ \left| R_1(s_i, a) - R_2(s_j, a) \right| + \gamma \left| \sum_{k=1}^{|\mathcal{S}_1|} \mathbb{P}_1(s_k | s_i, a) V_1^{(n)}(s_k) - \sum_{k=1}^{|\mathcal{S}_2|} \mathbb{P}_2(s_k | s_j, a) V_2^{(n)}(s_k) \right| \right\} \\
&\stackrel{(a)}{\leq} \max_a \{ |R_1(s_i, a) - R_2(s_j, a)| + \gamma W_1(\mathbb{P}_1(\cdot | s_i, a), \mathbb{P}_2(\cdot | s_j, a); d_n^{1-2}) \} \\
&= d_{n+1}^{1-2}(s_i, s_j), \quad \forall (s_i, s_j) \in \mathcal{S}_1 \times \mathcal{S}_2. \tag{40}
\end{aligned}$$

Here, steps (a) follows from the fact that $(V_1^{(n)}(s_k))_{k=1}^{|\mathcal{S}_1|}$ and $(V_2^{(n)}(s_k))_{k=1}^{|\mathcal{S}_2|}$ form a feasible, but not necessarily the optimal, solution to the dual LP in (4) for $W_1(\mathbb{P}_1(\cdot | s_i, a), \mathbb{P}_2(\cdot | s_j, a); d_n^{1-2})$.

Now from (38)-(40), we have $|V_1^{(n)}(s) - V_2^{(n)}(s')| \leq d_n^{1-2}(s, s')$, $\forall (s, s') \in \mathcal{S}_1 \times \mathcal{S}_2$, $\forall n \in \mathbb{N}$. Taking $n \rightarrow \infty$ yields the desired result.

C Proof of Theorem 4.1

This section provides a detailed proof of the regret bound for policy π transferred from \mathcal{M}_1 to \mathcal{M}_2 . By the triangle inequality, for any state $s_j \in \mathcal{S}_2$ and $s_i = f(s_j) \in \mathcal{S}_1$, we have

$$|V_2^*(s_j) - V_2^\pi(s_j)| \leq |V_2^*(s_j) - V_1^*(s_i)| + |V_1^*(s_i) - V_1^\pi(s_i)| + |V_1^\pi(s_i) - V_2^\pi(s_j)|. \tag{41}$$

Within the right-hand side of this inequality, the first summation term $|V_2^*(s_j) - V_1^*(s_i)|$ is upper bounded by $d^{1-2}(s_i, s_j)$ according to Theorem 3.3, and $|V_1^*(s_i) - V_1^\pi(s_i)|$ is upper bounded by $\max_{s \in \mathcal{S}_1} |V_1^*(s) - V_1^\pi(s)|$. For the last term, we have

$$\begin{aligned}
& |V_1^\pi(s_i) - V_2^\pi(s_j)| \\
&= \left| \sum_{a=1}^{|\mathcal{A}|} \pi(a|s_i) \left(R_1(s_i, a) + \gamma \sum_{k=1}^{|\mathcal{S}_1|} \mathbb{P}_1(s_k | s_i, a) V_1^\pi(s_k) \right) \right. \\
&\quad \left. - \sum_{a=1}^{|\mathcal{A}|} \pi(a|f(s_j)) \left(R_2(s_j, a) + \gamma \sum_{k=1}^{|\mathcal{S}_2|} \mathbb{P}_2(s_k | s_j, a) V_2^\pi(s_k) \right) \right| \\
&\leq \sum_{a=1}^{|\mathcal{A}|} \pi(a|s_i) \left(\left| R_1(s_i, a) - R_2(s_j, a) \right| + \gamma \left| \sum_{k=1}^{|\mathcal{S}_1|} \mathbb{P}_1(s_k | s_i, a) V_1^\pi(s_k) - \sum_{k=1}^{|\mathcal{S}_2|} \mathbb{P}_2(s_k | s_j, a) V_2^\pi(s_k) \right| \right) \\
&\leq \sum_{a=1}^{|\mathcal{A}|} \pi(a|s_i) \left(\left| R_1(s_i, a) - R_2(s_j, a) \right| + \gamma \left| \sum_{k=1}^{|\mathcal{S}_1|} \mathbb{P}_1(s_k | s_i, a) V_1^*(s_k) - \sum_{k=1}^{|\mathcal{S}_2|} \mathbb{P}_2(s_k | s_j, a) V_2^*(s_k) \right| \right) \\
&\quad + \gamma \sum_{a=1}^{|\mathcal{A}|} \pi(a|s_i) \left| \sum_{k=1}^{|\mathcal{S}_1|} \mathbb{P}_1(s_k | s_i, a) (V_1^*(s_k) - V_1^\pi(s_k)) \right| \\
&\quad + \gamma \sum_{a=1}^{|\mathcal{A}|} \pi(a|s_i) \left| \sum_{k=1}^{|\mathcal{S}_2|} \mathbb{P}_2(s_k | s_j, a) (V_2^*(s_k) - V_2^\pi(s_k)) \right|
\end{aligned}$$

$$\begin{aligned}
&\leq \max_a \left\{ \left| R_1(s_i, a) - R_2(s_j, a) \right| + \gamma \left| \sum_{k=1}^{|\mathcal{S}_1|} \mathbb{P}_1(s_k | s_i, a) V_1^*(s_k) - \sum_{k=1}^{|\mathcal{S}_2|} (\mathbb{P}(s_k | s_j, a) V_2^*(s_k)) \right| \right\} \\
&\quad + \gamma \max_{s \in \mathcal{S}_1} |V_1^*(s) - V_1^\pi(s)| + \gamma \max_{s \in \mathcal{S}_2} |V_2^*(s) - V_2^\pi(s)| \\
&\stackrel{(a)}{\leq} \max_a \{ |R_1(s_i, a) - R_2(s_j, a)| + \gamma W_1(\mathbb{P}_1(\cdot | s_i, a), \mathbb{P}_2(\cdot | s_j, a); d^{1-2}) \} \\
&\quad + \gamma \max_{s \in \mathcal{S}_1} |V_1^*(s) - V_1^\pi(s)| + \gamma \max_{s \in \mathcal{S}_2} |V_2^*(s) - V_2^\pi(s)| \\
&= d^{1-2}(s_i, s_j) + \gamma \max_{s \in \mathcal{S}_1} |V_1^*(s) - V_1^\pi(s)| + \gamma \max_{s \in \mathcal{S}_2} |V_2^*(s) - V_2^\pi(s)|. \tag{42}
\end{aligned}$$

Here, step (a) stems from the fact that, according to Theorem 3.3, $(V_1^*(s_k))_{k=1}^{|\mathcal{S}_1|}$ and $(V_2^*(s_k))_{k=1}^{|\mathcal{S}_2|}$ form a feasible, but not necessarily the optimal, solution to the dual LP in (4) for $W_1(\mathbb{P}_1(\cdot | s_i, a), \mathbb{P}_2(\cdot | s_j, a); d^{1-2})$. Combining the above inequalities on all three summation terms in (41) and taking the maximum of both sides, we have

$$\begin{aligned}
\max_{s' \in \mathcal{S}_2} |V_2^*(s') - V_2^\pi(s')| &\leq \underbrace{\max_{s' \in \mathcal{S}_2} d^{1-2}(f(s'), s')}_{\text{1st term}} + \underbrace{\max_{s \in \mathcal{S}_1} |V_1^*(s) - V_1^\pi(s)|}_{\text{2nd term}} \\
&\quad + \underbrace{\max_{s' \in \mathcal{S}_2} d^{1-2}(f(s'), s') + \gamma \max_{s \in \mathcal{S}_1} |V_1^*(s) - V_1^\pi(s)| + \gamma \max_{s' \in \mathcal{S}_2} |V_2^*(s') - V_2^\pi(s')|}_{\text{3rd term}} \\
&\leq 2 \max_{s \in \mathcal{S}_2} d^{1-2}(f(s), s) + (1 + \gamma) \max_{s \in \mathcal{S}_1} |V_1^*(s) - V_1^\pi(s)| + \gamma \max_{s' \in \mathcal{S}_2} |V_2^*(s') - V_2^\pi(s')|. \tag{43}
\end{aligned}$$

Rearranging the inequality yields the desired result.

D Proofs of Lax GBSM-based transfer bound

To prove the policy transfer bound based on lax GBSM, apart from the state mapping $f : \mathcal{S}_2 \rightarrow \mathcal{S}_1$, we need to define an additional action mapping $g : \mathcal{A}_1 \rightarrow \mathcal{A}_2$ for policy transfer between different action spaces. Then, we have

$$\begin{aligned}
&|V_1^\pi(s_i) - V_2^\pi(s_j)| \\
&= \left| \sum_{a=1}^{|\mathcal{A}_1|} \pi(a | s_i) (R_1(s_i, a) + \gamma \sum_{k=1}^{|\mathcal{S}_1|} \mathbb{P}_1(s_k | s_i, a) V_1^\pi(s_k)) \right. \\
&\quad \left. - \sum_{a=1}^{|\mathcal{A}_1|} \pi(a | f(s_j)) (R_2(s_j, g(a)) + \gamma \sum_{k=1}^{|\mathcal{S}_2|} \mathbb{P}_2(s_k | s_j, g(a)) V_2^\pi(s_k)) \right| \\
&\leq \sum_{a=1}^{|\mathcal{A}_1|} \left(\pi(a | s_i) (|R_1(s_i, a) - R_2(s_j, g(a))| \right. \\
&\quad \left. + \gamma \left| \sum_{k=1}^{|\mathcal{S}_1|} \mathbb{P}_1(s_k | s_i, a) V_1^\pi(s_k) - \sum_{k=1}^{|\mathcal{S}_2|} \mathbb{P}_2(s_k | s_j, g(a)) V_2^\pi(s_k) \right| \right) \\
&\leq \sum_{a=1}^{|\mathcal{A}_1|} \left(\pi(a | s_i) (|R_1(s_i, a) - R_2(s_j, g(a))| \right. \\
&\quad \left. + \gamma \left| \sum_{k=1}^{|\mathcal{S}_1|} \mathbb{P}_1(s_k | s_i, a) V_1^*(s_k) - \sum_{k=1}^{|\mathcal{S}_2|} \mathbb{P}_2(s_k | s_j, g(a)) V_2^*(s_k) \right| \right) \\
&\quad + \gamma \sum_{a=1}^{|\mathcal{A}_1|} \pi(a | s_i) \left| \sum_{k=1}^{|\mathcal{S}_1|} \mathbb{P}_1(s_k | s_i, a) (V_1^*(s_k) - V_1^\pi(s_k)) \right| \\
&\quad + \gamma \sum_{a=1}^{|\mathcal{A}_1|} \pi(a | s_i) \left| \sum_{k=1}^{|\mathcal{S}_2|} \mathbb{P}_2(s_k | s_j, g(a)) (V_2^*(s_k) - V_2^\pi(s_k)) \right| \\
&\leq \max_{a \in \mathcal{A}_1} \left\{ |R_1(s_i, a) - R_2(s_j, g(a))| \right. \\
&\quad \left. + \gamma \left| \sum_{k=1}^{|\mathcal{S}_1|} \mathbb{P}_1(s_k | s_i, a) V_1^*(s_k) - \sum_{k=1}^{|\mathcal{S}_2|} (\mathbb{P}(s_k | s_j, g(a)) V_2^*(s_k)) \right| \right\} \\
&\quad + \gamma \max_{s \in \mathcal{S}_1} |V_1^*(s) - V_1^\pi(s)| + \gamma \max_{s \in \mathcal{S}_2} |V_2^*(s) - V_2^\pi(s)|
\end{aligned}$$

$$\begin{aligned}
&\stackrel{(a)}{\leq} \max_{a \in \mathcal{A}_1} \min_{a' \in \mathcal{A}_2} \{ |R_1(s_i, a) - R_2(s_j, a')| + \gamma W_1(\mathbb{P}_1(\cdot | s_i, a), \mathbb{P}_2(\cdot | s_j, a'); d_{\text{Iax}}^{1-2}) \} \\
&\quad + \gamma \max_{s \in \mathcal{S}_1} |V_1^*(s) - V_1^\pi(s)| + \gamma \max_{s \in \mathcal{S}_2} |V_2^*(s) - V_2^\pi(s)| \\
&\leq H(\delta(d_{\text{Iax}}^{1-2}))(X_{s_i}, X'_{s_j}) + \gamma \max_{s \in \mathcal{S}_1} |V_1^*(s) - V_1^\pi(s)| + \gamma \max_{s \in \mathcal{S}_2} |V_2^*(s) - V_2^\pi(s)| \\
&= d_{\text{Iax}}^{1-2}(s_i, s_j) + \gamma \max_{s \in \mathcal{S}_1} |V_1^*(s) - V_1^\pi(s)| + \gamma \max_{s \in \mathcal{S}_2} |V_2^*(s) - V_2^\pi(s)|
\end{aligned}$$

Due to the introduction of max-min term via Hausdorff metric, step (a) requires that action mapping satisfies $g(a) = \arg \min_{a'} \delta((f(s'), a), (s', a'))$ for each s' and a .

E Proofs of on-policy GBSM-based Bound

Theorem E.1 (On-policy GBSM optimal value difference bound). *Let V_1^π and V_2^π denote the value functions with policy π in \mathcal{M}_1 and \mathcal{M}_2 , respectively. Then on-policy GBSM provides an upper bound for the difference between the value functions for any state pair $(s, s') \in \mathcal{S}_1 \times \mathcal{S}_2$:*

$$|V_1^\pi(s) - V_2^\pi(s')| \leq d_{\pi}^{1-2}(s, s'). \quad (44)$$

Proof. For the base case, we have

$$|V_1^{\pi, (0)}(s_i) - V_2^{\pi, (0)}(s_j)| = d_{\pi, 0}^{1-2}(s_i, s_j) = 0, \quad \forall (s_i, s_j) \in \mathcal{S}_1 \times \mathcal{S}_2. \quad (45)$$

By the induction hypothesis, we assume that for an arbitrary n ,

$$|V_1^{\pi, (n)}(s_i) - V_2^{\pi, (n)}(s_j)| \leq d_{\pi, n}^{1-2}(s_i, s_j), \quad \forall (s_i, s_j) \in \mathcal{S}_1 \times \mathcal{S}_2. \quad (46)$$

The induction follows

$$\begin{aligned}
&|V_1^{\pi, (n+1)}(s_i) - V_2^{\pi, (n+1)}(s_j)| \\
&= \left| \{ R_1^\pi(s_i) + \gamma \sum_{k=1}^{|\mathcal{S}_1|} \mathbb{P}_1^\pi(s_k | s_i) V_1^{\pi, (n)}(s_k) \} - \{ R_2^\pi(s_j) + \gamma \sum_{k=1}^{|\mathcal{S}_2|} \mathbb{P}_2^\pi(s_k | s_j) V_2^{\pi, (n)}(s_k) \} \right| \\
&\leq \left\{ |R_1^\pi(s_i) - R_2^\pi(s_j)| + \gamma \left| \sum_{k=1}^{|\mathcal{S}_1|} \mathbb{P}_1^\pi(s_k | s_i) V_2^{\pi, (n)}(s_k) - \sum_{k=1}^{|\mathcal{S}_2|} \mathbb{P}_2^\pi(s_k | s_j) V_2^{\pi, (n)}(s_k) \right| \right\} \\
&\leq \left\{ |R_1^\pi(s_i) - R_2^\pi(s_j)| + \gamma W_1(\mathbb{P}_1^\pi(\cdot | s_i), \mathbb{P}_2^\pi(\cdot | s_j); d_n^{1-2}) \right\} \\
&= d_{n+1}^{1-2}(s_i, s_j), \quad \forall (s_i, s_j) \in \mathcal{S}_1 \times \mathcal{S}_2. \quad (47)
\end{aligned}$$

Taking $n \rightarrow \infty$ yields the desired result. \square

Theorem E.2 (VFA error bound with non-optimal policy).

$$\max_s |V_1^\pi(s) - V_{[1]}^\pi(s)| \leq \max_s d_\pi^{1-[1]}(s, s) \leq \max_s \tilde{d}_\pi(s, [s]) / (1 - \gamma) \quad (48)$$

Proof. The first inequality follows directly from Theorem E.1, while the second is established using a derivation analogous to the proof of Theorem 4.4. \square

F Additional Numerical Results

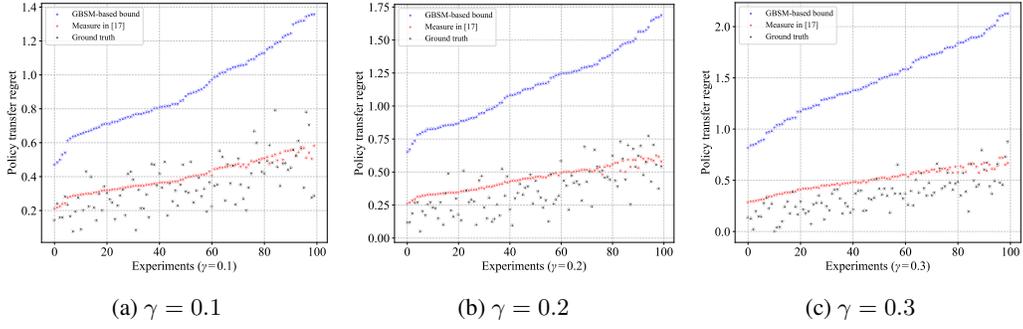


Figure 2: Experiments on random Garnet MDPs (policy transfer, $\gamma = 0.1$ to 0.3).

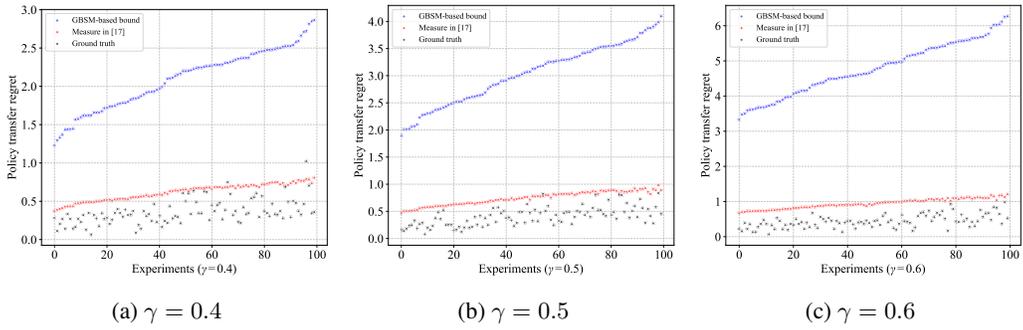


Figure 3: Experiments on random Garnet MDPs (policy transfer, $\gamma = 0.4$ to 0.6).

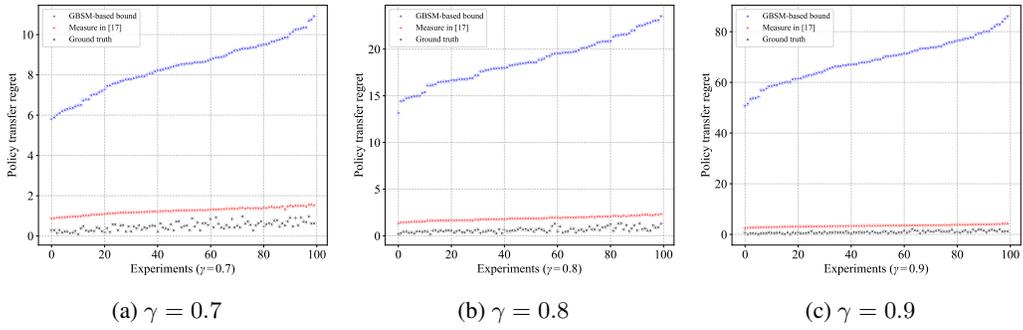


Figure 4: Experiments on random Garnet MDPs (policy transfer, $\gamma = 0.7$ to 0.9).

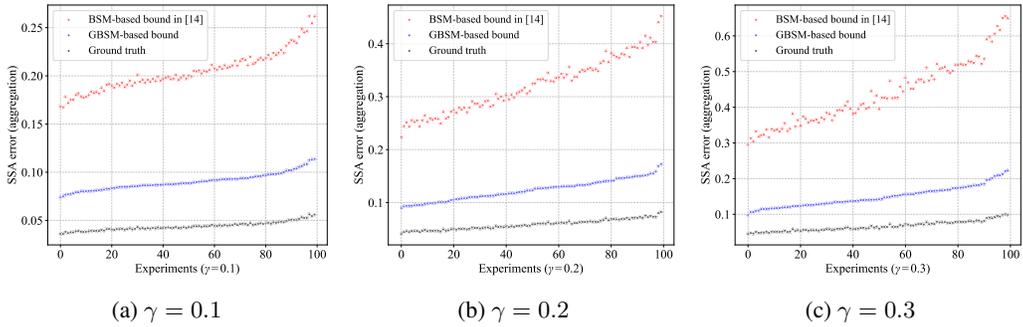


Figure 5: Experiments on random Garnet MDPs (SSA with aggregation, $\gamma = 0.1$ to 0.3).

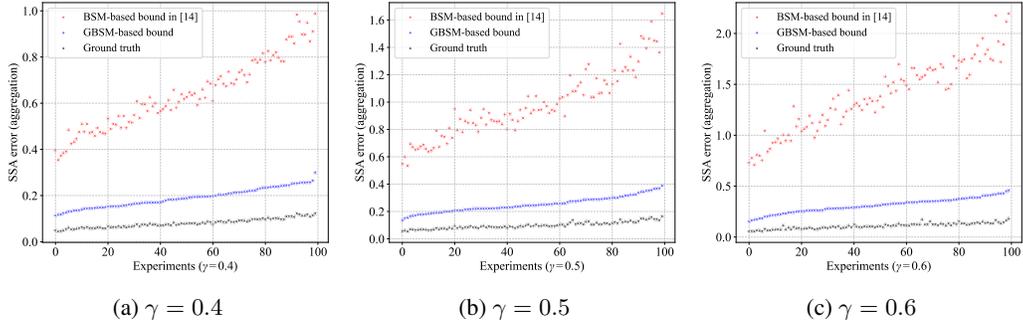


Figure 6: Experiments on random Garnet MDPs (SSA with aggregation, $\gamma = 0.4$ to 0.6).

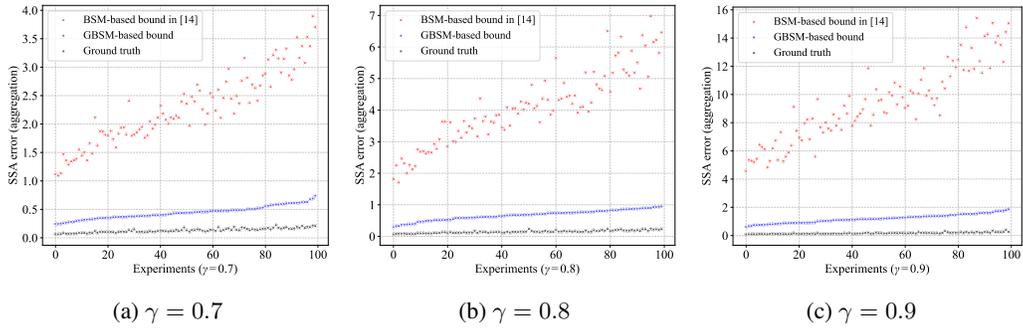


Figure 7: Experiments on random Garnet MDPs (SSA aggregation, $\gamma = 0.7$ to 0.9).

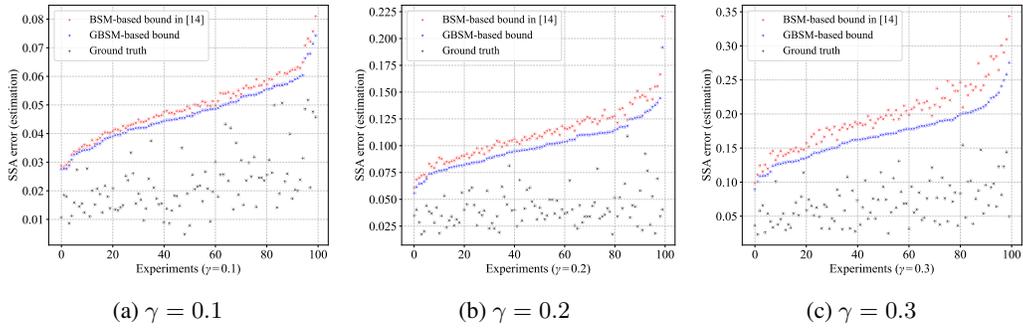


Figure 8: Experiments on random Garnet MDPs (SSA with estimation, $\gamma = 0.1$ to 0.3).

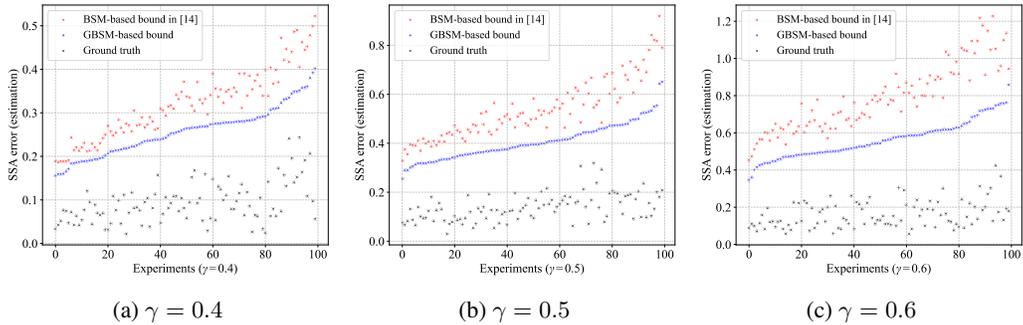


Figure 9: Experiments on random Garnet MDPs (SSA with aggregation, $\gamma = 0.4$ to 0.6).

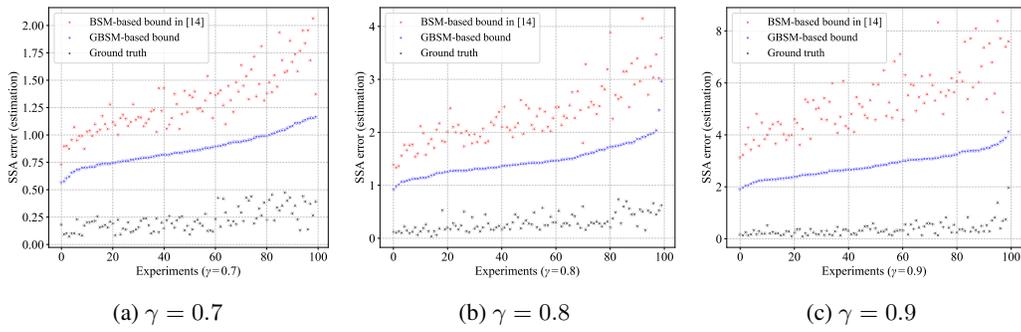


Figure 10: Experiments on random Garnet MDPs (SSA with aggregation, $\gamma = 0.7$ to 0.9).

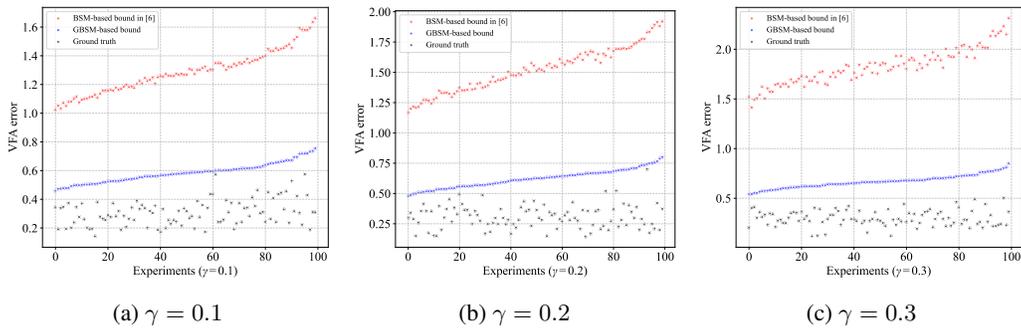


Figure 11: Experiments on random Garnet MDPs (VFA, $\gamma = 0.1$ to 0.3).

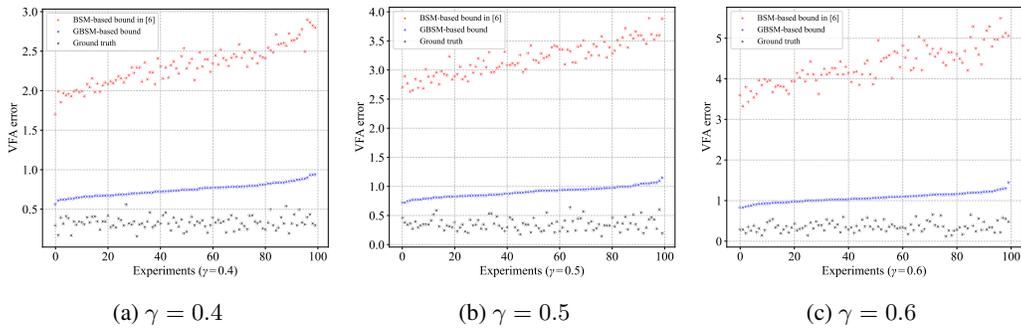


Figure 12: Experiments on random Garnet MDPs (VFA, $\gamma = 0.4$ to 0.6).

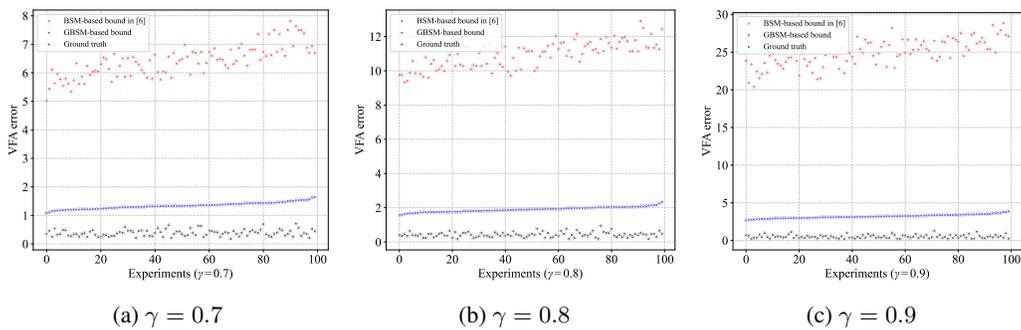


Figure 13: Experiments on random Garnet MDPs (VFA, $\gamma = 0.7$ to 0.9).