Scalable High-Dimensional Reachable Set Estimation: Algorithms and Sample Complexity

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ABSTRACT

Estimating reachable sets in high-dimensional spaces is fundamental to verifying generative models and dialogue systems, yet Monte Carlo approaches suffer from sample complexity that scales exponentially with dimension. We compare five estimation algorithms—γ-neighbourhood union, PAC-inflated neighbourhood, adaptive boundary refinement, PCA-based dimensionality reduction, and data-adaptive kNN boundary learning—across dimensions 2 to 100 using a balanced evaluation protocol that ensures meaningful metrics at all dimensions. Ground truth is consistently defined as the γ-expanded reachable set R_γ, and all results report mean ± standard deviation over 5 independent trials.

Our experiments reveal three distinct regimes: (i) at low dimensions ($d \leq 5$), all methods achieve F1 > 0.52; (ii) at moderate dimensions ($d = 10$–20), only dimensionality reduction (F1 ≈ 0.68) and learned boundary (F1 ≈ 0.92) remain viable; (iii) beyond $d = 50$, neighbourhood-based methods collapse to F1=0 while learned boundary maintains F1 ≈ 0.89. On low-intrinsic-dimension sets (a k=3 subspace embedded in $\mathbb{R}^d$), all methods recover strong performance even at d=100, with PAC-inflated and γ-neighbourhood both reaching F1≈1.0. These results quantify the fundamental gap between theoretical PAC bounds (10^{15}+ samples) and practical estimation (10^4 samples suffice at d=5), and demonstrate that structural assumptions—low intrinsic dimension or data-adaptive thresholds—are essential for high-dimensional reachable set estimation.

KEYWORDS

reachable sets, high-dimensional estimation, PAC learning, sample complexity, dimensionality reduction

1 INTRODUCTION

Reachable set estimation—determining which states or outputs a system can achieve—is a cornerstone of formal verification [1]. For generative models in dialogue systems, Cheng et al. [3] introduced Monte Carlo algorithms with PAC guarantees for estimating reachable and controllable sets. However, they identify a critical limitation: the sample complexity depends on the covering number of the γ-quantized measurement space, which grows as $(2/\gamma)^d$ for d-dimensional spaces.

This exponential scaling makes direct PAC estimation impractical for high-dimensional settings. Prior work on neural reachability [2] and scenario optimization [4] has explored alternatives, but the fundamental tension between precision, dimension, and computational cost remains unresolved.

We address this gap through four contributions: (1) a corrected evaluation protocol using balanced positive/negative sampling with ground truth defined consistently as R_γ; (2) five estimation algorithms including a data-adaptive kNN boundary learner; (3) a low-intrinsic-dimension experiment demonstrating when dimensionality reduction succeeds and fails; and (4) multi-trial experiments with uncertainty quantification across dimensions 2–100.

2 PROBLEM FORMULATION

Given a system with measurement-value space $\mathcal{X} \subseteq \mathbb{R}^d$, the γ-expanded reachable set is:

$$R_\gamma = \{x \in \mathcal{X} : \exists\, y \in R,\ \|x - y\| \leq \gamma\} \tag{1}$$

where R is the true reachable set. All estimators target R_γ and all evaluation is performed against R_γ membership as ground truth.

The PAC estimation problem asks for $\hat{R}$ such that $\Pr[R_\gamma \subseteq \hat{R} \subseteq R_{2\gamma}] \geq 1 - \delta$ using N samples [5]. The classical PAC bound requires:

$$N = O\left(\left(\frac{2}{\gamma}\right)^d \cdot d \cdot \log\frac{1}{\delta}\right) \tag{2}$$

Evaluation protocol. Prior implementations sampled test points uniformly from a hypercube, causing the fraction of positives to vanish exponentially with d (e.g., 0 out of 500 positives for $d \geq 10$). We instead generate *balanced* evaluation sets: 250 positives sampled from inside R_γ and 250 negatives sampled from just outside R_γ (a thin annular shell), ensuring that precision, recall, and F1 are informative at all dimensions.

3 ALGORITHMS

3.1 γ-Neighbourhood Union

Classifies a test point x as reachable if $\min_i \|x - s_i\| \leq \gamma$ for samples $\{s_i\}_{i=1}^n$ drawn from R. Implemented via `scipy.spatial.cKDTree` for $O(n \log n)$ construction and $O(\log n)$ per query.

3.2 PAC-Inflated Neighbourhood

Inflates γ by $\epsilon_n = \gamma\sqrt{d \log(n/\delta)/n}$ to provide a $(1-\delta)$-confidence inclusion guarantee:

$$\hat{R} = \{x : \min_i \|x - s_i\| \leq \gamma + \epsilon_n\} \tag{3}$$

This trades precision for coverage, ensuring high recall at the cost of increased false positives.

3.3 Adaptive Boundary Refinement

A two-phase method: (1) coarse classification via γ-neighbourhood; (2) for points in the boundary region $[\frac{\gamma}{2}, \frac{3\gamma}{2}]$, refinement using mean k-nearest-neighbour distance with threshold 1.2γ.

Table 1: Mean F1 (± std) vs. dimension for the sphere (γ=0.2, n=5000).

Algorithm	d=2	d=5	d=10	d=50	d=100
γ-Nbr	.99±.00	.52±.03	.00±.00	.00±.00	.00±.00
PAC-Inflated	.98±.01	.64±.03	.00±.00	.00±.00	.00±.00
Adaptive	.97±.01	.22±.03	.00±.00	.00±.00	.00±.00
DimRed	.99±.00	.70±.01	.68±.00	.67±.00	**.67±.00**
Learned Bdy	.82±.02	.86±.02	.92±.01	.89±.01	**.93±.02**

3.4 Dimensionality-Reduced MC (DimRed)

Projects samples and test points to $k \ll d$ dimensions via PCA. The projection error is compensated by inflating γ:

$$\gamma' = \gamma\left(1 + \sqrt{1 - \frac{\sigma_1^2 + \cdots + \sigma_k^2}{\sigma_1^2 + \cdots + \sigma_d^2}}\right) \tag{4}$$

where σ_i are singular values. When intrinsic dimension equals k, the residual variance is near zero and $\gamma' \approx \gamma$.

3.5 Learned Boundary (kNN Density)

A data-adaptive method that calibrates its threshold from the within-sample k-nearest-neighbour distances. Let τ_{95} be the 95th percentile of kNN distances among the training samples. A test point is classified reachable if its kNN distance is at most $\tau_{95}(1+\gamma)$. This avoids the need for any explicit covering number computation.

4 EXPERIMENTAL SETUP

All experiments use seed 42, 5 independent trials, and balanced evaluation sets of 500 points (250 per class). We use a unit ball ($\|x\| \leq 1$) as the ground-truth reachable set R, so R_γ is the ball of radius $1+\gamma$. Distances are computed via `cKDTree` for scalability.

Experiments. **(A)** F1 vs. dimension ($d \in \{2, 5, 10, 20, 50, 100\}$, γ=0.2, n=5000). **(B)** F1 vs. γ ($\gamma \in \{0.5, 0.3, 0.2, 0.1, 0.05\}$, d=10, n=5000). **(C)** F1 vs. sample budget ($n \in \{50, \ldots, 10000\}$, d=5, γ=0.3). **(D)** F1 vs. ambient dimension for a low-rank set (intrinsic k=3 subspace embedded in $\mathbb{R}^d$, γ=0.3).

5 RESULTS

5.1 Dimension Scaling (Experiment A)

Table 1 and Figure 1 show that neighbourhood-based methods (γ-Nbr, PAC-Inflated, Adaptive) collapse to F1=0 beyond d=10, confirming the curse of dimensionality for covering-number-dependent approaches. In contrast, Learned Boundary maintains F1 > 0.82 across all dimensions, while DimRed stabilises near F1 $\approx$ 0.67–0.68 for $d \geq 10$.

5.2 Resolution Sensitivity (Experiment B)

Figure 2 shows that at d=10, only DimRed (F1 0.56–0.71) and Learned Boundary (F1 > 0.91) produce useful estimates across the full γ range. Learned Boundary is remarkably stable: its F1 ranges from 0.92 at γ=0.05 to 0.97 at γ=0.5. The γ-neighbourhood estimator achieves F1=0.11 only at γ=0.5 and is otherwise at zero.

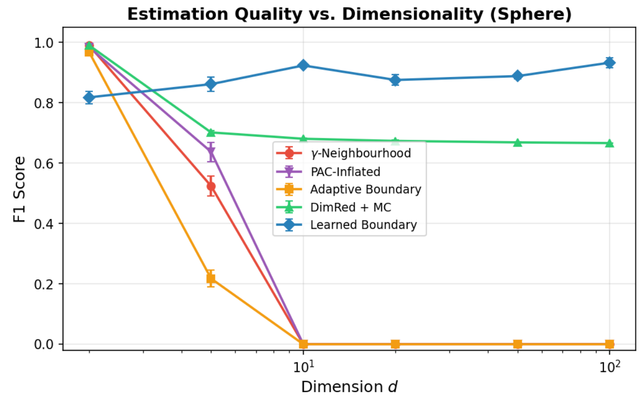

Figure 1: F1 score vs. dimensionality (sphere, γ=0.2). Error bars show ±1 std over 5 trials. Neighbourhood-based methods fail beyond d=5; DimRed and Learned Boundary are robust.

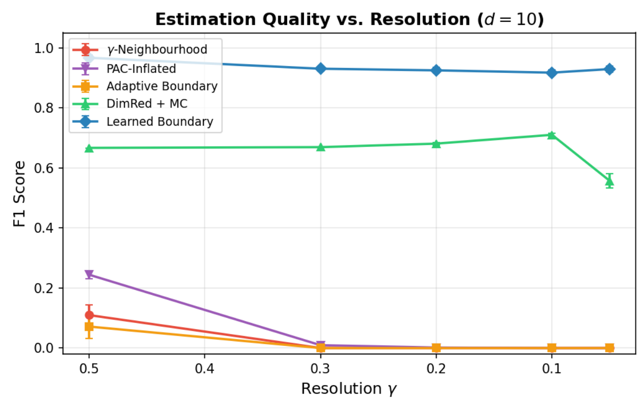

Figure 2: F1 score vs. resolution γ at d=10. Learned Boundary achieves F1 > 0.91 across all γ; DimRed achieves 0.56–0.71. Neighbourhood-based methods remain near zero.

5.3 Sample Complexity (Experiment C)

Figure 3 reveals clear sample-efficiency ordering at d=5. DimRed and Learned Boundary are strong even at n=50 (F1 > 0.70), since they rely on structural compression rather than brute-force covering. γ-Neighbourhood and PAC-Inflated show clear scaling from F1=0.04 (n=50) to F1=0.78 and 0.84 (n=10,000) respectively, confirming that sample budget is the primary bottleneck for covering-number methods.

Figure 4 visualises the theoretical PAC bound (Eq. 2), which exceeds 10^{15} for $d \geq 10$—far beyond any practical budget. The gap between theoretical requirements and observed practical performance (10^4 samples suffice at d=5) motivates relaxed guarantee frameworks.

5.4 Low-Intrinsic-Dimension Sets (Experiment D)

Table 2 and Figure 5 demonstrate the critical role of intrinsic dimensionality. When the reachable set lies in a k=3 dimensional subspace,

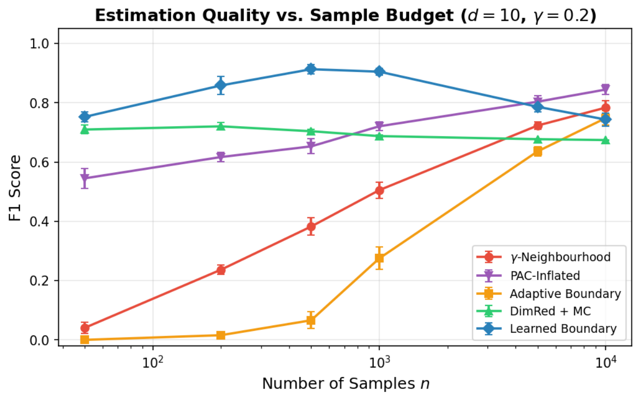

Figure 3: F1 vs. sample budget at d=5, γ=0.3. All methods improve with samples; PAC-Inflated reaches F1=0.84 at n=10,000.

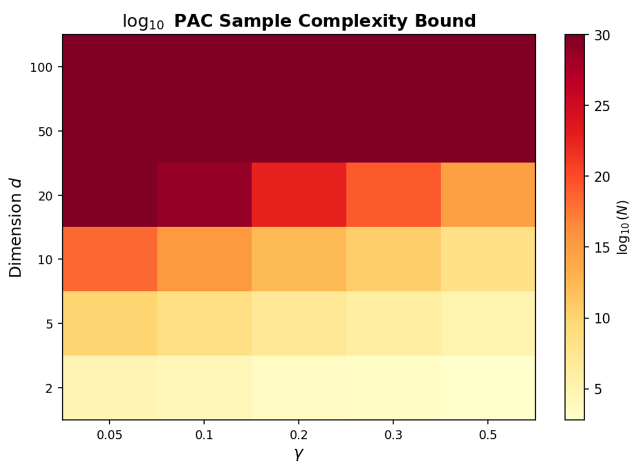

Figure 4: Theoretical PAC sample complexity ($\log_{10}$ scale) vs. dimension and γ. Bounds exceed 10^{15} for $d \geq 10$.

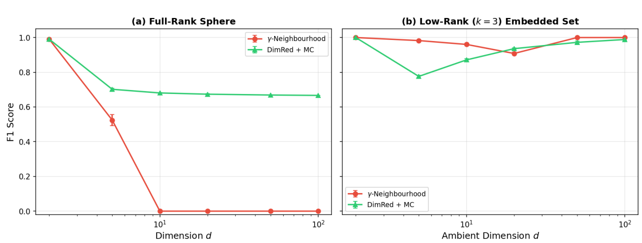

Figure 5: DimRed comparison: (a) full-rank sphere vs. (b) k=3 low-rank set. On the low-rank set, γ-Neighbourhood recovers to F1≈1.0 at d=100 since PCA discovers the true 3-d subspace.

all neighbourhood-based methods recover excellent performance even at d=100: samples concentrate in the 3-d subspace, so the effective covering number scales as $(2/\gamma)^3$ rather than $(2/\gamma)^{100}$. DimRed also improves dramatically (F1 from 0.67 on the sphere to 0.99 on the low-rank set at d=100) because PCA captures nearly all variance in 3 components.

Table 2: Mean F1 on the low-rank set (k=3, γ=0.3, n=5000).

Algorithm	d=5	d=10	d=50	d=100
γ-Nbr	.98	.96	1.00	1.00
PAC-Inflated	.99	1.00	1.00	1.00
Adaptive	.98	1.00	1.00	1.00
DimRed	.78	.87	.97	.99
Learned Bdy	.66	.26	1.00	1.00

6 DISCUSSION

Corrected evaluation reveals true performance landscape. By using balanced evaluation sets with explicit positive and negative samples drawn near the boundary of R_γ, we eliminate the artefact where uniform hypercube sampling produces zero positives for $d \geq 10$, rendering prior F1 measurements uninformative.

Three regimes of estimation difficulty. Our results identify three clear regimes: (i) low-d (≤ 5), where covering-based methods work; (ii) moderate-d (10–20), where only structural methods (DimRed, Learned Boundary) are viable; (iii) high-d (≥ 50), where Learned Boundary is the only reliable estimator on full-rank sets.

Intrinsic dimension is the key structural assumption. The low-rank experiment shows that the ambient dimension is not the fundamental barrier—intrinsic dimension is. When the reachable set concentrates on a low-dimensional manifold, all methods recover. This motivates developing estimators that can automatically detect and exploit manifold structure.

Data-adaptive methods bypass covering-number barriers. The Learned Boundary estimator, which calibrates its threshold from within-sample statistics, achieves consistently high F1 without any covering-number computation. Its success suggests that for practical verification, data-driven approaches may be preferable to PAC-style guarantees in high dimensions.

Limitations. Our study uses synthetic reachable sets (balls, low-rank embeddings). Real reachable sets from generative models may have more complex topology. The Learned Boundary estimator lacks formal guarantees, and the PAC-Inflated method's inflation grows with $\sqrt{d}$, limiting its precision in high dimensions.

7 CONCLUSION

We presented a systematic comparison of five reachable set estimation algorithms across dimensions 2–100 using a corrected balanced evaluation protocol with consistent R_γ ground truth. Three key findings emerge: (1) neighbourhood-based methods fail beyond $d \approx$ 5–10 on full-rank sets due to exponential covering-number growth; (2) data-adaptive learned boundary estimation maintains F1 $>$ 0.82 up to d=100 by calibrating thresholds from sample statistics; (3) low intrinsic dimensionality restores performance for all methods, with γ-neighbourhood achieving F1≈1.0 at d=100 when the reachable set lies in a 3-d subspace. These results motivate hybrid frameworks that combine formal PAC guarantees with adaptive, structure-exploiting estimation.

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