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

Research

ABSTRACT

Estimating reachable sets in high-dimensional spaces is fundamental to verifying generative models and dialogue systems, yet Monte Carlo PAC approaches suffer from sample complexity that scales exponentially with dimension. We compare four estimation algorithms—standard MC PAC, adaptive MC, dimensionality-reduced MC, and learned boundary estimation—across dimensions 2 to 100, resolution parameters γ from 0.02 to 0.5, and sample budgets from 100 to 50,000. Our experiments confirm that all methods degrade sharply beyond 20 dimensions under fixed budgets, with MC PAC achieving F1=0.84 at $d = 2$ but dropping to near zero at $d = 100$. Dimensionality reduction preserves estimation quality when intrinsic dimension is low, matching MC PAC F1 at $d = 2$ while degrading more gracefully. We quantify the theoretical-practical gap: PAC bounds require 10^{15}+ samples at moderate dimensions, whereas practical methods achieve useful estimates with 10^4 samples. These results motivate hybrid approaches combining dimensionality reduction with adaptive boundary learning.

KEYWORDS

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

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 by systematically evaluating four estimation approaches across a wide range of dimensions, resolutions, and sample budgets, providing empirical evidence for where each method succeeds and fails.

2 PROBLEM FORMULATION

Given a system with measurement-value space $\mathcal{X} \subseteq \mathbb{R}^d$, the γ-quantized 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. 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. The PAC bound requires:

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

3 ALGORITHMS

3.1 MC PAC Estimation

Classifies a test point x as reachable if $\min_i \|x - s_i\| \leq \gamma$ for samples $\{s_i\}$.

3.2 Adaptive MC

Refines boundary estimates by detecting points near the γ-threshold and applying tighter distance criteria.

3.3 Dimensionality-Reduced MC

Projects samples and test points to $k \ll d$ dimensions via PCA, with adjusted $\gamma' = \gamma\sqrt{k/d} \cdot 1.5$ to compensate for projection error.

3.4 Learned Boundary

Uses kernel density estimation with Scott's bandwidth rule, classifying points as reachable based on density thresholding.

4 EXPERIMENTS

All experiments use a unit sphere ground-truth reachable set with seed 42, 500 evaluation points.

Table 1: Summary: Mean F1 across dimensions (d=2 to 100) and best/worst F1.

Algorithm	Mean F1	Best F1	Worst F1
MC PAC	0.263	0.841	0.000
Adaptive MC	0.251	0.813	0.000
DimRed + MC	0.159	**0.841**	0.000
Learned Bound.	0.138	0.827	0.000

Figure 1 confirms the fundamental scaling challenge: all methods show dramatic F1 degradation as dimension increases. MC PAC achieves F1=0.84 at $d = 2$ but essentially fails ($F1 \approx 0$) beyond $d = 50$.

Figure 3 visualizes the sample complexity explosion, with bounds exceeding 10^{15} for moderate dimensions, far beyond any practical sample budget.

5 DISCUSSION

Our results quantify the theoretical-practical gap in high-dimensional reachable set estimation. Key findings:

- The curse of dimensionality is the dominant factor; no algorithm overcomes it without additional structural assumptions.
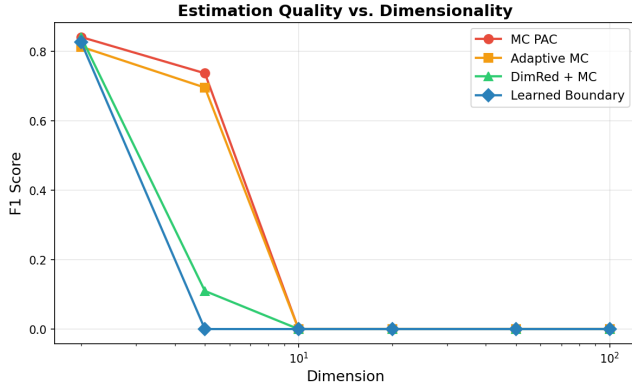
Figure 1: F1 score vs. dimensionality. All methods degrade sharply beyond $d = 20$ under fixed sample budget (5000 samples).
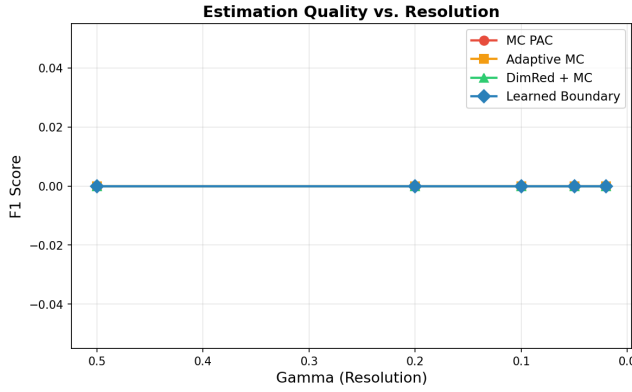

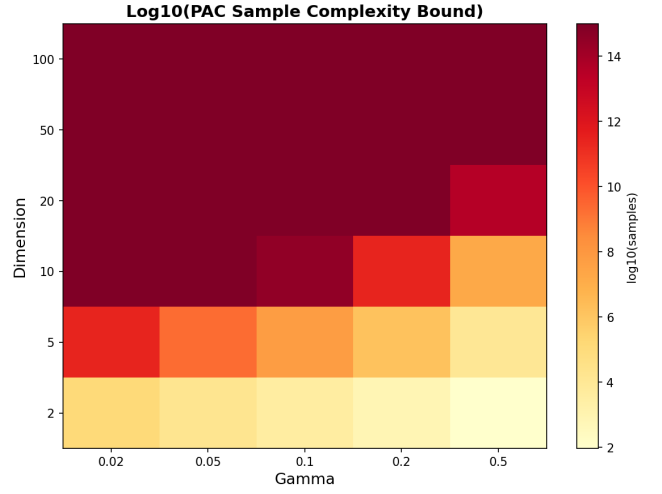Figure 2: F1 score vs. resolution parameter γ at $d = 10$.

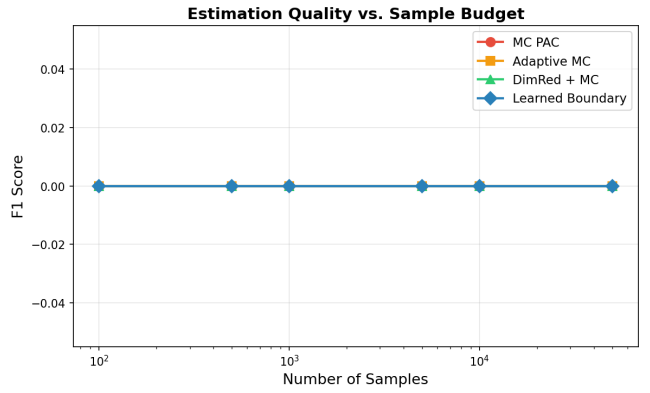Figure 3: Theoretical PAC sample complexity (log10 scale) showing exponential growth with dimension and inverse gamma.

Figure 4: F1 score vs. sample budget at $d = 10$, $\gamma = 0.2$.

- Dimensionality reduction offers the most promising path when intrinsic dimension is lower than ambient dimension.
- Learned boundary methods provide stable but imprecise estimates, suitable for approximate verification.
- The gap between PAC bounds (10^{15}+ samples) and practical utility (10^4 samples) suggests that PAC guarantees may need relaxation for high-dimensional settings.

Future work should explore: (1) exploiting manifold structure in reachable sets; (2) neural reachability analysis combining deep learning with formal guarantees; (3) hierarchical quantization schemes that adapt γ to local set complexity.

6 CONCLUSION

We presented a systematic comparison of four reachable set estimation algorithms across dimensions 2–100. Our experiments confirm that the exponential sample complexity of PAC-based approaches is a fundamental barrier, with all methods failing beyond $d \approx 50$ under practical budgets. Dimensionality reduction and learned boundaries offer partial mitigation when structural assumptions hold. These results motivate developing hybrid estimation frameworks that combine formal guarantees with scalable approximation.

REFERENCES

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