



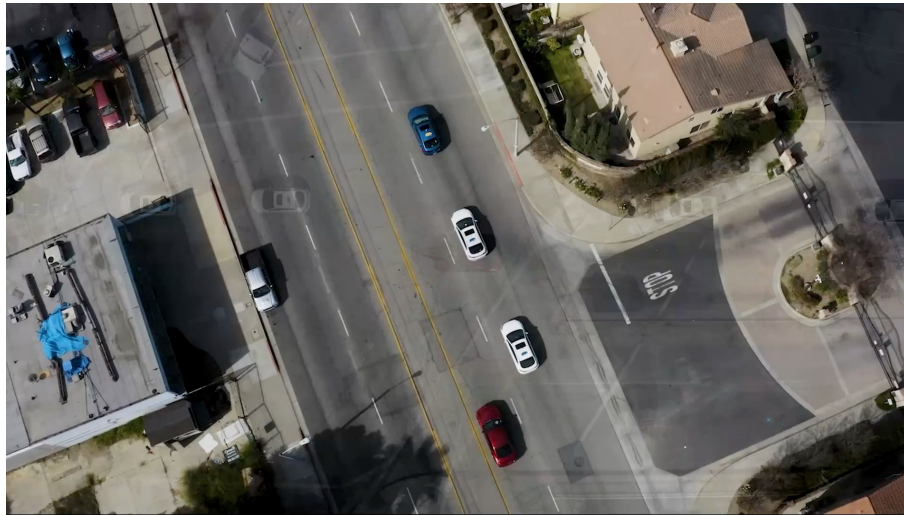
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Scalable Safe Set Methods for Control and Verification with Learning

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Overview

Reachable and invariant sets are critical for formal verification of safety and other requirements in autonomous systems.



Problem: Standard methods for estimating these sets do not scale to large system models.

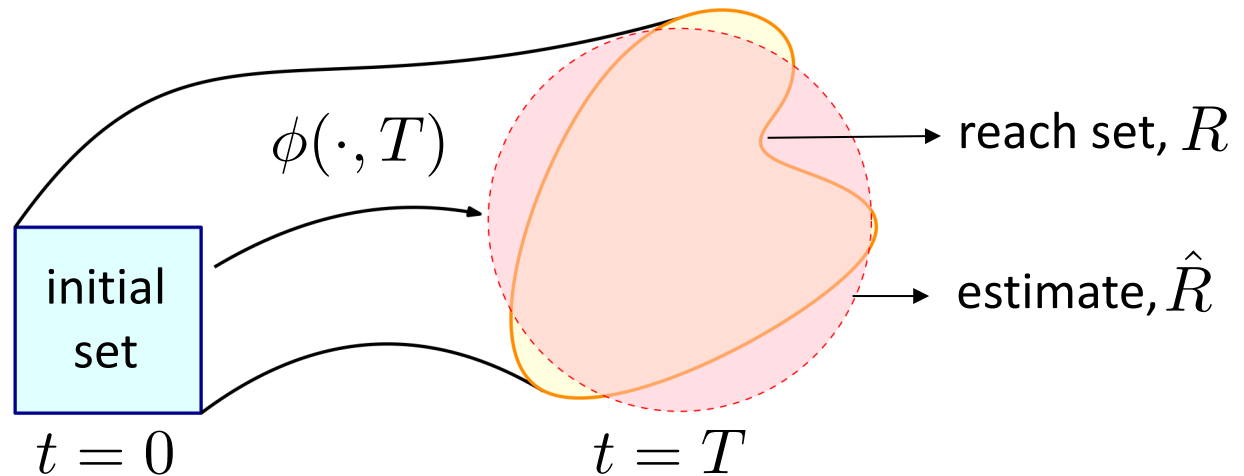
Approach in this talk: Use sample trajectories and *generalize* to unsampled ones using statistical learning.

Outline

1. Forward reachability with scenario optimization
2. Forward reachability with Christoffel functions
3. Probabilistic invariance for Gaussian Process (GP) state-space models

1. Forward Reachability with Scenario Optimization

Goal: Develop a data-driven reachability method that samples trajectories and provides a probabilistic containment guarantee.



Given a probability distribution on the initial set, the solution map induces a probability measure for the exact reachable set.

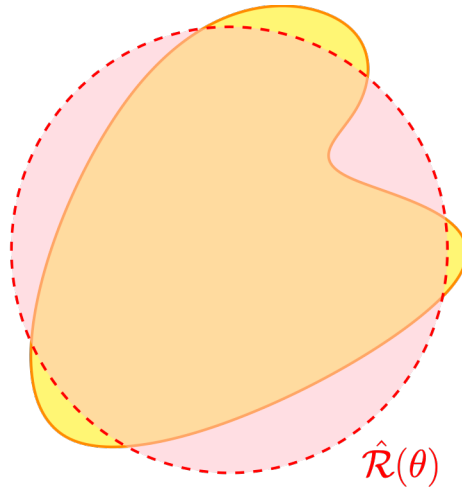
Find the smallest set from a parameterized family $\hat{R}(\theta)$ that contains $1 - \epsilon$ of the reachable set under this measure.

1. Forward Reachability with Scenario Optimization

Chance-
constrained
optimization
problem

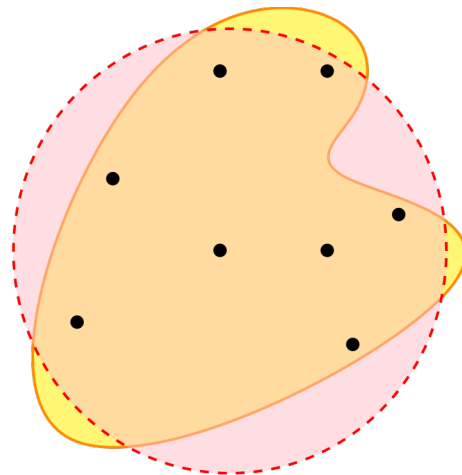


Approximate
solution by
scenario
optimization



Minimize $\text{Vol}(\text{circle})$
 θ

subject to $P(\text{orange region}) \geq 1 - \epsilon$



Minimize $\text{Vol}(\text{circle})$
 θ

subject to $\text{dots} \in \text{circle}$

1. Forward Reachability with Scenario Optimization

Given a parameterized class of approximating sets:

$$\hat{R}(\theta) = \{x : g(x, \theta) \leq 0\}, \quad \theta \in \mathbb{R}^{n_\theta}$$

and a volume proxy $\text{Vol}(\theta)$.

Scenario Optimization:

$$\begin{aligned} \min_{\theta} \quad & \text{Vol}(\theta) \\ \text{s.t.} \quad & g(d_i, \theta) \leq 0, \quad i = 1, \dots, N \end{aligned}$$

where $d_i = \phi(x_i, T)$ are successors of N iid samples $\{x_i\}_{i=1}^N$ from the given probability distribution on the initial set.

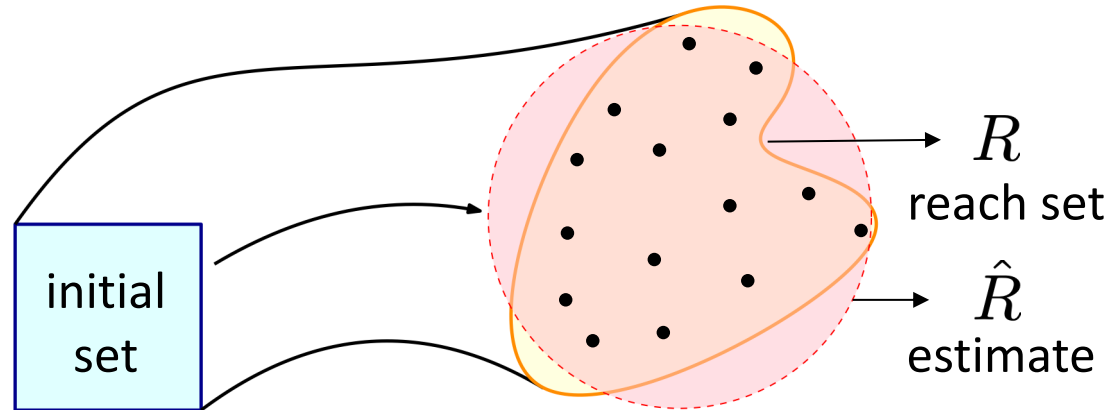
Note: convex problem if $\text{Vol}(\cdot)$ and $g(x, \cdot)$ are convex

Example: $g(A, b, x) = \|Ax - b\| - 1, \quad \theta = (A, b), \quad A \succ 0$

(norm ball) $\text{Vol}(\theta) = -\log \det A$

1. Forward Reachability with Scenario Optimization

How many samples do we need for $\hat{R}$ to cover $1 - \epsilon$ of R ?



Thm: Assume $g(x, \cdot)$ convex. Given $\delta \in (0, 1)$ we can state with $1 - \delta$ confidence that $\hat{R}$ contains measure $1 - \epsilon$ of reach set R if:

$$N \geq \frac{1}{\epsilon} \frac{e}{1 - e} \left(\log \frac{1}{\delta} + n_{\theta} \right)$$

More precisely, the sample bound above guarantees:

$$P_R^N(\{d_1, \dots, d_N\} : P_R(\hat{R}(d_1, \dots, d_N)) \geq 1 - \epsilon) \geq 1 - \delta$$

1. Forward Reachability with Scenario Optimization

Next task: eliminate the convexity requirement so we can generate complex shapes with few parameters, e.g. using RBFs:

$$g(x, \underbrace{\mu, \sigma, \gamma}_{\theta}) = \sum_{n=1}^N e^{-\frac{1}{2}(x-\mu_n)^2/\sigma_n^2} - \gamma$$
$$\text{Vol}(\theta) = \sum_{n=1}^N \sigma_n^2$$

Drawback: Number of samples can't be determined a priori. Samples collected in batches until accuracy passes threshold.

Approach 1: Wait-and-judge scenario optimization

- + Major reduction in sample complexity
- Requires resolving the optimization for every scenario

Approach 2: Holdout method

- + Improves accuracy and reduces computation dramatically
- Requires test set, adding to sample complexity

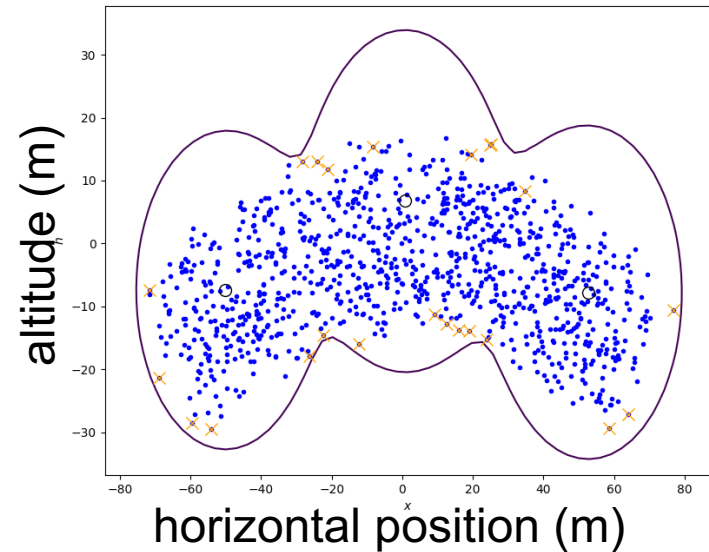
1. Forward Reachability with Scenario Optimization

Example: Quadrotor

$$\ddot{x} = u_1 K \sin(\theta),$$

$$\ddot{h} = -g + u_1 K \cos(\theta),$$

$$\ddot{\theta} = -d_0 \theta - d_1 \dot{\theta} + n_0 u_2$$



Holdout Method:	Training (N)	Testing (M)	$\text{Vol}(\hat{R}(\theta))$	ϵ
	$N = 10$	$M = 2990$	11.50	0.765
	$N = 50$	$M = 2950$	22.97	0.280
	$N = 100$	$M = 2900$	24.29	0.120
	$N = 1000$	$M = 2000$	27.74	0.019
	$N = 1500$	$M = 1500$	27.19	0.026
	$N = 2000$	$M = 1000$	27.85	0.031
	$N = 2900$	$M = 100$	27.81	0.187
	$N = 2950$	$M = 50$	27.30	0.384
	$N = 2990$	$M = 10$	28.27	0.874
Wait and Judge:	$N = 3000$		27.80	0.051

Runtimes:

Holdout:

~40 sec

Wait and judge:

~ 5.5 hr

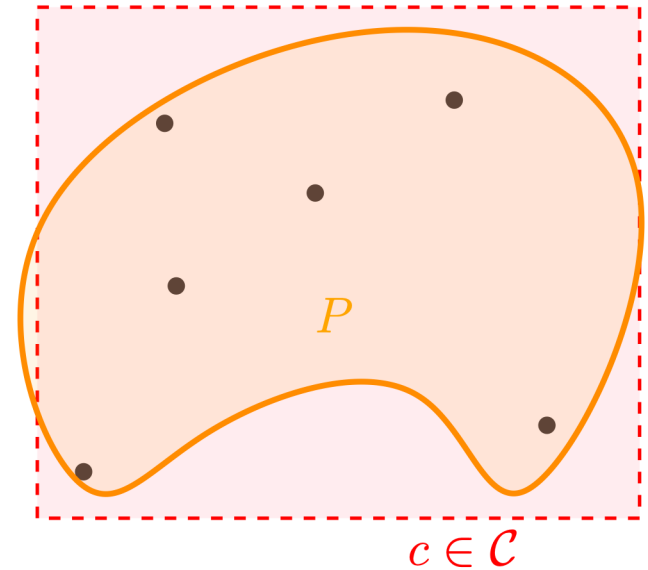
2. Forward Reachability with Christoffel Functions

Empirical Risk Minimization setup:

- i.i.d. samples $d_1, \dots, d_N \sim P$
- a class of sets $C \subseteq 2^{\mathcal{X}}$
- loss function $\ell : \mathcal{X} \times C \rightarrow \{0, 1\}$
- risk $r(c) = \mathbb{E}_P[\ell(d, c)], c \in C$

and empirical risk:

$$\hat{r}(c) = \frac{1}{N} \sum_{i=1}^d \ell(d_i, c)$$



$$\begin{aligned} \ell(\bullet, \boxed{}) &= \mathbb{1}\{\bullet \notin \boxed{}\} \\ r(\boxed{}) &= 1 - P(\boxed{}) \end{aligned}$$

- For reachability, C : class of reach set estimates,
 $\ell(d, c)$: indicator function that returns 1 when $d \notin c$
 $r(c)$: probability that a new sample not enclosed in c
Choose c to enclose all d_i so $\hat{r}(c) = 0$

2. Forward Reachability with Christoffel Functions

If the class $\mathcal{C}$ has finite Vapnik-Chervonenkis (VC) dimension, we can derive a bound for $r(c)$ that decreases with N .

Theorem (adapted from Alamo et al. 2009):

If VC dimension $\leq m$ and

$$N \geq \frac{5}{\epsilon} \left(\log \frac{4}{\delta} + m \log \frac{40}{\epsilon} \right)$$

then, with confidence $1 - \delta$, we can say that the estimate c contains measure $1 - \epsilon$ of the actual reach set.

Lemma: For an m -dimensional vector space $\mathbb{V}$ of functions $g : \mathbb{R}^n \rightarrow \mathbb{R}$, the class of sublevel sets of g has VC dimension m .

2. Forward Reachability with Christoffel Functions

The empirical inverse **Christoffel function** of order k is the degree $2k$ polynomial

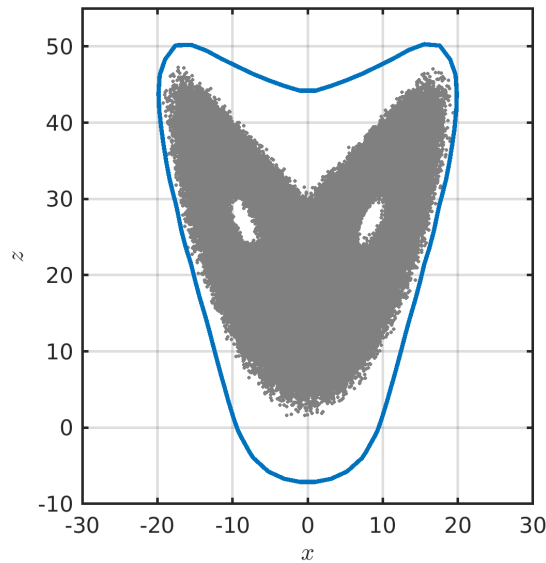
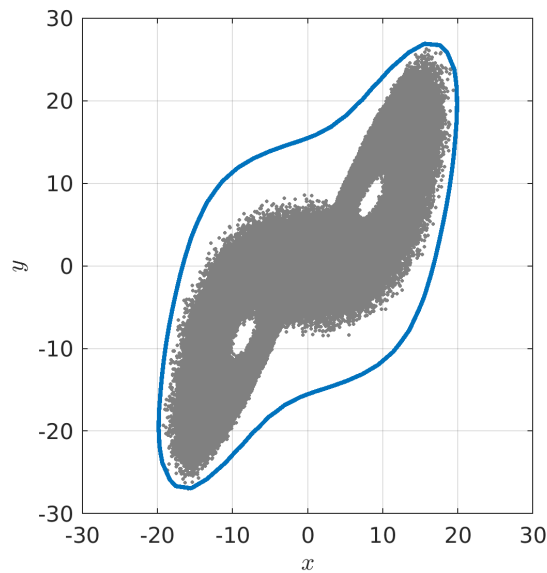
$$C_k(x) = \underbrace{z_k(x)^\top}_{\text{vector of monomials}} \underbrace{\left(\frac{1}{N} \sum_{i=1}^N z_k(d_i) z_k(d_i)^\top \right)^{-1}}_{\text{empirical moment matrix}} z_k(x).$$

Use sublevel set, with $\text{level} = \max_i C_k(d_i)$ as reach set estimate.
VC dimension $m \leq \binom{n_x + 2k}{n_x}$ so theorem above is applicable.

Why Christoffel functions?

- sublevel sets known for support-approximating quality in ML
- can morph into complex shapes (e.g., holes or disconnected)

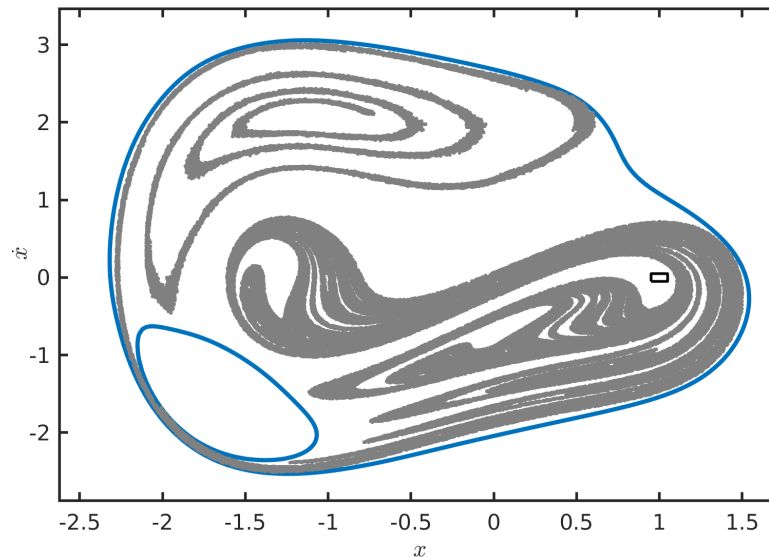
2. Forward Reachability with Christoffel Functions



Lorenz oscillator

$$n_x = 3, k = 5$$

$$N = 193,391$$



Duffing oscillator

$$n_x = 2, k = 10$$

$$N = 156,626$$

$$(\epsilon = 0.05, \delta = 10^{-9})$$

3. Probabilistic Invariance for GP State-Space Models

Gaussian Process (GP): Collection of random variables $\mathbf{f}(x)$ indexed by x , where any finite subset is jointly Gaussian.

Mean: $m(x) = \mathbb{E}[\mathbf{f}(x)]$

Covariance: $k(x, x') = \mathbb{E}[(\mathbf{f}(x) - m(x))(\mathbf{f}(x') - m(x'))]$

Covariance called stationary if it depends only on $|x - x'|$
e.g., $k(x, x') = \exp(-|x - x'|^2/2)$

For any collection $\{x_1, \dots, x_n\}$:

$$\begin{bmatrix} \mathbf{f}(x_1) \\ \vdots \\ \mathbf{f}(x_n) \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} m(x_1) \\ \vdots \\ m(x_n) \end{bmatrix}, \begin{bmatrix} k(x_1, x_1) & \cdots & k(x_1, x_n) \\ \vdots & \ddots & \vdots \\ k(x_n, x_1) & \cdots & k(x_n, x_n) \end{bmatrix} \right)$$

3. Probabilistic Invariance for GP State-Space Models

GP State-Space Model:

$$x_{k+1} = Ax_k + Bu_k + g(x_k, u_k) + w_k, \quad x_k \in \mathbb{R}^n$$

$$g_i \sim \text{GP}(0, k_i) \text{ with stationary } k_i$$

$$w_k \sim \mathcal{N}(0, Q)$$

Conditioning on data $\mathcal{D} = \{(\bar{x}_j, \bar{u}_j), \bar{x}_j^+\}_{j=1}^N$ yields posterior:

$$g(x_k, u_k) | \{x_k, u_k, \mathcal{D}\} \sim \mathcal{N}(\mu(x_k, u_k), \Sigma(x_k, u_k))$$

where μ, Σ depend on $\mathcal{D}, \{k_i\}_{i=1}^n$.

Using stationarity we can find bounds:

$$\|\mu(x, u)\| \leq \bar{\mu} \quad \forall x, u$$

$$\Sigma(x, u) \preceq \bar{\Sigma} \quad \forall x, u$$

3. Probabilistic Invariance for GP State-Space Models

With feedback $u = Lx$ the closed-loop system becomes:

$$x_{k+1} = (A + BL)x_k + d_k + v_k(x_k)$$

$$\mathbb{E}[v_k(x_k)|x_k] = 0, \quad \text{Cov}[v_k(x_k)|x_k] \preceq \bar{\Sigma} + Q$$

$$\|d_k\| \leq \bar{\mu}$$

Given $W \succeq 0$ define ellipsoid $\mathcal{E}(W) = \{W^{1/2}x : \|x\| \leq 1\}$

Theorem (Probabilistic Invariance): If we can find a set $X \subset \mathbb{R}^n$ s.t.

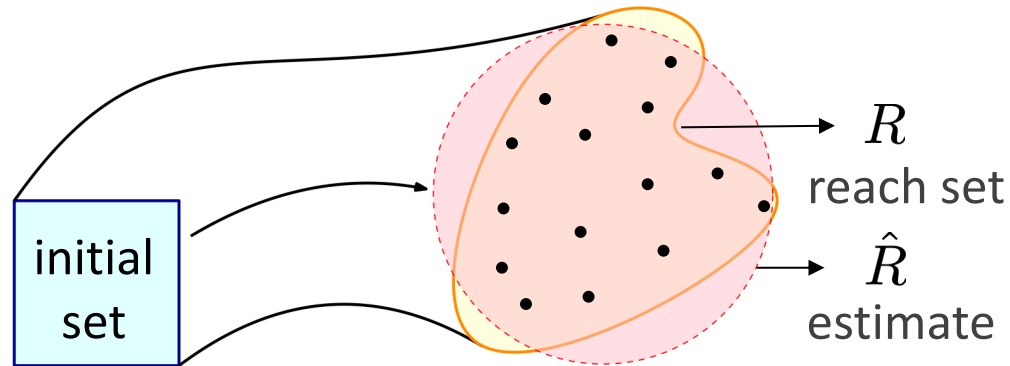
$$(A + BL) X \oplus \mathcal{E}(\bar{\mu}^2 I) \oplus \mathcal{E}\left(\frac{n}{1-p}(\bar{\Sigma} + Q)\right) \subseteq X \quad (\dagger)$$

Then: $x_o \in X \implies \Pr(x_k \in X) \geq p \quad \forall k \geq 1$

We formulate a semidefinite program to search for L and an ellipsoidal X satisfying $(\dagger)$. We then maximize p via bisection.

Conclusions

- Proposed a sampling approach for scalable estimation of reachable and invariant sets.



- To generalize from samples to unsampled trajectories, we used probabilistic structure and regularity of sets.
- Past work emphasized forward reachability. Now exploring backward reachable and controlled invariant sets. Essential for characterizing safe envelopes for autonomous systems.
- Gaussian Processes are promising for blending models and data. Demonstrated their use for probabilistic set invariance.

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