Continuous Reinforcement Learning for Delayed Dynamical Systems

A Path Signature-Based Representation Approach

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Agenda

1. Motivation
2. Theoretical Background
3. Continuous Time Reinforcement Learning Algorithms
4. Experiments
5. Limitations and Future Work

Motivation

Controlling Delayed Differential Equations (DDEs)

Ubiquitous in:

- Chemical engineering
- Population dynamics
- Network control
- ...

	ODE	DDE
Form	$\dot{x} = f(t, x(t))$	$\dot{x} = f(t, x(t), x(t - \tau_1), ..., x(t - \tau_n))$
Example	$\dot{x} = -x(t)$	$\dot{x} = -x(t) + x(t - \tau)$

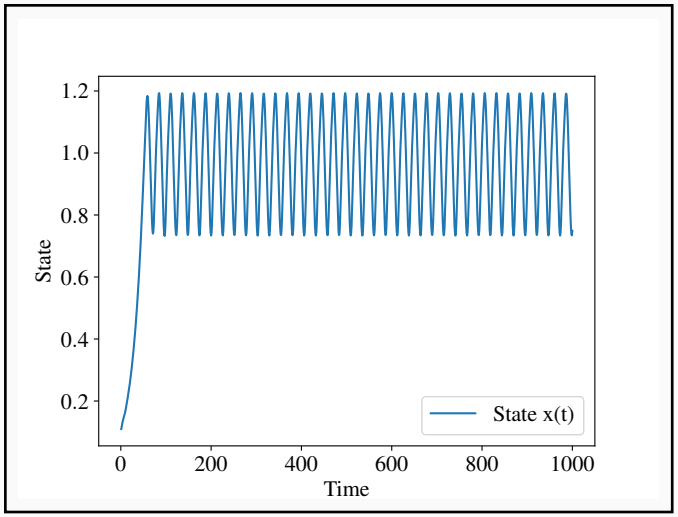
with $n \in \mathbb{N}$, $\tau_1, ..., \tau_n \in \mathbb{R}_+^*$

Problem: Usually no simple closed form solution to a DDE.

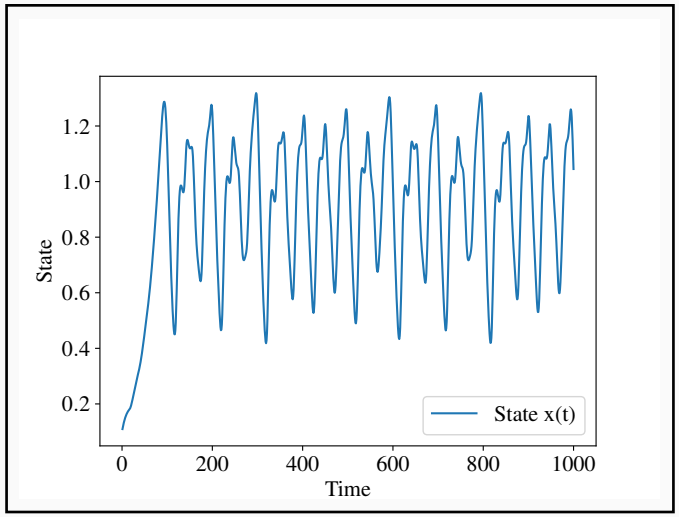
Uniqueness of solution: Up to an initial condition $x_0 : [-\tau_{\max}, 0] \to \mathbb{R}$.

Controlling Delayed Differential Equations (DDEs)

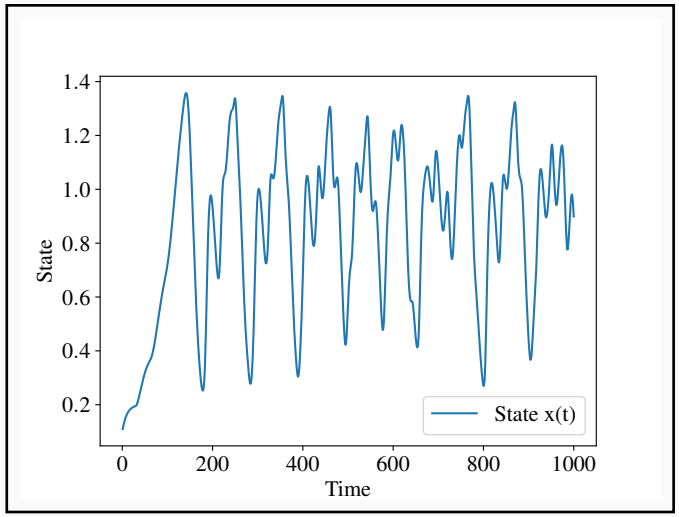
Mackey-Glass equation: $\forall t \in \mathbb{R}, \dot{x}(t) = -\mu x(t) + \frac{p x(t-\tau)}{1+x(t-\tau)^n}$ (n, μ and p fixed here). Used for modelling of healthy or pathological behaviour.



(a) $\tau = 8$



(b) $\tau = 17$



(c) $\tau = 30$

Figure 1: Mackey-Glass system for different delays (uncontrolled)

Controlling Delayed Differential Equations (DDEs)

Why are delayed systems complex to stabilize?

- Current position is not enough $\Rightarrow$ **we need knowledge of the past trajectory**
- RL framed as a Markov Decision Process ($x_{t+1} = f(x_t)$) $\Rightarrow$ **algorithms must be adapted**

Topic of this thesis: Stabilize delayed systems position to minimal energy fixed points (control)

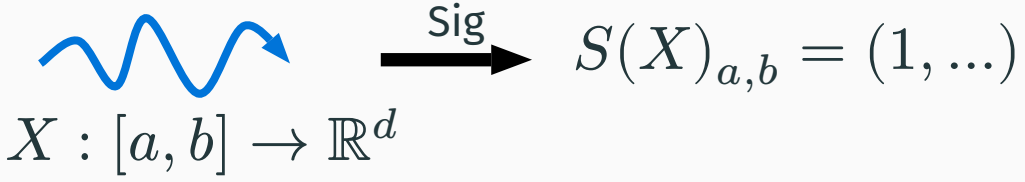
Research questions:

- Can we adapt RL algorithm to Non-Markovian dynamics?
- **How to represent the state?** (here the history function)

Theoretical Background

What is a Path Signature?

The signature of a path encodes its geometrical properties, it is a powerful feature-extractor that has been used in machine learning with promising results[1].



Input: a path $X \implies \mathcal{C}^1$ function from an interval to $\mathbb{R}^d$

Output: Infinite-size tensor with coefficients encoding the geometrical properties of the path

[1] Fermanian et al., "Framing RNN as a Kernel Method"; Kidger et al., "Deep Signature Transforms".

What is a Path Signature?

What are the coefficients?

- Take $(i_1, ..., i_N) \in \{1, ..., d\}^N$
- **Signature coefficient** associated to this tuple:

$$S_{[a,b]}^{(i_1,...,i_N)}(X) = \int_{a<u_1<...<u_n<b} ... \int \dot{X}_{i_1}(u_1)...\dot{X}_{i_N}(u_N)du_1...du_N$$

- Concatenate each coeff for $I \in \{1, ..., d\}^N$, $N \in \mathbb{N}^*$ in lexicographical order
- **Truncated Signature** (compression): stop at $N \leq \text{threshold}$

What is a Path Signature?

A more visual explanation Terms of depth (length of tuple) 1 are simply $S^{(i)}_{[a,b]}(X) = X^{(i)}(b) - X^{(i)}(a)$. Terms of depth 2 are represented in Figure 2[2]

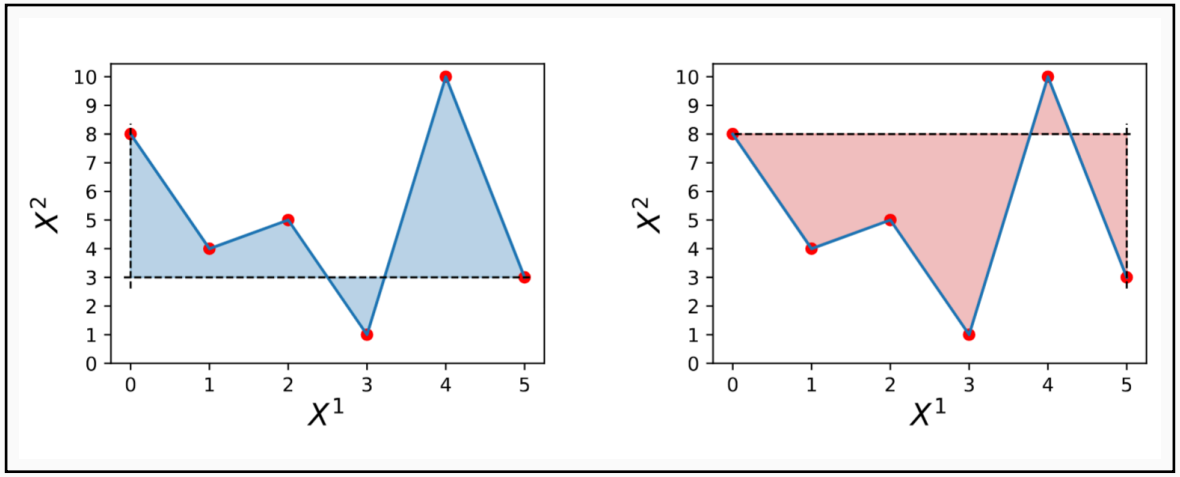


Figure 2: Signature representation for first terms $S^{(1,2)}(X)$ and $S^{(2,1)}(X)$

Deeper terms are harder to represent.

[2] Chevyrev and Kormilitzin, "A Primer on the Signature Method in Machine Learning".

What is a Path Signature?

A useful theorem[3]

For all $X : [a, b] \to \mathbb{R}^d$ $\mathcal{C}^1$ path, let $f : \mathbb{R}^d \to \mathbb{R}$ a continuous function. We define the time-augmented path $\tilde{X}(s) = (X(s), s)$ for $s \in [a, b]$.

For all $\varepsilon > 0$, there exists a linear operator $\mathcal{L}$ such that:

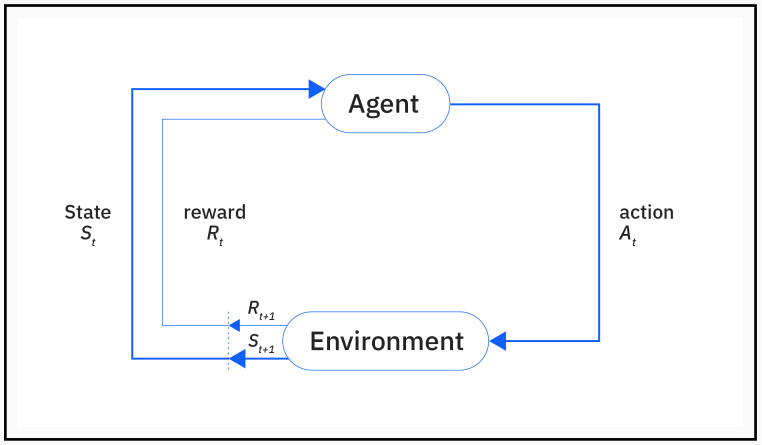
$$\left\| f(\tilde{X}) - \mathcal{L}(S(\tilde{X})) \right\| < \varepsilon$$

A similar theorem exists for truncated signatures[4].

[3] Arribas, "Derivatives Pricing Using Signature Payoffs".

[4] Chevyrev and Kormilitzin, "A Primer on the Signature Method in Machine Learning".

Discrete & Continuous Reinforcement Learning



- The Agent interacts with the environment with actions u
- u depends on x ($u(x)$ for us) $\Rightarrow$ state changes.
- Agent receives a reward $r(x,u) = \lambda_x \|x(t)\|_2^2 + \lambda_u \|u(x(t))\|_2^2$

	Value Function	Bellman equation
Discrete	$V^u(x(t)) = \sum_{i=t}^{\infty} \gamma^i r(x(i), u(x(i)))$	$V^*(x(t)) = \max_{u \in \mathcal{U}} (r(x(t),u) + \gamma V^*(x(t+1))$
Continuous	$V^u(x(t)) = \int_t^{\infty} e^{\frac{t-s}{\gamma}} r(x(s), u(x(s)))ds$	$\max_{u \in \mathcal{U}} \left(r(x(t),u) + \dot{V}^*(x(t)) \right) = -\frac{1}{\gamma} V^*(x(t))$

Continous Time RL $\Rightarrow$ well-suited for physical systems (high-frequency, different discretisation...).

Continuous Reinforcement Learning for Delayed Systems

How does the (Hamilton-Jacobi) Bellman equation translates to delayed systems?

Non-Markovian $\Rightarrow$ state of the system at t is $x_t : s \to x(t+s), s \in [-h, 0]$

HJB for DDEs/FDEs[5]:

$$\forall t, \quad \max_{u \in \mathcal{U}} (r(x_t, u) + L_u V(x_t)) = \frac{1}{\gamma} V(x_t)$$

with $L_u V(x_t) = \lim_{\Delta t \to 0} \frac{V\left(x_{t+\Delta_t}\right) - V(x_t)}{\Delta t}$

Now, how do we **learn** u and V?

[5] Kolmanovskii and Myshkis, Applied Theory of Functional Differential Equations.

Continuous Time Reinforcement Learning Algorithms

Plugging Signatures

How do we compute $V(x_t)$ and $u(x_t)$? $\Longrightarrow$ Signature approximation: $V(x_t) \approx \phi^\top S^N_{[-h,0]}(x_t)$ and $u(x_t) \approx \theta^\top S^N_{[-h,0]}(x_t)$.

Time derivative: $L_u V(x_t) = \phi^\top L_u S(x_t) = \phi^\top \lim_{\Delta t \to 0} \frac{S_{[-h,0]}(x_{t+\Delta t}) - S_{[-h,0]}(x_t)}{\Delta t}$

Can be approximated in two ways:

- $L_u S(x_t) \approx \frac{S_{[-h,0]}(x_{t+\Delta t}) - S_{[-h,0]}(x_t)}{\Delta t} \rightarrow$ compute both signature (not expensive)
- $L_u S(x_t) = S(x_t) \otimes \dot{x}(t) - \dot{x}(t-h) \otimes S(x_t)^{(*)} \rightarrow \dot{x}(t) \approx \frac{x(t+\Delta t) - x(t)}{\Delta t}$

$(*)$The proof for this equality is done using Chen's identity.[6]

[6] Chen, "Iterated Integrals and Exponential Homomorphisms".

Value-Gradient (VG)

Value-Gradient idea: learn the Value function and compute the optimal command using the learned $\hat{V}$.

- Minimize Temporal Difference $\delta(x_t) = r(x_t, u(x_t)) + L_u V(x_t) - \frac{1}{\gamma} V(x_t)$.
- Linear Quadratic Cost $\Rightarrow$ finding u is a simple optimisation problem.

With Signature-based Value function:

$$u^* = \frac{1}{2} R^{-1} g(x_t)^\top \nabla_{x(t)} V(x_t)$$

with $\nabla_{x(t)} V(x_t)$ the derivative of the Value Function at the extremity of the path $x(t)$, $g(x_t)$ the input function

Continuous Actor-Critic

- Actor $\Rightarrow$ control u
- Critic $\Rightarrow$ learn estimated Value Function $\hat{V}$.
- Critic updated with Bellman equation
- Actor updated with TD error (from Critic)

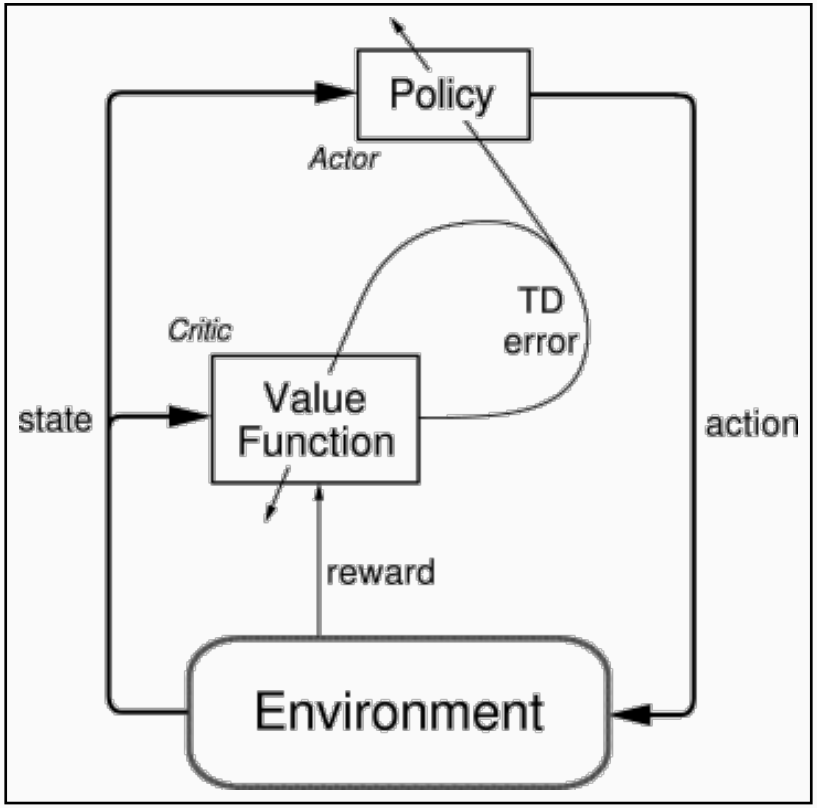


Figure 3: Actor Critic explained, from R. Sutton blog

Continuous Time Actor-Critic, delayed version

How do we adapt the Actor-Critic to Non-Markovian framework?

- Based on K. Doya's Continuous Time RL algorithms.[7]
- Instead of considering $x(t)$ as your state, take $x_t : s \mapsto x(t+s)$ for $s \in [-\tau_{\max}, 0]$ as your system state.
- Value is updated by minimizing the loss $\frac{1}{2}\delta(x_t)^2$ (like Value-Gradient).
- Actor update: $w_a \leftarrow w_a + \frac{n}{\sigma}\frac{\partial u}{\partial w_a} \Rightarrow$ **no noise implies no update**.

[7] Doya, "Reinforcement Learning in Continuous Time and Space".

Implementation

Environment:
- DDE solver compatible with RL
- RK4 scheme with linear interpolation.

Signatures:
- JAX library `signax`
- Full signature is recomputed each step (quick)

Training:
- Whole framework is coded in JAX $\Rightarrow$ compatible with the backpropagation with `signax`.

Experiments

Experimental Setup

3 different systems:

- **Simple 2D linear system:** $\dot{x} = Ax(t) + A_1 x(t-\tau) + Bu \rightarrow$ show developed methods are able to stabilize the systems
- **Mackey-Glass (chaotic 1D system):** $\dot{x} = -\mu x(t) + \frac{px(t-\tau)}{1+x(t-\tau)^n} \rightarrow$ Study behaviour on chaotic system and performance gains
- **Chemical reactor (nonlinear 4D system)**[8] $\rightarrow$ Evaluate performances on real systems & compare with literature

Each system is tested for different seeds and compared to CTAC without signatures.

[8] Dadebo and Luus, "Optimal Control of Time-Delay Systems by Dynamic Programming".

Metrics & Training

How to evaluate performances?

- **Cumulative cost**: $\int_{T_0}^{T_f} r(x,u)dt$. The lower is the better. Cost that plateaus $\Longrightarrow$ rewards going to 0 $\Longrightarrow$ system is stabilized around the origin $\Longrightarrow$ **success**.
- **State Norm** $t \mapsto \|x(t)\|_2$

Training (cluster)

- **2D system**: 1 min/run
- **Mackey-Glass**: 5 min/run to 20 min/run (dep. delay & depth)
- **Chemical Reactor**: 30 min/run

Chemical Reactor study

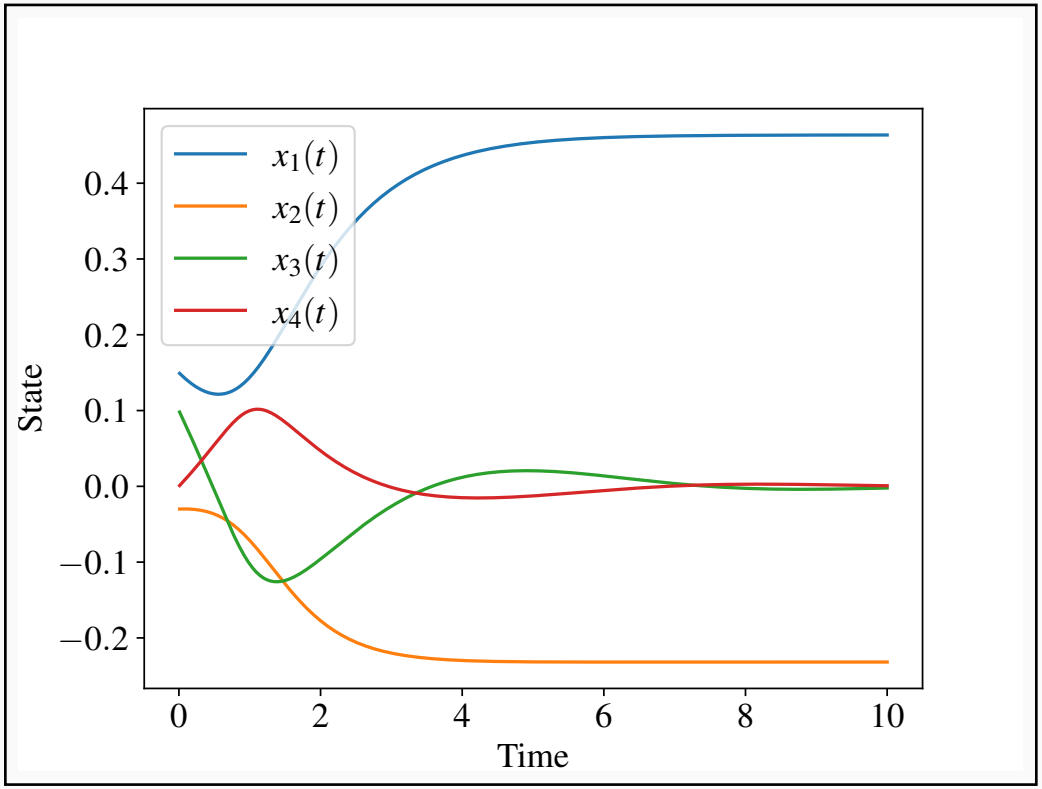


Figure 4: Chemical reactor trajectory

- $$\begin{cases} \dot{x}_1 = 0.5 - x_1(t) - R_1 \\ \dot{x}_2 = -2(x_2(t) + 0.25) - u_1(t)(x_2(t) + 0.25) + R_1 \\ \dot{x}_3 = x_1(t-\tau) - x_3(t) - R_2 + 0.25 \\ \dot{x}_4 = x_2(t-\tau) - 2x_4(t) - u_2(t)(x_4(t) + 0.25) + R_2 - 0.25 \end{cases}$$

$$\begin{cases} R_1 = (x_1(t) + 0.5)\exp\left(\frac{25x_2(t)}{x_2(t)+2}\right) \\ R_2 = (x_3(t) + 0.25)\exp\left(\frac{25x_4(t)}{x_4(t)+2}\right) \end{cases}$$

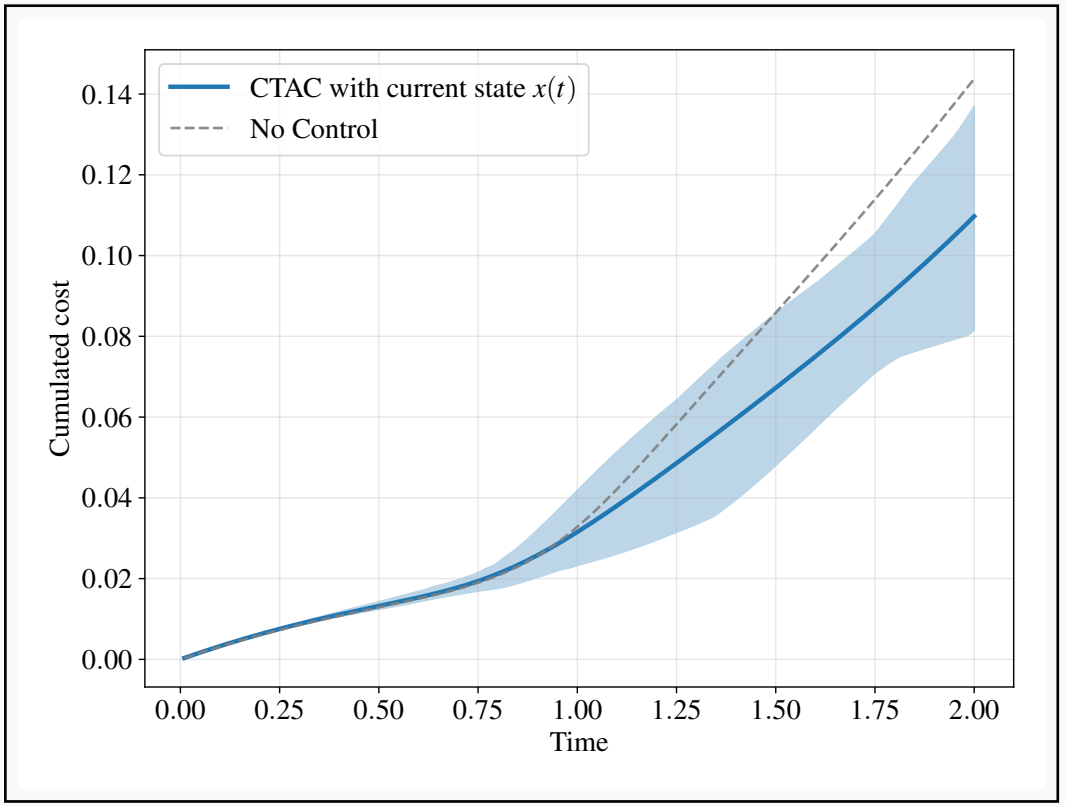
- 4D non linear system
- Optimize: $I = \int_0^2 r(x(t), u(x(t)))dt$
- **Baseline**: Dynamic Programming result $I = 0.024$

Chemical Reactor Instabilities

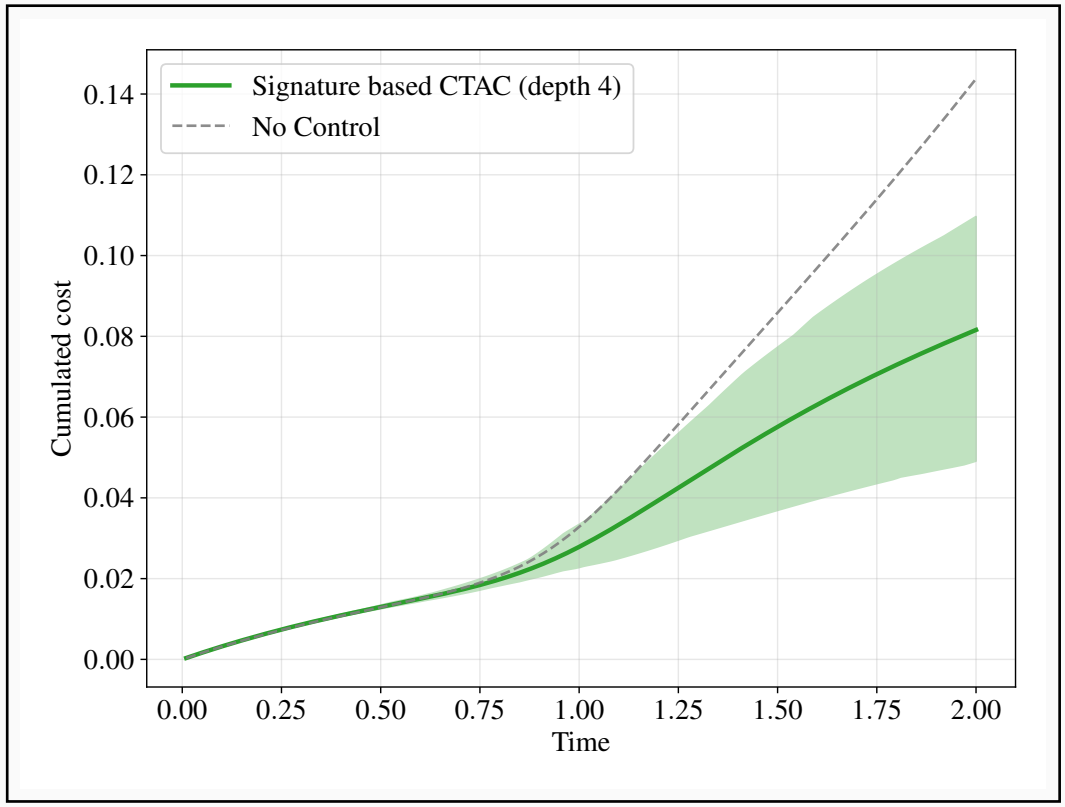
Technique	Bad perf. (%)	NaN (%)	Total rem. (%)	Best perf.	Mean perf. and std
CTAC with aug. position $(x(t), x(t-\tau))$	82.35	**0.00**	82.35	0.059	0.12 ± 0.024
CTAC with current position $x(t)$	54.90	**0.00**	54.90	0.037	0.11 ± 0.024
CTAC sig. depth 2	3.92	**0.00**	3.92	0.032	0.087 ± 0.023
CTAC sig. depth 3	**0.00**	**0.00**	**0.00**	0.036	0.085 ± 0.024
CTAC sig. depth 4	1.96	**0.00**	1.96	0.038	0.082 ± 0.024
VG sig. depth 2	47.06	**0.00**	47.06	0.036	0.11 ± 0.022
VG sig. depth 3	66.67	4.00	70.59	**0.027**	**0.073 ± 0.038**
VG sig. depth 4	52.94	**0.00**	52.94	0.032	0.076 ± 0.033
VG sig. depth 2 with more noise	16.00	**0.00**	16.00	0.030	0.11 ± 0.022
VG sig. depth 3 with more noise	34.00	4.00	38.00	0.031	**0.073 ± 0.038**
VG sig. depth 4 with more noise	40.00	**0.00**	40.00	0.037	0.076 ± 0.033

Table 1: Comparison of techniques on the chemical process: seed removal statistics and performance metrics.

Chemical Reactor results: mean



(a) CTAC with current state



(b) CTAC with signatures (depth 4)

Figure 5: Comparison of mean and quantiles (10-90 %) values for various techniques on the chemical reaction system **conditional on success**

Chemical Reactor results: best shot

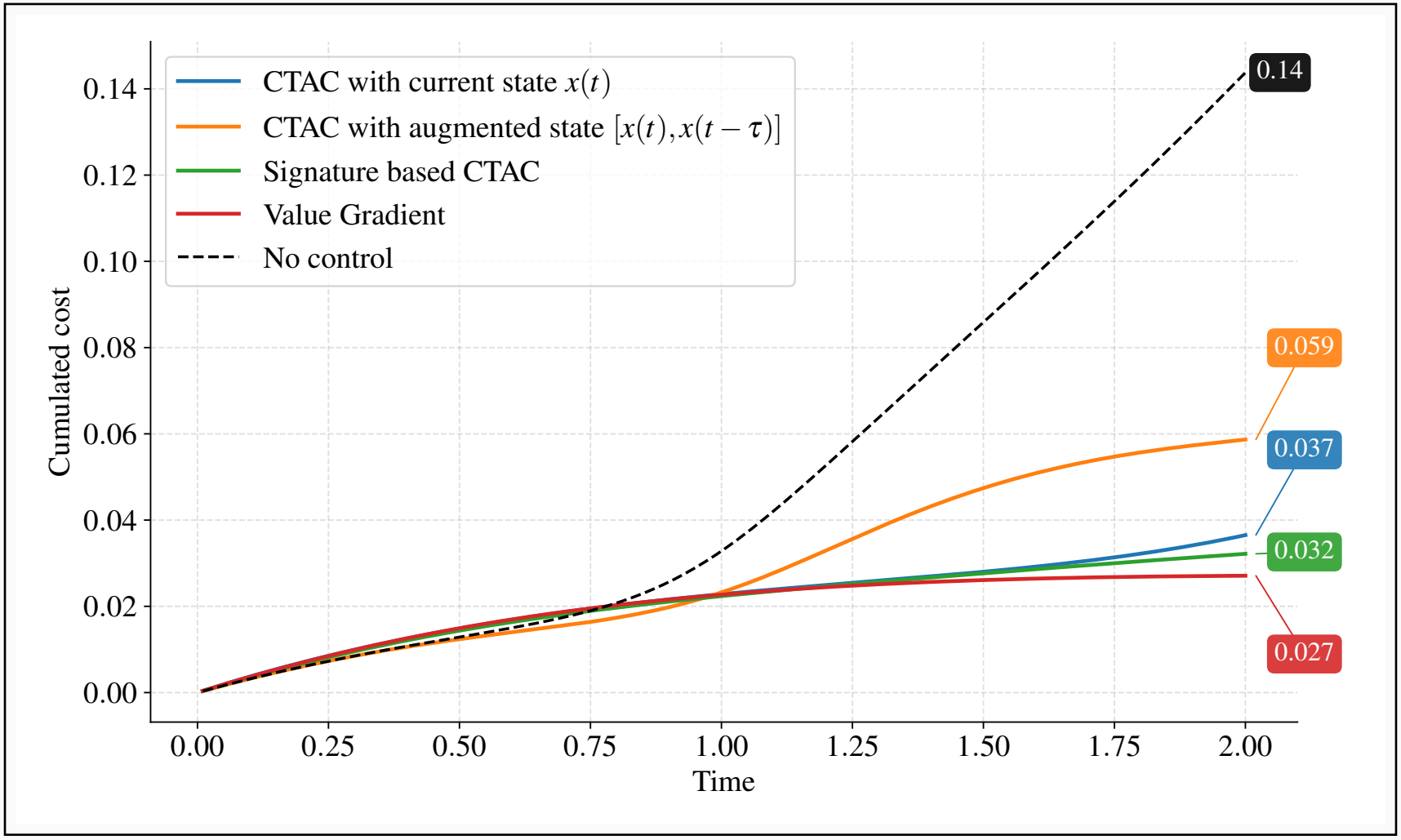


Figure 6: Best cumulative cost for various RL techniques. **Baseline: 0.024**

Limitations and Future Work

What can cause the Instabilities?

- **Curse of dimensionality**: number of signature coefficients grows as d^N, (N the depth, d system dimension). $d = 4, N = 4 \Rightarrow 4096$ coeffs (with time augmentation).
- **CTAC estimation of time derivative**: Finite difference scheme $\Rightarrow$ noisy.
- **VG convergence**: VG gets unstable as the Value Function error converges
- **Lots of Hyperparameters**:
  - lots of different parameters to play with
  - finding the sweet spot is computationally expensive.

Future Work

- **Analyse the algorithms analytically**: convergence bounds, more insights on instabilities...
- **Technical and engineering tricks**: Can we add some machine learning techniques to prevent gradient explosion?
- **Plug more complex networks?**: Current Signature & Machine Learning literature do nor use such simple approximation function: plug a Multi Layer Perceptron?
- **Partially observed systems**: Takens Theorem allows to link partially observed systems to delayed systems $\Longrightarrow$ Use the signatures on PO systems without the struggle of the delayed mechanics.

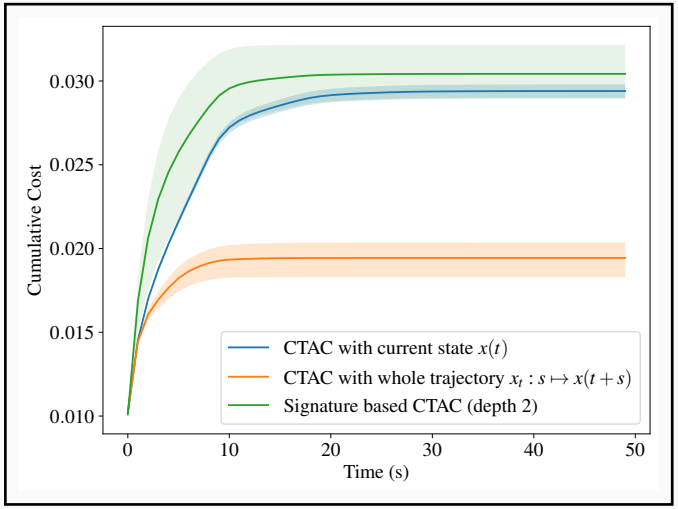
Conclusion

Conclusion

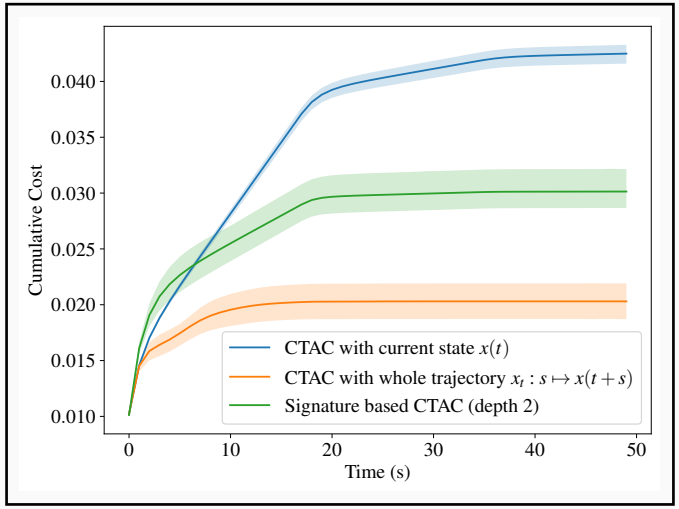
- Two algorithms for Reinforcement Learning for Delayed Systems, promising results on complex systems (chemical reactor)
- Formulation of the problem using Signatures, update rule for both algorithms
- Delayed Systems simulator and Environment to perform RL

Thank you for your attention!

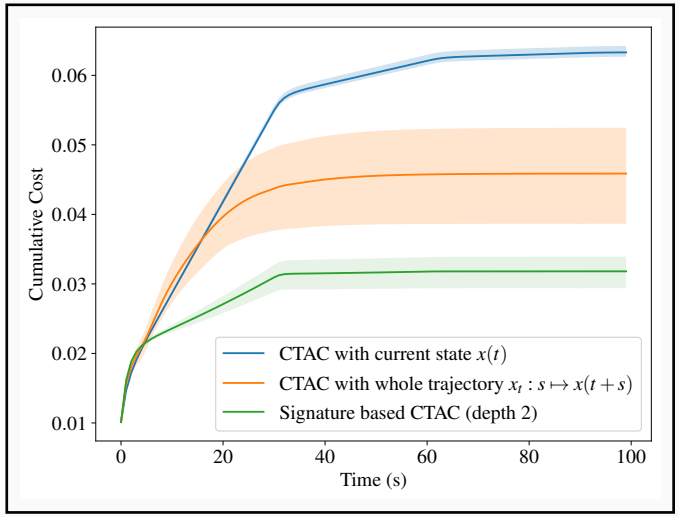
Mackey-Glass analysis



(a) $\tau = 8$



(b) $\tau = 17$



(c) $\tau = 30$

Figure 7: Comparison of cumulative cost (mean and 90% quantiles) on Mackey-Glass system for different control techniques over 10 seeds

More insights on instabilities

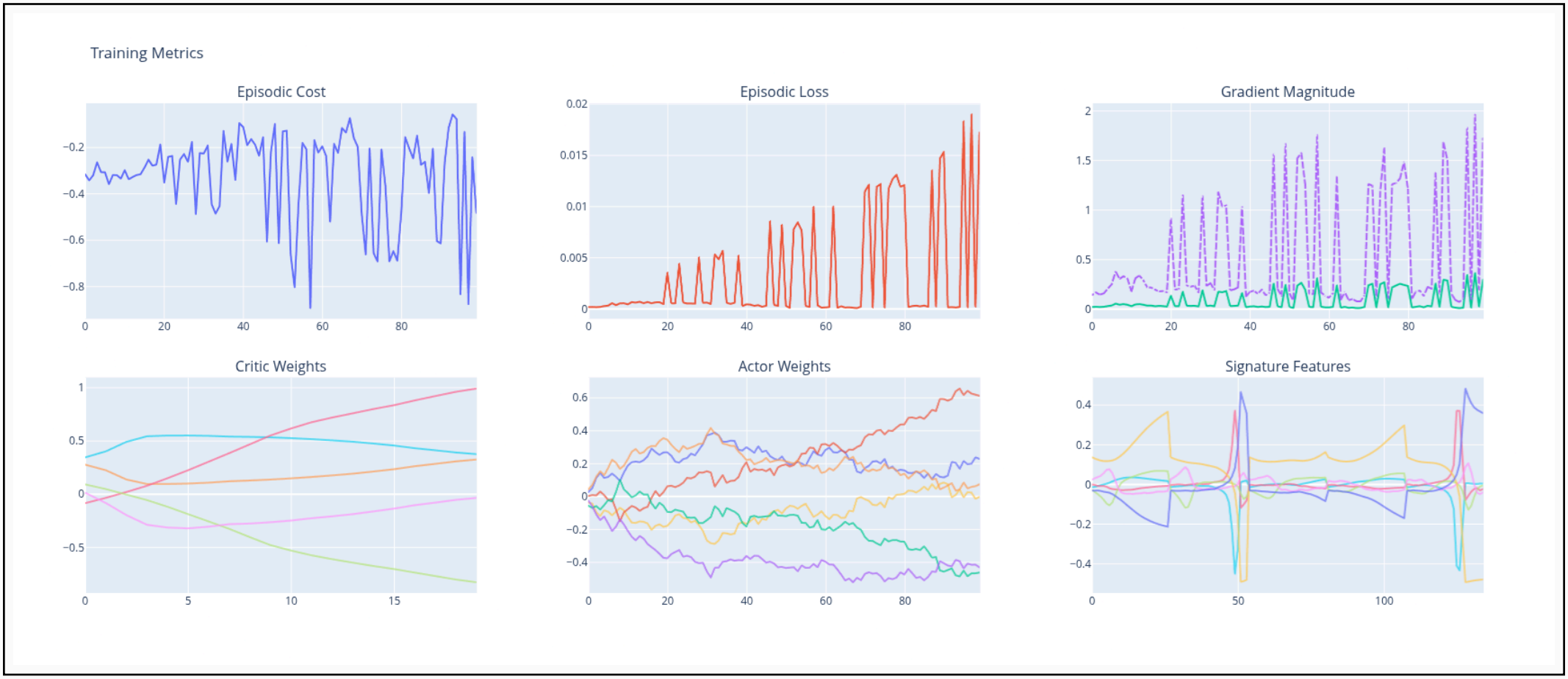


Figure 8: Training on Chemical Reactor, CTAC depth 2

More insights on instabilities

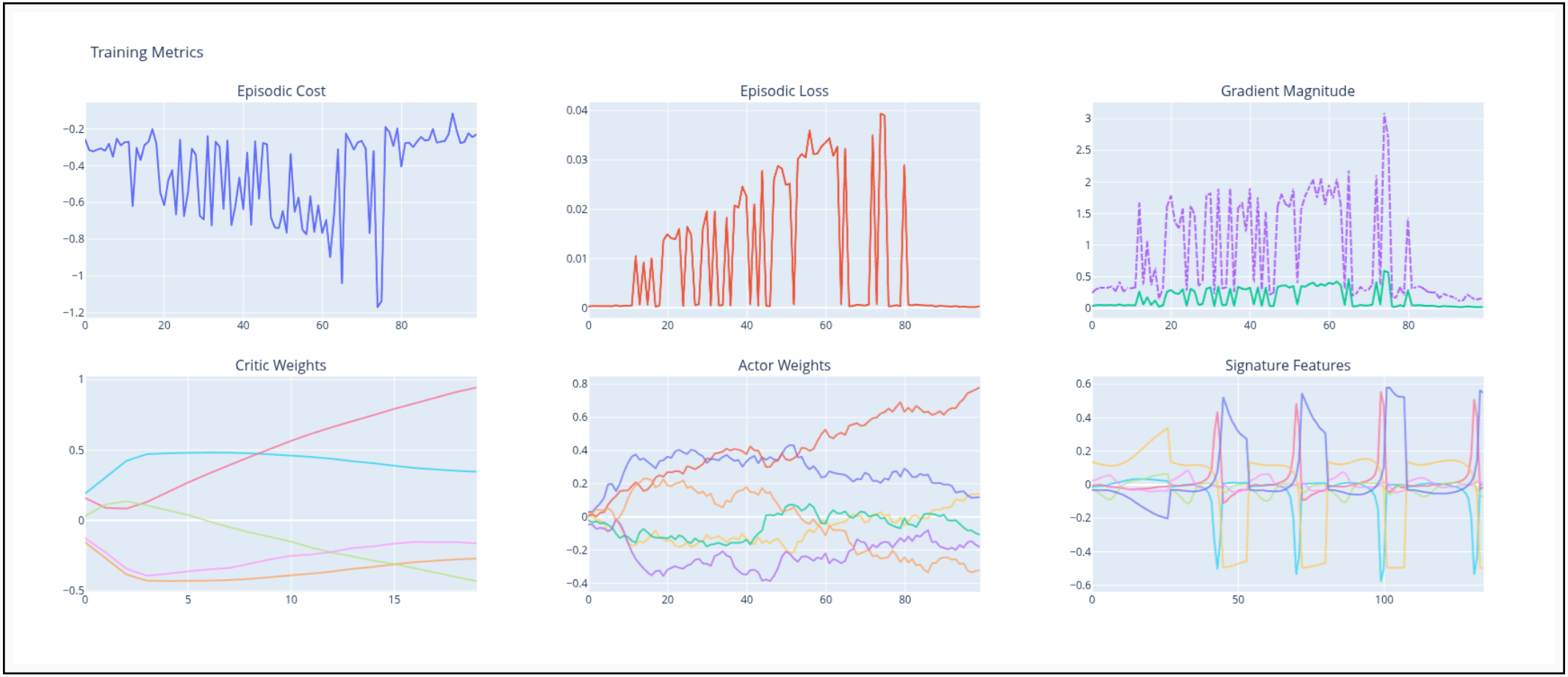


Figure 9: Training on Chemical Reactor, CTAC depth 3

More insights on instabilities

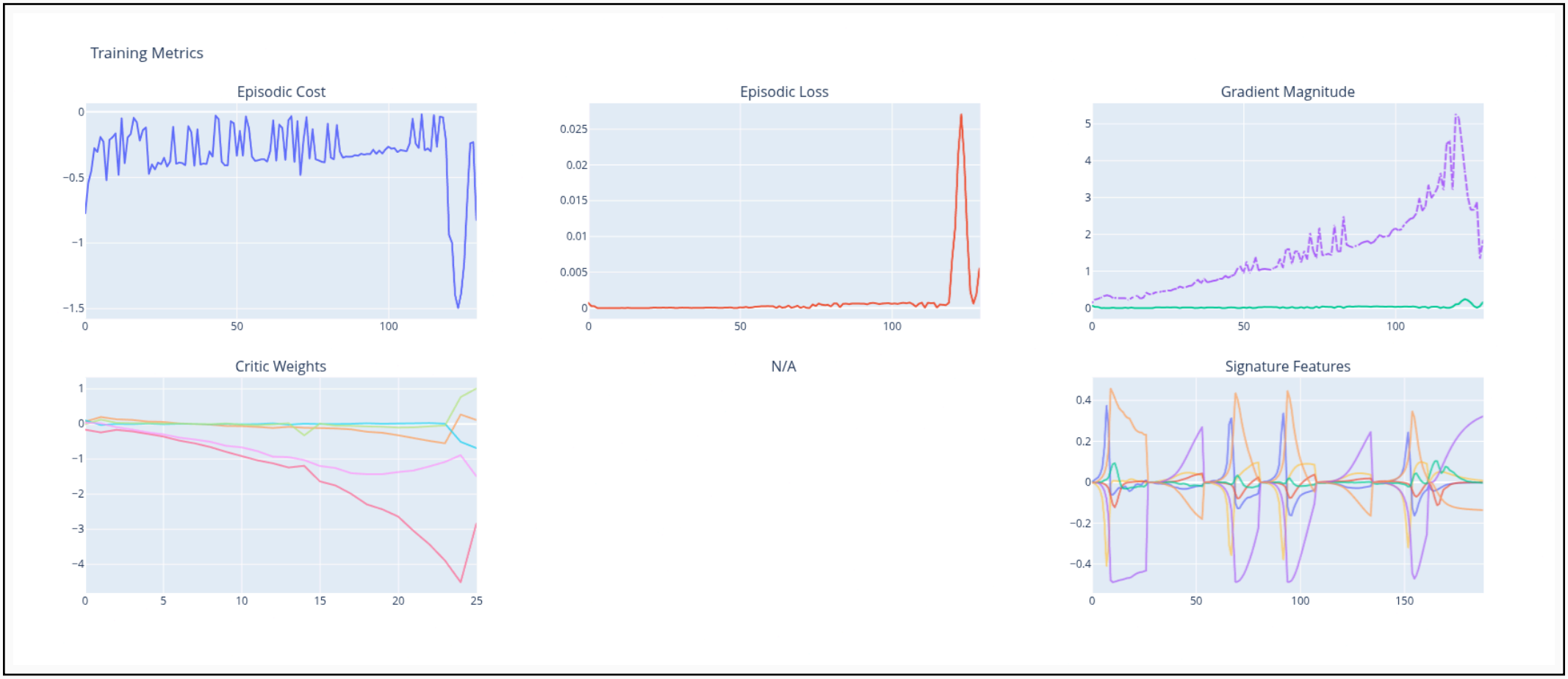


Figure 10: Training on Chemical Reactor, VG depth 2

CTAC algorithm

Algorithm 1: Continuous Time Actor Critic

Initialisation: actor function A with weights w_a and critic function V with weights
1 w_c, noise std σ, discretisation Δt, environment with step function dependent of Δt.

2 **while** not finished

3 $n \leftarrow$ random noise, std $= \sigma$

4 $x_{t+\Delta t}, r_t \leftarrow \text{step}_{\Delta t}(x_t, u + n)$

5 compute $V(x_t)$ and $V(x_{t+\Delta t})$

6 $\delta_t \leftarrow \frac{V(x_t) - V(x_{t+\Delta t})}{\Delta t} + r_t - \frac{1}{\gamma} V(x_t)$ temporal difference

7 $w_c \leftarrow w_c + \eta_c \delta_t \frac{\partial V(x_t)}{\partial w_c}$

8 $w_a \leftarrow w_a + \frac{n}{\sigma} \frac{\partial A}{\partial w_a}$

Value Gradient Algorithm

Algorithm 2: Functional Value Gradient

Initialisation: Critic function V with weights w_c, noise std σ, discretisation Δt,
environment with step function dependent of Δt, matrix $g(x_t)$, learning rate $\eta_c > 0$.

while not finished

- $\nabla_{x(t)} V(x_t) \leftarrow \frac{\partial V(x_t)}{x_t} \mid_{t=0}$
- $u \leftarrow \frac{1}{2} R^{-1} g(x_t)^\top \nabla_{x(t)} V(x_t)$
- $n \leftarrow$random noise, std $= \sigma$
- $x_{t+\Delta t}, r_t \leftarrow \text{step}_{\Delta t}(x_t, u + n)$
- compute $V(x_t)$ and $V(x_{t+\Delta t})$
- $\delta_t \leftarrow \frac{V(x_t) - V(x_{t+\Delta t})}{\Delta t} + r_t - \frac{1}{\tau} V(x_t)$ temporal difference
- $w_c \leftarrow w_c + \eta_c \delta_t \frac{\partial V(x_t)}{\partial w_c}$

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