Generalizing to New Physical Systems via Context-Informed Dynamics Model

Matthieu Kirchmeyer*[1,2], Yuan Yin*[1], Jérémie Donà[1], Nicolas Baskiotis[1], Alain Rakotomamonjy[2,3], Patrick Gallinari[1,2]

*Equal Contribution [1]Sorbonne Université, ISIR, MLIA [2]Criteo AI Lab [3]Université de Rouen, LITIS

{matthieu.kirchmeyer,yuan.yin}@sorbonne-universite.fr

SORBONNE UNIVERSITÉ CRÉATEURS DE FUTURS DEPUIS 1257 · CRITEO · ICML International Conference On Machine Learning

Motivation

- Neural dynamics models are successful but generalize poorly out-of-distribution.
- Limitation if applied to real-world problems e.g.
  - *disease diffusion prediction in new countries*
  - *heart dynamics modelling for new patients*
  - *weather prediction for new spatial regions*
- *CoDA*: first principled solution to this problem

Problem Setting

We consider systems described by a differential eq.:

$$\mathrm{d}x(t)/\mathrm{d}t = f(x(t))$$

- $x(t)$ is the state at t
- f unknown dynamics describing the evolution of x
  - *defined by context e.g. parameters, forcing*
  - *defines trajectories:* $x(t) = x_0 + \int_0^t f(x(\tau))\mathrm{d}\tau$

We learn a neural dynamics model g_θ across contexts.

- We leverage several different environments:
  - *environment* $e \in \mathcal{E} \Leftrightarrow$ *physical context*
  - *trajectories* $\mathcal{D}^e$ *of corresponding dynamics* f^e
- Training: environments $\mathcal{E}_{\mathrm{tr}}$ with *reasonable* data
- Adaptation: environments $\mathcal{E}_{\mathrm{ad}}$ with *scarce* data
- Task: generalize to new trajectories of $\mathcal{E}_{\mathrm{ad}}$

CoDA Framework

Adaptation Rule

$\forall e, \theta^e \triangleq \theta^c + \delta\theta^e$, θ^c shared; $\delta\theta^e$ env. specific

Locality

$$\min_{\theta^c, \{\delta\theta^e\}} \sum_{e\in\mathcal{E}} \|\delta\theta^e\|^2 \text{ s.t. } \forall t \; \frac{\mathrm{d}x^e(t)}{\mathrm{d}t} = g_{\theta^c+\delta\theta^e}(x^e(t))$$

- Fast adaptation by constraining θ^c
- Hypothesis space constrained around θ^c

Low-rank adaptation via hypernetwork

$$\forall e, \theta^e \triangleq \theta^c + W\xi^e \quad (\delta\theta^e \triangleq W\xi^e)$$

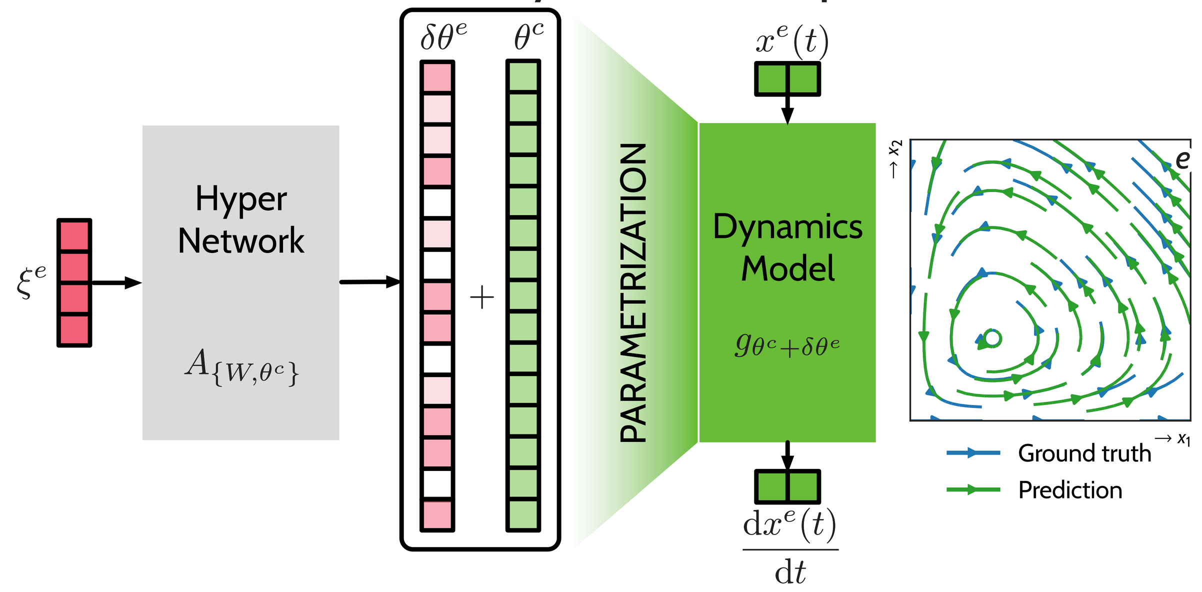
Smaller adaptation space ($d_\xi \ll d_\theta$)

Theoretical Motivation

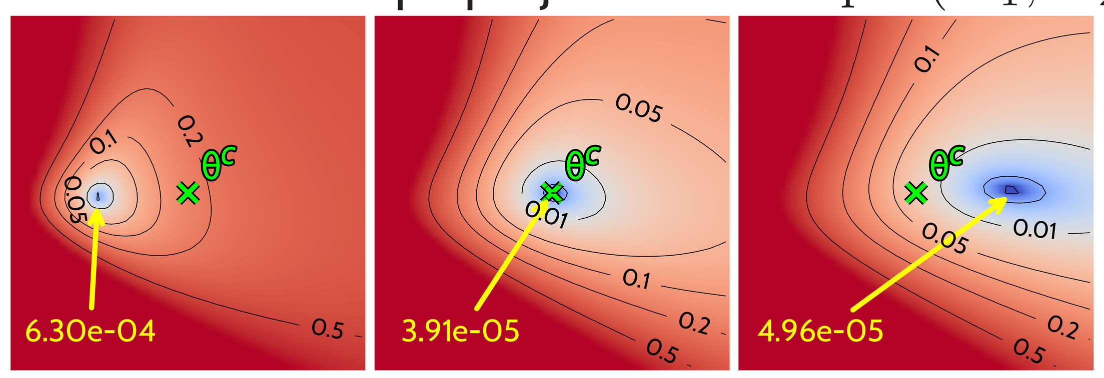
Proposition 1 (Low-rank gradients). *For linearly parameterized dynamics with d_p parameters, $\forall\theta^c \in \mathbb{R}^{d_\theta}$, $\dim(\mathrm{Span}(\{\nabla_\theta\mathcal{L}(\theta^c, \mathcal{D}^e)\}_{e\in\mathcal{E}})) \leq d_p \ll d_\theta$.*

Visualization

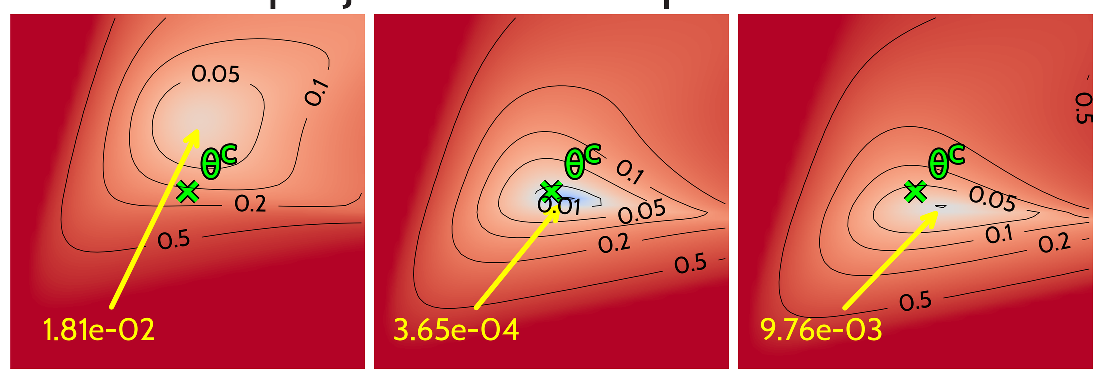
Context-Informed Dynamics Adaptation (*CoDA*)



CoDA's loss landscape projected onto $\mathrm{Span}(W_1, W_2)$



ERM's loss projected onto top 2 SVD directions



- Smooth loss with a single minimum across $\mathcal{E}$
- Proximity of local loss optimas to θ^c
- Low minimal loss of optimas of *CoDA* w.r.t. ERM

Constrained Optimization

Training: $\displaystyle\min_{\theta^c, W, \{\xi^e\}_{\mathcal{E}_{\mathrm{tr}}}} \sum_{e\in\mathcal{E}_{\mathrm{tr}}} \mathcal{L}(\theta^c + W\xi^e, \mathcal{D}^e) + \|W\xi^e\|^2$

Adaptation: $\displaystyle\min_{\{\xi^e\}_{\mathcal{E}_{\mathrm{ad}}}} \sum_{e\in\mathcal{E}_{\mathrm{ad}}} \mathcal{L}(\theta^c + W\xi^e, \mathcal{D}^e) + \|W\xi^e\|^2$

- $\mathcal{L}(\theta, \mathcal{D}^e) = \sum_{i=1}^{N_{tr}} \sum_{t_k} \left\|(x^{e,i} - \tilde{x}^{e,i})(t_k)\right\|_2^2$
  $\tilde{x}^{e,i}(t_k) = x^{e,i}(t_{k-1}) + \int_{t_{k-1}}^{t_k} g_\theta(\tilde{x}^{e,i}(\tau))\mathrm{d}\tau$
- $\|W\xi^e\|^2 \rightarrow \lambda_\xi\|\xi^e\|_2^2 + \lambda_\Omega\Omega(W)$
  ℓ_2: $\Omega(W) = \|W\|_2$ $\quad \ell_1$: $\Omega(W) = \sum_{i=1}^{d_\theta}\|W_{i,\cdot}\|_2$

Experimental Setting

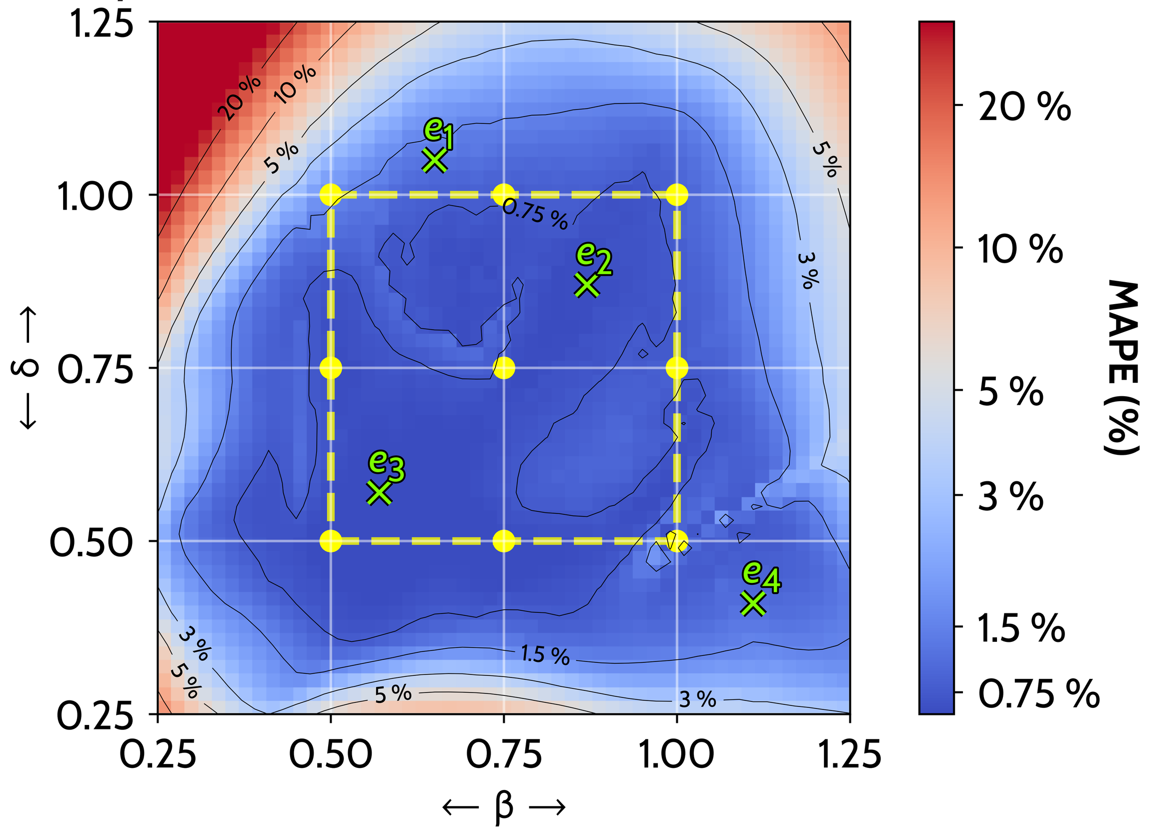
- ODE: Lotka-Volterra (`LV`), Glycolitic Oscillator (`GO`)
- PDE: Gray-Scott (`GS`), Navier-Stokes (`NS`)
- d_p parameters vary between physical systems
- Various architecture for dynamics model g_θ
  ODE → *MLP*   *PDE* → *ConvNet, FNO*

Results

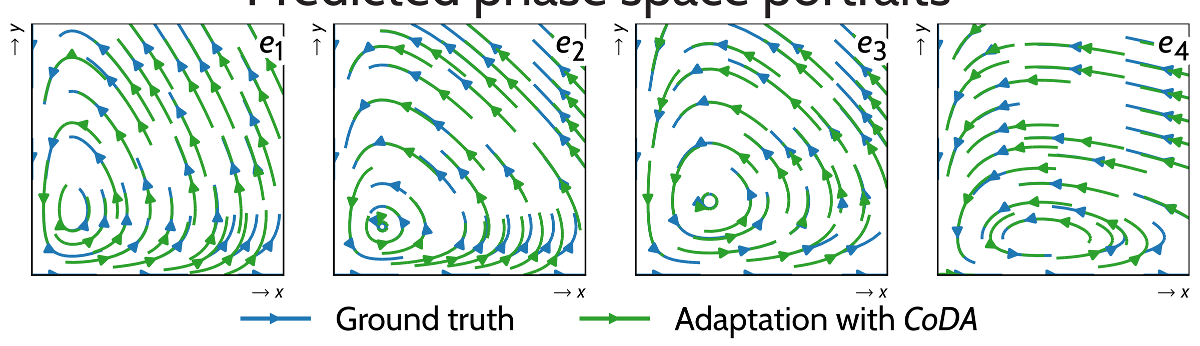
Evaluation on new test trajectories: In-Domain ($\mathcal{E}_{\mathrm{tr}}$) and 1-shot Adaptation ($\mathcal{E}_{\mathrm{ad}}$, $N_{ad} = 1$)

Test MSE (↓)	`LV` ($\times 10^{-5}$)		`GO` ($\times 10^{-4}$)		`GS` ($\times 10^{-3}$)		`NS` ($\times 10^{-4}$)	
	In-Domain	Adaptation	In-Domain	Adaptation	In-Domain	Adaptation	In-Domain	Adaptation
MAML	60.3±1.3	3150±940	57.3±2.1	1081±62	3.67±0.53	2.25±0.39	68.0±8.0	51.1±4.0
LEADS	3.70±0.27	47.61±12.47	31.4±3.3	113.8±41.5	2.90±0.76	1.36±0.43	14.00±1.55	28.60±7.23
CAVIA-FiLM	4.38±1.15	8.41±3.20	4.44±1.46	3.87±1.28	2.81±1.15	1.43±1.07	23.2±12.1	22.60±9.88
CAVIA-Concat	2.43±0.66	6.26±0.77	5.09±0.35	2.37±0.23	2.67±0.48	1.62±0.85	25.50±6.31	26.00±8.24
CoDA-ℓ_2	1.52±0.08	1.82±0.24	2.45±0.38	1.98±0.06	1.01±0.15	0.77±0.10	9.40±1.13	10.30±1.48
CoDA-ℓ_1	**1.35±0.22**	**1.24±0.20**	**2.20±0.26**	**1.86±0.29**	**0.900±0.057**	**0.74±0.10**	**8.35±1.71**	**9.65±1.37**

Adaptation MAPE (↓) with *CoDA*-ℓ_1 on `LV` ($\bullet$ $\mathcal{E}_{\mathrm{tr}}$)



Predicted phase space portraits



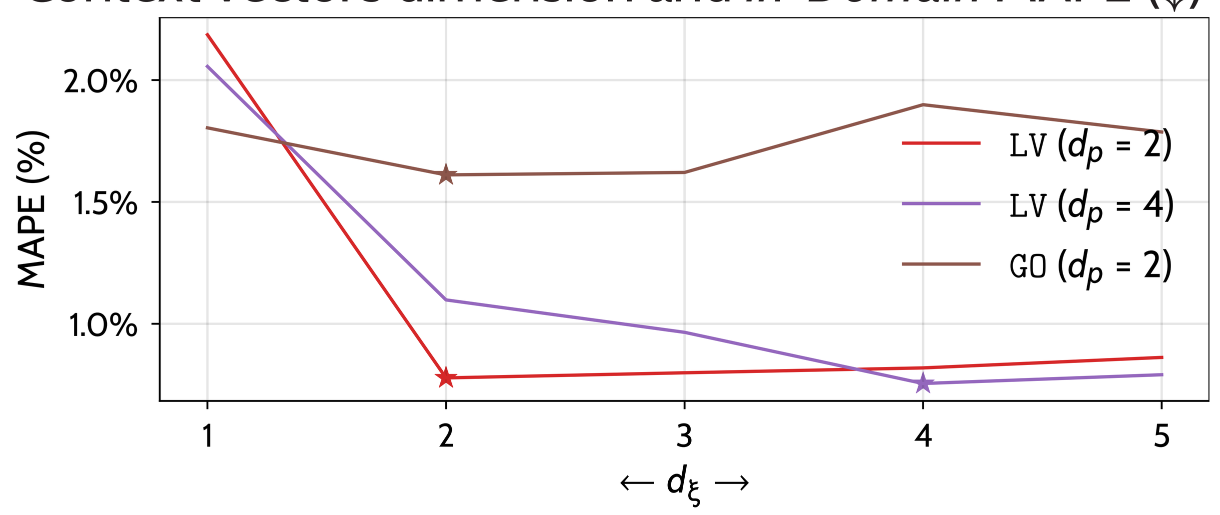
$$\texttt{LV} \quad \frac{\mathrm{d}x}{\mathrm{d}t} = \alpha x - \beta xy \qquad \frac{\mathrm{d}y}{\mathrm{d}t} = \delta xy - \gamma y$$

x: prey
y: predator

Sample efficiency and impact of number of adaptation trajectories N_{ad} on *Adaptation* MSE (↓) on `LV`

Test MSE $\times 10^{-5}$	1	5	10
MAML	3150±940	239±16	173±10
LEADS	47.61±12.47	19.89±7.23	19.42±3.52
CoDA-ℓ_1	**1.24±0.20**	**1.21±0.18**	**1.20±0.17**

Context vector's dimension and *In-Domain* MAPE (↓)



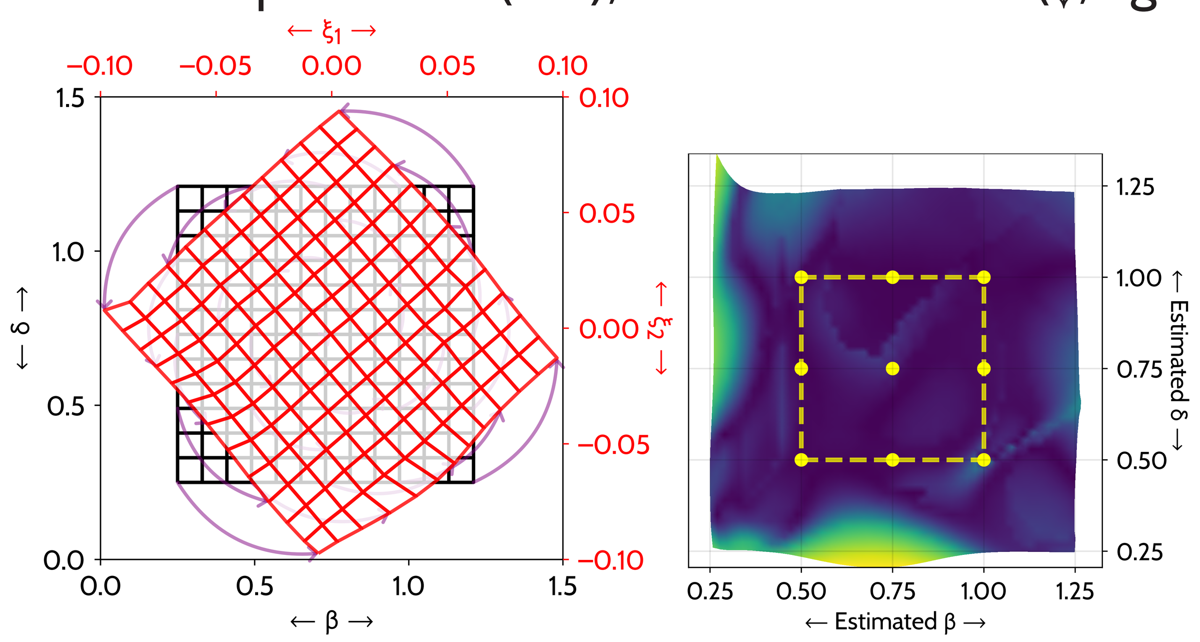
ℓ_2 locality and layer importance for *In-Domain* MSE (↓)

In-Domain	`LV` ($\times 10^{-5}$)		`GO` ($\times 10^{-4}$)	
MSE (↓)	W/o ℓ_2	With ℓ_2	W/o ℓ_2	With ℓ_2
Full	2.28±0.29	1.52±0.08	2.98±0.71	2.45±0.38
FirstLayer	2.25±0.29	2.41±0.23	2.38±0.71	**2.12±0.55**
LastLayer	1.86±0.24	**1.27±0.03**	28.40±0.60	28.40±0.64

System Parameter Estimation

- Learn correspondence between context vectors ⊞ and *known* system parameters ⊞ on $\mathcal{E}_{\mathrm{tr}}$
- Apply the correspondence to $\mathcal{E}_{\mathrm{ad}}$ to infer parameters

`LV` - correspondence (left); estimation MAPE (↓, right)



`NS` estimation MAPE (↓)