Marrying Causal Representation Learning and Dynamical Systems for Science

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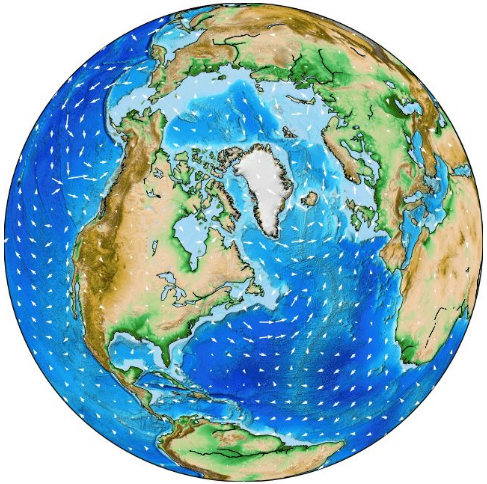
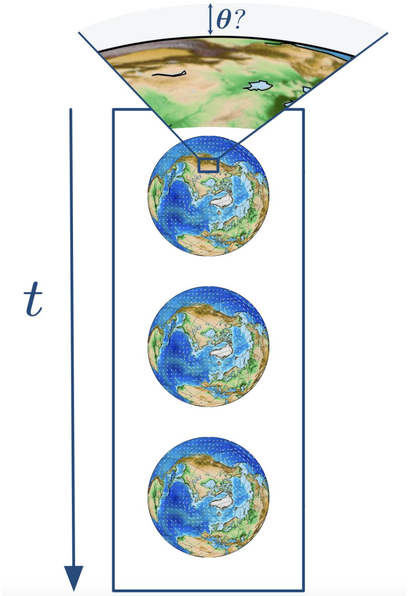
Causal Learning and AI

Motivation

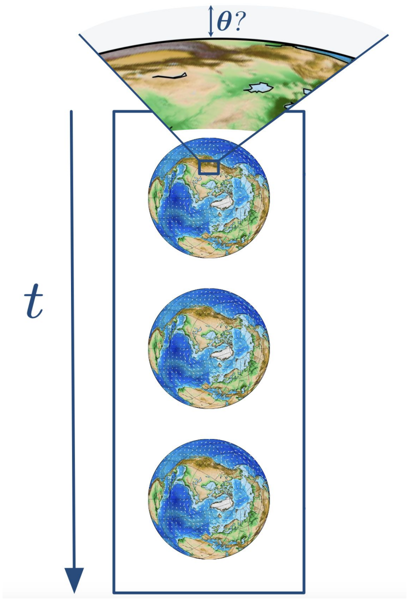
Goal: Answer scientific questions that are related to underlying physical parameters from complex dynamical systems





Problem Formulation

ODE System: $\dot{\mathbf{x}}(t) = f_\theta(\mathbf{x}(t))$



How much do we know about the system?

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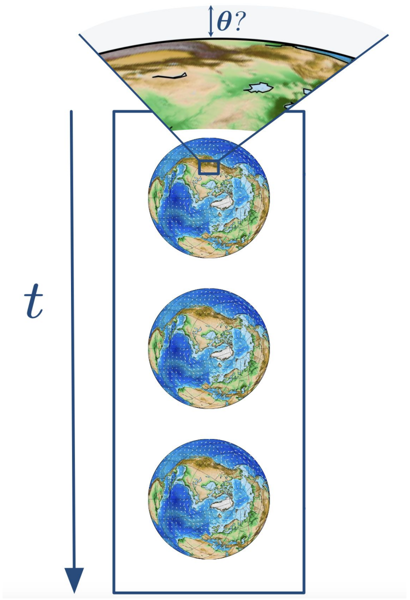
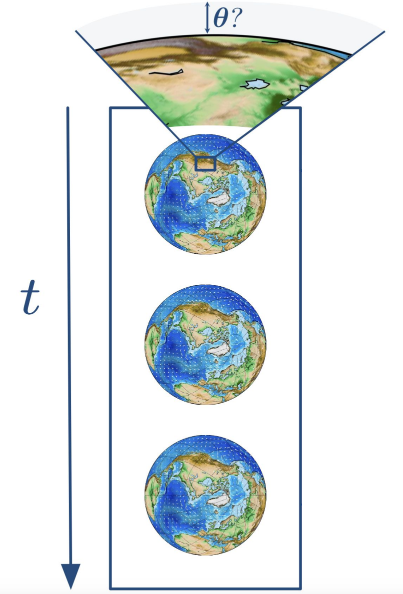


System f_θ given by field experts

If the functional form of the system is known

ODE System: $\dot{\mathbf{x}}(t) = f_\theta(\mathbf{x}(t))$



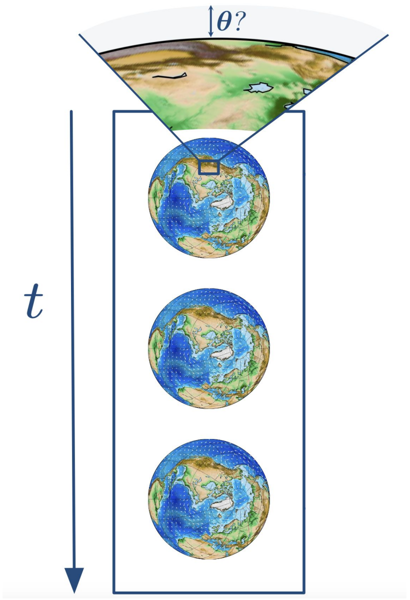
Corollary 1 (Full identifiability with known f)

$$\hat{\boldsymbol{\theta}} \in \operatorname{argmin} \left\| F(\hat{\boldsymbol{\theta}}) - \mathbf{x} \right\|_2^2 \tag{1}$$

fully-identifies *the ground truth parameter θ.*

If the functional form of the system is unknown

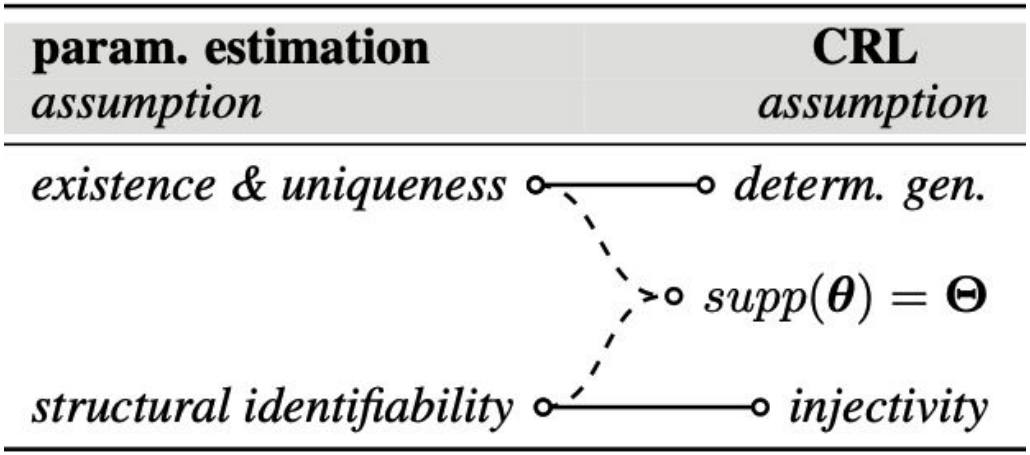
ODE System: $\dot{\mathbf{x}}(t) = f_\theta(\mathbf{x}(t))$



System f_θ unknown → CRL approaches

Why can we use CRL for system identification?

The ground assumptions between these two fields align



Edward L Ince. Ordinary differential equations. Courier Corporation, 1956.
Ror Bellman and Karl Johan Åström. On structural identifiability. Mathematical biosciences, 7(3-4): 329–339, 1970.

Identifiability for Unknown Systems

(e.g. with Multiview CRL)

Corollary 2 (Identifiability without known f)

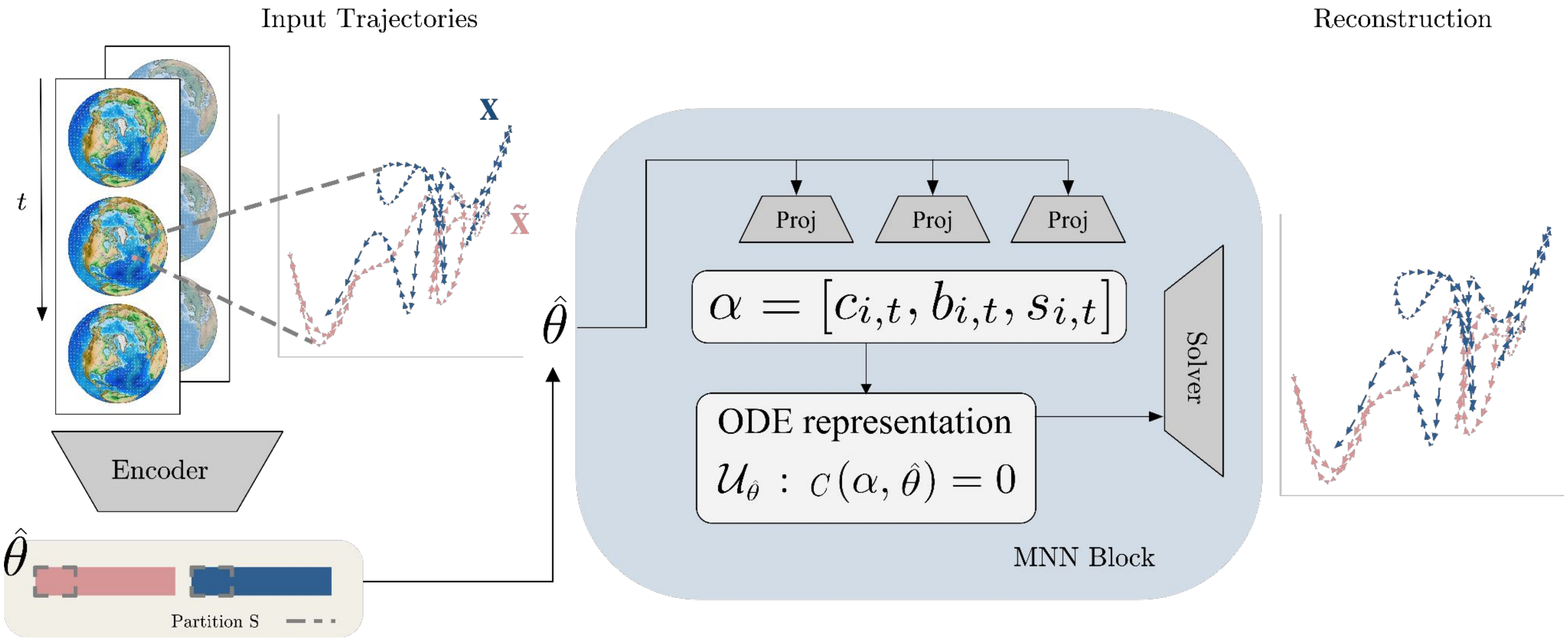
$$g, \hat{F} \in \operatorname{argmin} \mathbb{E}_{\mathbf{x},\tilde{\mathbf{x}}} \underbrace{\|g(\mathbf{x})_S - g(\tilde{\mathbf{x}})_S\|_2^2}_{\text{Alignment}} + \underbrace{\|\hat{F}(g(\mathbf{x})) - \mathbf{x}\|_2^2 + \|\hat{F}(g(\tilde{\mathbf{x}})) - \tilde{\mathbf{x}}\|_2^2}_{\text{Sufficiency}}, \quad (2)$$

then the parameter θ is partially identified by g up to a diffeomorphism in the statistical setting.

**The choice of alignment can be generalized --"Unifying Causal Representation Learning with the Invariance Principle" Yao et al. 2024*

Model Architecture

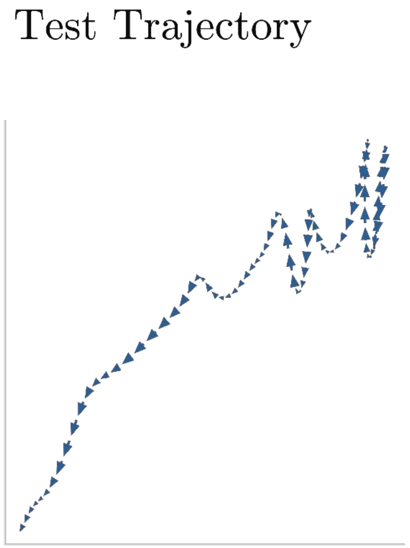
A general recipe for CRL-integrated system identifier



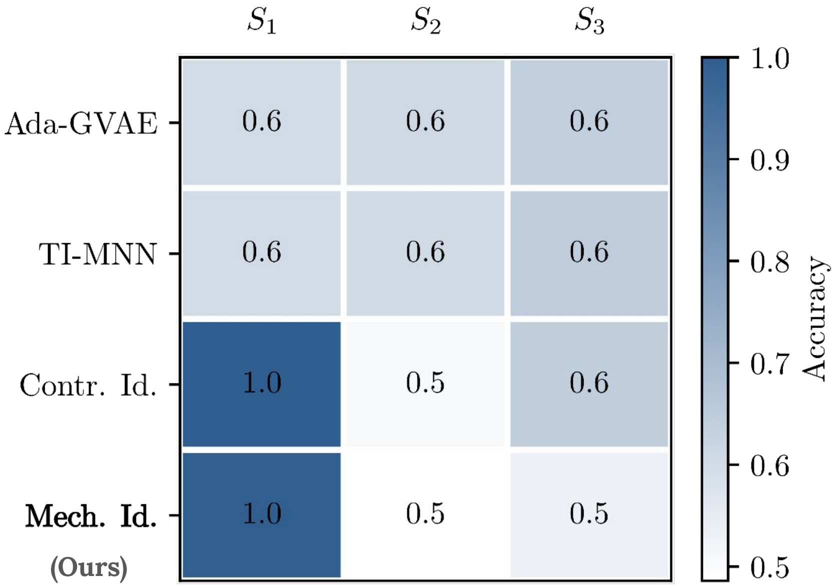
"Mechanistic Neural Networks for Scientific Machine Learning", Pervez et al. ICML 2024; "Scalable Mechanistic Neural Networks" Chen et al. 2024

Wind Simulation: Efficiently Extracting Downstream Features

Goal: Discriminating air layer thickness by wind observations



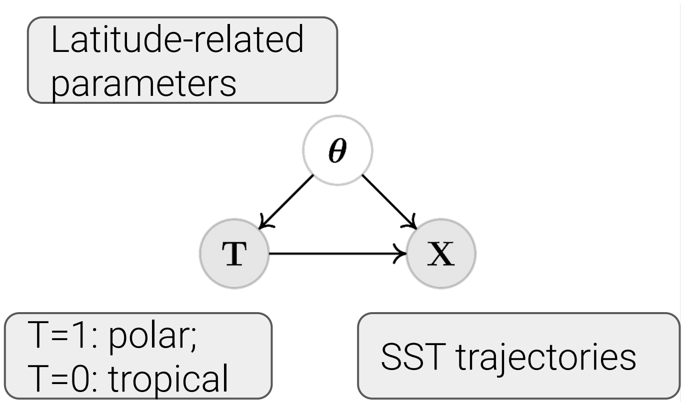
θ?

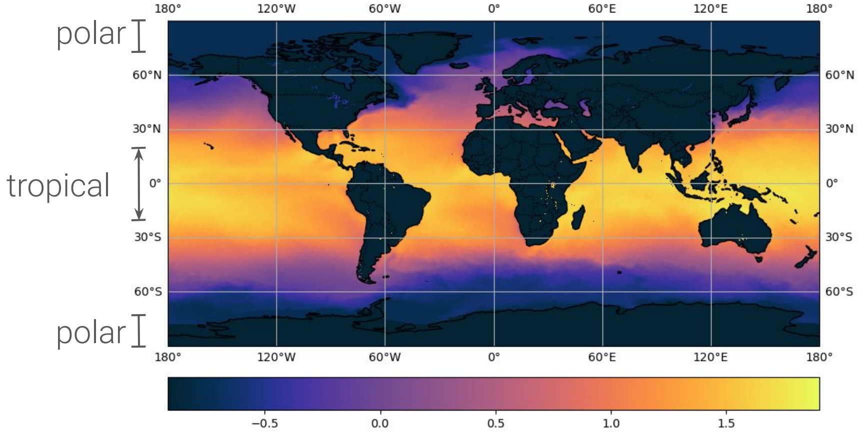


Sea Surface Temperature: Estimating Pre-treatment Covariates

Goal: Isolating latitude-related parameters for reliable ATE estimation

$$\mathrm{ATE} = \mathbb{E}[\mathbf{X}_1 - \mathbf{X}_0 \mid \theta]$$





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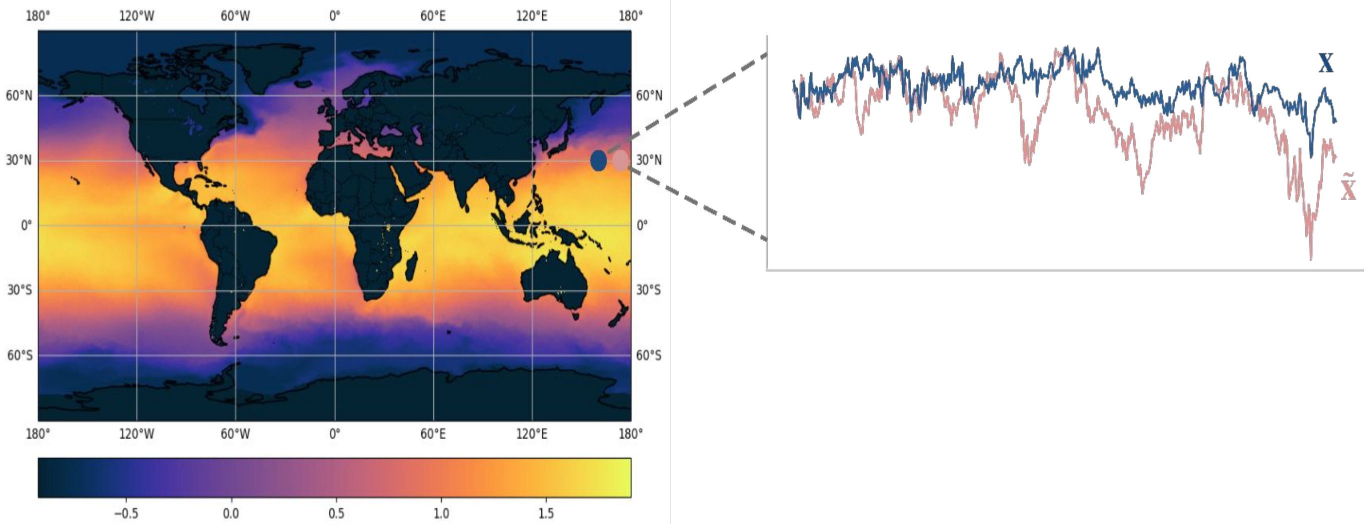

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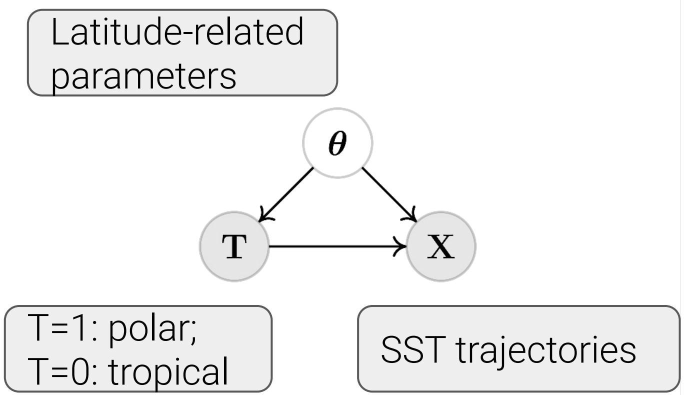

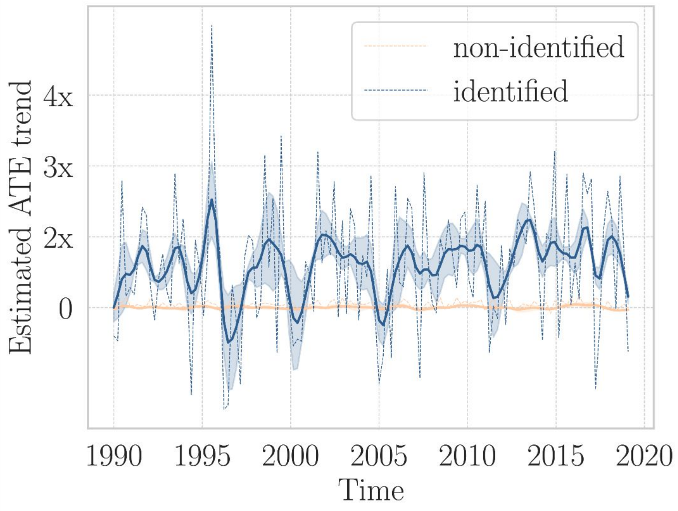

“The arctic has warmed nearly four times faster than the globe since 1979”, Rantanen et al., Nature Communications Earth & Environment 2022.

Conclusion

CRL Identifiability approaches can be applied beyond traditional causal models and facilitate scientific discoveries.

Thank you!