Missing Nodes

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RESEARCH ARTICLE | JANUARY 19 2022

Inferring network structure with unobservable nodes from time series data

Mengyuan Chen; Yan Zhang; Zhang Zhang; Lun Du; Shuo Wang; Jiang Zhang

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Network structures play important roles in social, technological, and biological systems. However, the observable nodes and connections in real cases are often incomplete or unavailable due to measurement errors, private protection issues, or other problems. Therefore, inferring the complete network structure is useful for understanding human interactions and complex dynamics. The existing studies have not fully solved the problem of the inferring network structure with partial information about connections or nodes. In this paper, we tackle the problem by utilizing time series data generated by network dynamics. We regard the network inference problem based on dynamical

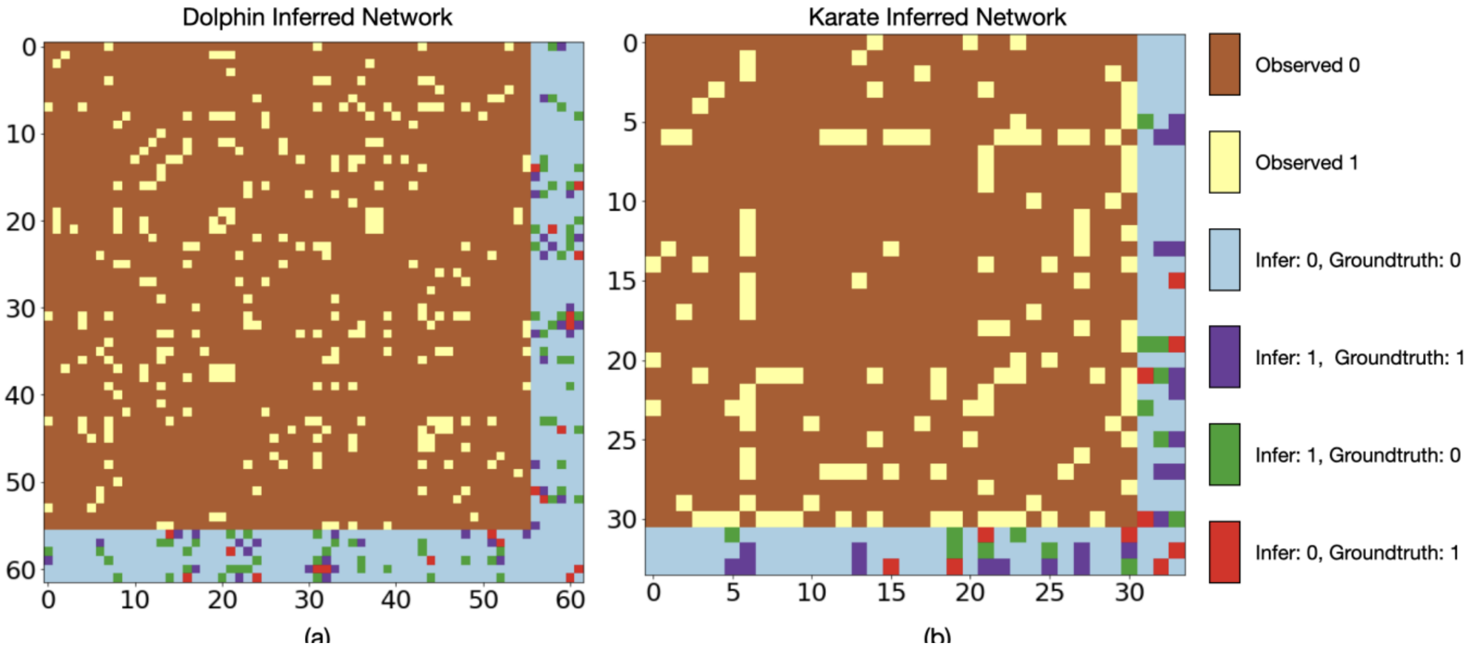

TABLE III. Network completion without structural information

Dynamics	Network	Nodes-Missing nodes	Missing AUC	Reconstruction AUC	All AUC
Discrete	Karate	34-3	0.7602	0.9930	0.9524
	Dolphins	62-6	0.8237	0.9989	0.9766
	Email-partial	143-14	0.5899	0.9819	0.9231
	ER	100-10	0.8923	0.9908	0.9850
	WS	100-10	0.8622	0.9883	0.9957
	BA	100-10	0.9189	0.9956	0.9875
Binary	ER	100-10	0.8585	0.9931	0.9717
	WS	100-10	0.8979	0.9943	0.9808
	BA	100-10	0.8863	0.9795	0.9776

https://arxiv.org/pdf/2202.10144.pdf

Learning hidden interactions

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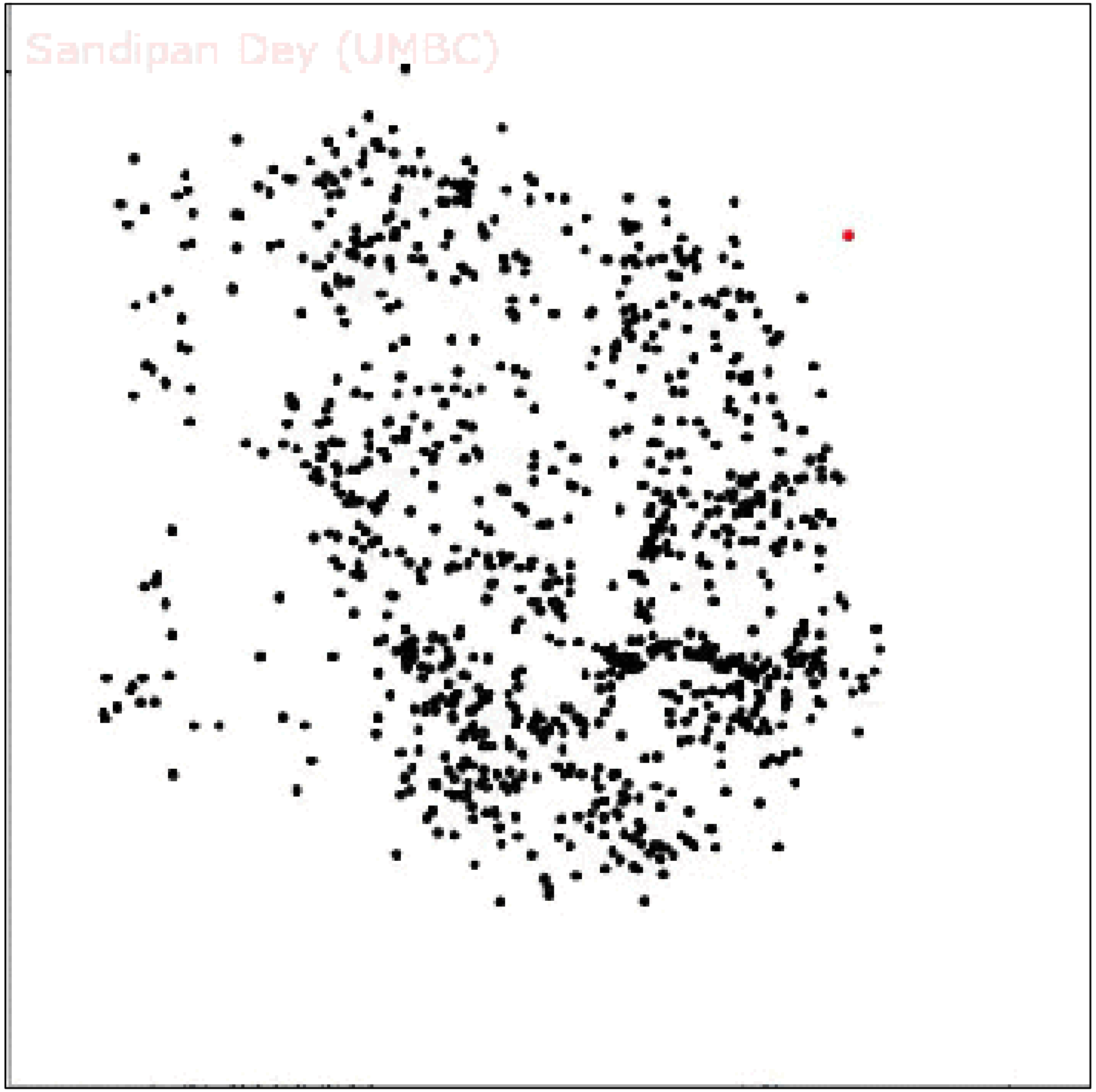
Unraveling hidden interactions in complex systems with deep learning

Seungwoong Ha & Hawoong Jeong

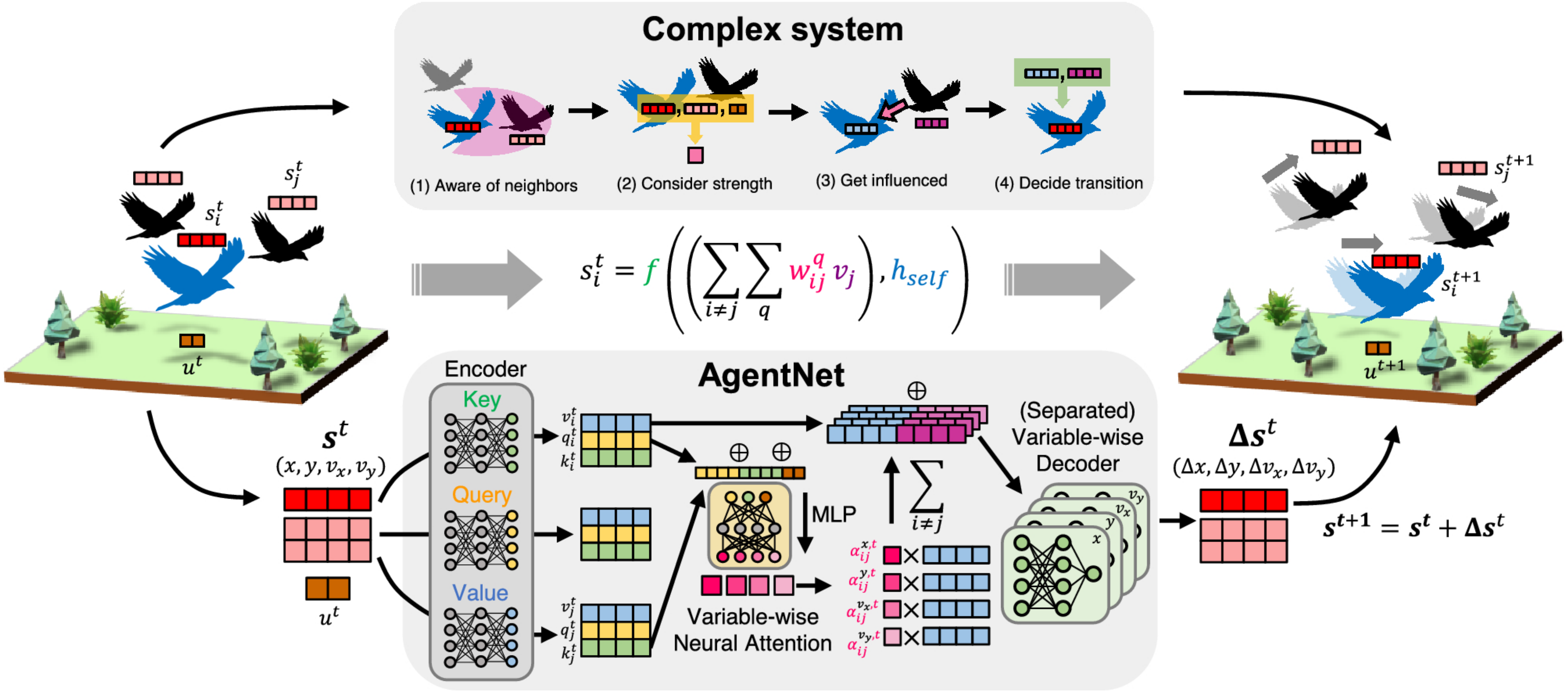
Scientific Reports **11**, Article number: 12804 (2021) | Cite this article

Boid Model

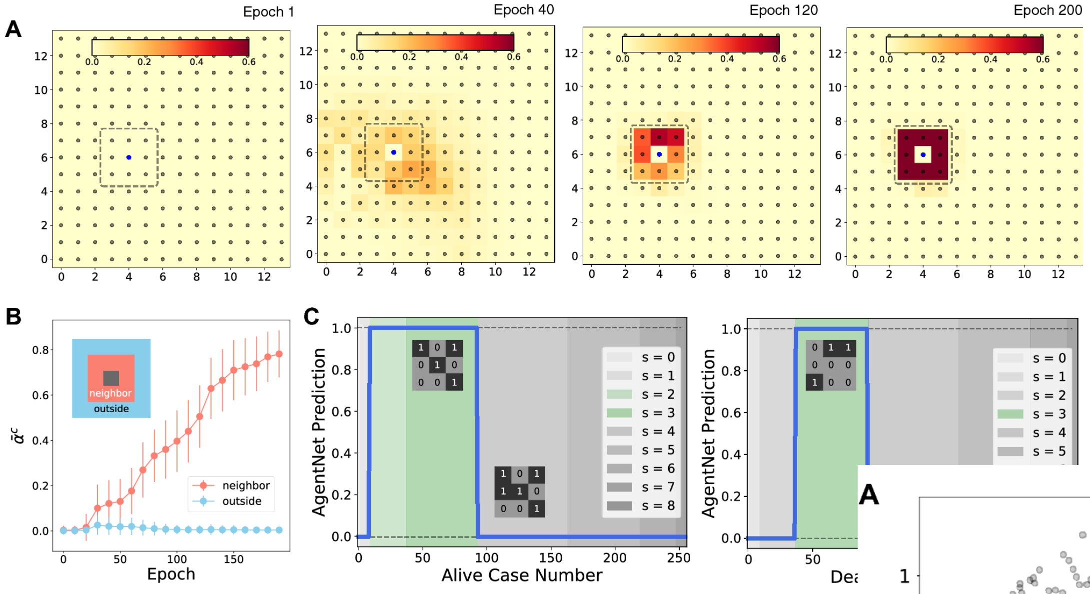
- Boid model
- Each boid follows 3 rules
  - Cohesion
  - Alignment
  - Separation

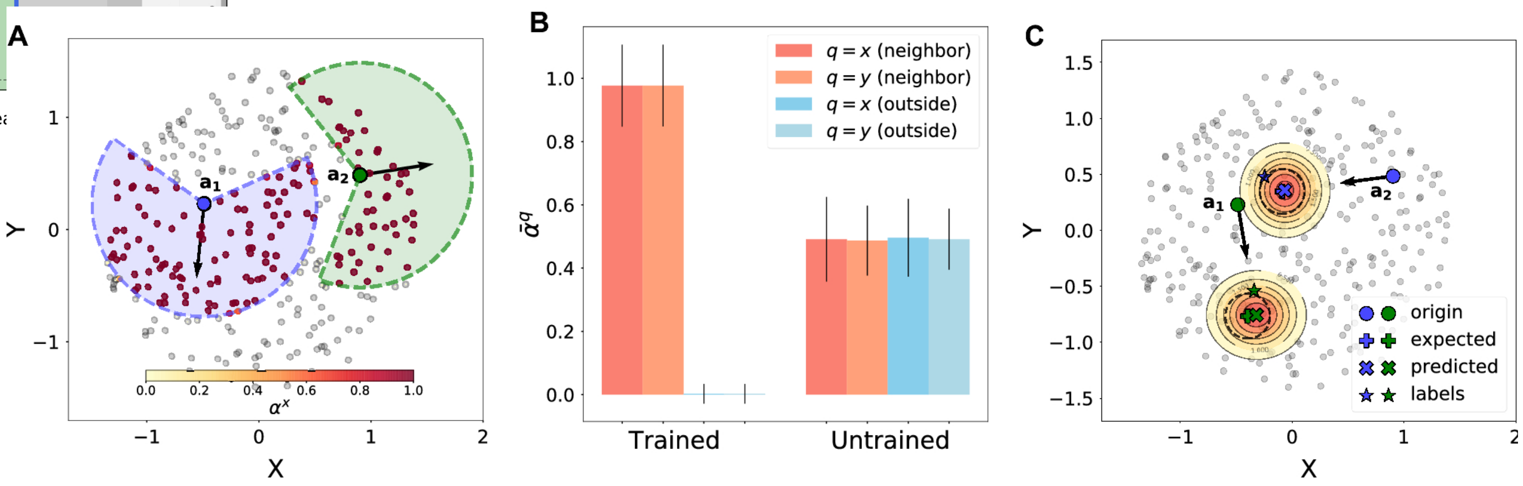


Self-attention



Self-attention visualization

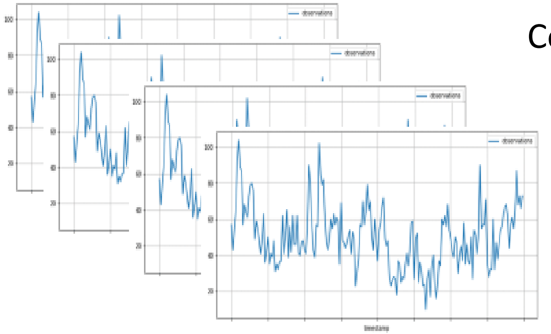




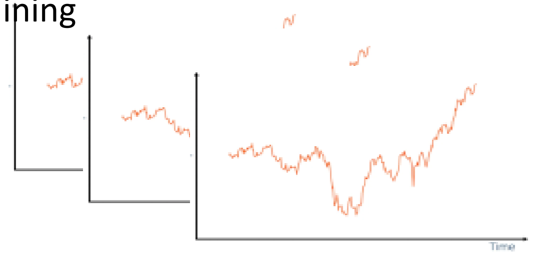
Outline

- AI for complex systems
  - Complex Systems and Modelling Methods
  - Representation & Generation
  - Dynamics Learning
  - Network Reconstruction
  - Multi-scale Modelling
  - Simulation, optimization, and control
- Complexity science for AI

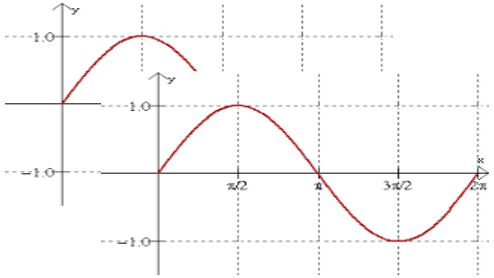
Multi-scale Modelling



Coarse Graining



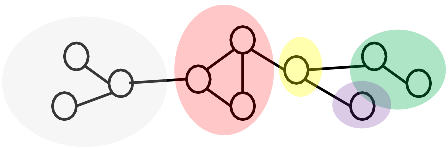
Coarse Graining

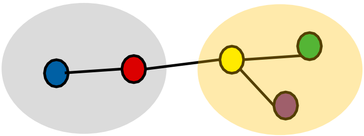


Automated Modelling

Automated Modelling

Automated Modelling





$$\frac{dX_S}{dt} = f_S(X_S)$$

$$\frac{dX_M}{dt} = f_M(X_M)$$

$$\frac{dX_L}{dt} = f_L(X_L)$$

Station - City

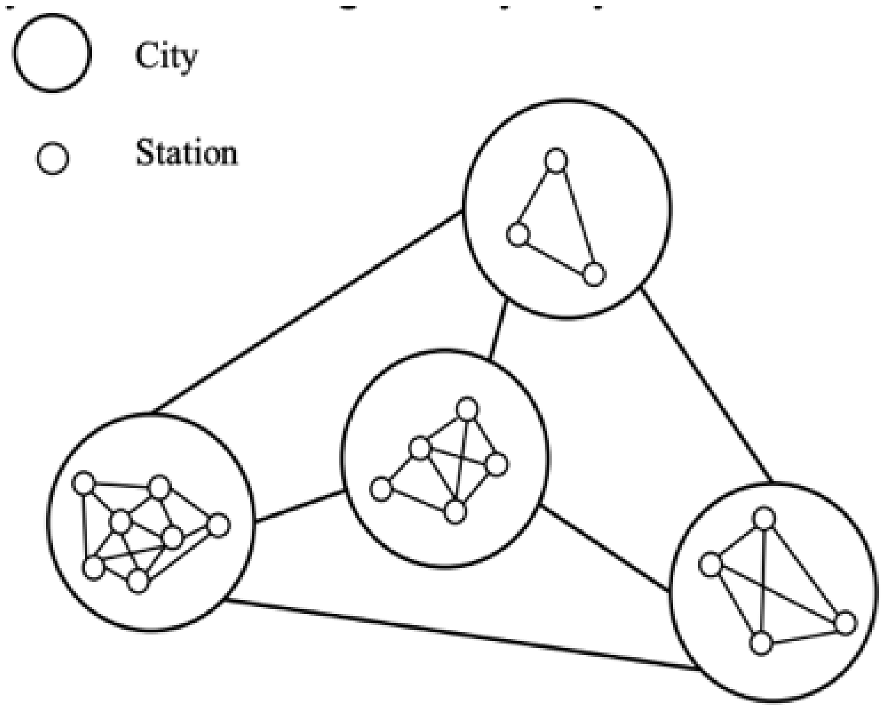
HighAir: A Hierarchical Graph Neural Network-Based Air Quality Forecasting Method

Jiahui Xu, Ling Chen, Mingqi Lv, Chaoqun Zhan, Sanjian Chen, and Jian Chang

Abstract—**Accurately forecasting air quality is critical to protecting general public from lung and heart diseases. This is a challenging task due to the complicated interactions among distinct pollution sources and various other influencing factors. Existing air quality forecasting methods cannot effectively model the diffusion processes of air pollutants between cities and monitoring stations, which may suddenly deteriorate the air quality of a region. In this paper, we propose HighAir, i.e., a hierarchical graph neural network-based air quality forecasting method, which adopts an encoder-decoder architecture and considers complex air quality influencing factors, e.g., weather and land usage. Specifically, we construct a city-level graph and station-level graphs from a hierarchical perspective, which can consider city-level and station-level patterns, respectively. We design two strategies, i.e., upper delivery and lower updating, to implement the inter-level interactions, and introduce message passing mechanism to implement the intra-level interactions. We dynamically adjust edge weights based on wind direction to model the correlations between dynamic factors and air quality. We compare HighAir with the state-of-the-art air quality forecasting**

since the air pollution path of urban atmosphere consists of emission and diffusion processes [1]–[3], air quality has complex dependencies in spatial and temporal dimensions, which are difficult to capture. Second, air quality is affected by multi-source complex factors, e.g., weather and land usage [4], and the corresponding knowledge needs to be extracted from data sources.

Existing methods for air quality forecasting can be roughly divided into two categories: physical model based methods and machine learning based methods. Physical model based methods exploit domain knowledge to simulate the physical and chemical processes of air pollutants, e.g., street canyon models [5], [6] and Gaussian plume models [7]. These methods are usually based on domain knowledge and the generalization abilities of them are limited. Machine learning based methods leverage a data-driven process to learn complex relationships between inputs and outputs. To capture temporal dependencies,



https://arxiv.org/abs/2101.04264v1

Skeleton-based action recognition

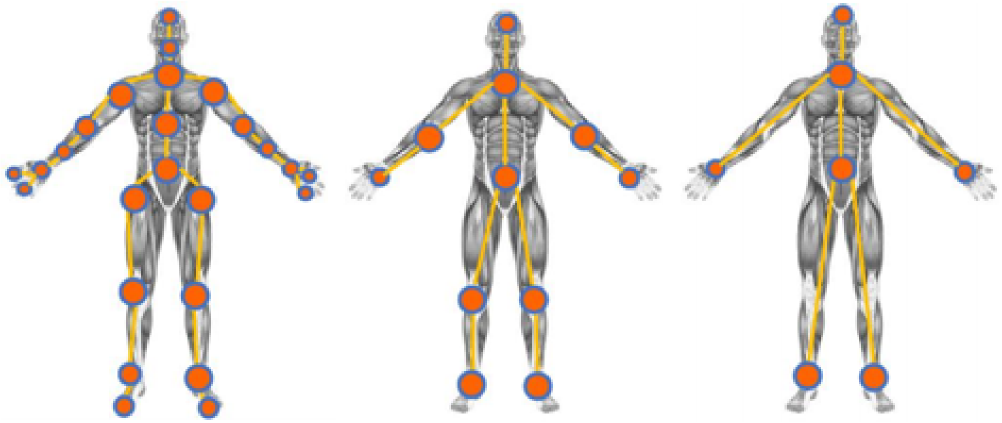
Multi Scale Temporal Graph Networks for Skeleton-Based Action Recognition

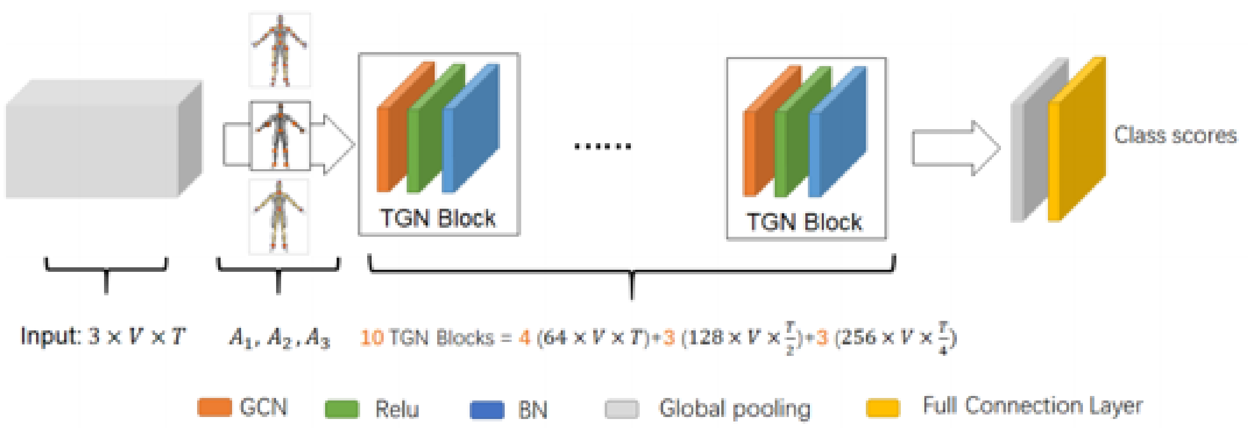
Tingwei Li[1], Ruiwen Zhang[2], Qing Li[1]

[1]Department of Automation Tsinghua University, Beijing, China
[2]Department of Computer Science Tsinghua University, Beijing, China

Abstract

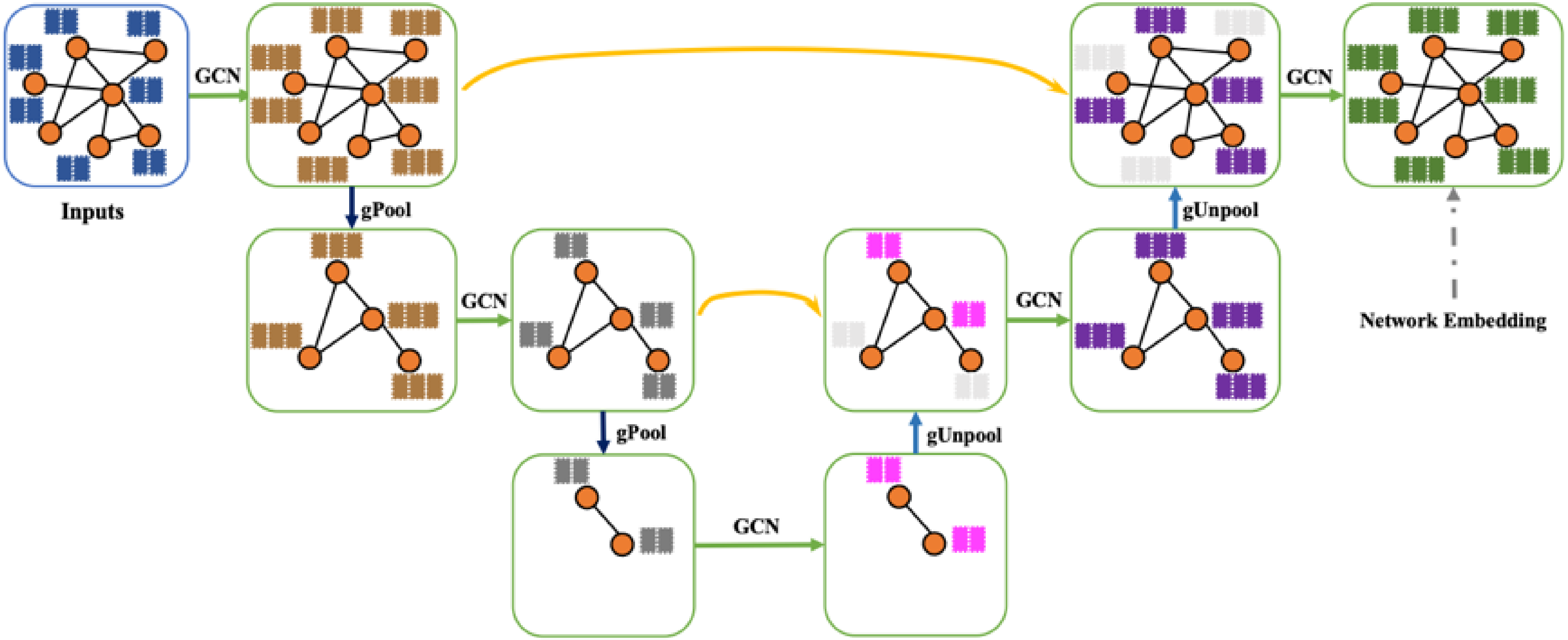
Graph convolutional networks (GCNs) can effectively capture the features of related nodes and improve the performance of model. More attention is paid to employing GCN in Skeleton-Based action recognition. But existing methods based on GCNs have two problems. First, the consistency of temporal and spatial features is ignored for extracting features node by node and frame by frame. To obtain spatiotemporal features simultaneously, we design a generic representation of skeleton sequences for action recognition and propose a novel model called Temporal Graph Networks (TGN). Secondly, the adjacency matrix of graph describing the relation of joints are mostly depended on the physical connection between joints. To appropriate describe the relations between joints in skeleton graph, we propose a multi-scale graph strategy, adopting a full-scale graph, part-scale graph and core-scale graph to capture the local features of each joint and the contour features of important joints. Experiments were carried out on two large datasets and results show that TGN with our graph strategy outperforms state-of-the-art methods.





https://arxiv.org/abs/2206.13028

Graph U-Net



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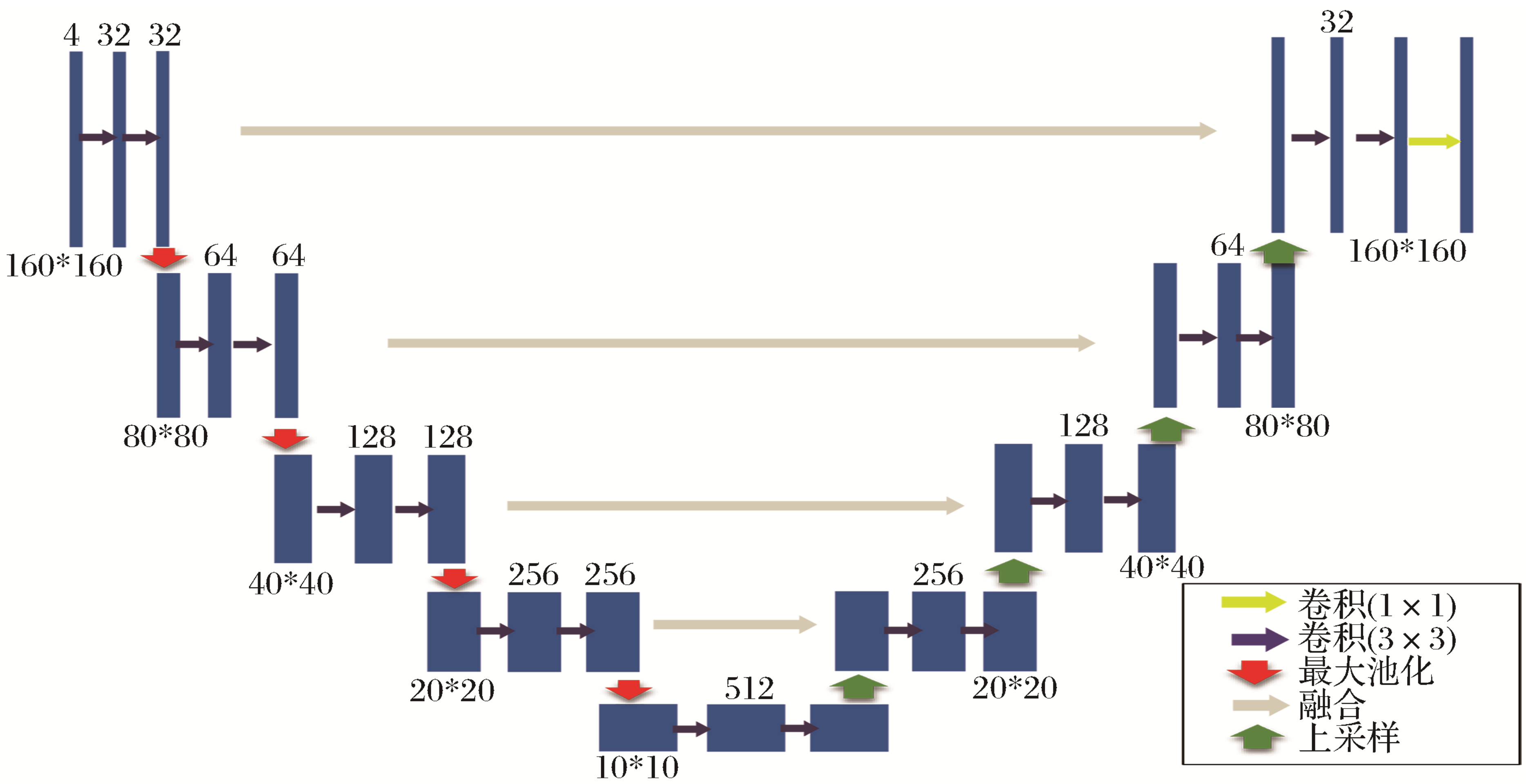
U-Net



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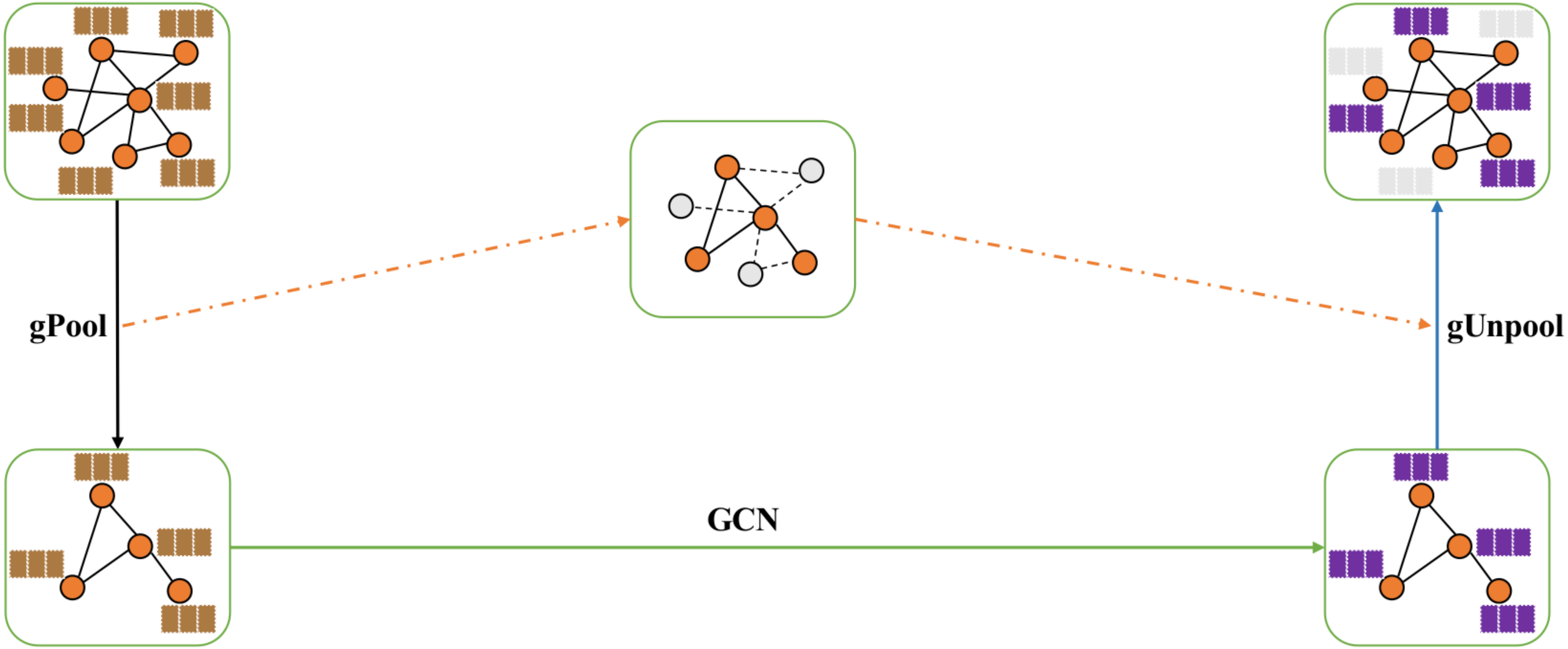
How to Down Sampling a Graph?



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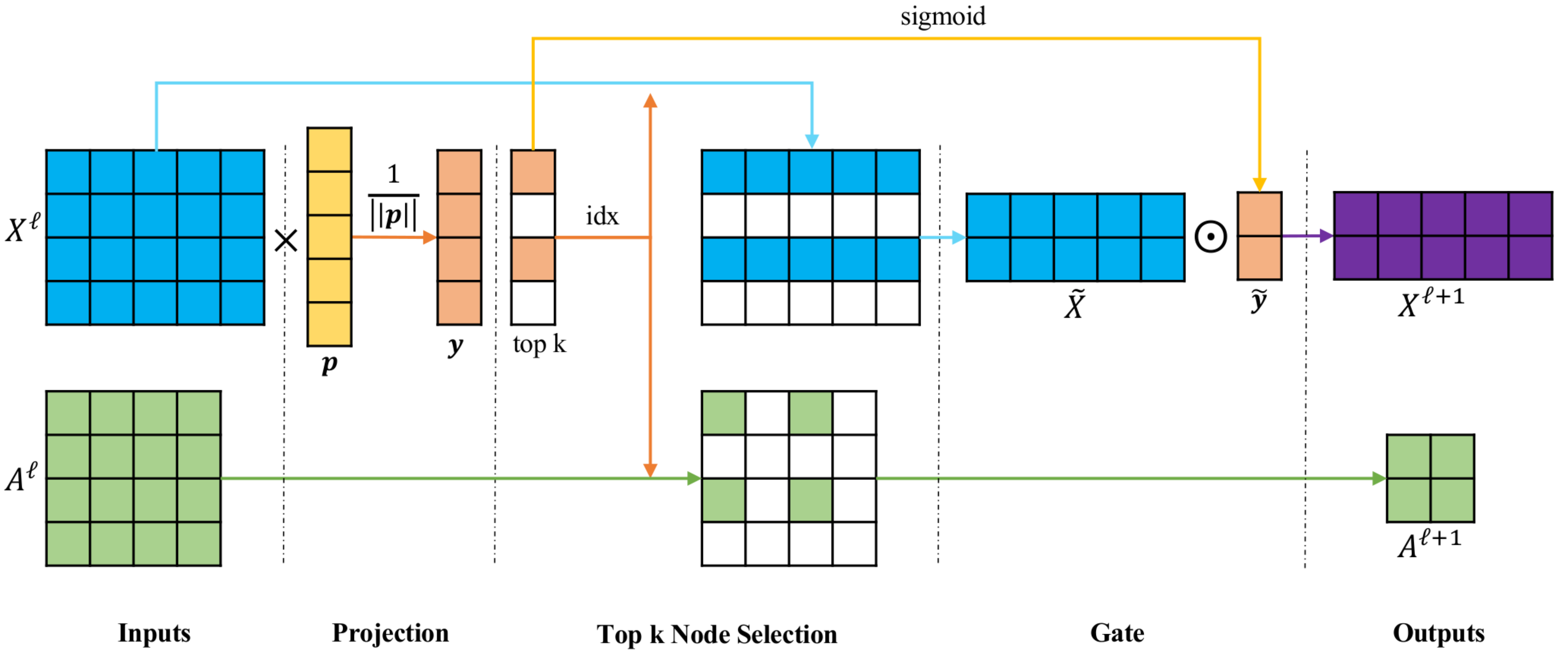
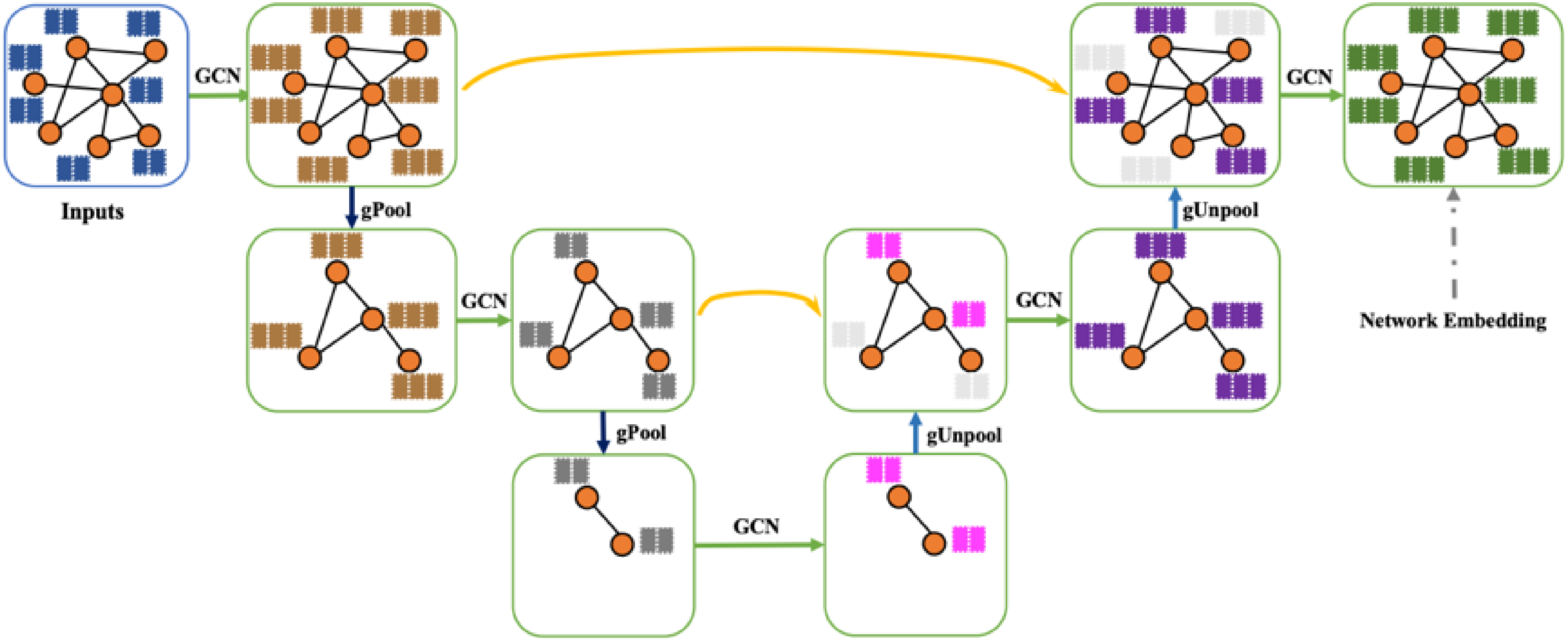
How to Down Sampling a Graph?



$$
\begin{aligned}
\mathbf{y} &= \mathrm{X}^\ell \mathbf{p}^\ell / \|\mathbf{p}^\ell\| \\
\mathrm{idx} &= \mathrm{rank}(\mathbf{y}, \mathrm{k}) \\
\tilde{\mathbf{y}} &= \mathrm{sigmoid}(\mathbf{y}(\mathrm{idx})) \\
\tilde{\mathrm{X}}^\ell &= \mathrm{X}^\ell(\mathrm{idx}, :) \\
\mathrm{A}^{\ell+1} &= \mathrm{A}^\ell(\mathrm{idx}, \mathrm{idx}) \\
\mathrm{X}^{\ell+1} &= \tilde{\mathrm{X}}^\ell \odot (\tilde{\mathbf{y}} \mathbf{1}_\mathrm{C}^\mathrm{T})
\end{aligned}
$$

https://arxiv.org/abs/1905.05178

Whole Picture



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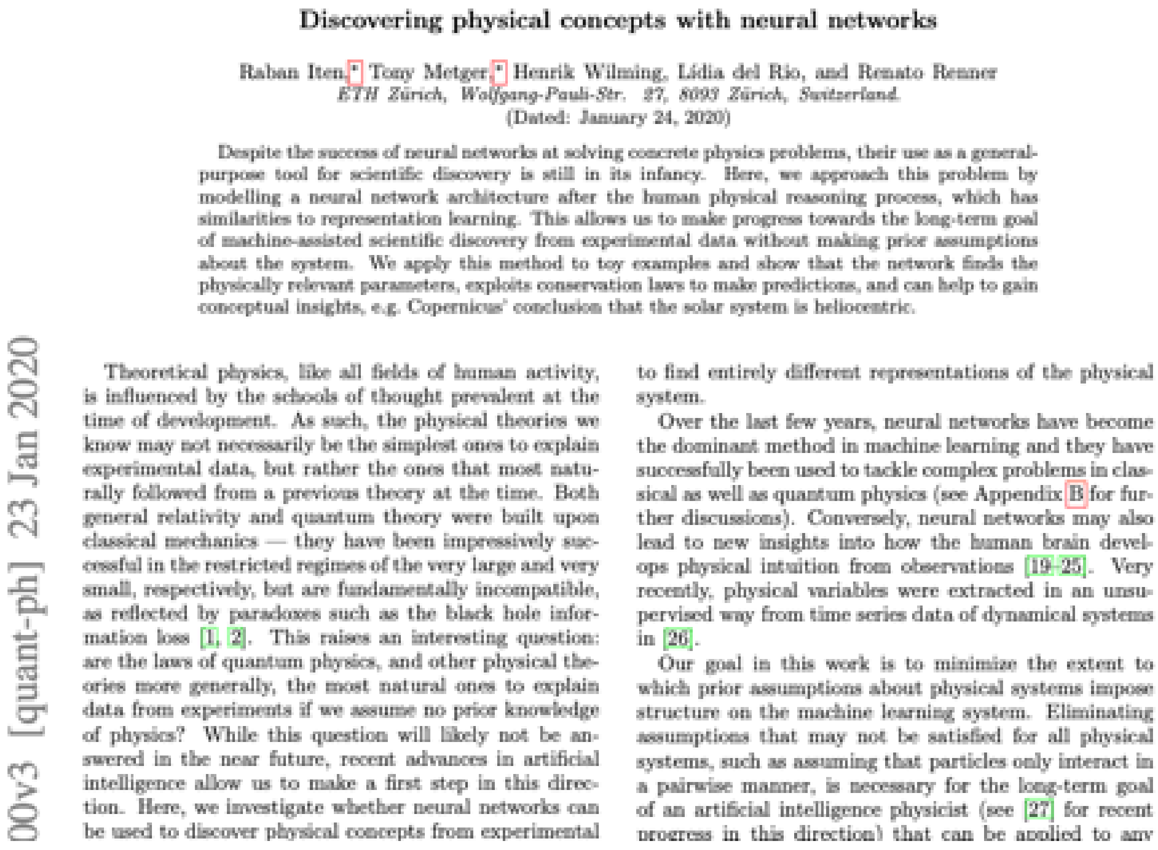
Learning More Effective Dynamics on Macro-scale



Discovering physical concepts with neural networks

Raban Iten,* Tony Metger,* Henrik Wilming, Lídia del Rio, and Renato Renner
ETH Zürich, Wolfgang-Pauli-Str. 27, 8093 Zürich, Switzerland.
(Dated: January 24, 2020)

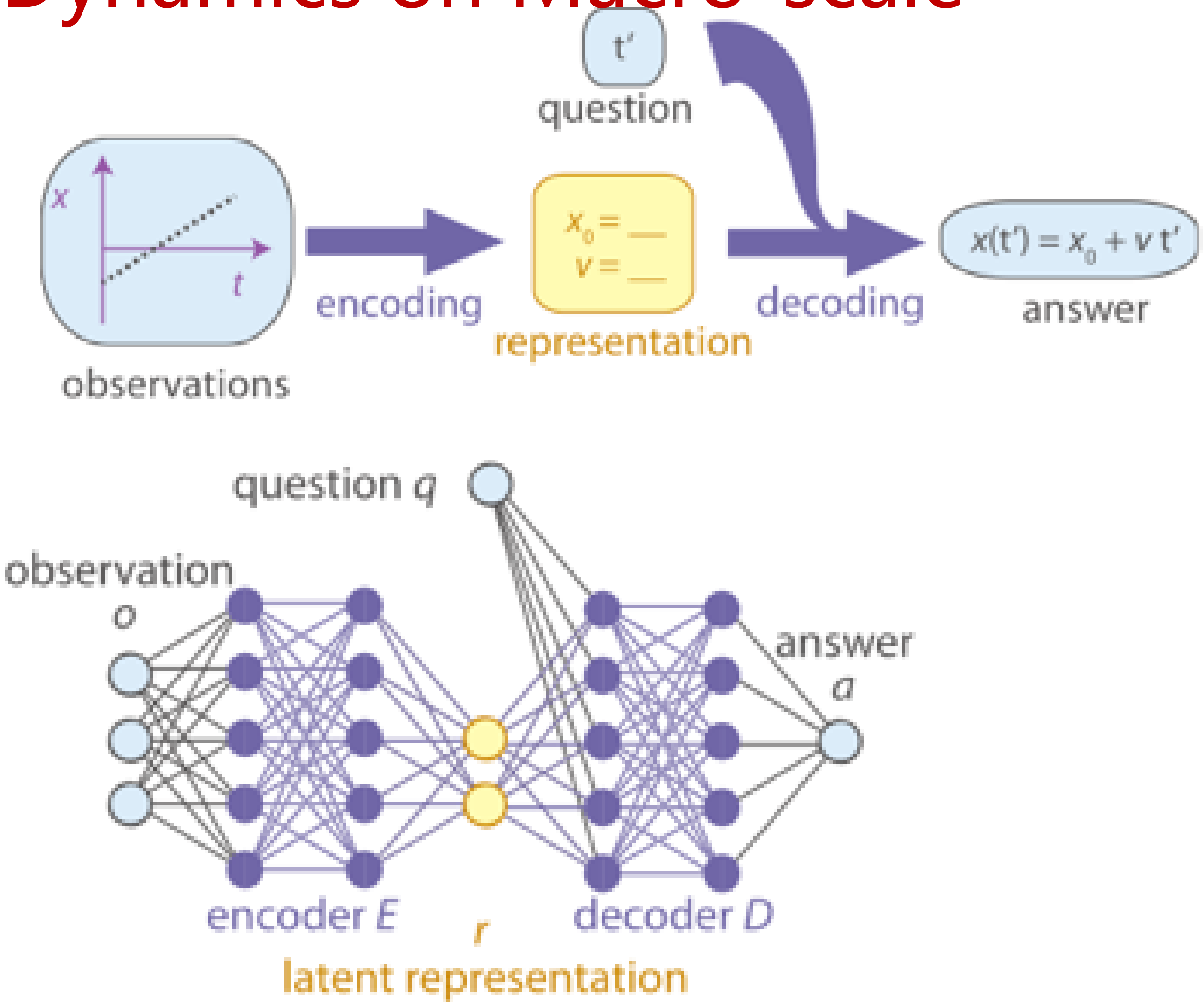
Despite the success of neural networks at solving concrete physics problems, their use as a general-purpose tool for scientific discovery is still in its infancy. Here, we approach this problem by modelling a neural network architecture after the human physical reasoning process, which has similarities to representation learning. This allows us to make progress towards the long-term goal of machine-assisted scientific discovery from experimental data without making prior assumptions about the system. We apply this method to toy examples and show that the network finds the physically relevant parameters, exploits conservation laws to make predictions, and can help to gain conceptual insights, e.g. Copernicus' conclusion that the solar system is heliocentric.

00v3 [quant-ph] 23 Jan 2020

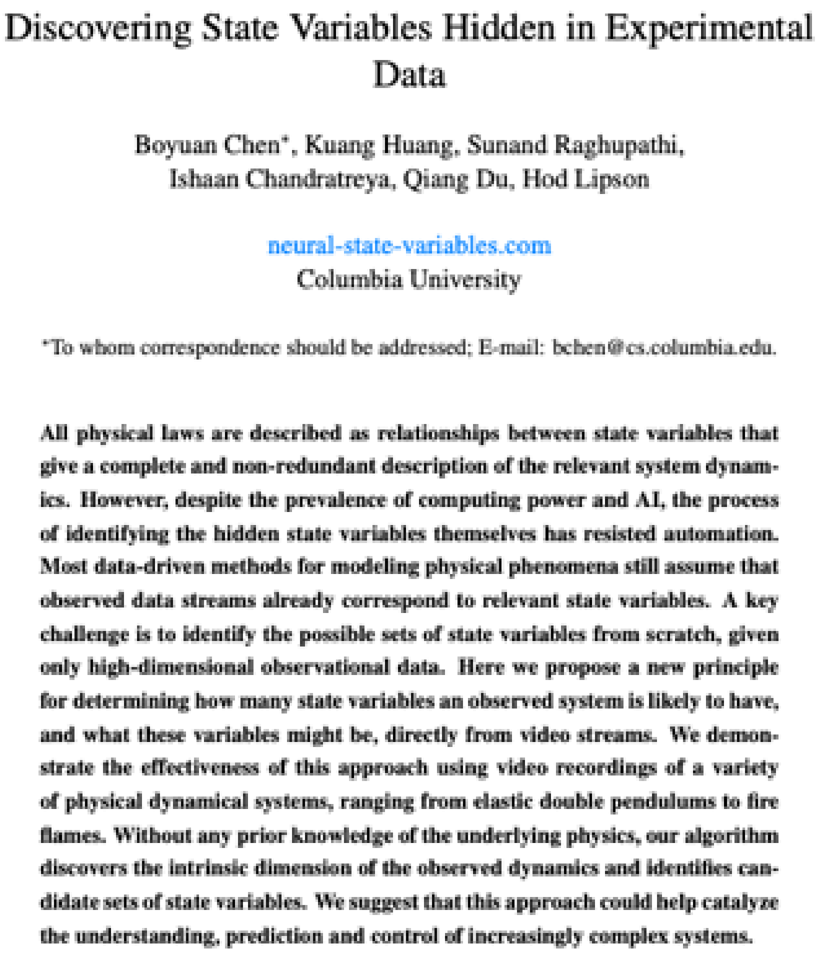
Theoretical physics, like all fields of human activity, is influenced by the schools of thought prevalent at the time of development. As such, the physical theories we know may not necessarily be the simplest ones to explain experimental data, but rather the ones that most naturally followed from a previous theory at the time. Both general relativity and quantum theory were built upon classical mechanics — they have been impressively successful in the restricted regimes of the very large and very small, respectively, but are fundamentally incompatible, as reflected by paradoxes such as the black hole information loss [1, 2]. This raises an interesting question: are the laws of quantum physics, and other physical theories more generally, the most natural ones to explain data from experiments if we assume no prior knowledge of physics? While this question will likely not be answered in the near future, recent advances in artificial intelligence allow us to make a first step in this direction. Here, we investigate whether neural networks can be used to discover physical concepts from experimental data to find entirely different representations of the physical system.

Over the last few years, neural networks have become the dominant method in machine learning and they have successfully been used to tackle complex problems in classical as well as quantum physics (see Appendix B for further discussions). Conversely, neural networks may also lead to new insights into how the human brain develops physical intuition from observations [19–25]. Very recently, physical variables were extracted in an unsupervised way from time series data of dynamical systems in [26].

Our goal in this work is to minimize the extent to which prior assumptions about physical systems impose structure on the machine learning system. Eliminating assumptions that may not be satisfied for all physical systems, such as assuming that particles only interact in a pairwise manner, is necessary for the long-term goal of an artificial intelligence physicist (see [27] for recent progress in this direction) that can be applied to any



Learning More Effective Dynamics on Macro-scale



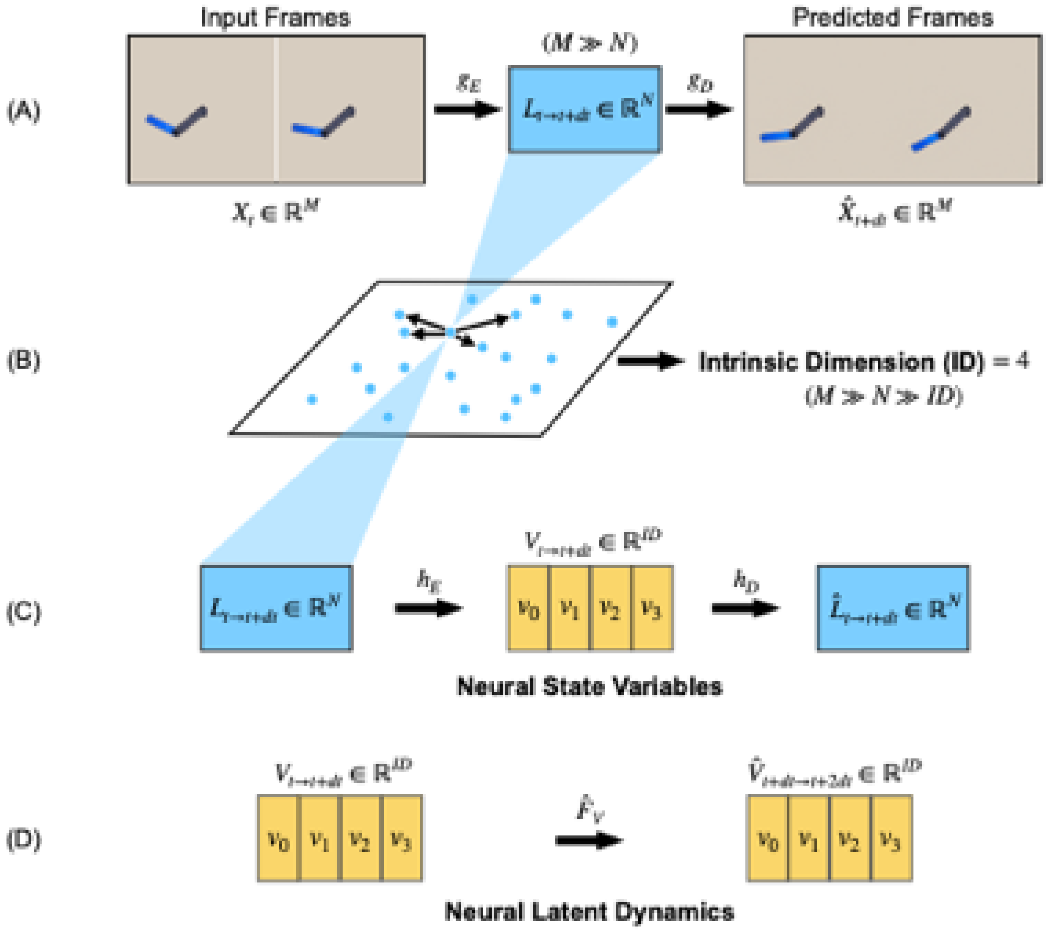
Discovering State Variables Hidden in Experimental Data

Boyuan Chen*, Kuang Huang, Sunand Raghupathi, Ishaan Chandratreya, Qiang Du, Hod Lipson

neural-state-variables.com
Columbia University

*To whom correspondence should be addressed; E-mail: bchen@cs.columbia.edu.

All physical laws are described as relationships between state variables that give a complete and non-redundant description of the relevant system dynamics. However, despite the prevalence of computing power and AI, the process of identifying the hidden state variables themselves has resisted automation. Most data-driven methods for modeling physical phenomena still assume that observed data streams already correspond to relevant state variables. A key challenge is to identify the possible sets of state variables from scratch, given only high-dimensional observational data. Here we propose a new principle for determining how many state variables an observed system is likely to have, and what these variables might be, directly from video streams. We demonstrate the effectiveness of this approach using video recordings of a variety of physical dynamical systems, ranging from elastic double pendulums to fire flames. Without any prior knowledge of the underlying physics, our algorithm discovers the intrinsic dimension of the observed dynamics and identifies candidate sets of state variables. We suggest that this approach could help catalyze the understanding, prediction and control of increasingly complex systems.



https://arxiv.org/abs/2112.10755

Learning More Effective Dynamics on Macro-scale

STABILITY PRESERVING DATA-DRIVEN MODELS WITH LATENT DYNAMICS

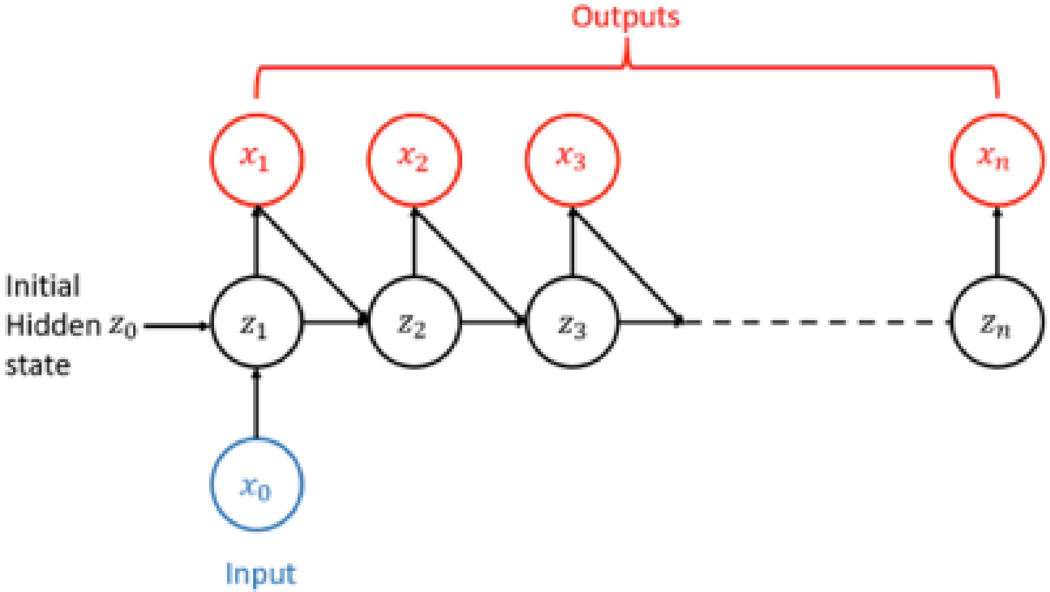
YUSHUANG LUO AND XIANTAO LI AND WENRUI HAO

ABSTRACT. In this paper we introduce a data-driven modeling approach for dynamics problem with latent variables. The state space of the proposed model includes artificial latent variables, in addition to observed variables that can be fit to a given data set. We present a model framework where the stability of the coupled dynamics can be easily enforced. The model is implemented by recurrent cells and trained using back propagation through time. Numerical examples using benchmark tests from order reduction problems demonstrate the stability of the model and the efficiency of the recurrent cell implementation. As applications, two fluid-structure interaction problems are considered to illustrate the accuracy and predictive capability of the model.

1. INTRODUCTION

Forecasting the long-time behavior of a complex system based on short-time data series is a long-standing problem in many scientific domains, e.g., spacecraft designing [1] and meteorology [2]. One particular challenge is due to the fact that there are hidden (latent) dynamics that are not directly observed. More specifically, the dynamics of the observed quantities is the result of continuous interactions with the latent dynamics. In addition, choosing an appropriate ODE model to fit is also crucial to the effectiveness of the method. One well established framework for constructing an effective model is reduced-order modeling (ROM), where one starts with an underlying full-order model (FOM), and derive an a reduced model, often by subspace projections [3, 4, 5]. With certain guaranteed approximation properties, the reduced models are able to efficiently capture the input-output

rXiv:2204.11744v1 [math.OC] 20 Apr 2022



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Learning More Effective Dynamics on Macro-scale

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Multiscale simulations of complex systems by learning their effective dynamics

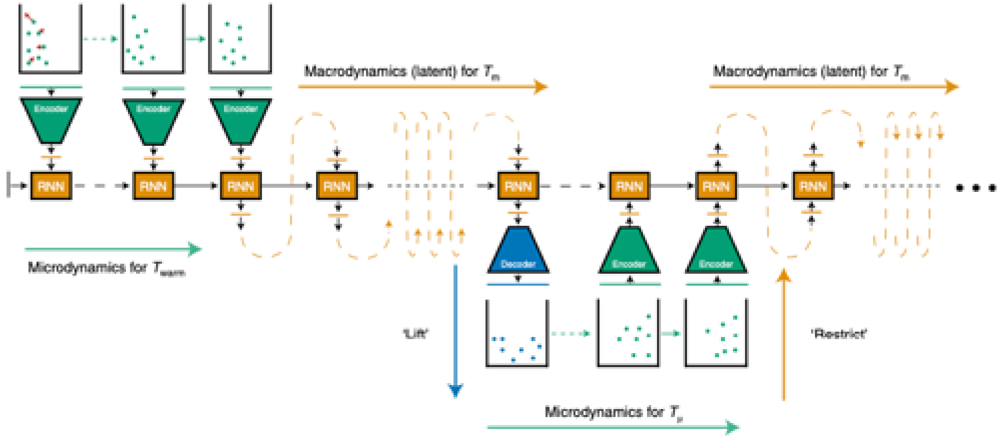
Pantelis R. Vlachas[1,2], Georgios Arampatzis[1,2], Caroline Uhler[3] and Petros Koumoutsakos[1,2] ✉

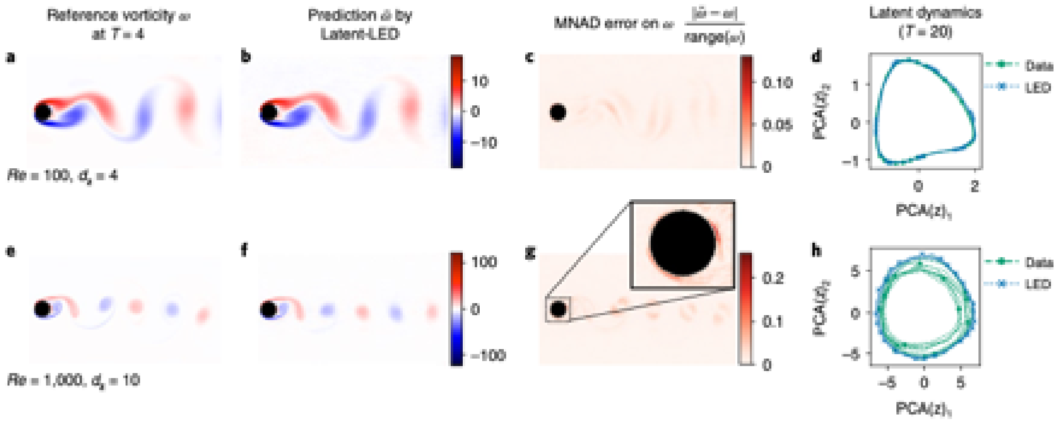
Predictive simulations of complex systems are essential for applications ranging from weather forecasting to drug design. The veracity of these predictions hinges on their capacity to capture effective system dynamics. Massively parallel simulations predict the system dynamics by resolving all spatiotemporal scales, often at a cost that prevents experimentation, while their findings may not allow for generalization. On the other hand, reduced-order models are fast but limited by the frequently adopted linearization of the system dynamics and the utilization of heuristic closures. Here we present a novel systematic framework that bridges large-scale simulations and reduced-order models to learn the effective dynamics of diverse, complex systems. The framework forms algorithmic alloys between nonlinear machine learning algorithms and the equation-free approach for modelling complex systems. Learning the effective dynamics deploys autoencoders to formulate a mapping between fine- and coarse-grained representations and evolves the latent space dynamics using recurrent neural networks. The algorithm is validated on benchmark problems, and we find that it outperforms state-of-the-art reduced-order models in terms of predictability, and large-scale simulations in terms of cost. Learning the effective dynamics is applicable to systems ranging from chemistry to fluid mechanics and reduces the computational effort by up to two orders of magnitude while maintaining the prediction accuracy of the full system dynamics. We argue that learning the effective dynamics provides a potent novel modality for accurately predicting complex systems.

Some of the most important scientific advances and engineering designs are founded on the study of complex systems that exhibit dynamics spanning multiple spatiotemporal scales. Examples include protein dynamics[1], morphogenesis[2], brain dynamics[3], climate[4], ocean dynamics[5] and social systems[6]. Over the last 50 years, simulations have become a key component of these studies thanks to a confluence of advances in computing architectures, numerical methods and software. Large-scale simulations have led to unprecedented insight, acting as in silico microscopes[7] or telescopes to reveal the dynamics of galaxy formations[8]. At the same time, these simulations have led to the understanding that resolving the full range of spatiotemporal scales in such complex systems will remain out of reach for the foreseeable future.

In recent years there have been intense efforts to develop effi- dynamics. The fine-scale dynamics are obtained by judiciously 'lifting' the coarse scales to return to the fine-scale description of the system and repeat. When the EFF reproduces trajectories of the original system, the identified low-order dynamics represent the intrinsic system dynamics, also called effective dynamics, inertial manifold[18,19] or reaction coordinates in molecular kinetics.

While it is undisputed that the EFF, HMM, FLAVOR and related frameworks have revolutionized the field of multiscale modelling and simulation, we identify two critical issues that currently limit their potential. First, the accuracy of propagating the coarse-grained/latent dynamics hinges on the employed time integrators. Second, the choice of information transfer, particularly from coarse- to fine-scale dynamics in lifting, affects the forecasting capacity of the methods.





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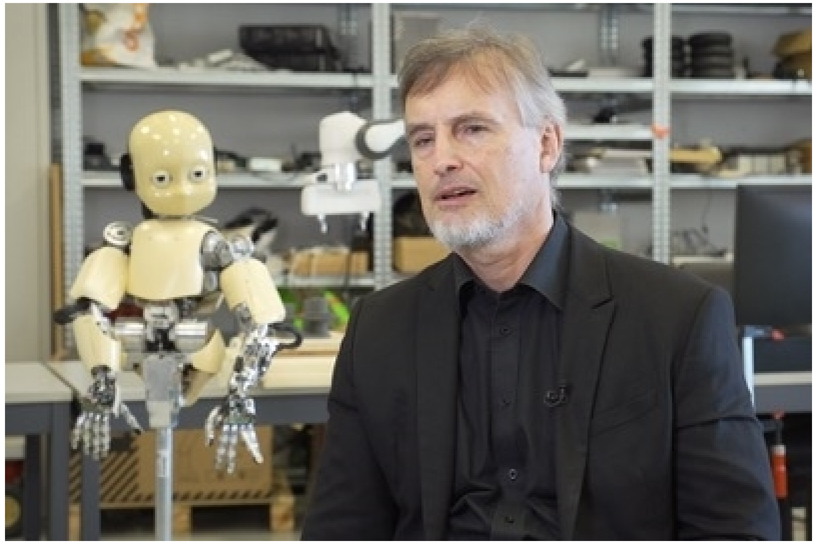
World Models



World Models

David Ha [1] Jürgen Schmidhuber [2 3]

Abstract

We explore building generative neural network models of popular reinforcement learning environments. Our *world model* can be trained quickly in an unsupervised manner to learn a compressed spatial and temporal representation of the environment. By using features extracted from the world model as inputs to an agent, we can train a very compact and simple policy that can solve the required task. We can even train our agent entirely inside of its own hallucinated dream generated by its world model, and transfer this policy back into the actual environment.

An interactive version of this paper is available at `https://worldmodels.github.io`

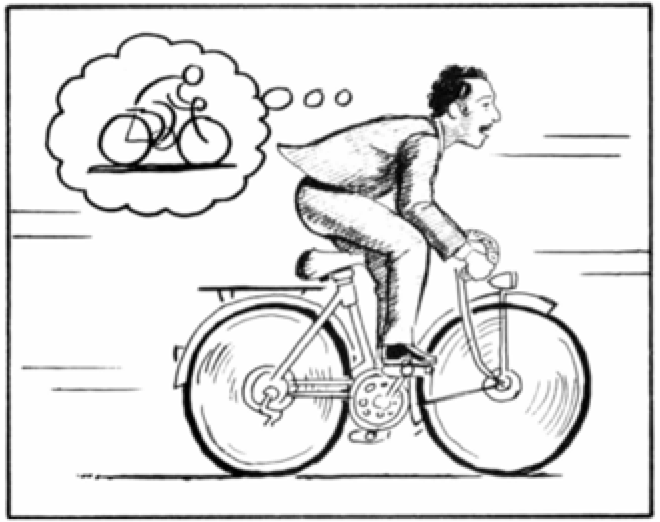
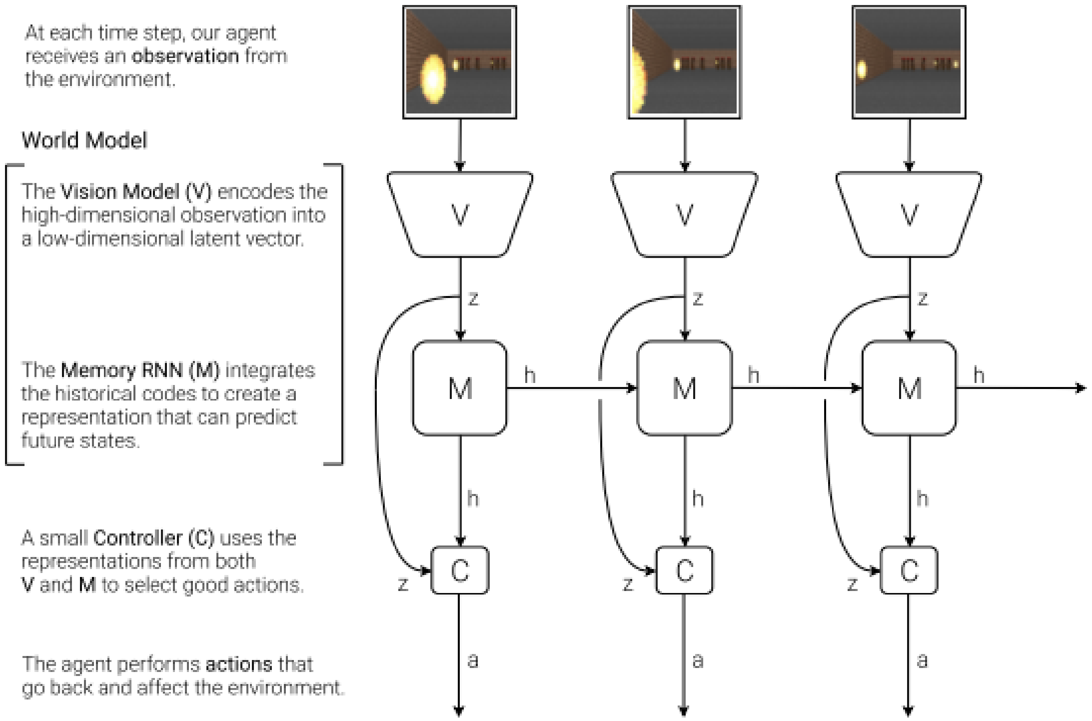
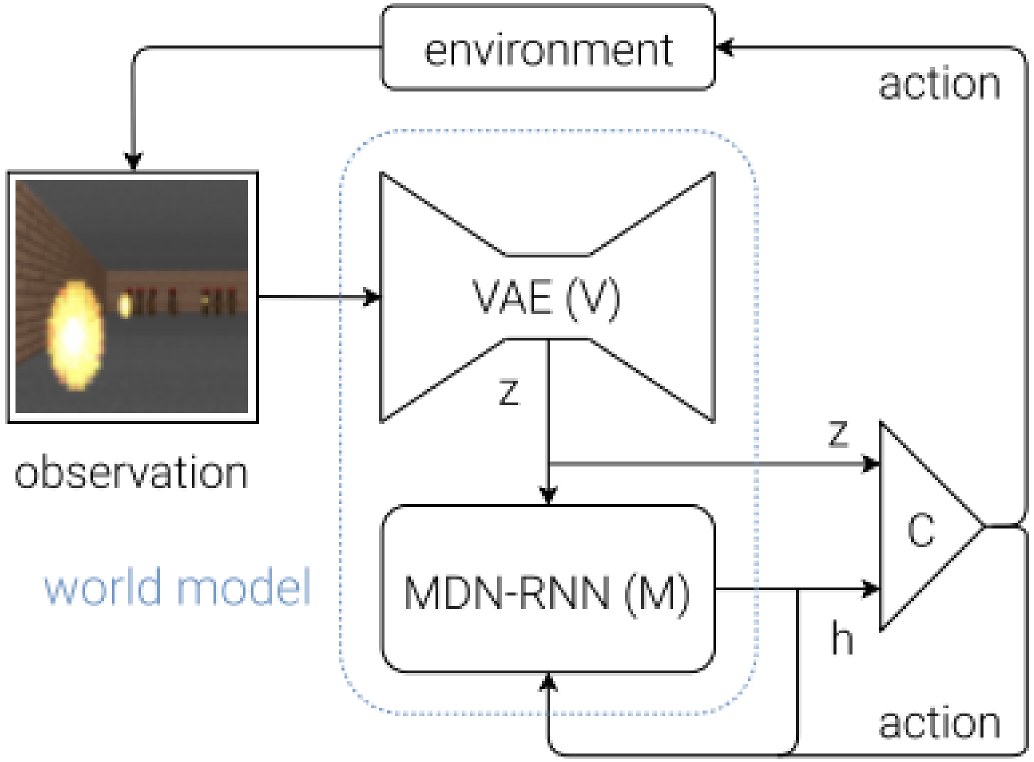


Figure 1. A World Model, from Scott McCloud's *Understanding Comics.* (McCloud, 1993; E, 2012)

https://arxiv.org/pdf/1803.10122.pdf

World Models



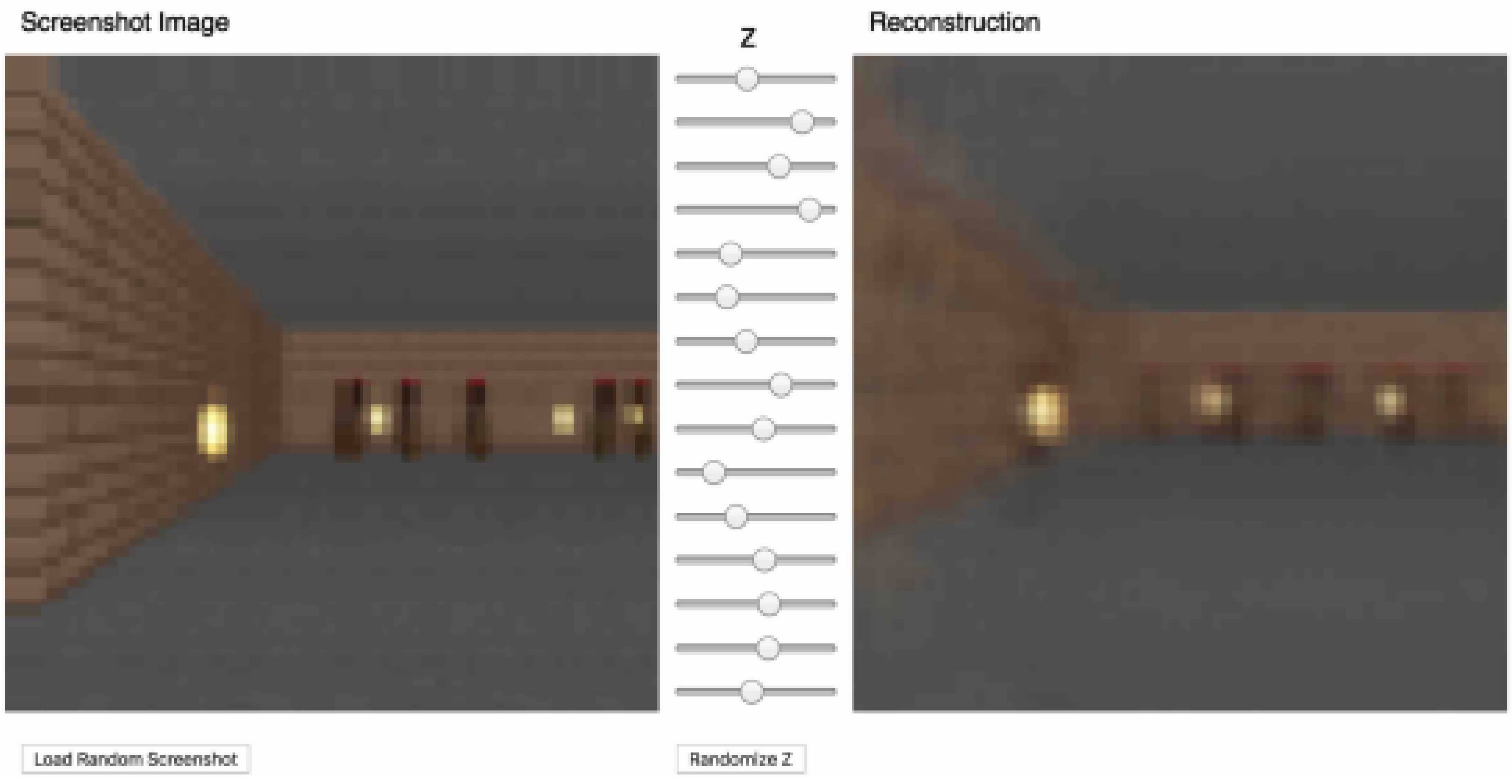


https://arxiv.org/pdf/1803.10122.pdf

World Models

1. Collect 10,000 rollouts from a random policy.
2. Train VAE (V) to encode each frame into a latent vector $z \in \mathcal{R}^{64}$, and use V to convert the images collected from (1) into the latent space representation.
3. Train MDN-RNN (M) to model $P(z_{t+1}, d_{t+1} \mid a_t, z_t, h_t)$.
4. Define Controller (C) as $a_t = W_c\ [z_t\ h_t]$.
5. Use CMA-ES to solve for a W_c that maximizes the expected survival time inside the virtual environment.
6. Use learned policy from (5) on actual environment.

MODEL	PARAMETER COUNT
VAE	4,446,915
MDN-RNN	1,678,785
CONTROLLER	1,088



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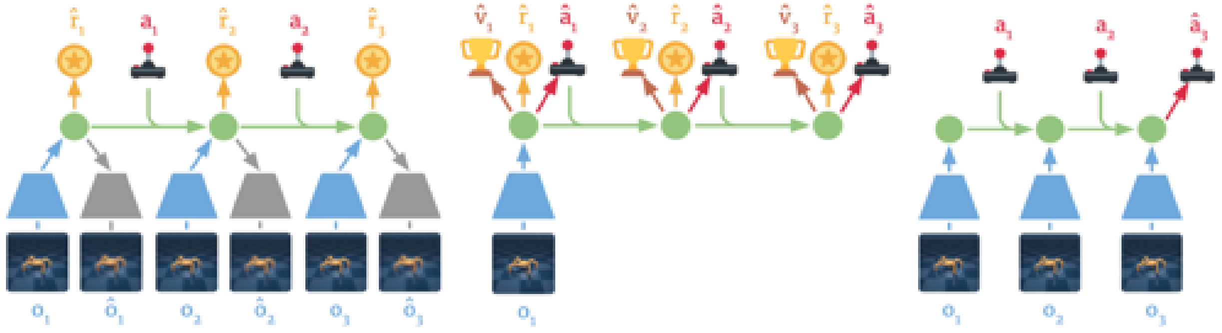
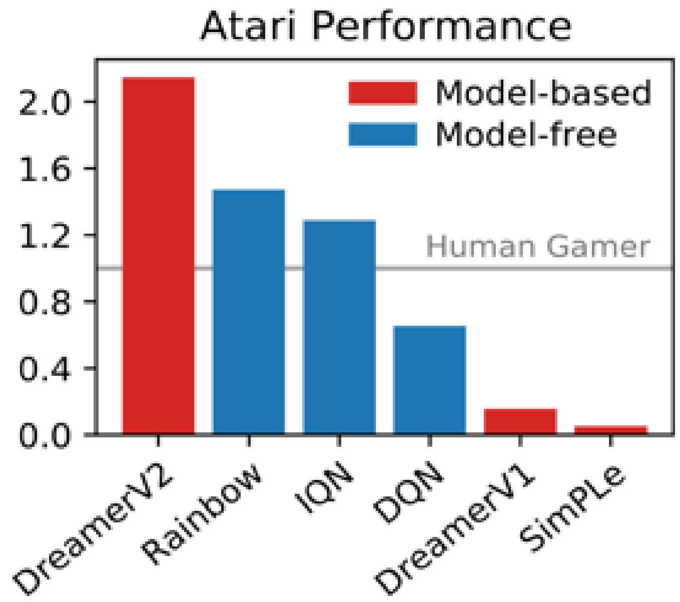
Dreamers

Components of DreamerV1:



(a) Learn dynamics from experience (b) Learn behavior in imagination (c) Act in the environment

DreamerV2 is the first agent that learns purely within a world model to achieve human-level Atari performance



Atari benchmark of 55 games with sticky actions at 200M steps.

Model improvement?

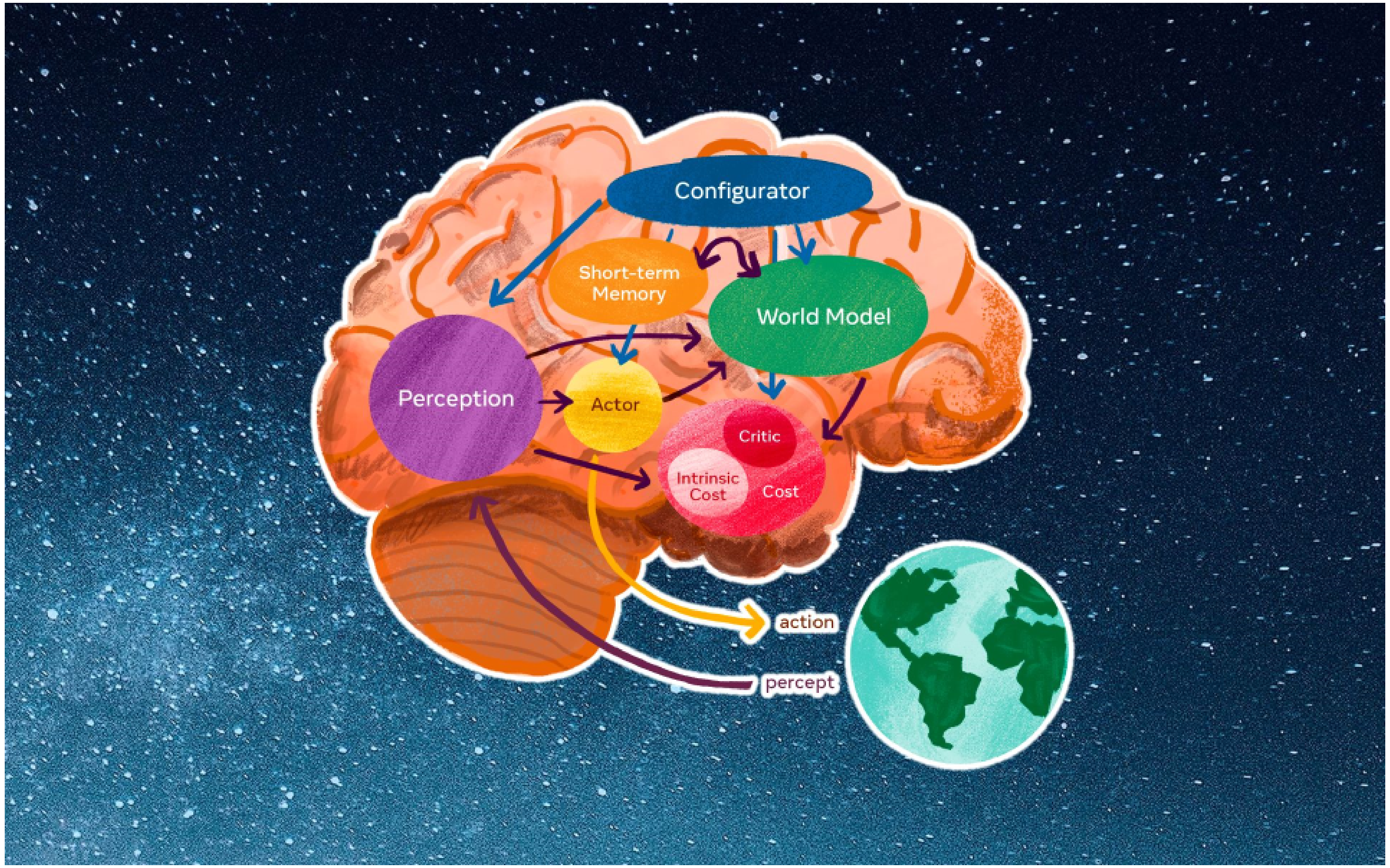
- change Gaussian latents to categorical variables.
- balancing terms within the KL loss

【DreamerV2 ICLR2021】 Hafner D, Lillicrap T, Norouzi M, et al. Mastering atari with discrete world models[J]. arXiv preprint arXiv:2010.02193, 2020.

【DreamerV1 ICLR2020】 Hafner D, Lillicrap T, Ba J, et al. Dream to control: Learning behaviors by latent imagination[J]. arXiv preprint arXiv:1912.01603, 2019.

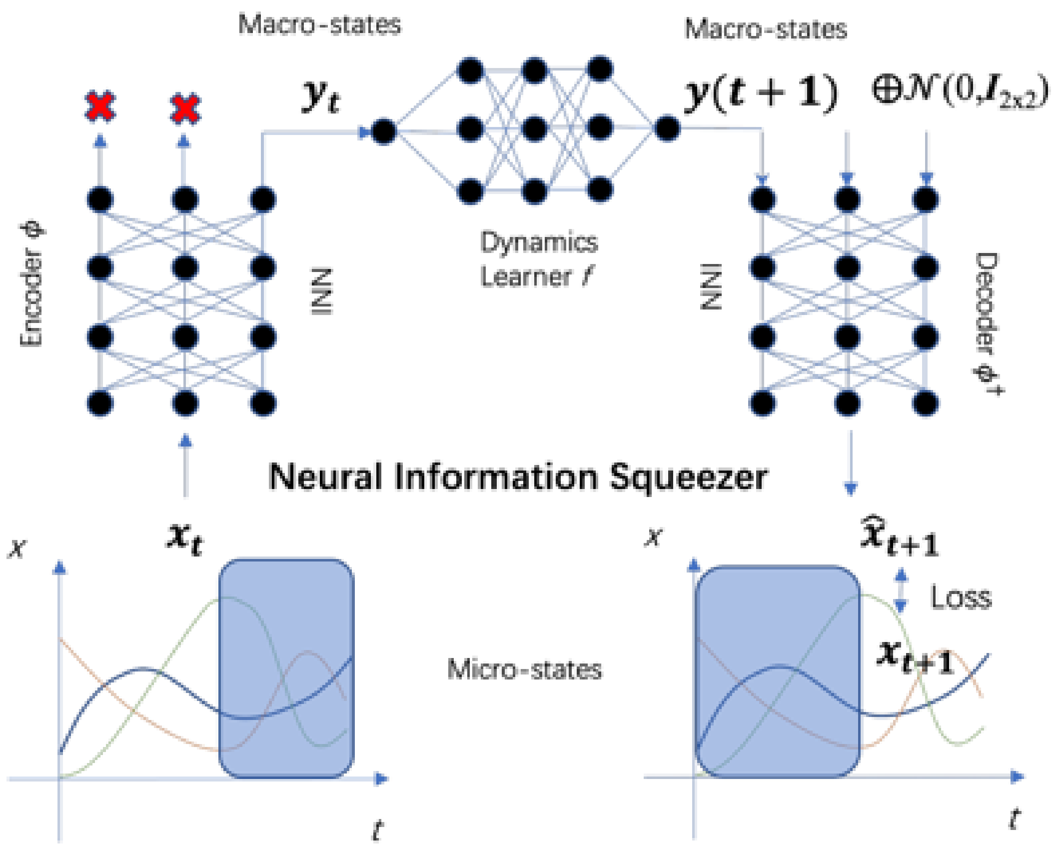
https://arxiv.org/pdf/1912.01603.pdf

Yann Lecun’ s world model



https://openreview.net/pdf?id=BZ5a1r-kVsf

Neural Information Squeezer

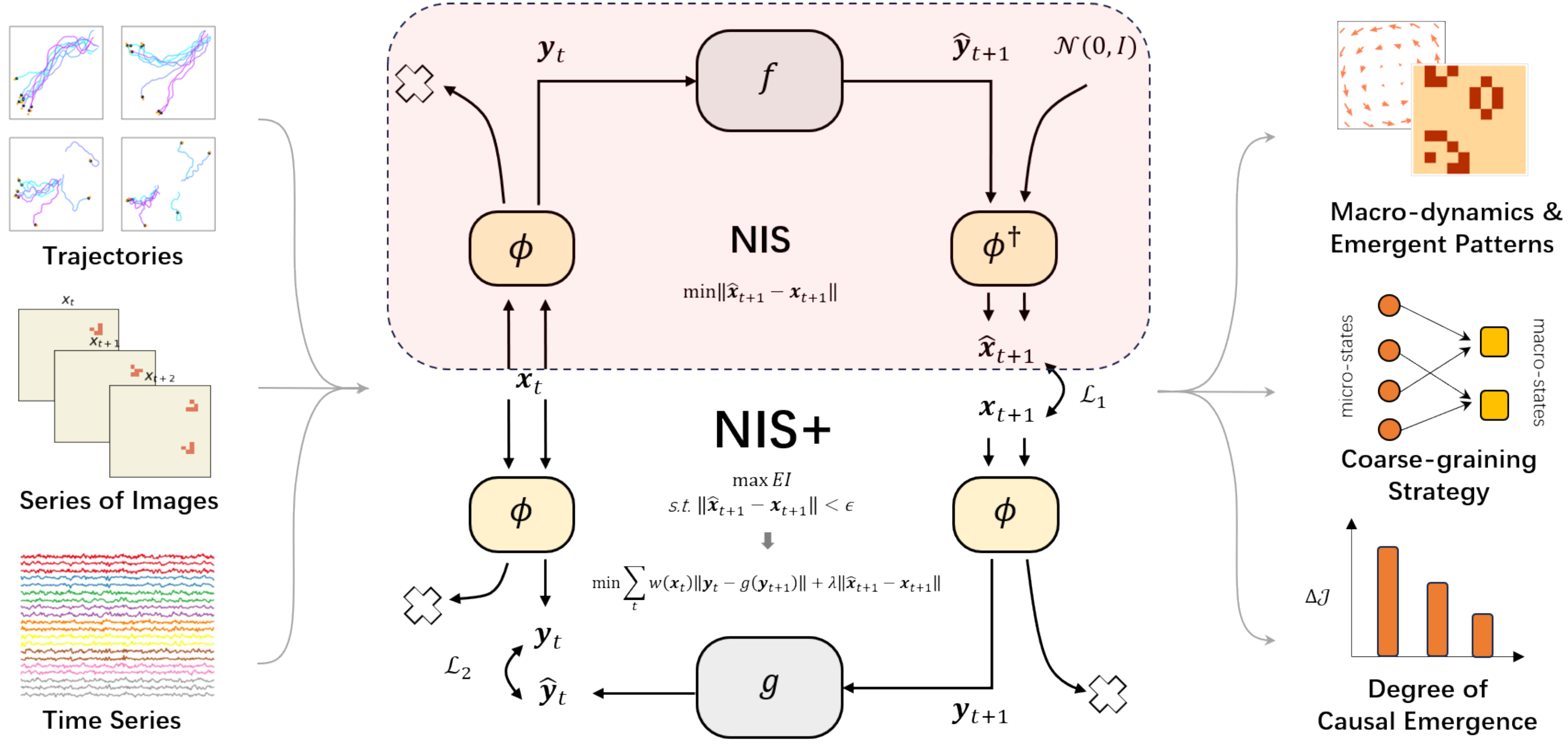


$$\max_{\psi,g,M} EI(g)$$

$$s.t. \left\| {\psi_\alpha}^{-1}\left[g_\beta\left(\chi(\psi_\alpha(X_t))\right), \xi_t\right] - X_{t+1} \right\| < \epsilon$$

https://arxiv.org/abs/2201.10154

Neural Information Squeezer +



(a). Input (b). Framework (c). Output

Yang et al. Finding emergence in data by maximizing effective information

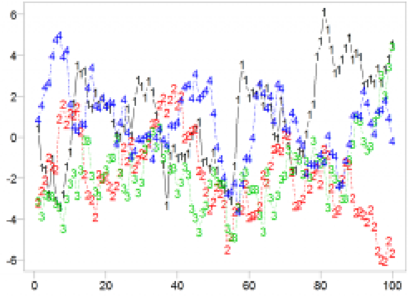
Outline

- AI for complex systems
  - Complex Systems and Modelling Methods
  - Representation & Generation
  - Dynamics Learning
  - Network Reconstruction
  - Multi-scale Modelling
  - Simulation, optimization, and control
- Complexity science for AI

Automated Modelling of Complex Systems

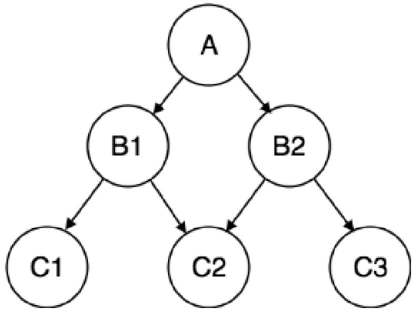
Complex System

Behavior (observations)



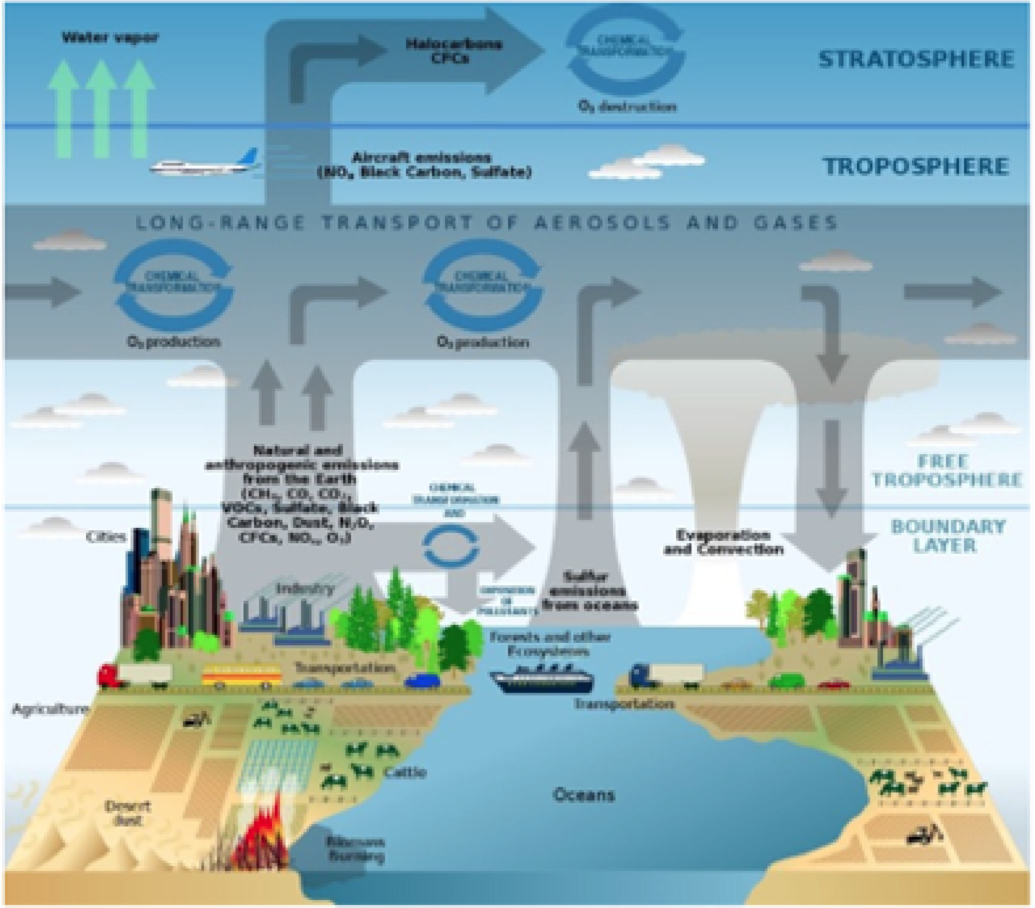
AI systems

Models

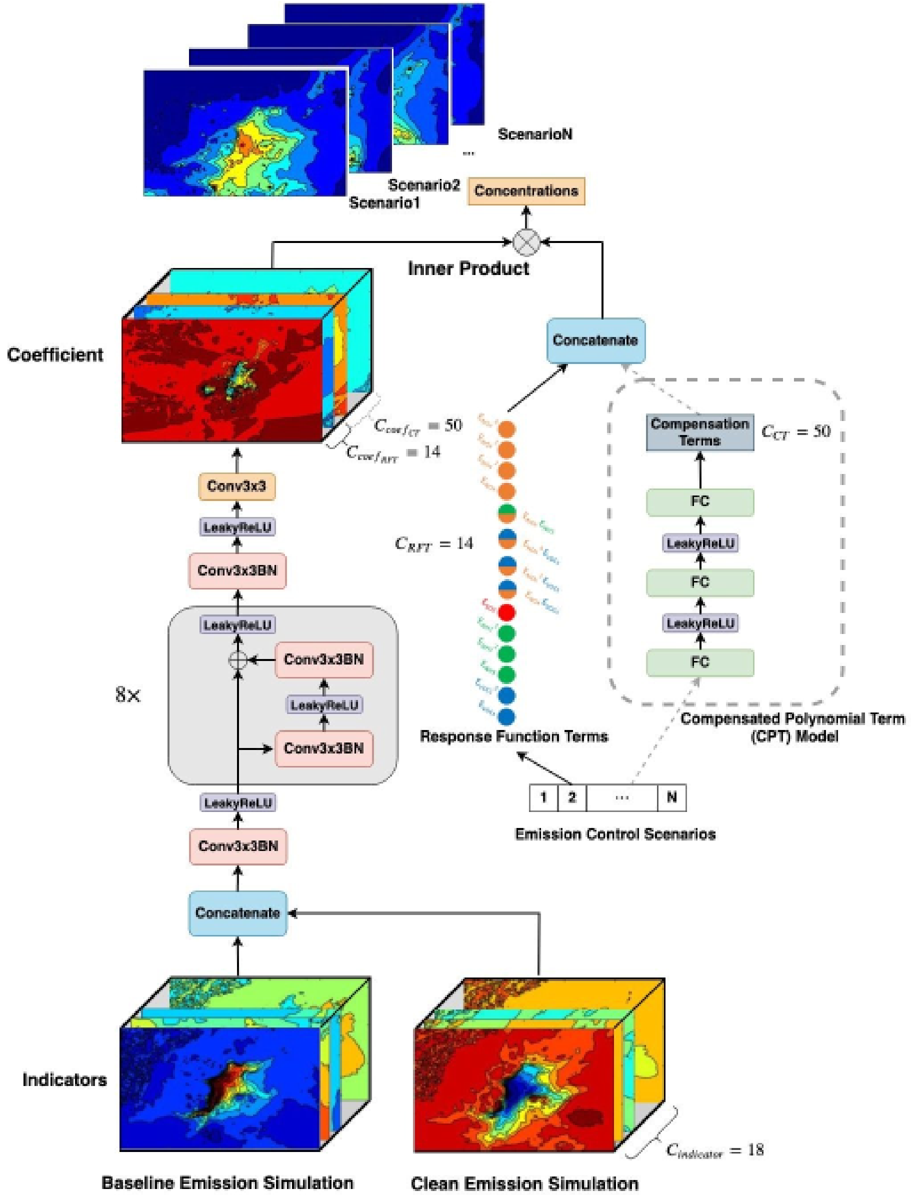


Prediction, Simulation,
Optimization, Controls

Surrogate Model - DeepRSM

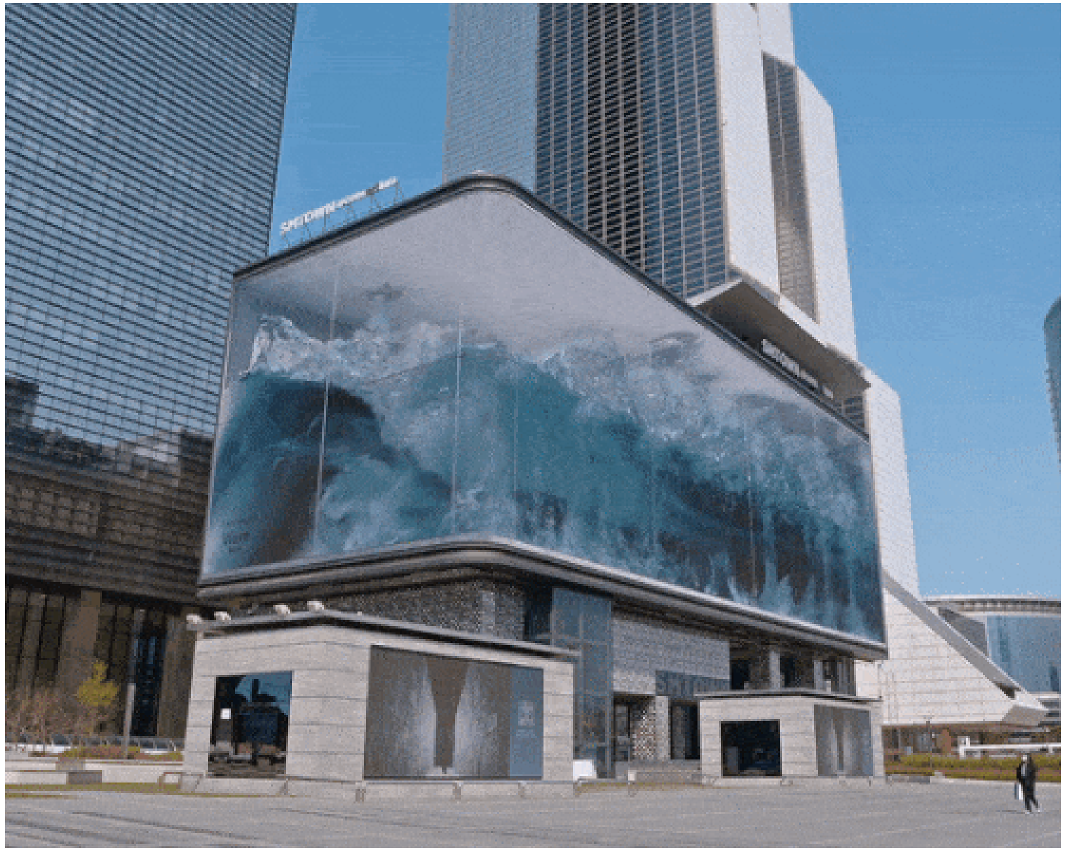


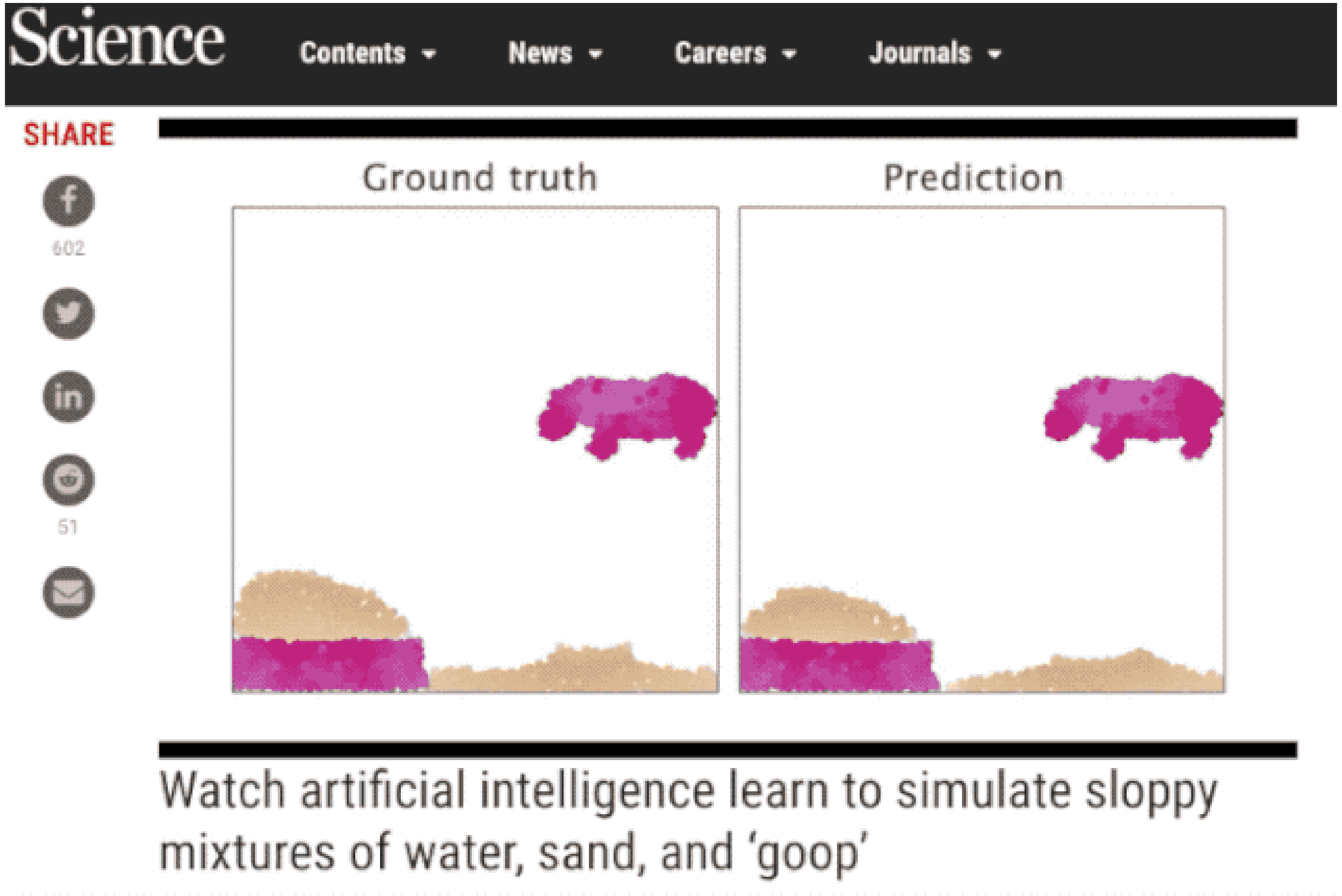
大气化学传输模型（CTM）



[1] Xing J, Zheng S, Ding D, et al. Deep learning for prediction of the air quality response to emission changes[J]. Environmental Science & Technology, 2020.
[2] Cohen A J, Brauer M, Burnett R, et al. Estimates and 25-year trends of the global burden of disease attributable to ambient air pollution: an analysis of data from the Global Burden of Diseases Study 2015[J]. The Lancet, 2017, 389(10082): 1907-1918.

Learning to Simulate Complex Physics with Graph Networks





https://arxiv.org/abs/2002.09405

Influence maximization problem

- Finding the most **significant node** such that the influence could be maximized under the constraints of resource