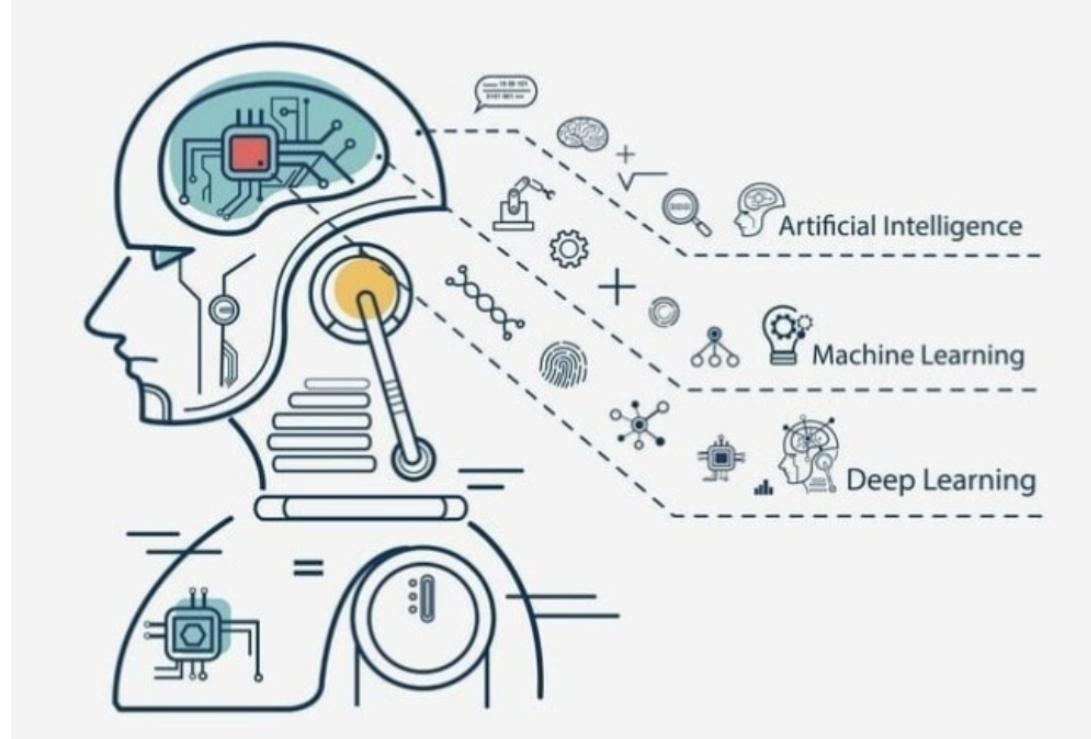


# AI and Complex Systems



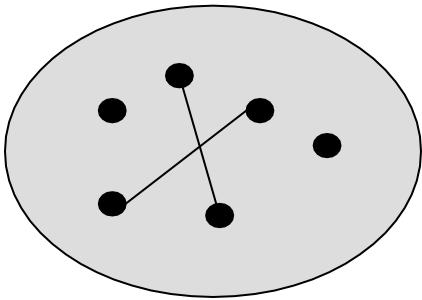
张江

北京师范大学系统科学学院教授  
集智俱乐部、集智学园创始人  
集智研究中心理事长

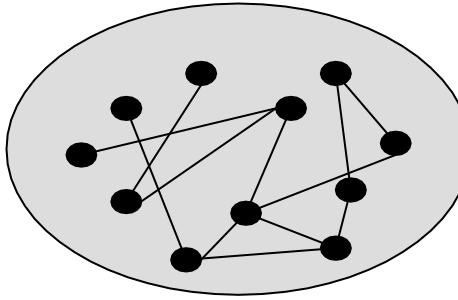
# What are Complex Systems?



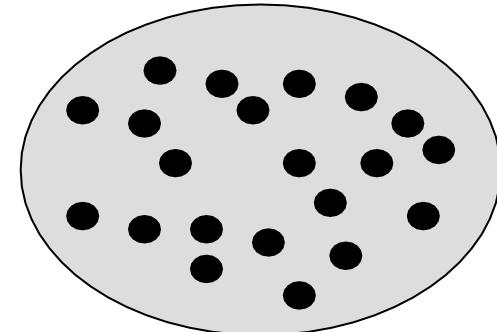
# What are Complex Systems?



简单系统



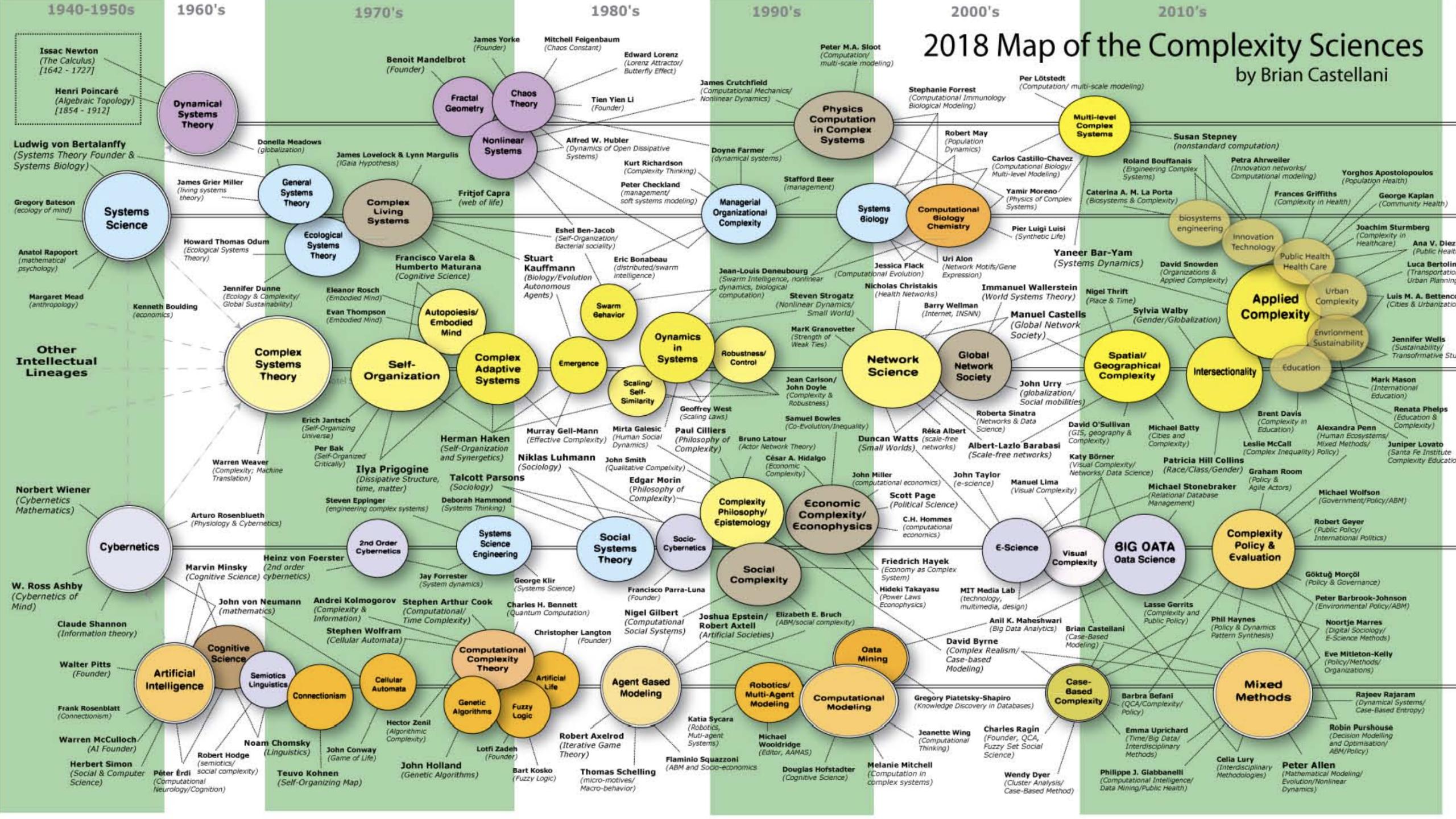
复杂系统



无组织的随机系统

# What is complexity science?





# (复杂) 系统科学的演进



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# What is complexity science?

涌现

统一性

统计

计算

适应性

随机

自相似

混沌

自组织

系统

非线性

反馈

量子

开放性

进化

整体论

适应

分形

混沌

演化

长程关联

网络

博弈

统计物理

还原论

优化

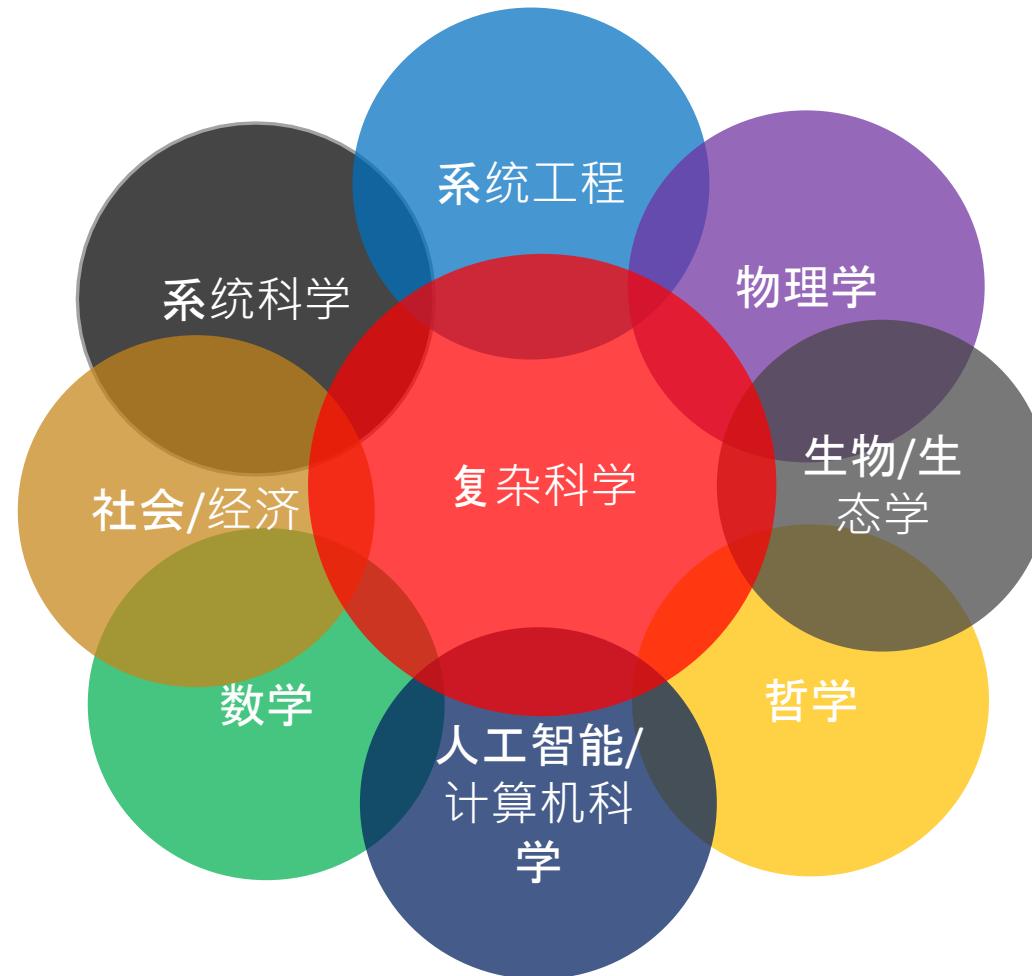
函数

平衡

对称



# What is complexity science?



# Outline

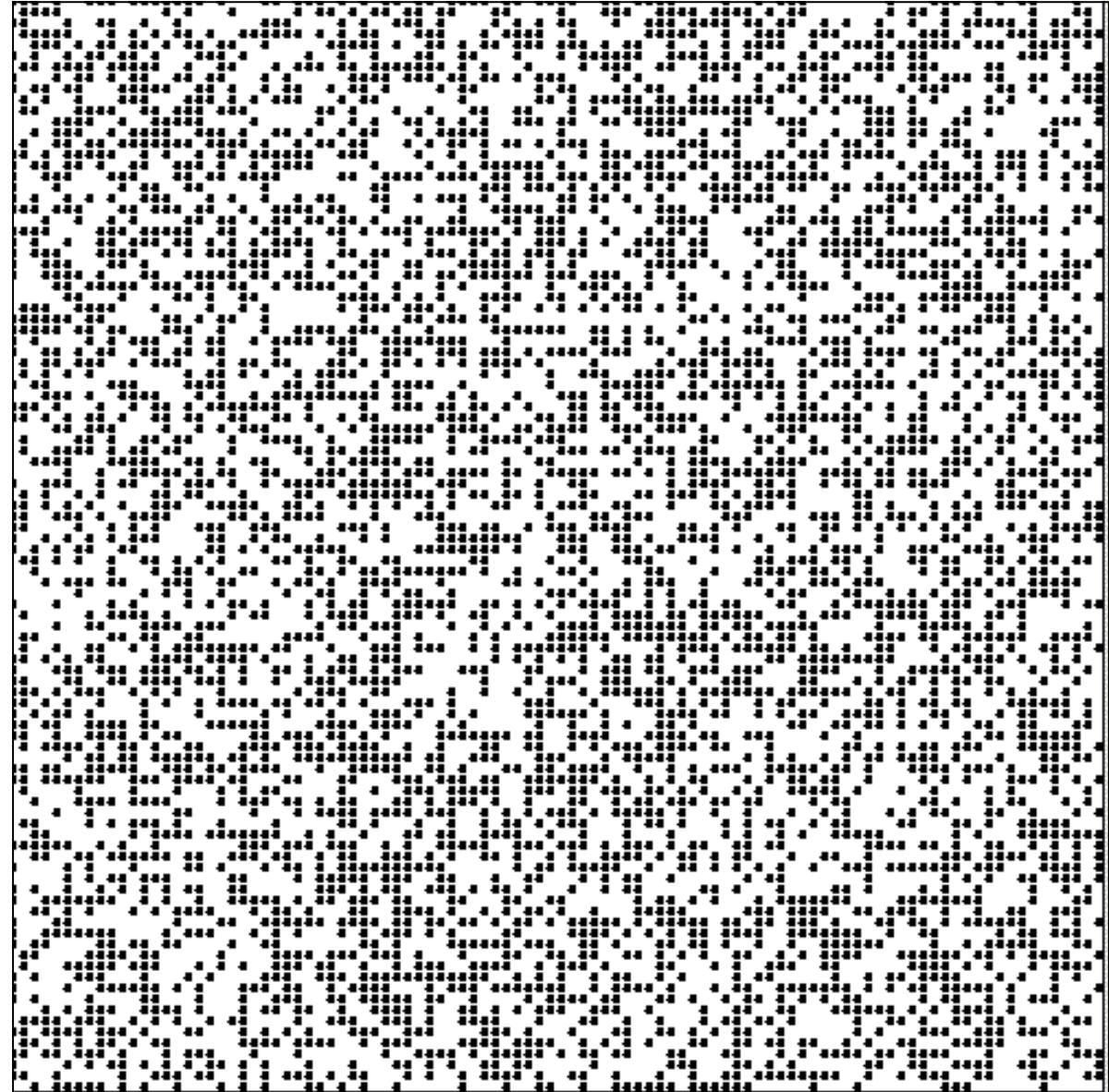
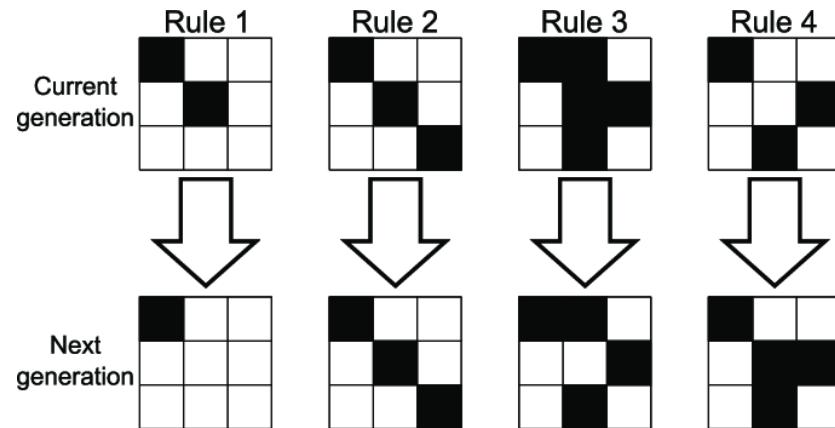
- AI for complex systems
- Complexity science for AI

# 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

# Game of Life

- Conway's GAME of LIFE
- Each cell has 8 neighbors
- Change color according to neighbors
- Studying complexity

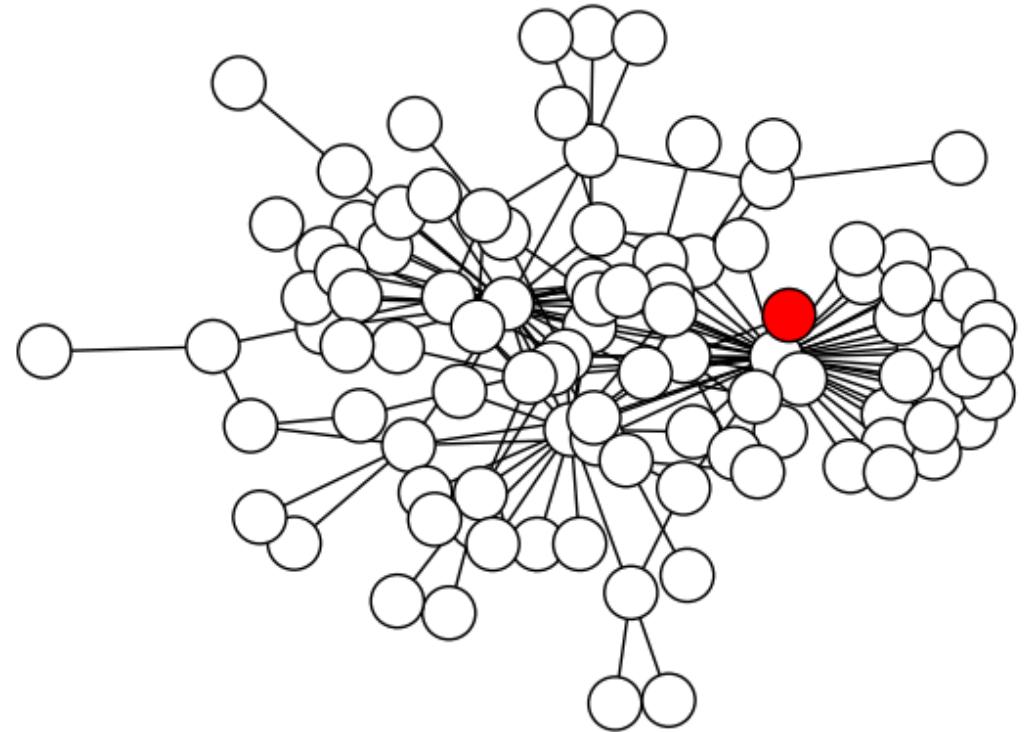


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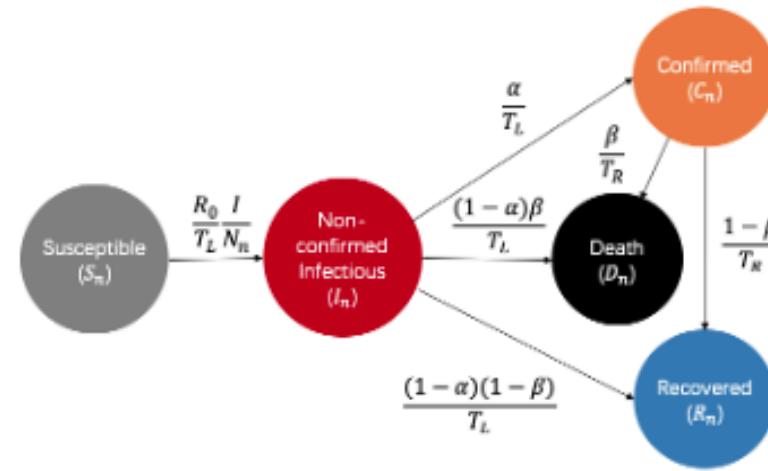
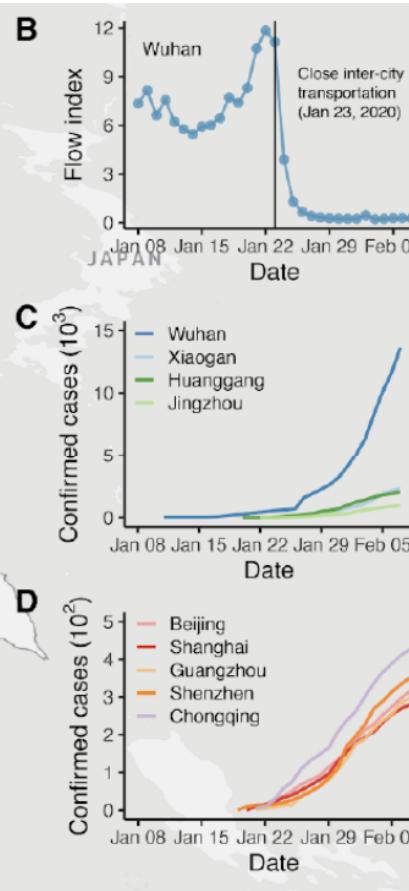
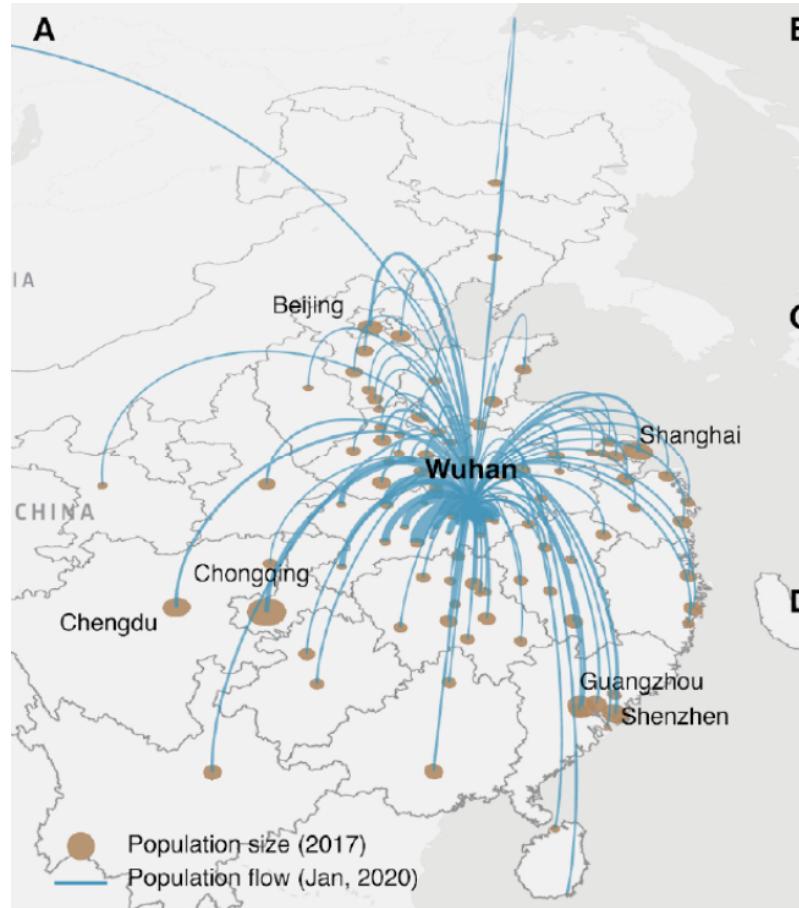
# SIR on Network

First infection = neighbour of highest degree node  
time = 0

- SIR model
- S node (white) can be infected by the infectious node (red)
- Infectious node can turn to recovered (grey)



# Epidemic



$$\frac{\partial s_n}{\partial t} = -\frac{R_0}{T_L} s_n i_n + \omega \sum_{m \neq n} P_{mn} (s_m - s_n)$$

$$\frac{\partial i_n}{\partial t} = \frac{R_0}{T_L} s_n i_n - \frac{\alpha}{T_L} i_n - \frac{1-\alpha}{T_L} i_n + \omega \sum_{m \neq n} P_{mn} (i_m - i_n)$$

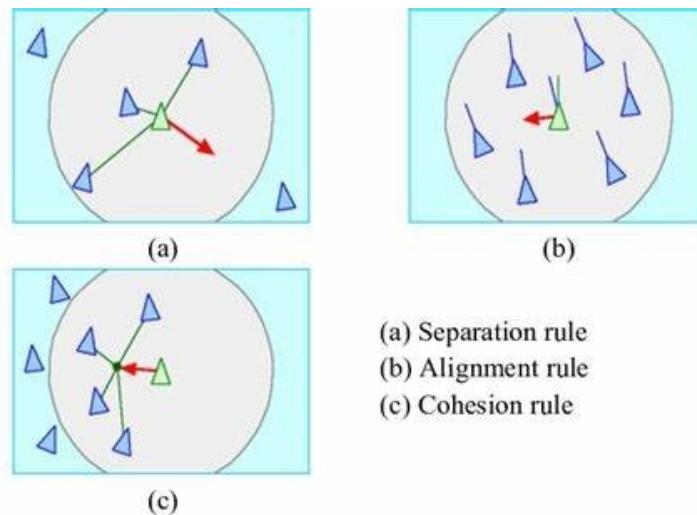
$$\frac{\partial c_n}{\partial t} = \frac{\alpha}{T_L} i_n - \frac{1}{T_R} c_n$$

$$\frac{\partial d_n}{\partial t} = \frac{\beta(1-\alpha)}{T_L} i_n + \frac{\beta}{T_R} c_n$$

$$r_n = 1 - s_n - j_n - c_n - d_n$$

# Boid Model

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



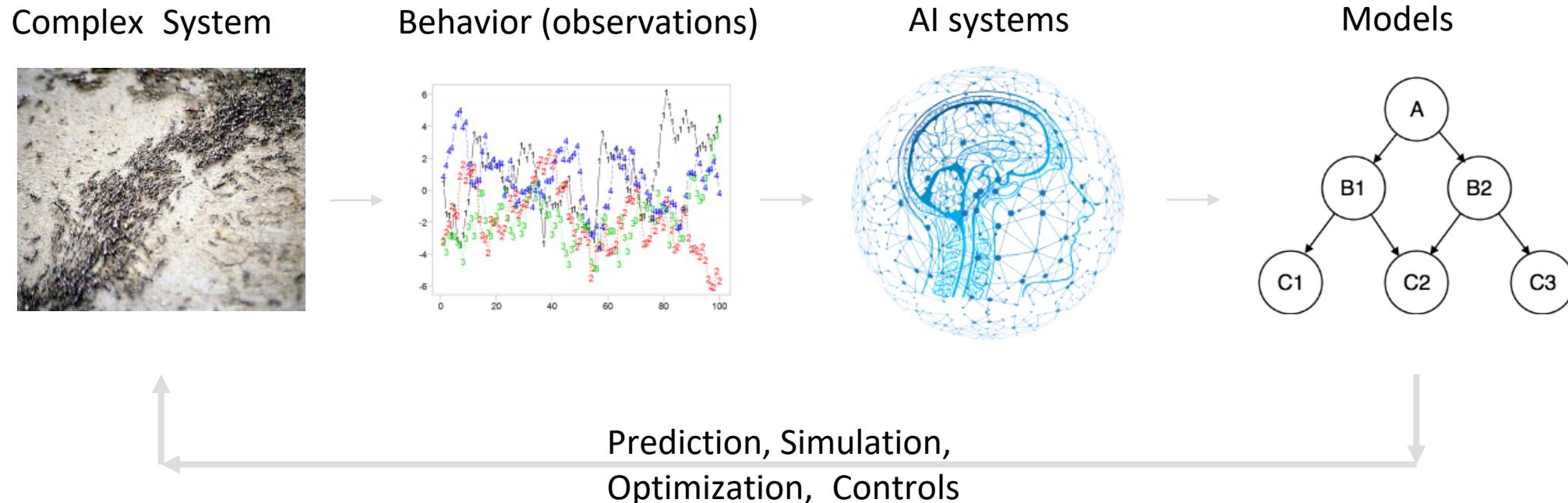
Sandipan Dey (UMBC)



# Summary

- Benefits:
  - Simple & concise
  - More insightful
  - More theoretical analysis
  - Cheap computation
- Drawbacks:
  - Too Simple to explain complex phenomenon
  - Difficult to incorporate real data
  - Poor prediction accuracy
  - Rely on Human Heuristics
  - Case by Case

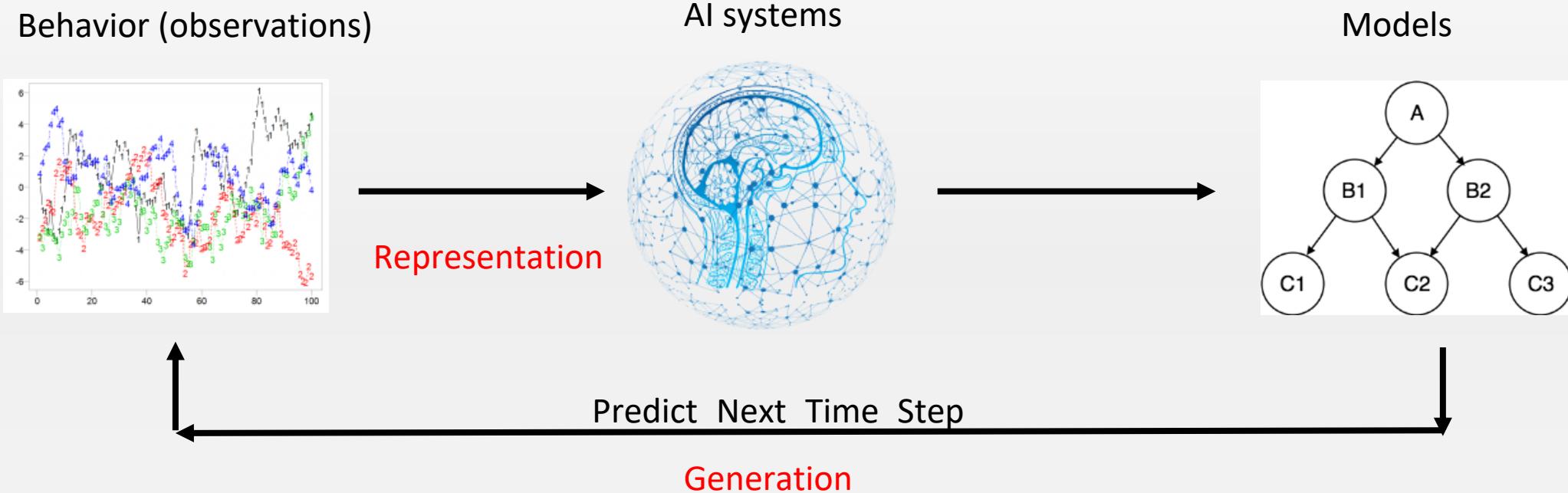
# Automated Modelling of Complex Systems



# Outline

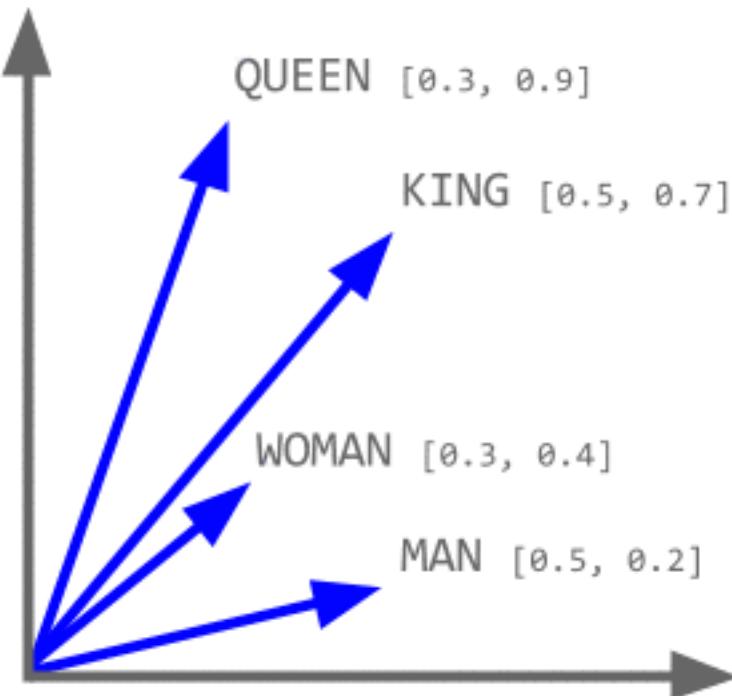
- AI for complex systems
  - Complex Systems and Modelling Methods
  - Representation & Generation
  - Dynamics Learning
  - Network Reconstruction
  - Multi-scale Modelling
  - Simulation, optimization, and control
- Complexity science for AI

# Representation & Generation

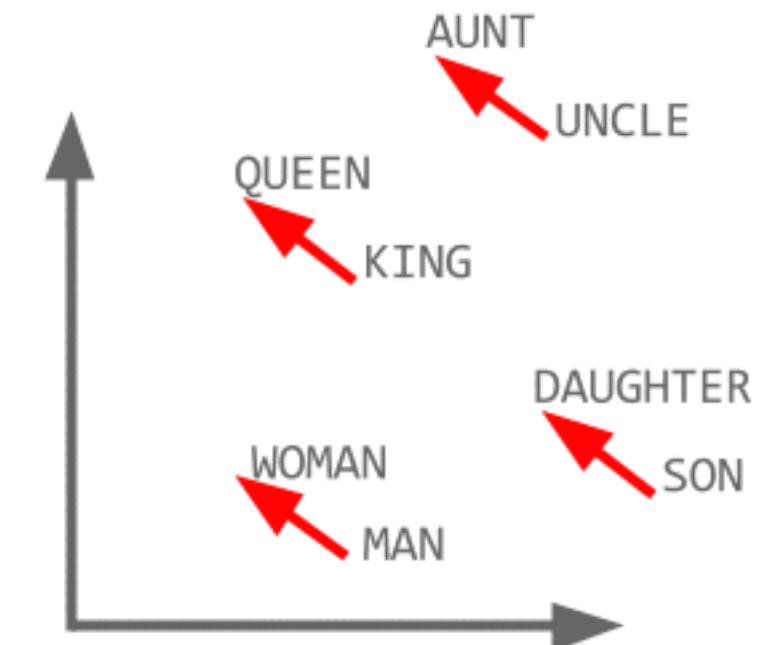
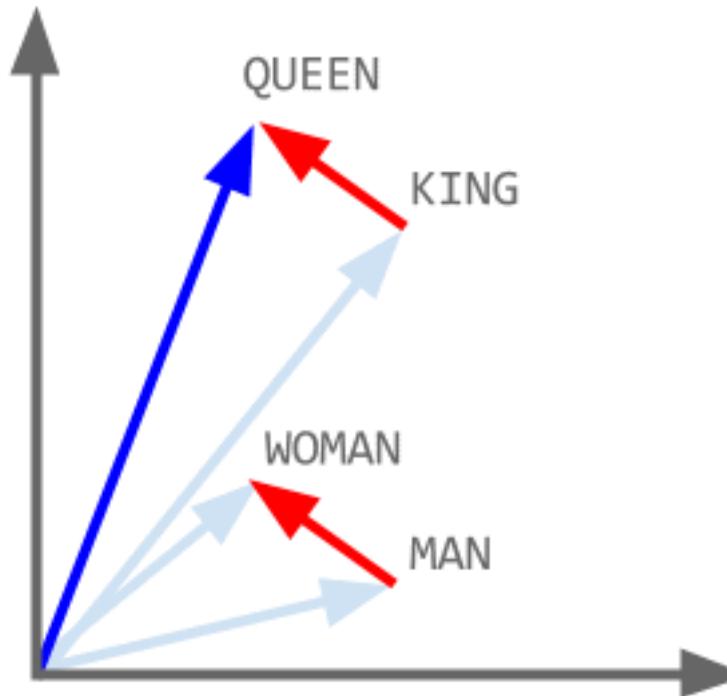


# Word2Vec

Load up the word vectors



So  $\text{king} + \text{man} - \text{woman} = \text{queen}$  Which is consistent across all words



# Generative AI



# Learning nonequilibrium statistical mechanics and dynamical phase transitions

nature communications

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Article | Open access | Published: 06 February 2024

## Learning nonequilibrium statistical mechanics and dynamical phase transitions

Ying Tang , Jing Liu, Jiang Zhang & Pan Zhang 

Nature Communications 15, Article number: 1117 (2024) | [Cite this article](#)

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### Abstract

Nonequilibrium statistical mechanics exhibit a variety of complex phenomena far from equilibrium. It inherits challenges of equilibrium, including accurately describing the joint distribution of a large number of configurations, and also poses new challenges as the distribution evolves over time. Characterizing dynamical phase transitions as an emergent behavior further requires tracking nonequilibrium systems under a control parameter. While a number of methods have been proposed, such as tensor networks for one-dimensional lattices, we lack a method for arbitrary time beyond the steady state and for higher

### (a) System and problem

Equilibrium statistical mechanics

Spin configurations  
 $\mathbf{x} = \{x_1, x_2, \dots, x_N\}$

Probability distribution  $P(\mathbf{x})$ ?

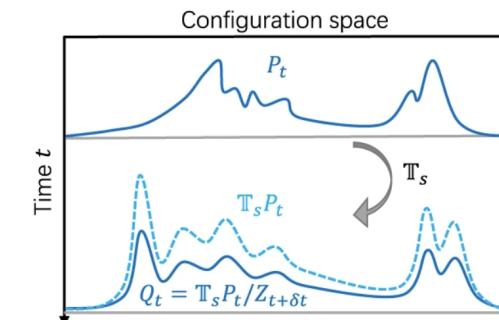


Nonequilibrium statistical mechanics

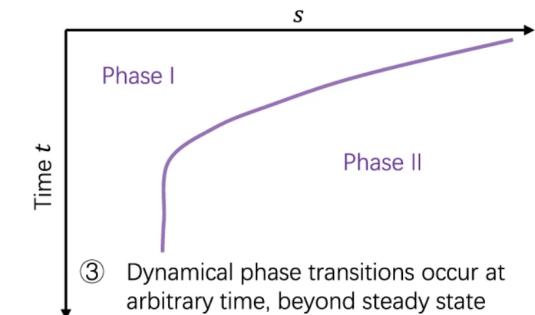
How does  $P_t(\mathbf{x})$  evolve?

### (b) Challenges to study dynamical phase transitions

- ① Transition operator  $\mathbb{T}_s$  gives unnormalized distribution, requiring  $Z_{t+\delta t}$  for normalization

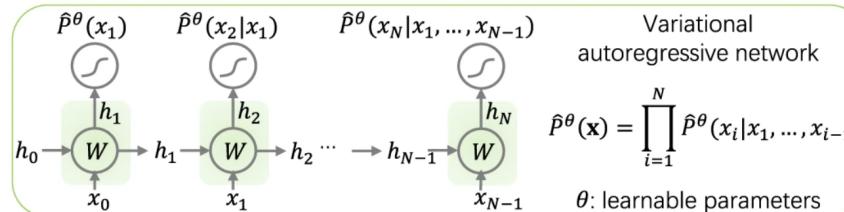


- ② Accurately track dynamics under a set values of the control parameter  $s$



- ③ Dynamical phase transitions occur at arbitrary time, beyond steady state

### (c) Method based on machine learning



Minimize loss function over time:

$$\mathcal{L}_{t+\delta t} = D_{KL}[\hat{P}_{t+\delta t}^\theta | \hat{Q}_t^\theta] - \ln Z_{t+\delta t}$$

Dynamical partition function:

$$-\ln Z_{t+\delta t} = \min_{\theta_{t+\delta t}} \mathcal{L}_{t+\delta t}$$

- ① Normalization constant ✓  
② Applicable to various  $s$  ✓  
③ Trackable at any time ✓

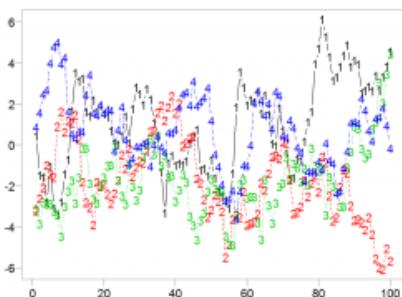
Uncover dynamical phase transitions over time

# Outline

- AI for complex systems
  - Complex Systems and Modelling Methods
  - Representation & Generation
  - Dynamics Learning
  - Network Reconstruction
  - Multi-scale Modelling
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# Problem Definition

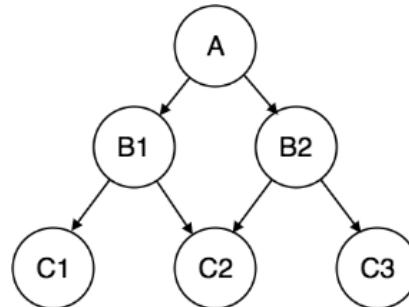
Behavior (observations)



AI systems



Models



Predict Next Time Step

## Takens's theorem

From Wikipedia, the free encyclopedia



This article includes a list of general [references](#), but it lacks sufficient corresponding [inline citations](#). Please help to improve this article by introducing more precise citations. (September 2020) ([Learn how and when to remove this template message](#))

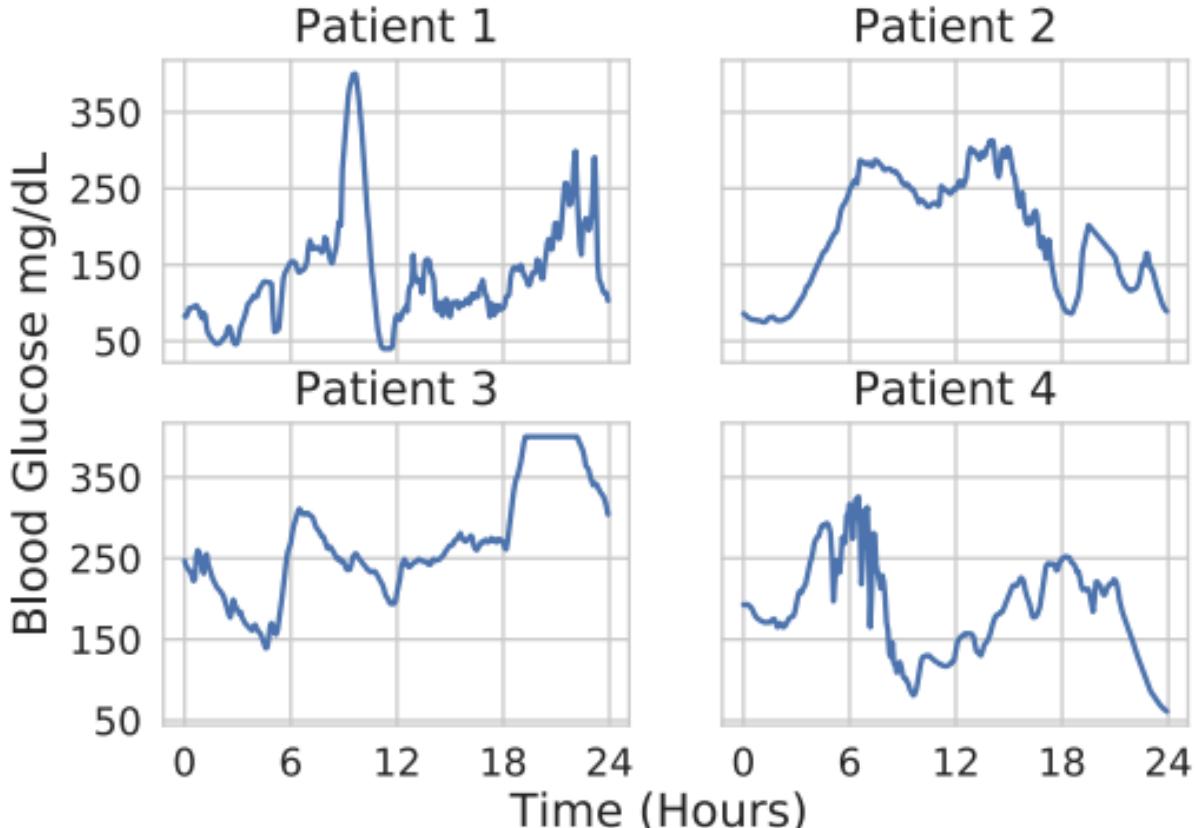
In the study of [dynamical systems](#), a [delay embedding theorem](#) gives the conditions under which a [chaotic dynamical system](#) can be reconstructed from a sequence of observations of the state of a dynamical system. The reconstruction preserves the properties of the dynamical system that do not change under smooth coordinate changes (i.e., [diffeomorphisms](#)), but it does not preserve the geometric shape of structures in phase space.

- Abstractor reconstruction
- Polynomial regression
- Compressed sensing
- Driving response
- Reservoir Computing
- Time series analysis...

[https://en.wikipedia.org/wiki/Takens's\\_theorem](https://en.wikipedia.org/wiki/Takens's_theorem)



# RNN based Dynamics Learning



053357v1 [es] [G] 14 Jun 2018

## Deep Multi-Output Forecasting

## Learning to Accurately Predict Blood Glucose Trajectories

Ian Fox<sup>1</sup>, Lynn Ang<sup>2</sup>, Mamta Jaiswal<sup>2</sup>, Rodica Pop-Busui<sup>2</sup>, Jenna Wiens<sup>1</sup>  
<sup>1</sup>CSE, University of Michigan, <sup>2</sup>Internal Medicine, University of Michigan

## ABSTRACT

In many forecasting applications, it is valuable to predict not only the value of a signal at a certain time point in the future, but also the values leading up to that point. This is especially true in clinical applications, where the future state of the patient can be less important than the patient's overall trajectory. This requires multi-step forecasting, a forecasting variant where one aims to predict multiple values in the future simultaneously. Standard methods to accomplish this can propagate error from prediction to prediction, reducing quality over the long term. In light of these challenges, we propose multi-output deep architectures for multi-step forecasting in which we explicitly model the distribution of future values of the signal over a prediction horizon. We apply these techniques to the challenging and clinically relevant task of blood glucose forecasting. Through a series of experiments on a real-world dataset consisting of 550K blood glucose measurements, we demonstrate the effectiveness of our proposed approaches in capturing the underlying signal dynamics. Compared to existing shallow and deep methods, we find that our proposed approaches improve performance individually and capture complementary information, leading to a large improvement over the baseline when combined (4.87 vs. 5.31 absolute percentage error (APE)). Overall, the results suggest the efficacy of our proposed approach in predicting blood glucose level and multi-step forecasting more generally.

## ACM Reference Format:

Ian Fox, Lynn Ang, Mamta Jaiswal, Rodica Pop-Busui, Jenna Wiens. 2018. Deep Multi-Output Explanations: Learning to Aggregate Predictions and Classifications. In *Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing*, Brussels, Belgium, October 11–15, 2018, Volume 1, pages 103–113.

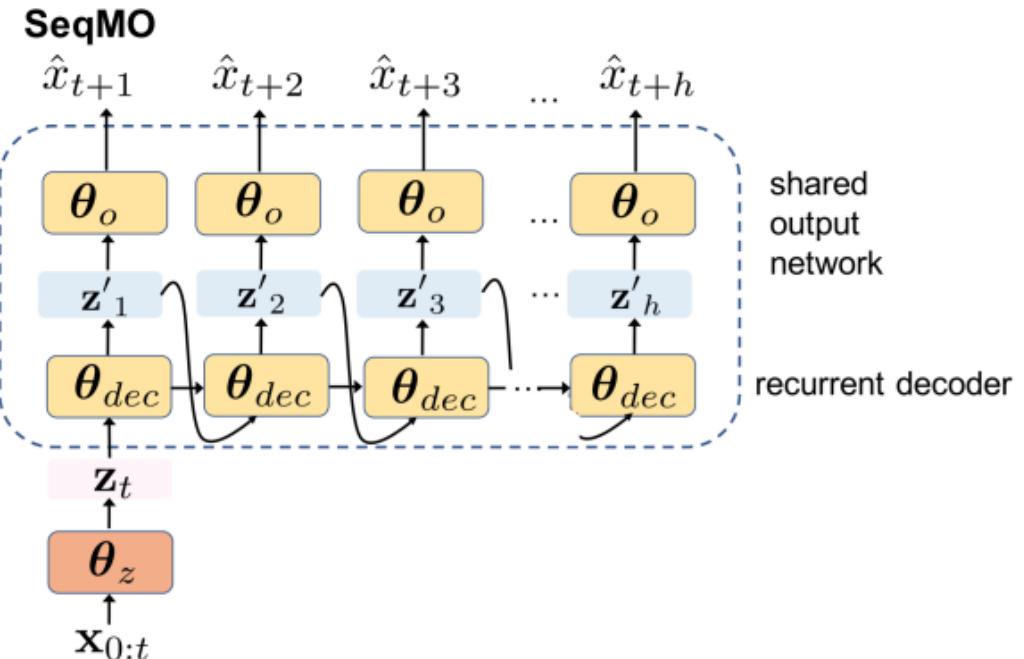
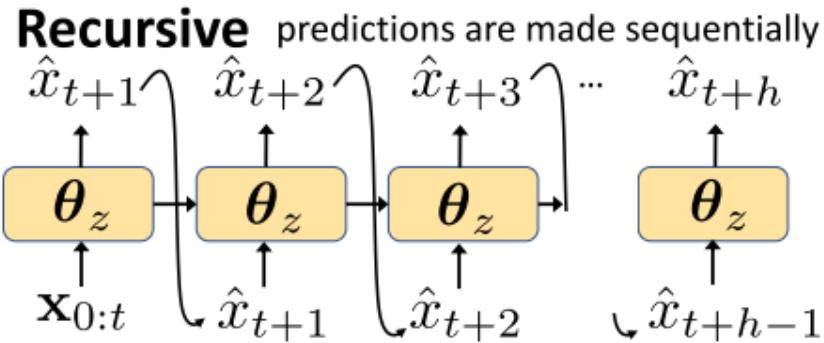
setting is inherently more difficult, since it requires modeling the joint probability of future measurements. While more challenging, if successful this joint modeling of observations within a sequence can improve overall performance. For example, while the word 'the' occurs often in English, the phrase 'the the the' does not.

Recursive approaches, in which a single-step forecaster predicts several values by using the current prediction to make the next prediction, are commonly used in multi-step forecasting [22]. However, such approaches often suffer from poor long term performance, since any error introduced will enter a positive feedback loop. Alternatively, multi-output forecasting aims to estimate multiple values at once. While no longer susceptible to the feedback issue, multi-output forecasting may not adequately capture dependencies among predictions.

We propose two complementary solutions to these issues. The first is a multi-output recurrent neural network where explicit temporal dependencies between outputs capture the relationships between the predictions. The second is a novel architecture that directly models the underlying generating function of the signal by learning a polynomial approximation for the outputs. The problem of error accumulation during sequence prediction has been previously studied in NLP [1, 13]. We distinguish ourselves from this past work by focusing on new models that alleviate this problem, as opposed to new training schemes.

We apply the proposed approaches to a challenging real-world forecasting problem (described below). Our main contributions can be summarized as followed:

# Recursive v.s. Multi-output



## Deep Multi-Output Forecasting

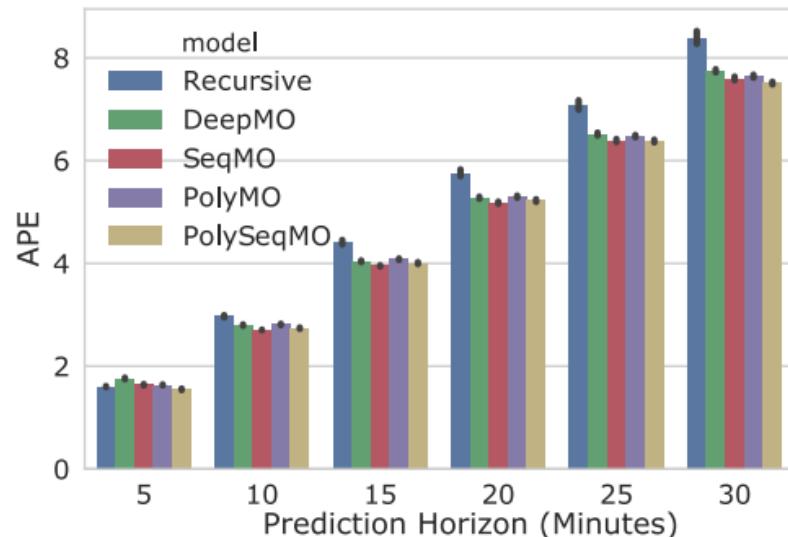
Learning to Accurately Predict Blood Glucose Trajectories

Ian Fox<sup>1</sup>, Lynn Ang<sup>2</sup>, Mamta Jaiswal<sup>2</sup>, Rodica Pop-Busui<sup>2</sup>, Jenna Wiens<sup>1</sup>

<sup>1</sup>CSE, University of Michigan, <sup>2</sup>Internal Medicine, University of Michigan

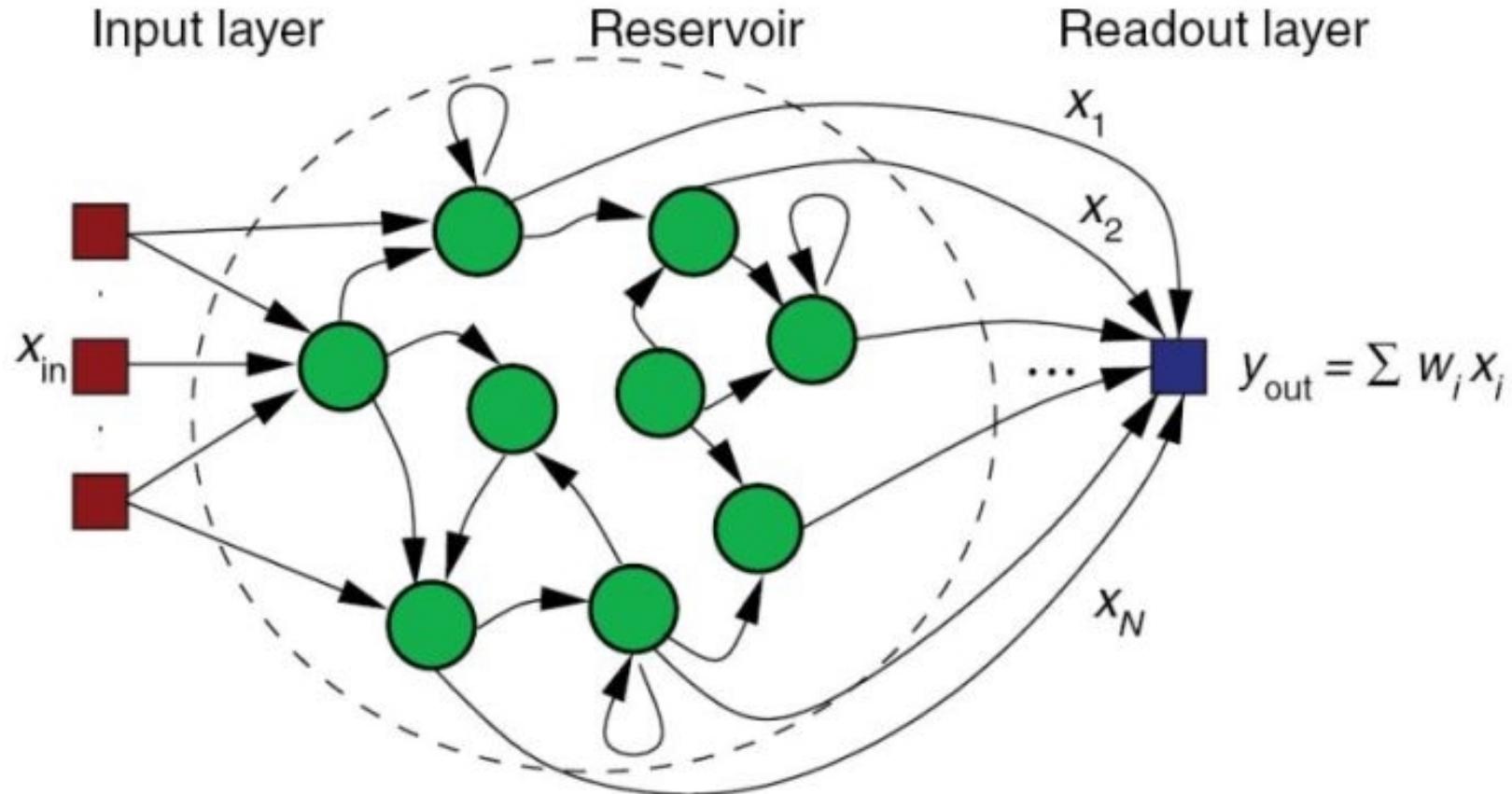
Forecasting with DeepMO involves transforming the input to a shared representation and then learning separate output networks for each time point in the prediction horizon  $h$ .

# Results



	Architecture	Full 39k	Event 3.1k	Hypo 1.2k	Hyper 1.9k
Shallow Baseline	Extrapolation	6.48 (0.21-42.12)	10.76 (1.42-63.98)	14.85 (1.89-86.81)	8.73 (1.30-36.87)
	RF: Rec	8.00 (0.62-40.83)	10.45 (1.99-65.21)	14.31 (2.73-91.12)	8.82 (1.85-30.42)
	RF: MO	5.18 (0.71-30.16)	10.64 (1.41-55.28)	17.88 (2.70-75.46)	8.20 (1.14-28.00)
Deep Baseline	Recursive	5.31 (0.00-29.32)	10.00 (1.45-46.22)	13.34 (2.17-62.86)	8.43 (1.24-30.49)
	DeepMO	5.01 (0.00-28.74)	9.93 (1.62-41.67)	12.91 (2.26-56.04)	8.52 (1.43-30.02)
Proposed	SeqMO	4.91 (0.00-28.95)	9.69 (1.51-41.54)	12.48 (2.28-54.02)	8.37 (1.29-29.46)
	PolyMO	4.95 (0.51-28.30)	9.79 (1.48-43.67)	12.49 (1.93-60.78)	8.46 (1.31-30.75)
	PolySeqMO	4.87 (0.48-27.80)	9.57 (1.43-43.59)	12.05 (2.03-60.90)	8.31 (1.24-29.76)
	PolySeqMO Ensemble	4.59 (0.41-21.12)	9.38 (1.35-42.34)	11.61 (1.99-59.89)	8.13 (1.18-29.49)

# Reservoir Computing



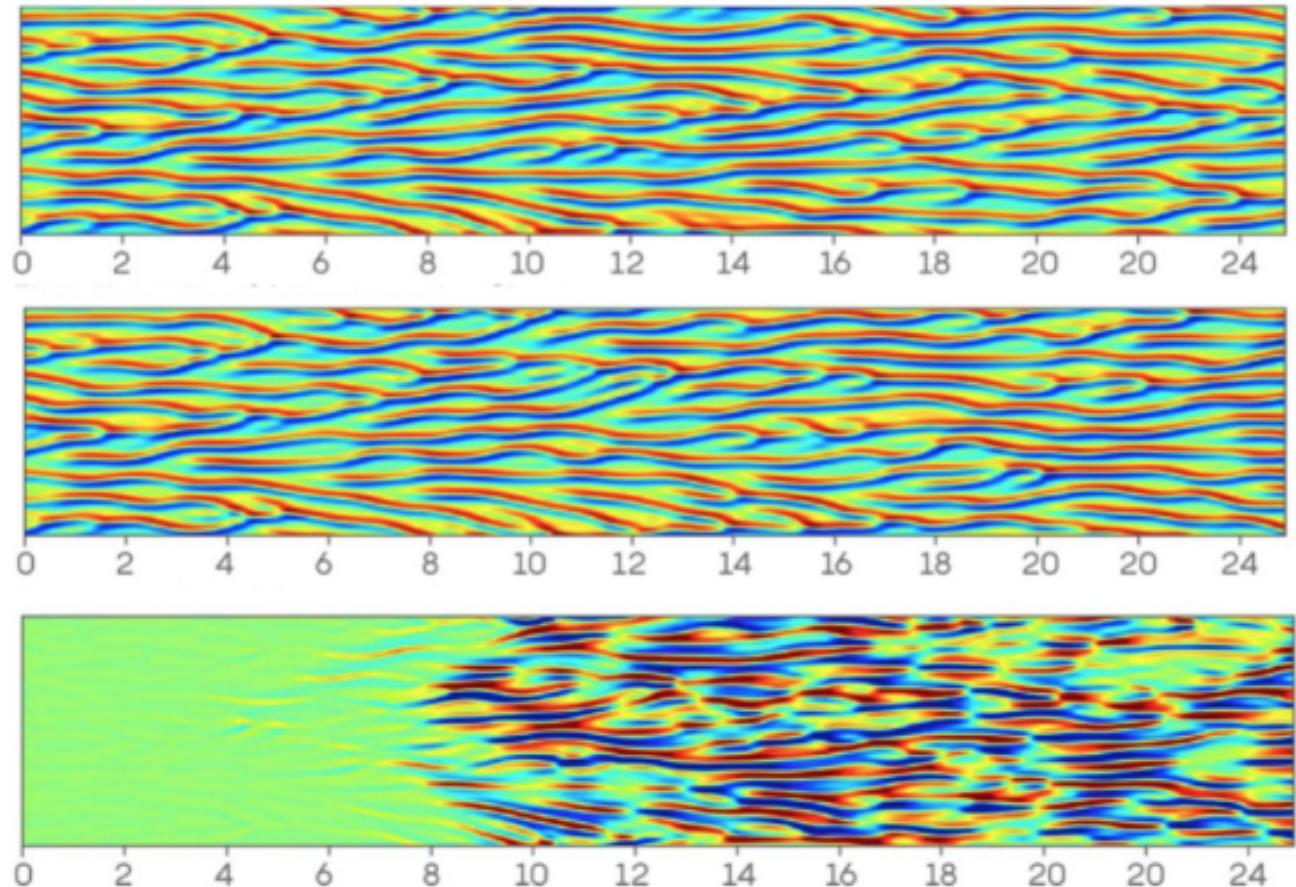
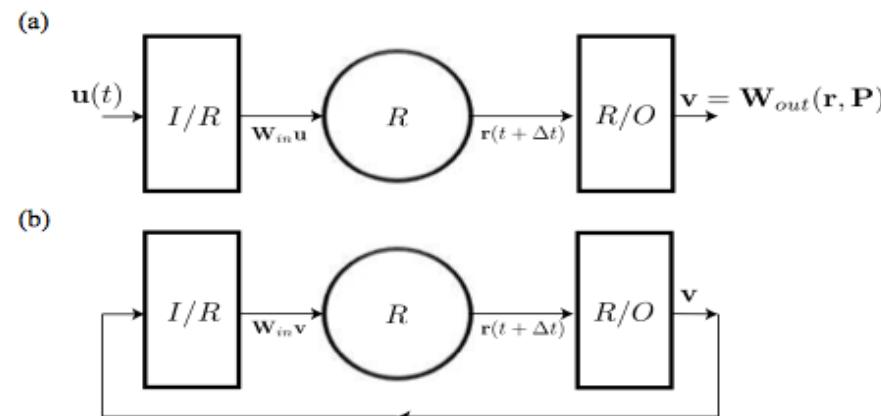
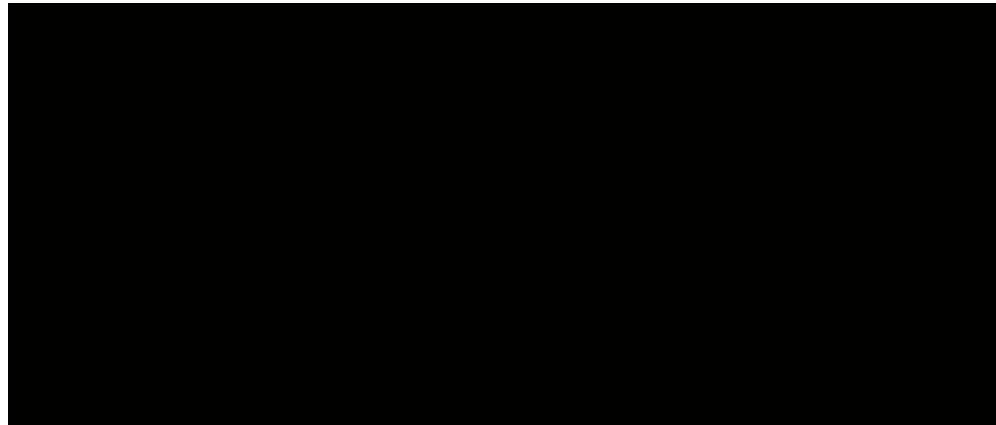
[https://en.wikipedia.org/wiki/Reservoir\\_computing](https://en.wikipedia.org/wiki/Reservoir_computing)



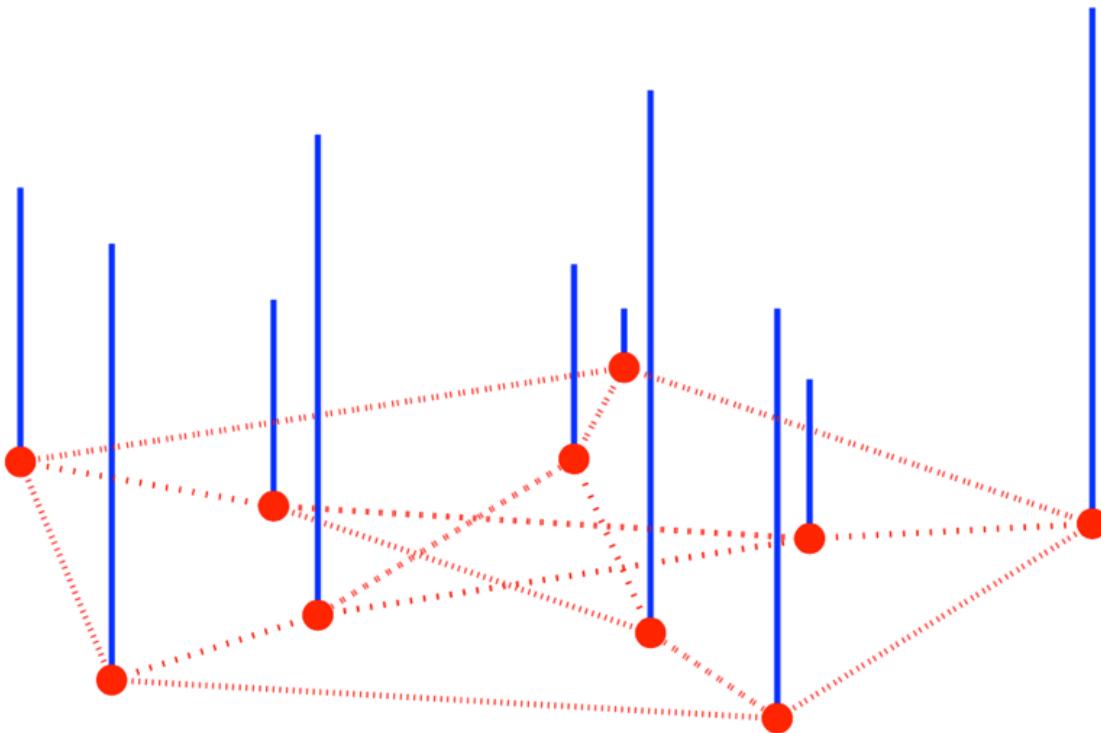
# Predict Chaotic Dynamics

Kuramoto-Sivashinsky equation:

$$u_t + \nabla^4 u + \nabla^2 u + \frac{1}{2} |\nabla u|^2 = 0$$



# Dynamics on Graph

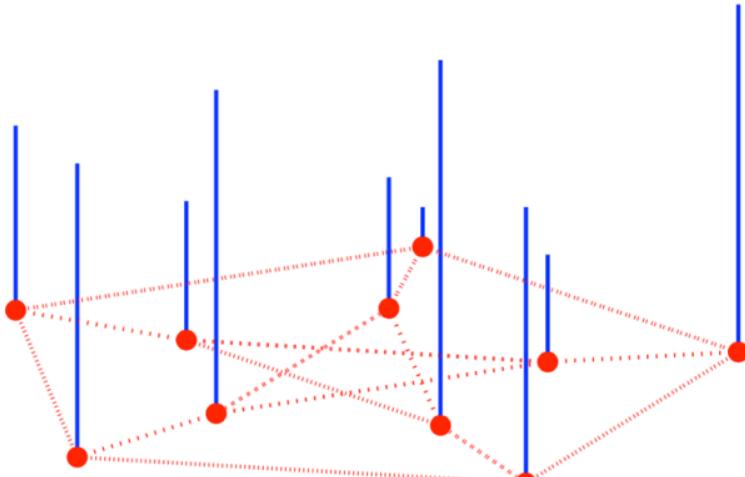


$$\frac{dX(t)}{dt} = f(X(t), A)$$

$$X(t) = (x_1(t), x_2(t), \dots, x_n(t))^T$$

$$X(t + 1) = F(X(t), A)$$

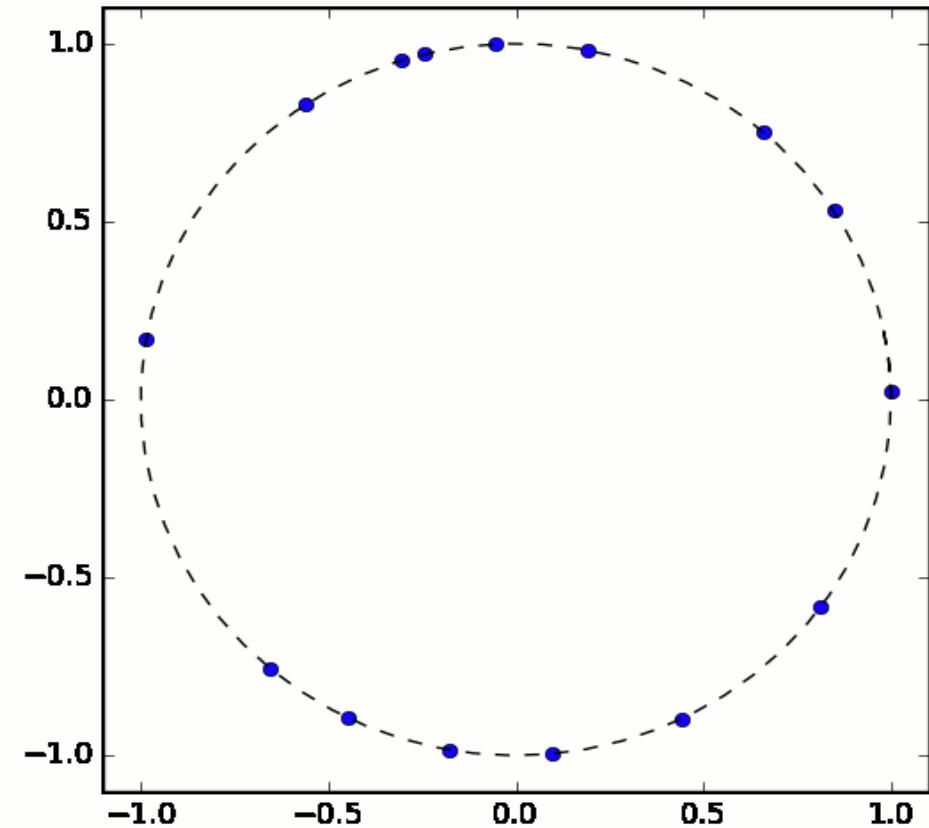
# Dynamics on Graph



$$\frac{dX(t)}{dt} = f(X(t), A)$$

$$X(t) = (x_1(t), x_2(t), \dots, x_n(t))^T$$

$$X(t+1) = F(X(t), A)$$



$$\frac{d\theta_i}{dt} = \omega_i + \frac{K}{N} \sum_{j=1}^N \sin(\theta_j - \theta_i), \quad i = 1 \dots N,$$