Differential Deep Learning on Graphs and its Applications

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This Tutorial

- www.calvinzang.com/DDLG_AAAI_2020.html
- AAAI-2020
- Friday, February 7, 2020, 2:00 PM -6:00 PM
- Sutton North, Hilton New York Midtown, NYC

This Tutorial

- **Molecular Graph Generation**: to generate novel molecules with optimized properties
  - Graph generation
  - Graph property prediction
  - Graph optimization
- ✓ **Learning Dynamics on Graphs**: to predict temporal change or final states of complex systems
  - Continuous-time dynamics prediction
  - Structured sequence prediction
  - Node classification/regression
- **Mechanism Discovery**: to find dynamical laws of complex systems
  - Density Estimation vs. Mechanism Discovery
  - Data-driven discovery of differential equations

Part 2: Neural Dynamics on Complex Networks

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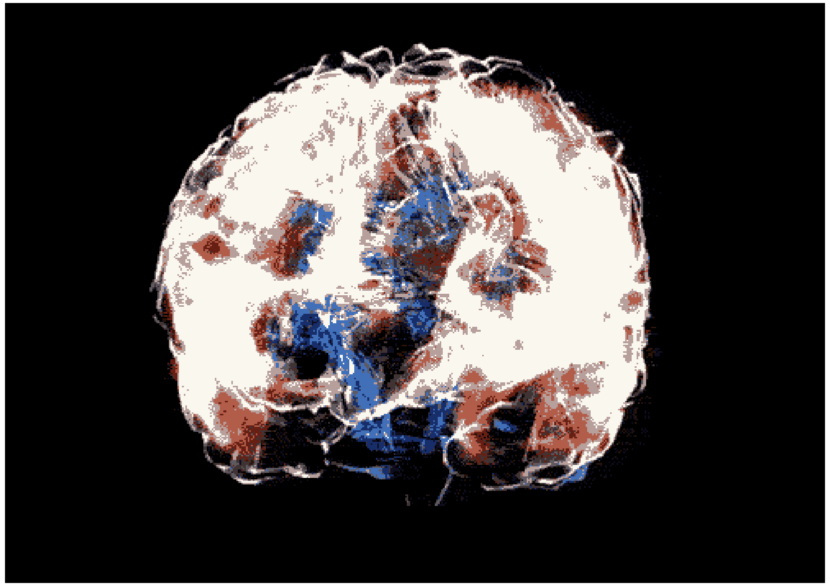
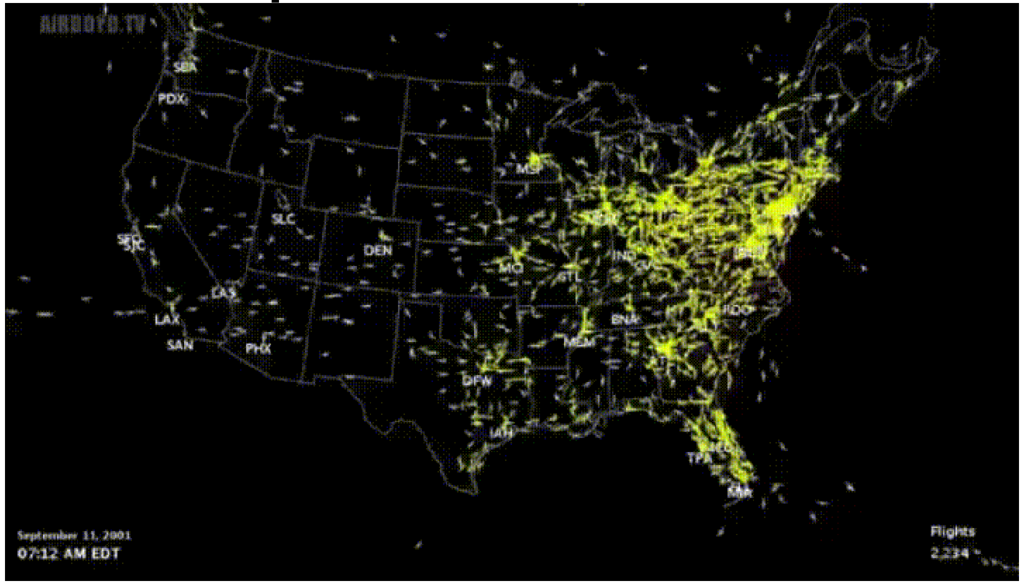
Structures and Dynamics of Complex Systems

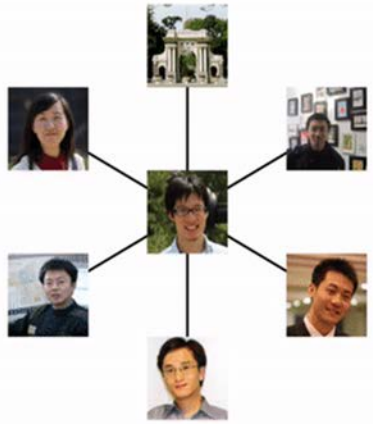
Brain and Bioelectrical flow



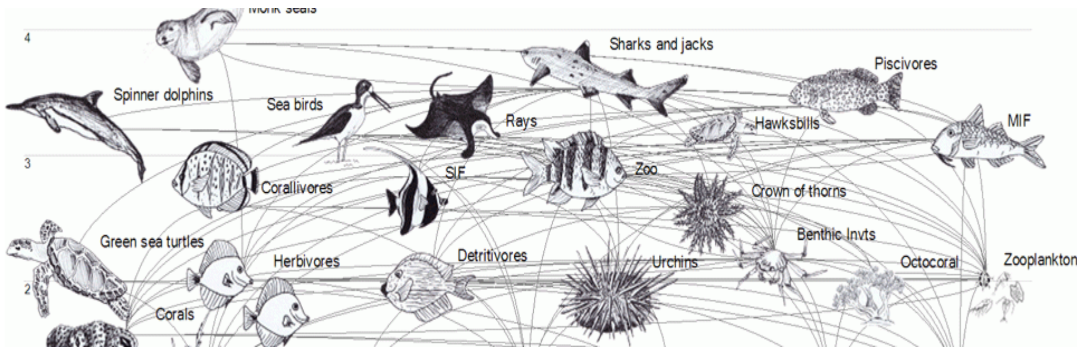
Transportation and Traffic flow



Social Networks and Information flow

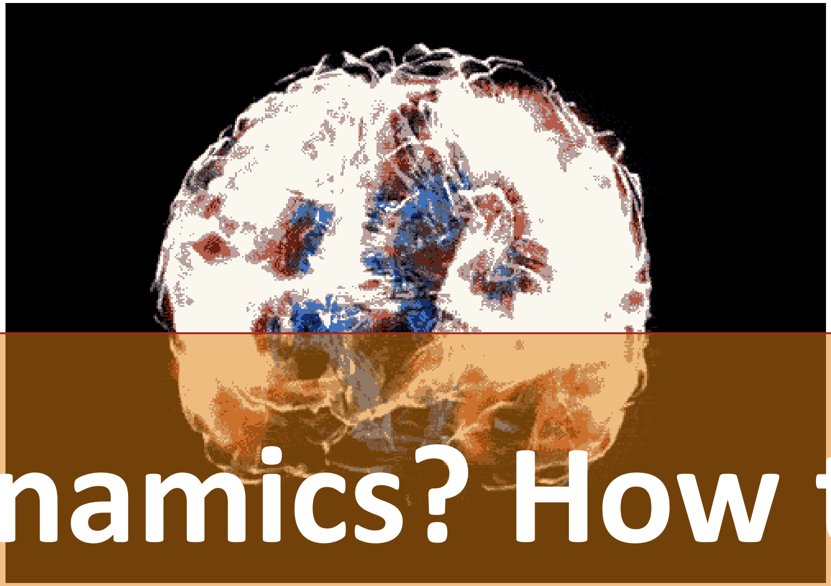


Ecological Systems and Energy flow



Problem: Learning Dynamics of complex systems

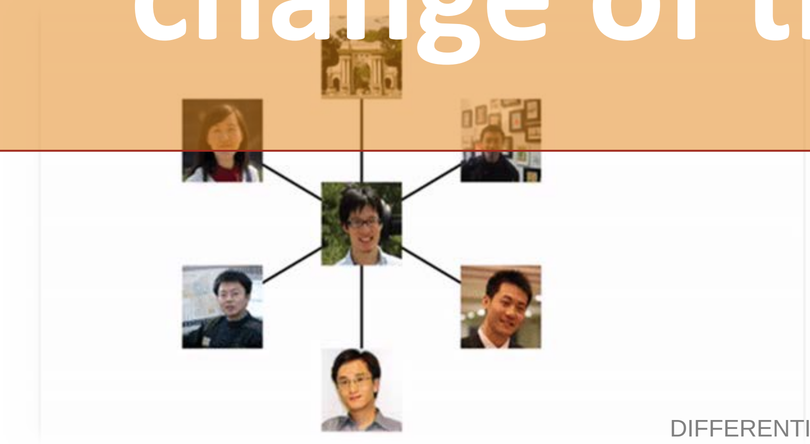
Brain and Bioelectrical flow



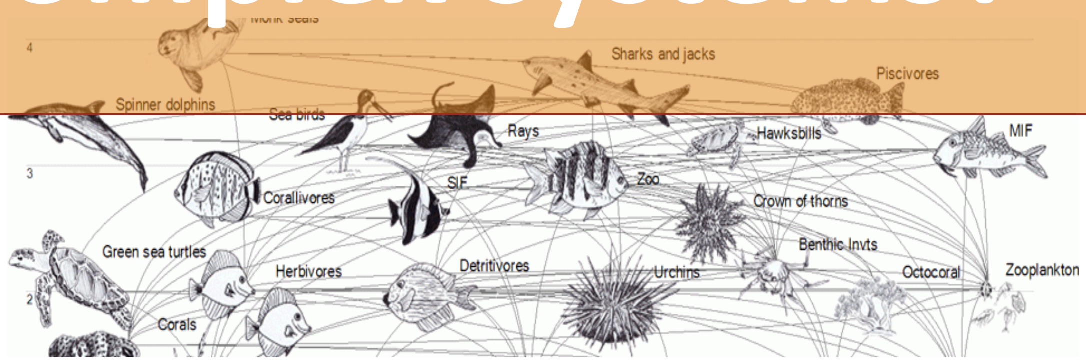
Transportation and Traffic flow

Dynamics? How to predict the temporal change of these complex systems?

Social Networks and Information flow



Ecological Systems and Energy flow



Problem: Math Formulation

❑Learning Dynamics on Graph

- Dynamics of nodes: $X(t) \in \mathbb{R}^{n*d}$ at t, where n is number of nodes, d is number of features, $X(t)$ changes over continuous time t.
- Graph: $G = (V, E)$, V are nodes, E are edges.
- How dynamics $\frac{dX(t)}{dt} = f(X(t), G, \theta, t)$ change on graph?

Problem: Prediction Tasks

- **Continuous-time network dynamics prediction:**
  - Input: G, $\left\{\widehat{X(t_1)}, \widehat{X(t_2)}, \ldots, \widehat{X(t_T)} \middle| 0 \leq t_1 < \cdots < t_T\right\}, t_1 < \cdots < t_T$ are arbitrary time moments
  - ?A model of dynamics on graphs $\frac{dX(t)}{dt} = f(X(t), G, \theta, t)$
  - Output: to predict $X(t)$ at an arbitrary time moment

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  - ? A model of dynamics on graphs $\frac{dX(t)}{dt} = f(X(t), G, \theta, t)$
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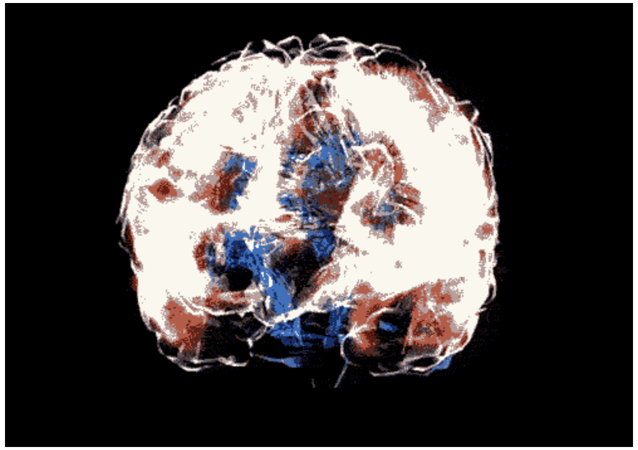
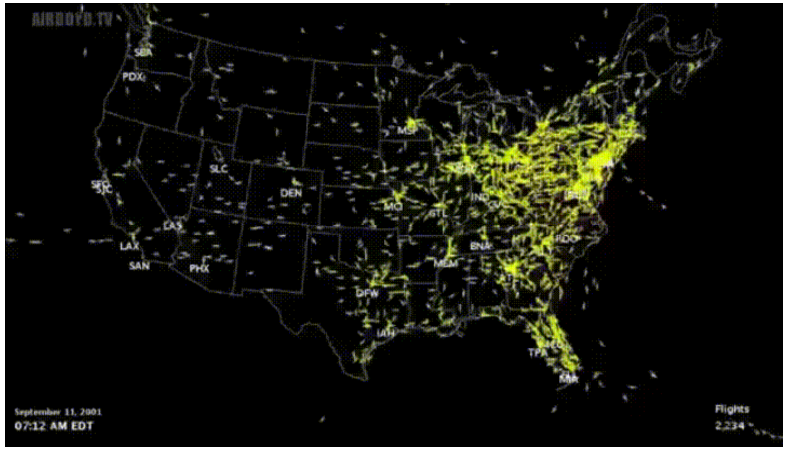
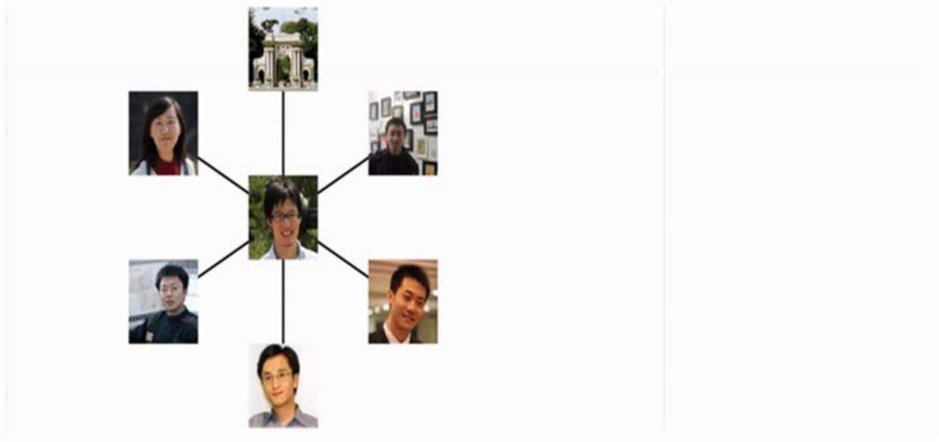
  - ? A model of dynamics on graphs $\frac{dX(t)}{dt} = f(X(t), G, \theta, t)$
  - Output: to predict $[X, Y]$

Why Dynamics Matter?

- **To understand, predict, and control real-world dynamic systems in engineering and science.**
  - Brain dynamics, traffic dynamics, social dynamics

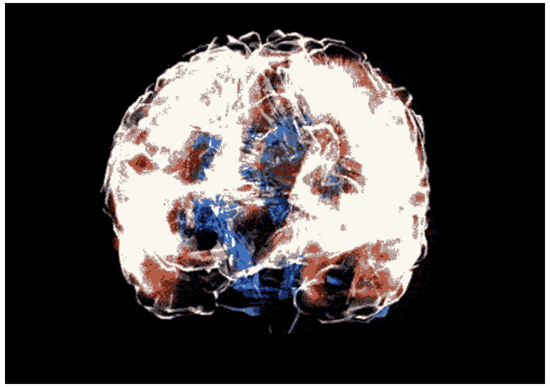






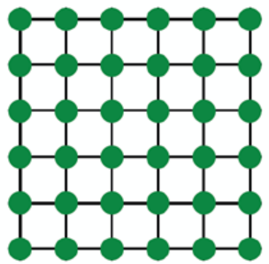
Challenges: Dynamics of Complex Systems

- **Complex systems:**
  - High-dimensionality and Complex interactions
  - ≥ 100 nodes, ≥ 1000 interactions
- **Dynamics:**
  - Continuous-time, Nonlinear
- **Structural-dynamic dependencies:**
  - Difficult to be modeled by simple mechanistic models

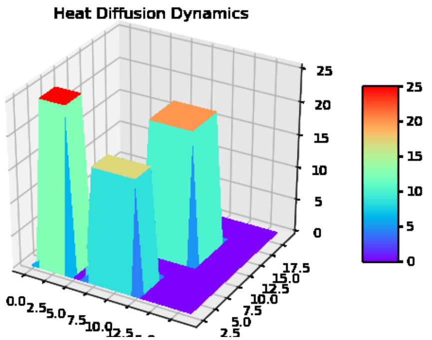


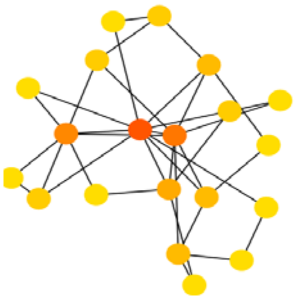
Challenges: Dynamics of Complex Systems

❑Examples of dynamics on graphs



+ Linear Dynamics →





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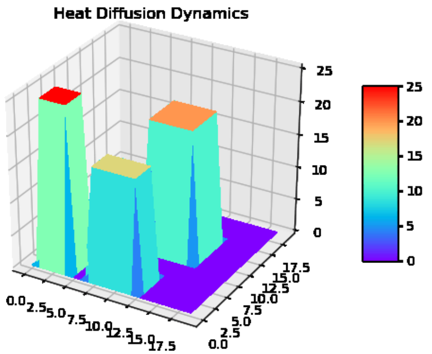
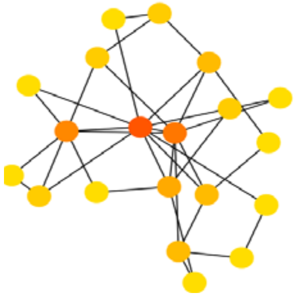
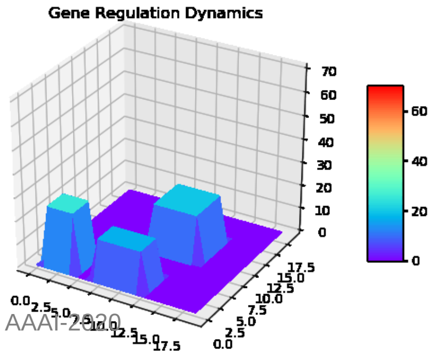




+ Non-Linear Dynamics →

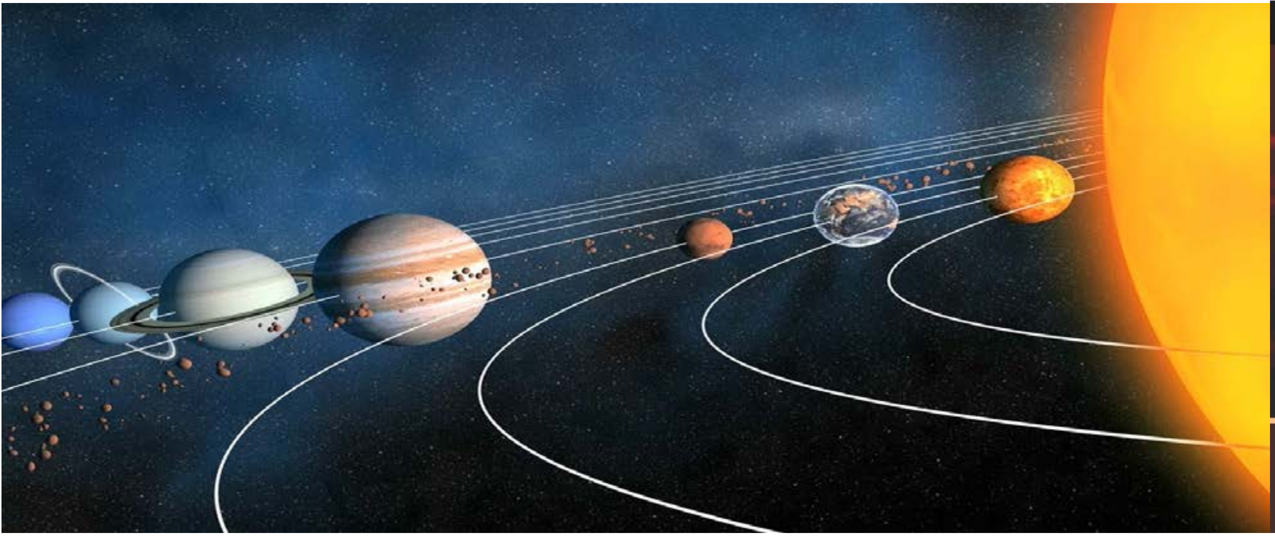


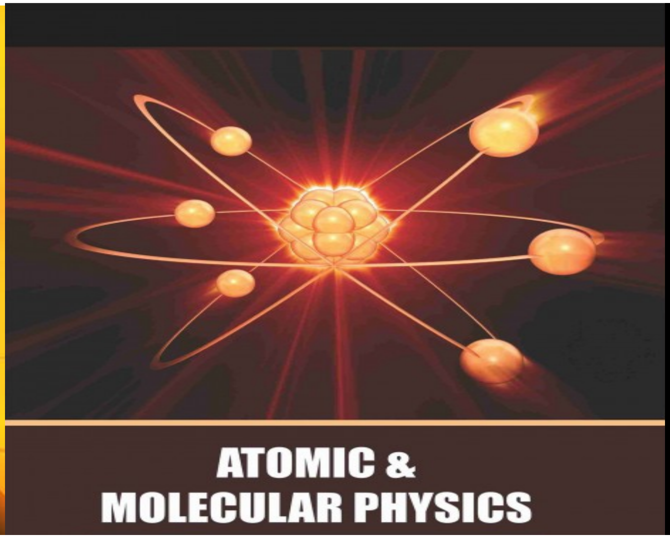
$\boldsymbol{f(X(t), G, \theta, t)}$

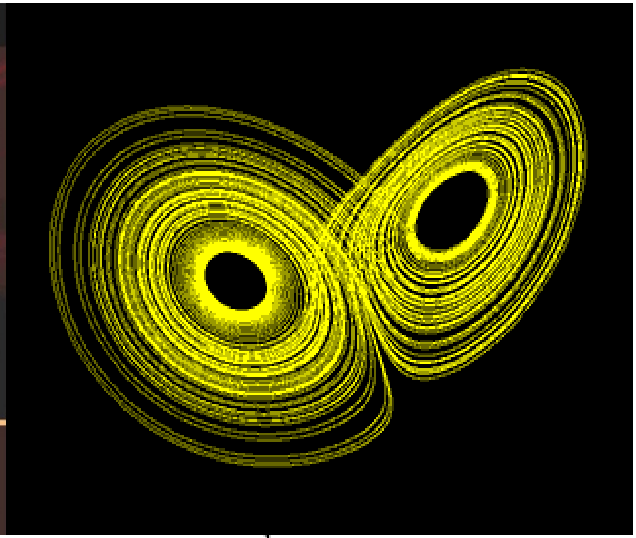
?

Related Works 1: Learning Continuous Time Dynamics

- **To learn continuous-time dynamics**
  - A clear knowledge of the mechanisms, small systems, few interaction terms, first principle from physical laws, mechanistic models,







Macro: $$\boldsymbol{F} = \frac{d(m\boldsymbol{v})}{dt}$$

Micro: $$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[\frac{-\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t)$$

Chaos: $$\frac{\mathrm{d}x}{\mathrm{d}t} = \sigma(y-x),$$ $$\frac{\mathrm{d}y}{\mathrm{d}t} = x(\rho - z) - y,$$ $$\frac{\mathrm{d}z}{\mathrm{d}t} = xy\ 14\beta z.$$

Data-driven Dynamics for Small Systems

- ❑ **Data-driven discovery of ODEs/ PDEs**
  - o **Sparse Regression**
  - o Residual Network
  - o Etc.
- ❑ **Small systems!**
  - o <10 nodes & interactions
  - o Combinatorial complexity
  - o Not for complex systems

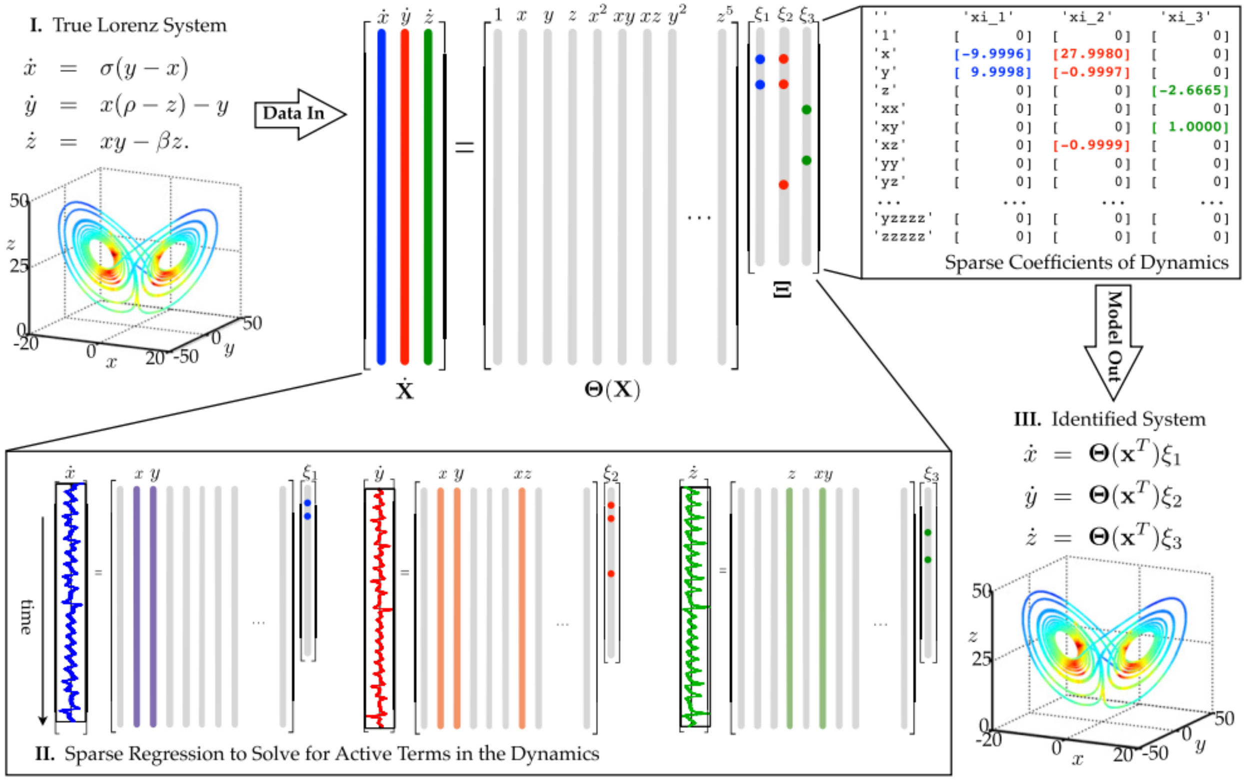


Image from: Brunton et al. 2016. [Discovering governing equations from data by sparse identification of nonlinear dynamical systems.](#) PNAS

Related Works 2: Structured Sequence Learning

- **Defined characteristics**
  - Dynamics on graphs are regularly-sampled with same time intervals
- **Temporal Graph Neural Networks**
  - RNN + CNN
  - RNN + GNN
    - X[t+1]=LSTM(GCN([t], G))
- **Limitations:**
  - Only ordered sequence instead of continuous physical time

Seo et al. 2016. Structured Sequence Modeling with Graph Convolutional Recurrent Networks.
Wu et al. 2019. A Comprehensive Survey on Graph Neural Networks

Related Works 3: Node (Semi-supervised) Classification/Regression

❑ Defined characteristics

- One-snapshot features and some labels on graphs
- Goal: to assign labels to each node

❑ Graph Neural Networks

- GCN,
- GAT, etc.

$$Z = f(X, A) = \mathrm{softmax}\Big(\hat{A}\ \mathrm{ReLU}\Big(\hat{A}XW^{(0)}\Big)\ W^{(1)}\Big)$$

$$\vec{h}'_i = \sigma\left(\frac{1}{K}\sum_{k=1}^{K}\sum_{j\in\mathcal{N}_i}\alpha_{ij}^k \mathbf{W}^k \vec{h}_j\right)$$

❑ Limitations

- 1 or 2 layers
- Lacking a continuous-time dynamics view
  - ❖ To spread features or labels on graphs
  - ❖ Continuous-time: more fine-grained control on diffusion

Kipf et al. 2016. Semi-Supervised Classification with Graph Convolutional Networks
Velickovic et al. 2017. Graph Attention Networks

Goal: A Unified Framework for All?

- **Continuous-time network dynamics prediction:**
  - Input: G, $\{\widehat{X(t_1)}, \widehat{X(t_2)}, \ldots, \widehat{X(t_T)} \mid 0 \leq t_1 < \cdots < t_T\}$, $t_1 < \cdots < t_T$ are arbitrary time moments
  - **?Model: dynamics on graphs** $\frac{d\boldsymbol{X}(\boldsymbol{t})}{d\boldsymbol{t}} = \boldsymbol{f}(\boldsymbol{X}(\boldsymbol{t}), \boldsymbol{G}, \boldsymbol{\theta}, \boldsymbol{t})$
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  - Output: to predict $[X, Y]$

Our Ideas

- **Differential Equation Systems**
  - Graphs and Differential Equations are general tools to describe structures and dynamics of complex systems
- **Deep Learning**
  - RNN, GNN, Temporal GNN, Res-Net etc. are the state-of-the-art computational tools driven by data
- **How to leverage Differential equation systems and Deep Learning?**

Neural Dynamics on Complex Networks (NDCN)

Differential Deep Learning

- Differential Equation systems: $\frac{d\boldsymbol{X}(\boldsymbol{t})}{d\boldsymbol{t}} = \boldsymbol{f}(\boldsymbol{X}(\mathbf{t}), \mathbf{G}, \boldsymbol{W}, \mathbf{t})$ is a graph neural network like structure.
- Differential Deep model: $X(\boldsymbol{t}) = \boldsymbol{X}(\mathbf{0}) + \int_{\mathbf{0}}^{\boldsymbol{t}} \boldsymbol{f}(\boldsymbol{X}(\boldsymbol{\tau}), \mathbf{G}, \boldsymbol{W}, \boldsymbol{\tau}) d\boldsymbol{\tau}$ for arbitrary time t
- Learned as following optimization problem:

$$
\begin{aligned}
\underset{W_*, b_*}{\operatorname{argmin}} \quad & \mathcal{L} = \int_0^T |X(t) - \hat{X(t)}|\, dt \\
\text{subject to} \quad & X_h(t) = \tanh\left(X(t)W_e + b_e\right)W_0 + b_0 \\
& \frac{dX_h(t)}{dt} = \operatorname{ReLU}\left(\Phi X_h(t) W + b\right), X_h(0) \\
& X(t) = X_h(t) W_d + b_d
\end{aligned}
$$

$\Phi = D^{-\frac{1}{2}}(D - A)D^{-\frac{1}{2}} \in \mathbb{R}^{n \times n}$

Neural Dynamics on Complex Networks (NDCN)

❑ Differential Deep Learning

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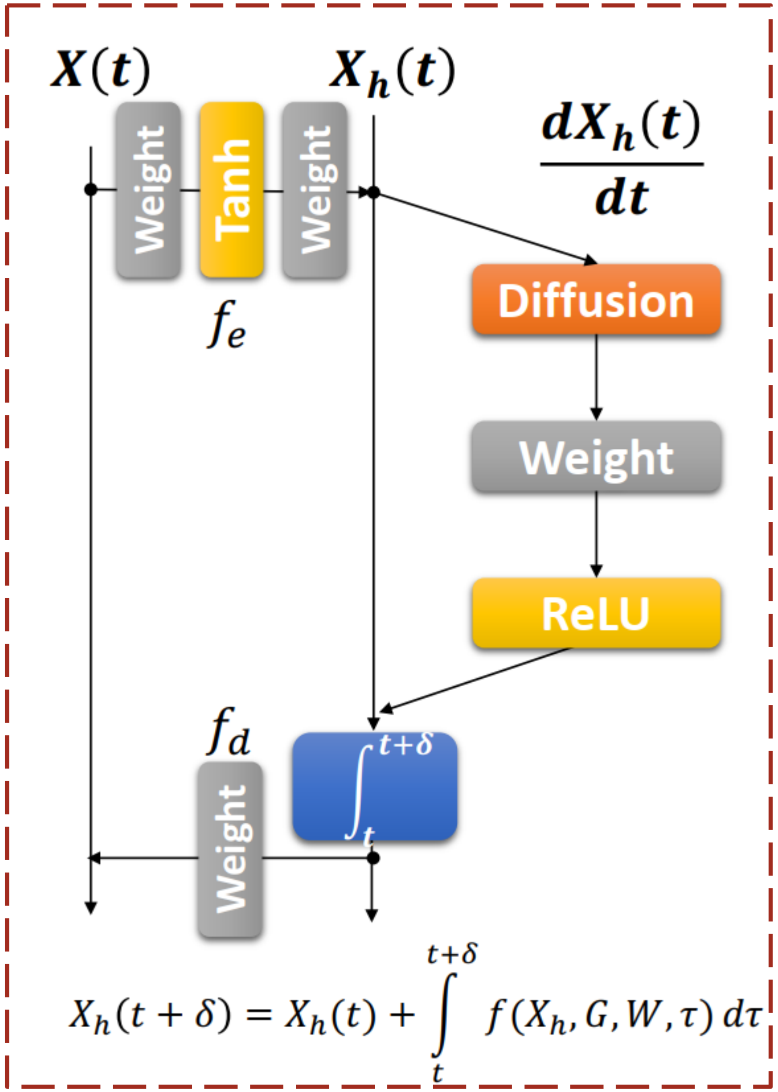
?



$\Phi = D^{-\frac{1}{2}}(D - A)D^{-\frac{1}{2}} \in \mathbb{R}^{n\times n}$

Interpretation from Residual Learning

❑ Deep Learning: f_* is a neural layer

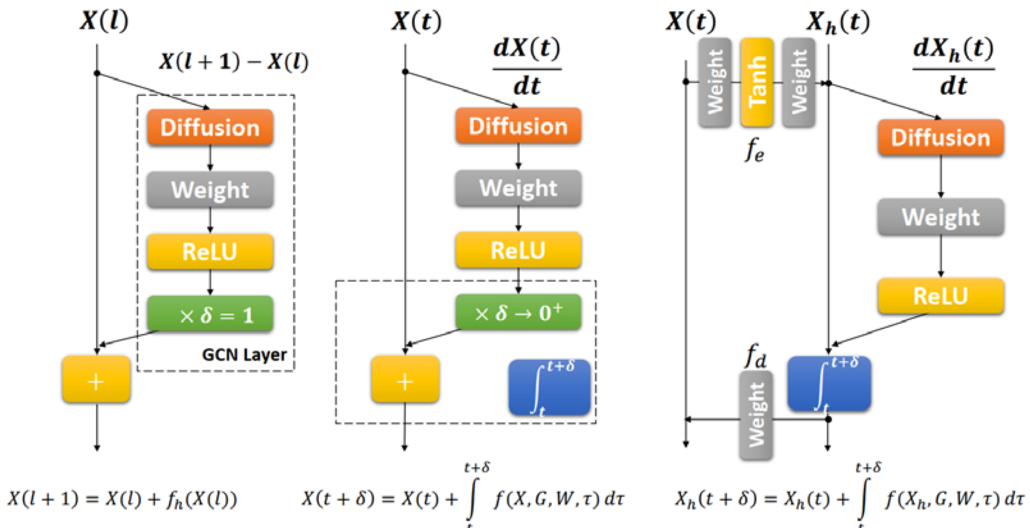
- Each layer: $X[l+1] = f_{l+1}(X[l])$
- Deep Model: $X[L] = f_L \circ \cdots \circ f_1(X[0])$,

❑ Residual Learning: deep

- Each layer: $\mathrm{X}[l+1] = \mathrm{X}[l] + \mathrm{f}_{l+1}(\mathrm{X}[l])$
- Deep Model: $X[L] = (f_L + I) \circ \cdots \circ (f_1 + I)(X[0])$

❑ Differential Deep Learning:

- Each time moment ("layer"): Instantaneous rate at t : $\frac{\mathrm{dX}}{\mathrm{dt}} = \mathrm{f}(\mathrm{X}(\mathrm{t}))$
  - ❖ Each Discrete layer vs. continuous time moment
  - ❖ Neural mapping vs. Neural Differential Equation Systems
- Continuous-time ("Deep") Model: $\mathrm{X}(\mathrm{t}) = \mathrm{X}(0) + \int_0^t \mathrm{f}(\mathrm{X}(\tau), \mathrm{W}, \tau) d\tau$ Integration over continuous-time
  - ❖ A sequence of mappings vs. continuous integration
  - ❖ Trajectory of dynamics



Residual **DE system** **NDCN**

$$\underset{W_*, b_*}{\operatorname{argmin}} \quad \mathcal{L} = \int_0^T |X(t) - \hat{X(t)}|\, dt$$

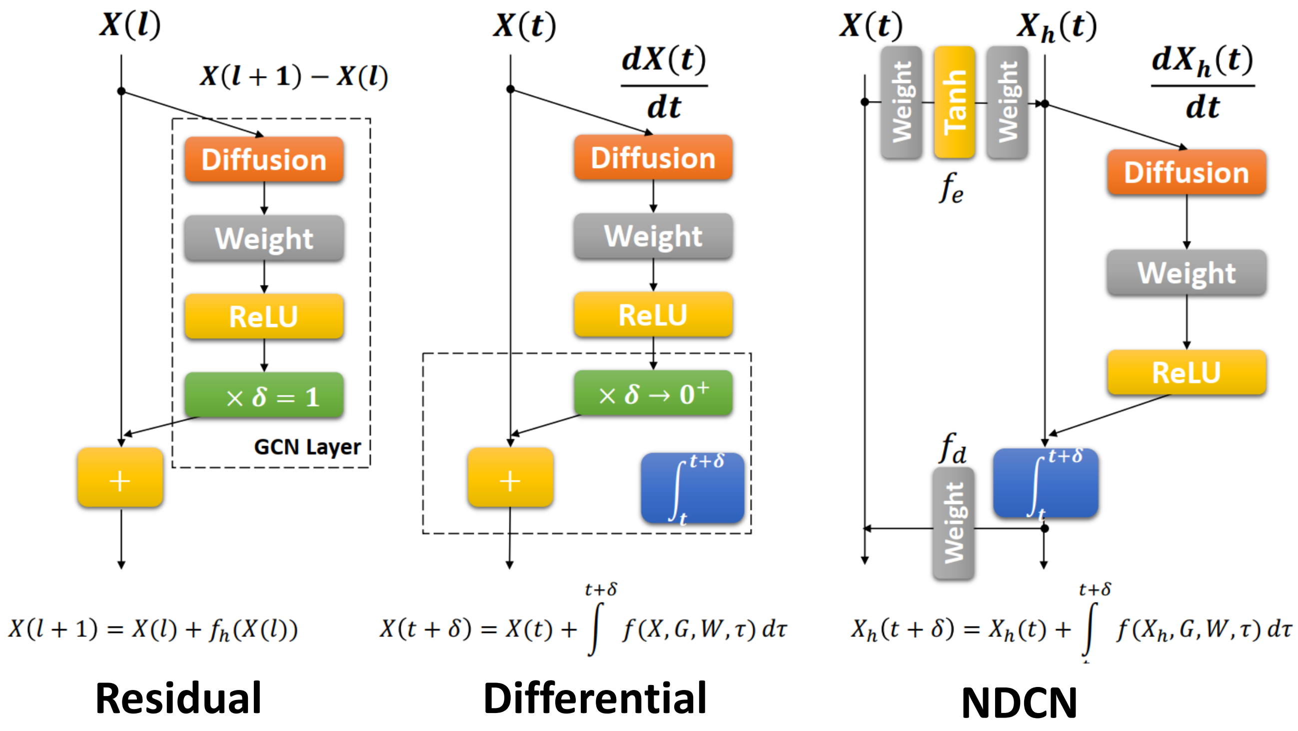
$$\text{subject to} \quad X_h(t) = \tanh\left(X(t) W_e + b_e\right) W_0 + b_0$$

$$\frac{dX_h(t)}{dt} = \mathrm{ReLU}\left(\Phi X_h(t) W + b\right), X_h(0)$$

$$X(t) = X_h(t) W_d + b_d$$

Interpretation from Graph Neural Networks

- **GNN, Residual-GNN, ODE-GNN, NDCN**
  - GNN: $X_{t+1} = f(G, X_t, \theta_t)$
  - Residual-GNN: $X_{t+1} = X_t + f(G, X_t, \theta_t)$
  - Differential-GNN: $X_{t+\delta} = X_t + \delta f(G, X_t, \theta_t), \delta \to 0$
    - $\frac{dX}{dt} = f(G, X_t, \theta_t)$
- **Our model is an Differential-GNN with continuous layer with real number depth.**



Interpretation from RNN and Temporal GNN

- **RNN, Temporal GNN and our model**
  - RNN or Temporal GNN
    - $h_t = f(h_{t-1}, x_t, \theta_t)$ or $h_t = f(h_{t-1}, G * x_t, \theta_t)$
    - $y_t = o(h_t, w_t)$
  - Residual RNN or Temporal GNN with skip connection
    - $h_t = h_{t-1} + f(h_{t-1}, x_t, \theta_t)$ or $h_t = h_{t-1} + f(h_{t-1}, G * x_t, \theta_t)$
    - $y_t = o(h_t, w_t)$
  - Differential RNN or Differential GNN
    - $\frac{dh_t}{dt} = f(h_t, x_t, \theta_t)$ or $\frac{dh_t}{dt} = f(h_t, G * x_t, \theta_t)$
    - $y_t = o(h_t, w_t)$
- **Our model is an Differential GNN**
    - Learning continuous-time network dynamics
    - Encompassing Temporal GNN by discretization
    - Encompassing RNN by not using graph convolution

Exp1: Learning Continuous-time Network Dynamics

❑The Problem:

- Input: $\{\widehat{X(t_1)}, \widehat{X(t_2)}, \ldots, \widehat{X(t_T)} \mid 0 \le t_1 < \cdots < t_T\}, t_1 < \cdots < t_T$ are **arbitrary time moments with different time intervals**
- Output: $X(t)$, t is an arbitrary time moment
  - ❖**interpolation** prediction: $t < t_T$ and $\neq \{t_1 < \cdots < t_T\}$
  - ❖**extrapolation** prediction: t $> t_T$

❑Setups:

- 120 irregularly sampled snapshots of network dynamics
- First 100: 80 for train 20 for testing interpolation
- Last 20: testing for extrapolation

Canonical Dynamics on Graphs in Physics and Biology

❑ Real-world Dynamics on Graph (adjacency matrix A)

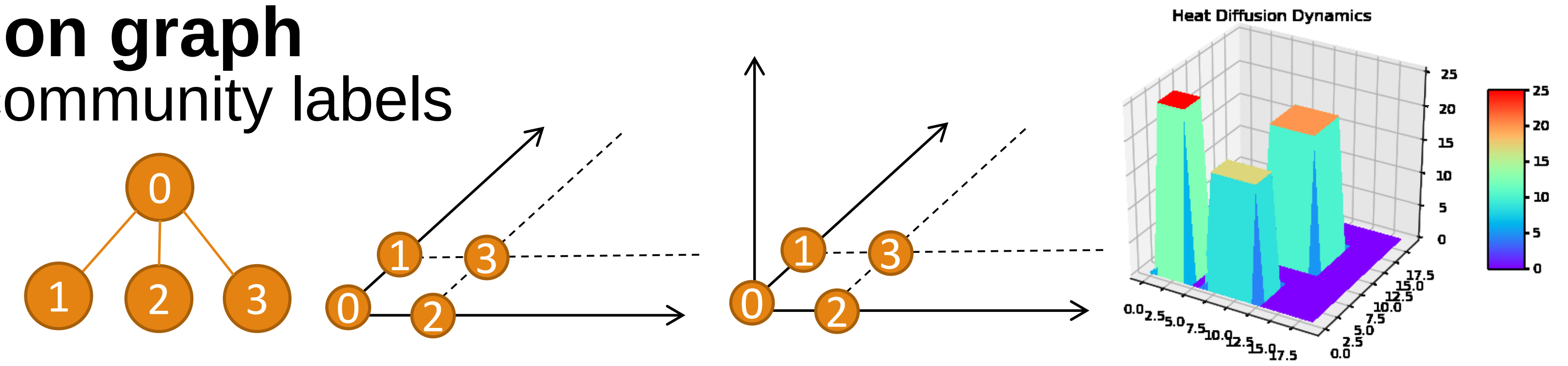
- **Heat diffusion**: $\frac{d\overrightarrow{x_i(t)}}{dt} = -k_{i,j}\sum_{j=1}^{n} A_{i,j}\left(\overrightarrow{x_i(t)} - \overrightarrow{x_j(t)}\right)$
- **Mutualistic interaction**: $\frac{d\overrightarrow{x_i(t)}}{dt} = b_i + \overrightarrow{x_i(t)}\left(1 - \frac{\overrightarrow{x_i(t)}}{k_i}\right)\left(\frac{\overrightarrow{x_i(t)}}{c_i} - 1\right) + \sum_{j=1}^{n} A_{i,j}\frac{\overrightarrow{x_i(t)} * \overrightarrow{x_j(t)}}{d_i + e_i\overrightarrow{x_i(t)} + h_j\overrightarrow{x_j(t)}}$
- **Gene regulatory**: $\frac{d\overrightarrow{x_i(t)}}{dt} = -b_i\overrightarrow{x_i(t)}^{f} + \sum_{j=1}^{n} A_{i,j}\frac{\overrightarrow{x_j(t)}^{h}}{\overrightarrow{x_j(t)}^{h} + 1}$

❑ Graphs

- Grid, Random, power-law, small-world, community, etc.

❑ Visualizing dynamics on graph

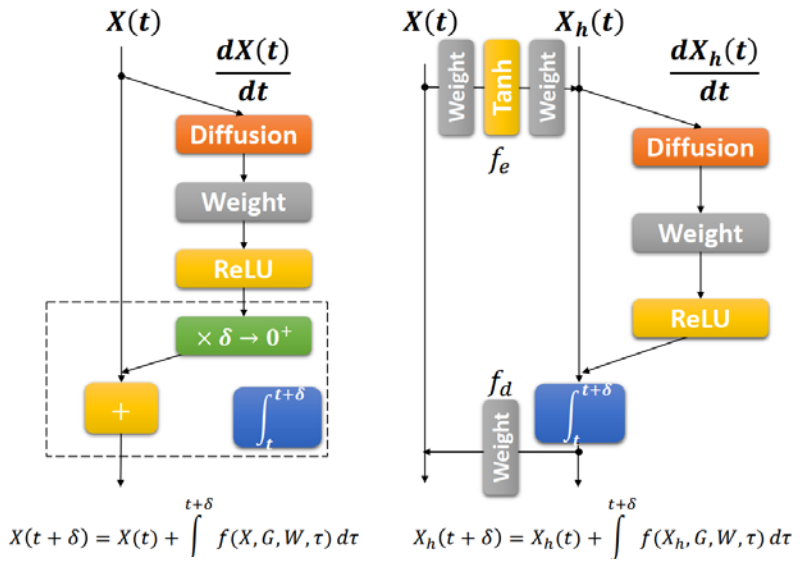
- Nodes are numbered by community labels
- Mapped into a $\mathbb{N}^2$ grid
- $X(t)^{n*1}$: $\mathbb{N}^2 \rightarrow \mathbb{R}$



Exp1: Learning Continuous-time Network Dynamics

❑Baselines: ablation models

- oDifferential-GNN
  - ❖No encoding layer
- oNeural ODE Network
  - ❖No graph diffusion
- oNDCN without control parameter *W*
  - ❖Determined dynamics



Differential **NDCN**

$$
\begin{aligned}
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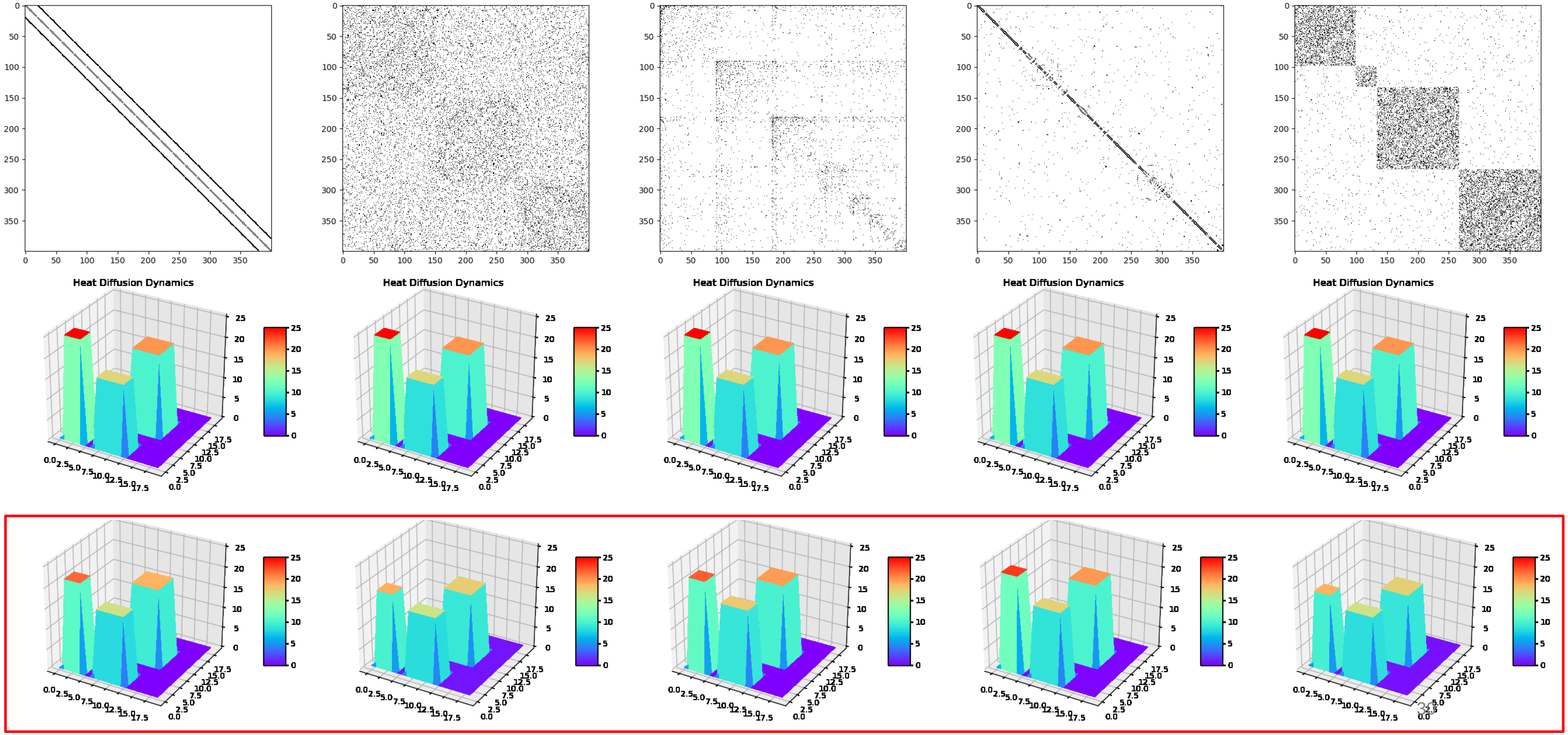
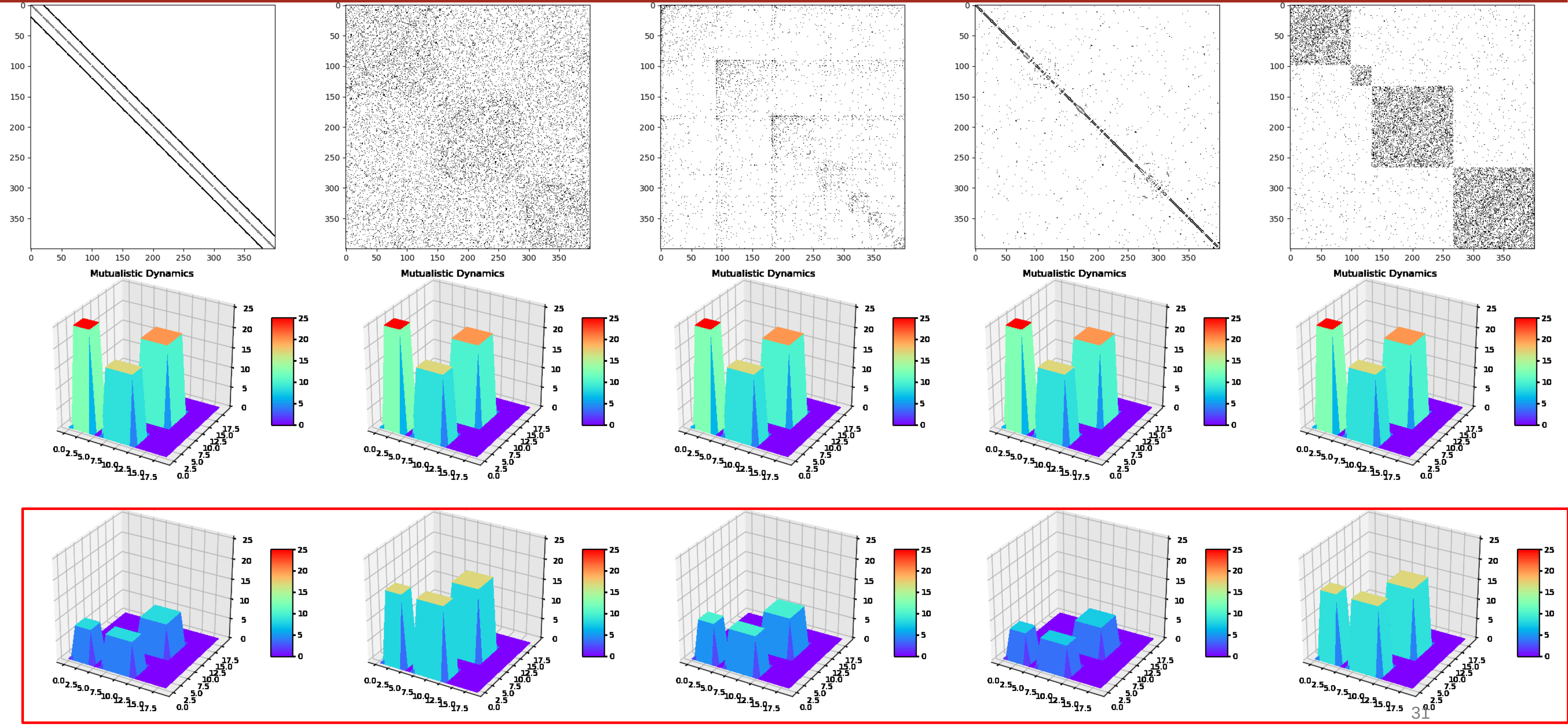
& X(t) = X_h(t)W_d + b_d
\end{aligned}
$$

Chen et al. 2019. Neural Ordinary Differential Equations. *NeurIPS*.

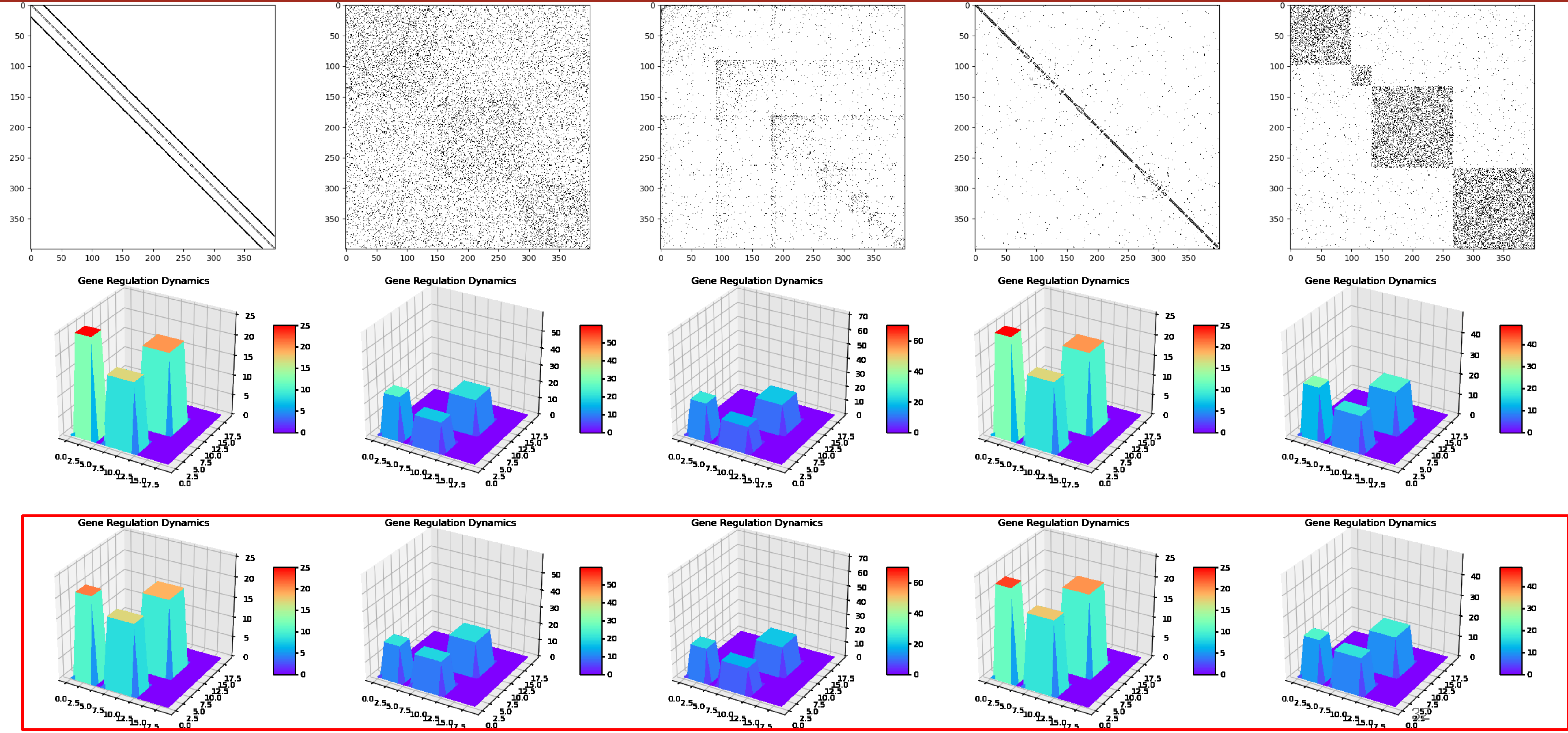
Exp1: Heat Diffusion on Different Graphs



Exp1: Mutualistic Dynamics on Different Graphs



Exp1: Gene Dynamics on Different Graphs



Exp1: Results for Continuous-time Extrapolation

- Mean Absolute Percentage Error
- 20 runs for 3 dynamics on 5 graphs
- Our model achieves lowest error

Table 1: **Continuous-time Extrapolation Prediction.** Our NDCN predicts different continuous-time network dynamics accurately. Each result is the normalized ℓ_1 error with standard deviation (in percentage %) from 20 runs for 3 dynamics on 5 networks by each method.

		Grid	Random	Power Law	Small World	Community
Heat Diffusion	No-Encode	29.9 ± 7.3	27.8 ± 5.1	24.9 ± 5.2	24.8 ± 3.2	30.2 ± 4.4
	No-Graph	30.5 ± 1.7	5.8 ± 1.3	6.8 ± 0.5	10.7 ± 0.6	24.3 ± 3.0
	No-Control	73.4 ± 14.4	28.2 ± 4.0	25.2 ± 4.3	30.8 ± 4.7	37.1 ± 3.7
	NDCN	$\mathbf{4.1 \pm 1.2}$	$\mathbf{4.3 \pm 1.6}$	$\mathbf{4.9 \pm 0.5}$	$\mathbf{2.5 \pm 0.4}$	$\mathbf{4.8 \pm 1.0}$
Mutualistic Interaction	No-Encode	45.3 ± 3.7	9.1 ± 2.9	29.9 ± 8.8	54.5 ± 3.6	14.5 ± 5.0
	No-Graph	56.4 ± 1.1	6.7 ± 2.8	14.8 ± 6.3	54.5 ± 1.0	9.5 ± 1.5
	No-Control	140.7 ± 13.0	10.8 ± 4.3	106.2 ± 42.6	115.8 ± 12.9	16.9 ± 3.1
	NDCN	$\mathbf{26.7 \pm 4.7}$	$\mathbf{3.8 \pm 1.8}$	$\mathbf{7.4 \pm 2.6}$	$\mathbf{14.4 \pm 3.3}$	$\mathbf{3.6 \pm 1.5}$
Gene Regulation	No-Encode	31.7 ± 14.1	17.5 ± 13.0	33.7 ± 9.9	25.5 ± 7.0	26.3 ± 10.4
	No-Graph	13.3 ± 0.9	12.2 ± 0.2	43.7 ± 0.3	15.4 ± 0.3	19.6 ± 0.5
	No-Control	65.2 ± 14.2	68.2 ± 6.6	70.3 ± 7.7	58.6 ± 17.4	64.2 ± 7.0
	NDCN	$\mathbf{16.0 \pm 7.2}$	$\mathbf{1.8 \pm 0.5}$	$\mathbf{3.6 \pm 0.9}$	$\mathbf{4.3 \pm 0.9}$	$\mathbf{2.5 \pm 0.6}$

Exp1: Results for Continuous-time Interpolation

- Interpolation is easier than extrapolation
- Our model achieves lowest error

Table 2: **Continuous-time Interpolation Prediction.** Our NDCN predicts different continuous-time network dynamics accurately. Each result is the normalized ℓ_1 error with standard deviation (in percentage %) from 20 runs for 3 dynamics on 5 networks by each method.

		Grid	Random	Power Law	Small World	Community
Heat Diffusion	No-Encode	32.0 ± 12.7	26.7 ± 4.4	25.7 ± 3.8	27.9 ± 7.3	35.0 ± 6.3
	No-Graph	41.9 ± 1.8	9.4 ± 0.6	18.2 ± 1.5	25.0 ± 2.1	25.0 ± 1.4
	No-Control	56.8 ± 2.8	32.2 ± 7.0	33.5 ± 5.7	40.4 ± 3.4	39.1 ± 4.5
	NDCN	$\mathbf{3.2 \pm 0.6}$	$\mathbf{3.2 \pm 0.4}$	$\mathbf{5.6 \pm 0.6}$	$\mathbf{3.4 \pm 0.4}$	$\mathbf{4.3 \pm 0.5}$
Mutualistic Interaction	No-Encode	28.9 ± 2.0	19.9 ± 6.5	34.5 ± 13.4	27.6 ± 2.6	25.5 ± 8.7
	No-Graph	28.7 ± 4.5	7.8 ± 2.4	23.2 ± 4.2	26.9 ± 3.8	14.1 ± 2.4
	No-Control	72.2 ± 4.1	22.5 ± 10.2	63.8 ± 3.9	67.9 ± 2.9	33.9 ± 12.3
	NDCN	$\mathbf{7.6 \pm 1.1}$	$\mathbf{6.6 \pm 2.4}$	$\mathbf{6.5 \pm 1.3}$	$\mathbf{4.7 \pm 0.7}$	$\mathbf{7.9 \pm 2.9}$
Gene Regulation	No-Encode	39.2 ± 13.0	14.5 ± 12.4	33.6 ± 10.1	27.7 ± 9.4	21.2 ± 10.4
	No-Graph	25.2 ± 2.3	11.9 ± 0.2	39.4 ± 1.3	15.7 ± 0.7	18.9 ± 0.3
	No-Control	66.9 ± 8.8	31.7 ± 5.2	40.3 ± 6.6	49.0 ± 8.0	35.5 ± 5.3
	NDCN	$\mathbf{5.8 \pm 1.0}$	$\mathbf{1.5 \pm 0.6}$	$\mathbf{2.9 \pm 0.5}$	$\mathbf{4.2 \pm 0.9}$	$\mathbf{2.3 \pm 0.6}$

Exp2: Structured Sequence Prediction

- **The Problem (Structured sequence prediction):**
  - Input: $\left\{\widehat{X[1]}, \widehat{X[2]}, \dots, \widehat{X[T]} \middle| 0 \leq 1 < \cdots < T\right\}, 1, ..T$ are regularly-sampled with same time intervals
    - with an emphasis on ordered sequence rather than time
  - Output: $X(t_T + M)$, next M steps
    - extrapolation prediction
- **Setups:**
  - 100 regularly sampled snapshots of network dynamics
  - First 80 for training, last 20 for testing

Exp2: Structured Sequence Prediction

- **Baselines: temporal-GNN models**
  - LSTM-GNN
    - X[t+1]=LSTM(GCN([t], G))
  - GRU-GNN
    - X[t+1]=GRU(GCN([t], G))
  - RNN-GNN
    - X[t+1]=RNN(GCN([t], G))

Seo et al. 2016. [Structured Sequence Modeling with Graph Convolutional Recurrent Networks.]
Wu et al. 2019. [A Comprehensive Survey on Graph Neural Networks]

Exp2: Structured Sequence Prediction

- **Results:**
  - Our model achieves lowest error with much less parameters
- **The learnable parameters:**
  - LSTM-GNN: 84,890, GRU-GNN: 64,770, RNN-GNN: 24,530
  - NDCN: 901

Table 3: **Regularly-sampled Extrapolation Prediction.** Our NDCN predicts different structured sequences accurately. Each result is the normalized ℓ_1 error with standard deviation (in percentage %) from 20 runs for 3 dynamics on 5 networks by each method.

		Grid	Random	Power Law	Small World	Community
Heat Diffusion	LSTM-GNN	12.8 ± 2.1	21.6 ± 7.7	12.4 ± 5.1	11.6 ± 2.2	13.5 ± 4.2
	GRU-GNN	11.2 ± 2.2	9.1 ± 2.3	8.8 ± 1.3	9.3 ± 1.7	7.9 ± 0.8
	RNN-GNN	18.8 ± 5.9	25.0 ± 5.6	18.9 ± 6.5	21.8 ± 3.8	16.1 ± 0.0
	NDCN	$\mathbf{4.3 \pm 0.7}$	$\mathbf{4.7 \pm 1.7}$	$\mathbf{5.4 \pm 0.4}$	$\mathbf{2.7 \pm 0.4}$	$\mathbf{5.3 \pm 0.7}$
Mutualistic Interaction	LSTM-GNN	51.4 ± 3.3	24.2 ± 24.2	27.0 ± 7.1	58.2 ± 2.4	25.0 ± 22.3
	GRU-GNN	49.8 ± 4.1	$\mathbf{1.0 \pm 3.6}$	12.2 ± 0.8	51.1 ± 4.7	$\mathbf{3.7 \pm 4.0}$
	RNN-GNN	56.6 ± 0.1	8.4 ± 11.3	12.0 ± 0.4	57.4 ± 1.9	8.2 ± 6.4
	NDCN	$\mathbf{29.8 \pm 1.6}$	$\mathbf{4.7 \pm 1.1}$	$\mathbf{11.2 \pm 5.0}$	$\mathbf{15.9 \pm 2.2}$	$\mathbf{3.8 \pm 0.9}$
Gene Regulation	LSTM-GNN	27.7 ± 3.2	67.3 ± 14.2	38.8 ± 12.7	13.1 ± 2.0	53.1 ± 16.4
	GRU-GNN	24.2 ± 2.8	50.9 ± 6.4	35.1 ± 15.1	11.1 ± 1.8	46.2 ± 7.6
	RNN-GNN	28.0 ± 6.8	56.5 ± 5.7	42.0 ± 12.8	14.0 ± 5.3	46.5 ± 3.5
	NDCN	$\mathbf{18.6 \pm 9.9}$	$\mathbf{2.4 \pm 0.9}$	$\mathbf{4.1 \pm 1.4}$	$\mathbf{5.5 \pm 0.8}$	$\mathbf{2.9 \pm 0.5}$

Exp3. Node Semi-suprvised Classification

The Problem:

- One-snapshot case
- Input: G, $X,$ part of labels $Y(X)$
- Output: To Complete $Y(X)$

Datasets:

- Table 11: Statistics for three real-world citation network datasets. N, E, D, C represent number of nodes, edges, features, classes respectively.

Dataset	N	E	D	C	Train/Valid/Test
Cora	$2,708$	$5,429$	$1,433$	7	140/500/1, 000
Citeseer	$3,327$	$4,732$	$3,703$	6	120/500/1, 000
Pubmed	$19,717$	$44,338$	500	3	60/500/1, 000

Exp3. Node Semi-suprvised Classification

❑Baselines

- oGraph Convolution Network (GCN)

$$Z = f(X, A) = \mathrm{softmax}\Big(\hat{A}\ \mathrm{ReLU}\Big(\hat{A}XW^{(0)}\Big)\,W^{(1)}\Big)$$

- oAttention-based GNN (AGNN)
- oGraph Attention Networks (GAT)

$$\vec{h}'_i = \sigma\left(\frac{1}{K}\sum_{k=1}^{K}\sum_{j\in\mathcal{N}_i}\alpha_{ij}^{k}\mathbf{W}^{k}\vec{h}_j\right)$$

Kipf et al. 2016. Semi-Supervised Classification with Graph Convolutional Networks
Velickovic et al. 2017. Graph Attention Networks

Exp3. Node Semi-suprvised Classification

❑Interpretation of model

- Input: G, $[X, Mask \odot Y]$, features and some node labels
- Output: To Complete Y
- Model: A graph dynamics to spread features and labels over time T
  - ❖ $\frac{d[X,Y]}{dt} = \mathrm{f}(\mathrm{G}, \mathrm{X}, \mathrm{Y}, \mathrm{W})$

$$\begin{aligned}
\underset{W_e, b_e, W_d, b_d}{\operatorname{argmin}} \quad & \mathcal{L} = \int_0^T \mathcal{R}(t)\, dt - \sum_{i=1}^{n} \sum_{k=1}^{c} \hat{Y}_{i,k}(T) \log Y_{i,k}(T) \\
\text{subject to} \quad & X_h(0) = \tanh\left(X(0) W_e + b_e\right) \\
& \frac{dX_h(t)}{dt} = \mathrm{ReLU}\left(\Phi X_h(t)\right) \\
& Y(T) = \mathrm{softmax}(X_h(T) W_d + b_d)
\end{aligned}$$

Exp3. Node Semi-suprvised Classification

❑Metrics
- Accuracy over 100 runs

❑Results
- Continuous-time dynamics on graphs
- Best results at time T=1.2
  - ❖Continuous depth/time
- Not using dropout

Table 4: Test mean accuracy with standard deviation in percentage (%) over 100 runs. Our NDCN model gives very competitive results compared with many GNN models.

Model	Cora	Citeseer	Pubmed
GCN	81.5	70.3	79.0
AGNN	83.1 ± 0.1	71.7 ± 0.1	$\mathbf{79.9 \pm 0.1}$
GAT	83.0 ± 0.7	72.5 ± 0.7	79.0 ± 0.3
NDCN	$\mathbf{83.3 \pm 0.6}$	$\mathbf{73.1 \pm 0.6}$	$\mathbf{79.8 \pm 0.4}$

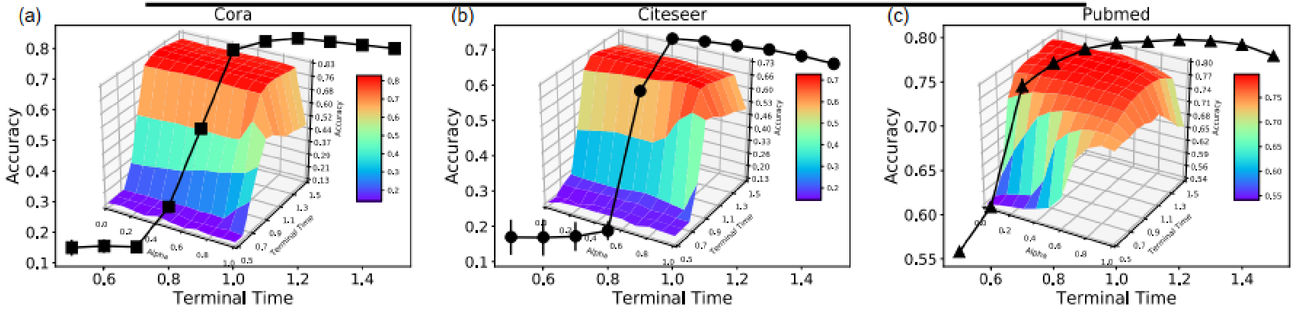


Figure 5: *Our NDCN model captures continuous-time dynamics.* Mean classification accuracy of 100 runs over terminal time when given a specific α. Insets are the accuracy over the two-dimensional space of terminal time and α

Summary

- **Our NDCN, a unified framework to solve**
  - Continuous-time network dynamics prediction:
  - Structured sequence prediction
  - Node regression/classification at final state

  good performance with less parameters.

- **Differential Deep Learning on Graphs**
  - A potential data-driven method to model structure and dynamics of complex systems in a unified framework

This Tutorial

- ❑ **Molecular Graph Generation**: to generate novel molecules with optimized properties
  - o Graph generation
  - o Graph property prediction
  - o Graph optimization
- ☑ **Learning Dynamics on Graphs**: to predict temporal change or final states of complex systems
  - o Continuous-time dynamics prediction
  - o Structured sequence prediction
  - o Node classification/regression
- ❑ **Mechanism Discovery**: to find dynamical laws of complex systems
  - o Density Estimation vs. Mechanism Discovery
  - o Data-driven discovery of differential equations

This Tutorial

- www.calvinzang.com/DDLG_AAAI_2020.html
- AAAI-2020
- **Friday, February 7, 2020, 2:00 PM -6:00 PM**
- **Sutton North, Hilton New York Midtown, NYC**

Thank You!

Weill Cornell Medicine

Differential Deep Learning on Graphs and its Applications

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