Differential Deep Learning on Graphs and its Applications

Chengxi Zang and Fei Wang
Weill Cornell Medicine
www.calvinzang.com

This Tutorial

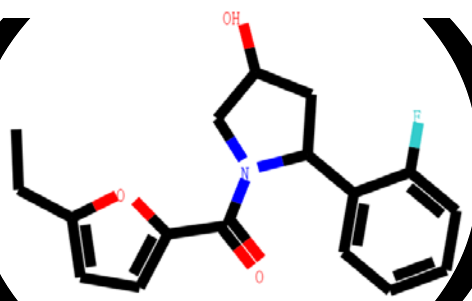
- www.calvinzang.com/DDLG_AAAI_2020.html
- AAAI-2020
- Friday, February 7, 2020, 2:00 PM -6:00 PM
- Sutton North, Hilton New York Midtown, NYC

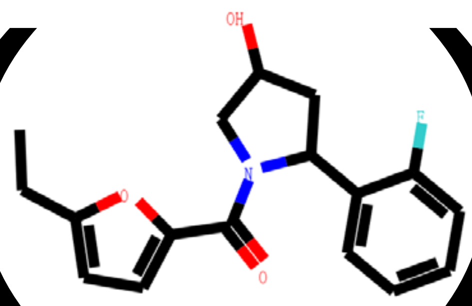
This Tutorial

- ☑ **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 network 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

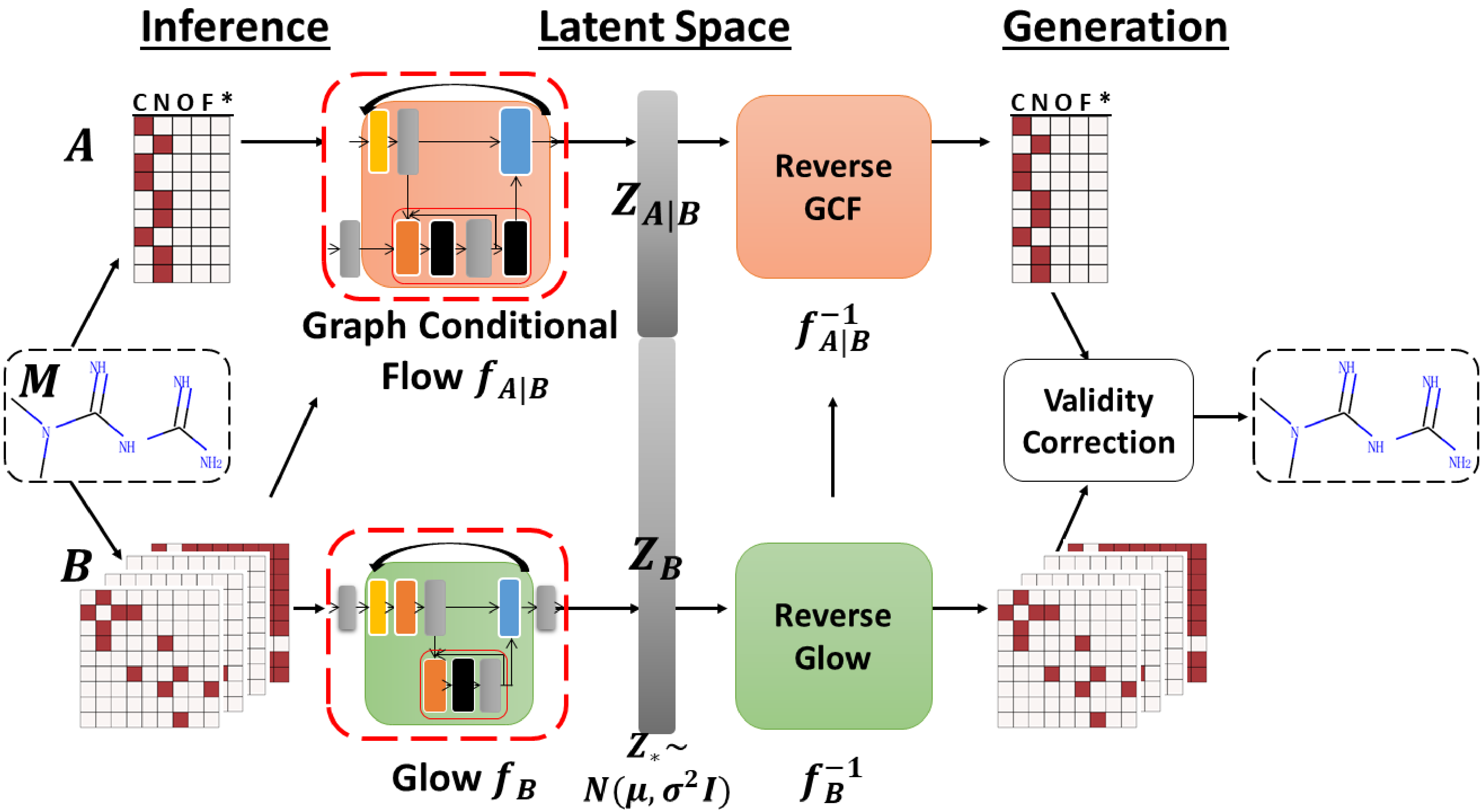
Molecular Graph Generation

- **Goal:** To generate novel molecules with optimized properties
- **Graph Analysis tasks**
  - Graph generation: $\mathrm{G} \sim \mathrm{P}(G)$
  - Graph property prediction: $f(G)$
  - Graph optimization: $\mathrm{G} \rightarrow \mathrm{G}'$ and $\mathrm{maximizing}\ f(G') - f(G)$

P()?

f()=?

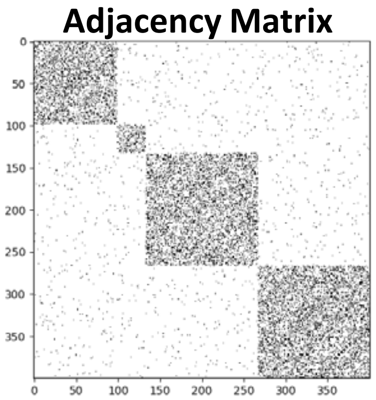
MoFlow: An Invertible Flow Model for Generating Molecular Graphs



Learning Dynamics on Graphs

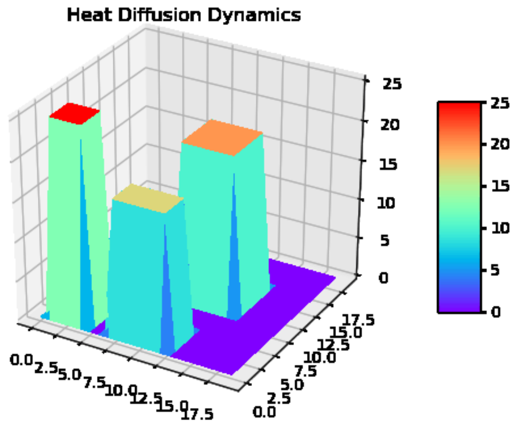
- **Goal: To predict temporal change or final states of complex systems**
- **Graph Analysis tasks**
  - Continuous-time network dynamics prediction $X(t)$
  - Structured sequence prediction $X[t+1]$
  - Node classification/regression $Y(X(T))$

Graph



+

Dynamic Process →



Dynamics of each nodes

?

Neural Dynamics on Complex Networks

❑Our Model :

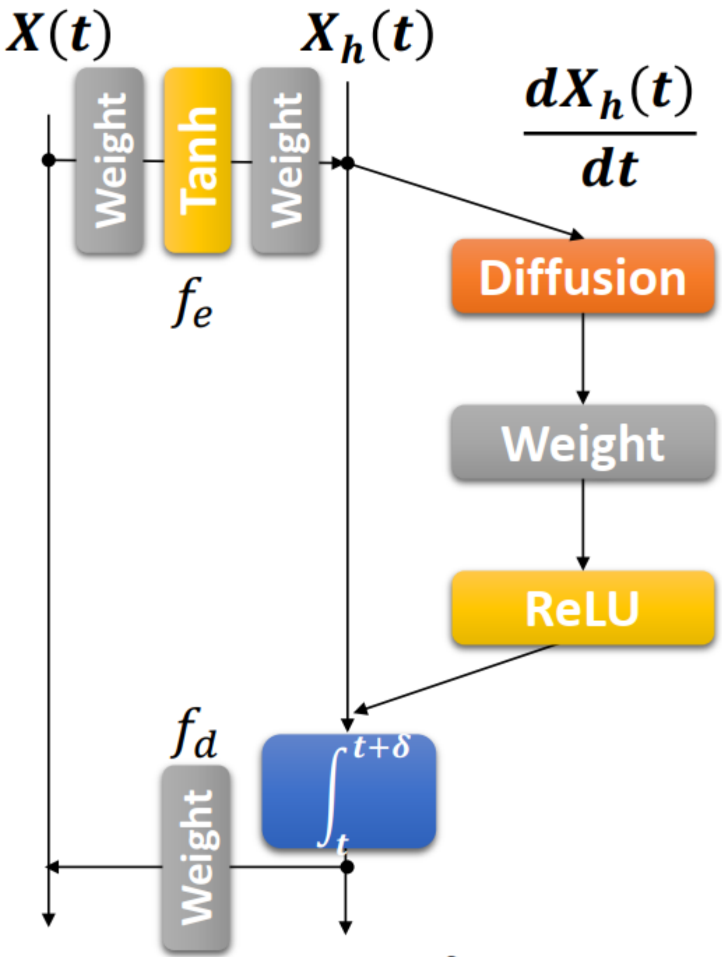
$$\underset{W_*, b_*}{\operatorname{argmin}} \quad \mathcal{L} = \int_0^T |X(t) - \hat{X(t)}| \, dt$$

subject to

$$X_h(t) = \tanh\Big(X(t)W_e + b_e\Big)W_0 + b_0$$

$$\frac{dX_h(t)}{dt} = \operatorname{ReLU}\Big(\Phi X_h(t)W + b\Big), X_h(0)$$

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

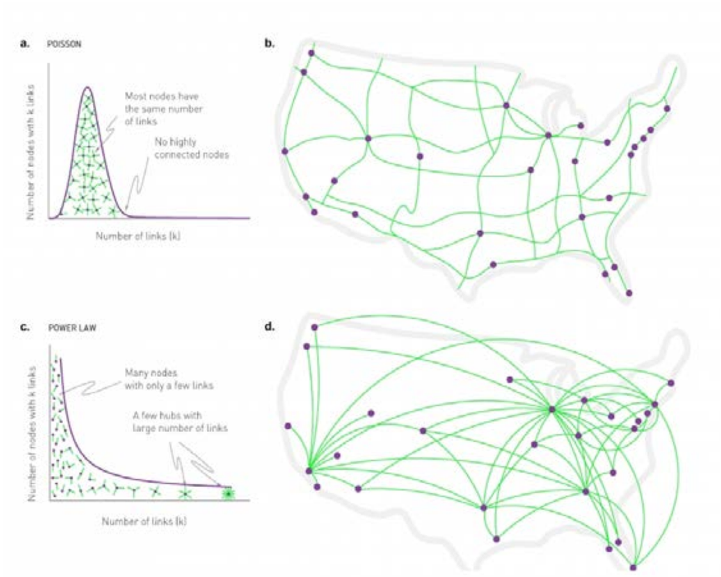


$$X_h(t+\delta) = X_h(t) + \int_t^{t+\delta} f(X_h, G, W, \tau)\, d\tau$$

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

Mechanism Discovery

- **Goals:** To find dynamical laws of complex systems
- **Graph Analysis tasks**
  - Density estimation vs. mechanism discovery
  - Data-driven discovery of differential equations



?

$$\frac{dX}{dt}$$

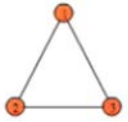
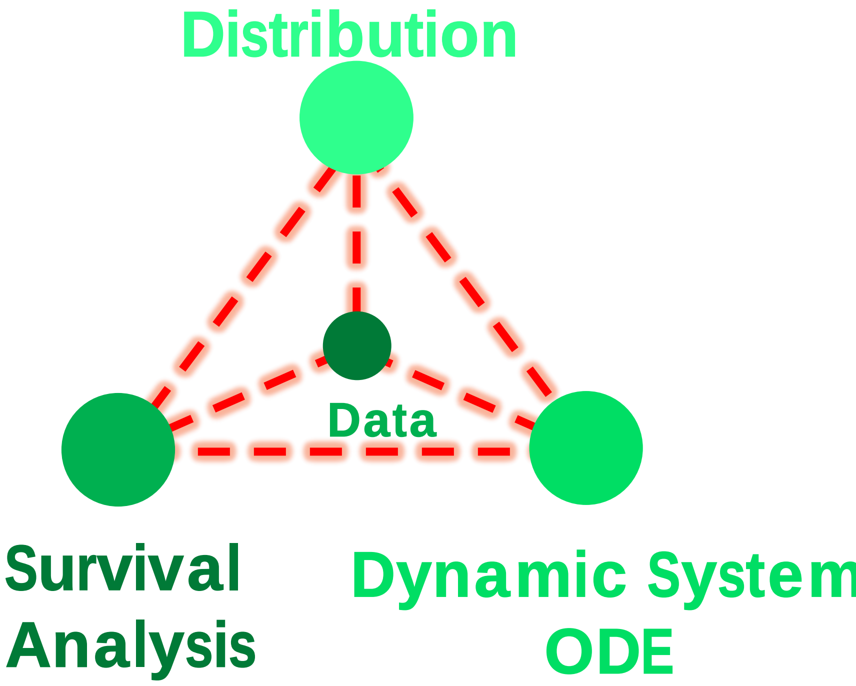
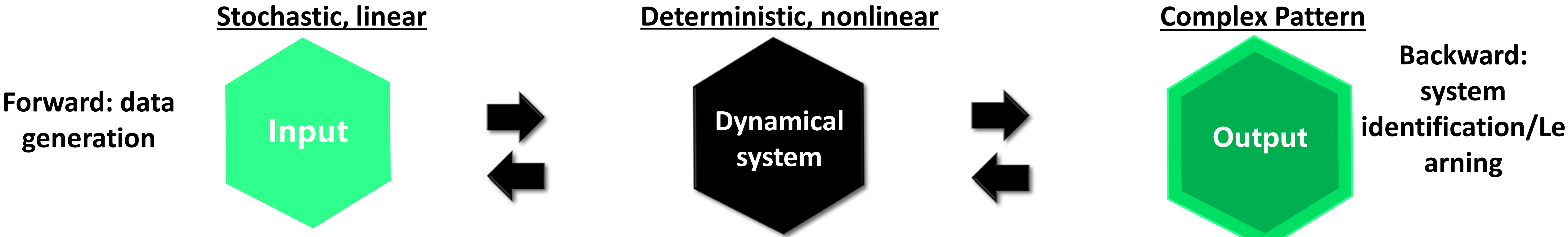


Image from http://networksciencebook.com/chapter/4#hubs

Dynamical Origins of Distribution Functions

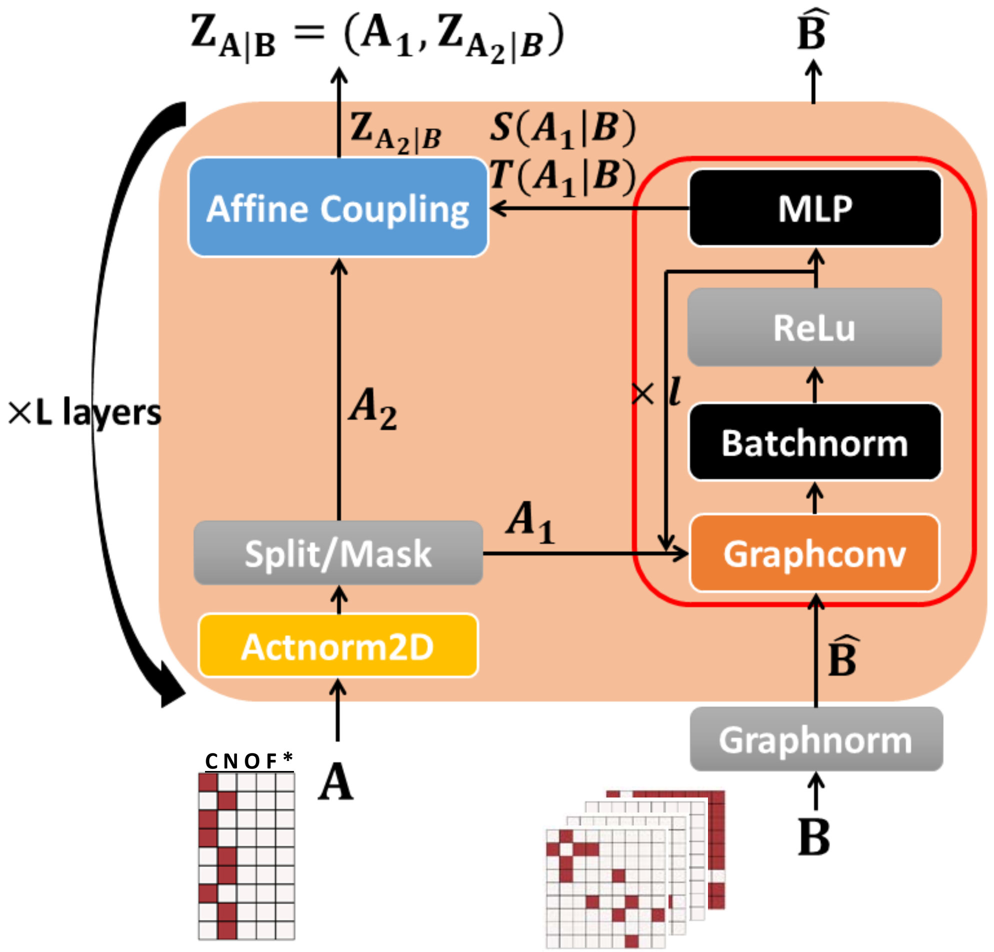
- A theorem constructing dynamic systems described by Differential Equations which generate the observed distribution





Some Practical Tips

- ❑ **Data preprocessing**
  - o Padding null atoms, augmenting null edges
- ❑ **Normalization matters**
  - o Graphnorm, batchnorm, actnorm
- ❑ **Stable flows with less reconstruction error**
  - o Normalization, sigmoid, checking each layer
- ❑ **Discrete mapping is faster than integration**
- ❑ **Split and coupling layer are very efficient invertible framework for graph convolution**
- ❑ **Visualizing dynamics on graphs**
- ❑ **Thinking physical meanings of differential equations**



Differential Deep Learning on Graphs

- **Graphs and Differential Equations are general tools to describe structures and dynamics of complex systems**
- **Inspired by the Differential Equations, we can design and analyze Deep Models**
- **For applications on graphs (our focus), including:**
  - Molecular Graph Generation
  - Learning dynamics of complex systems
  - Mechanism discovery

in a data-driven manner

More Directions

- **Deep Learning → Differential Equations**
  - **Analysis**
    - Math analysis tools
    - Concepts in dynamic system and control: stability, robustness, complexity, resilience, etc.
  - Modeling Continuous-time process
    - Physical meaning. The laws of nature are expressed as differential equations.
- **Differential Equations → Deep Learning**
  - **Design**
    - There are many dynamical systems and differential equations.
    - Discretization of continuous time-varying neural dynamics → Deep Neural Networks
    - DNNs implemented by modern auto-differentiation softwares are more flexible, expressive and efficient
  - Generative models and Invertible structures

More Directions

- **Applications**
  - Network medicine
  - **Drug discovery**
  - Molecular dynamics
  - Urban computing
  - **Social networks**
  - Recommendation
  - Etc. (structures + dynamics)

Thank You!

Differential Deep Learning on Graphs and its Applications

Chengxi Zang and Fei Wang
Weill Cornell Medicine
www.calvinzang.com