Differential Deep Learning on Graphs and its Applications

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This Tutorial

- AAAI-2020
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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 network 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
Molecular Graph Generation

- **Goal:** To generate novel molecules with optimized properties

- **Graph Analysis tasks**
  - Graph generation: $G \sim P(G)$
  - Graph property prediction: $f(G)$
  - Graph optimization: $G \rightarrow G'$ and maximizing $f(G') - f(G)$

$$P \left( \begin{array}{c} \text{molecule 1} \\ \text{molecule 2} \end{array} \right) ? \quad f \left( \begin{array}{c} \text{molecule 1} \\ \text{molecule 2} \end{array} \right) = ?$$
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 $Y(X(T))$

![Adjacency Matrix](Image)

Graph + Dynamic Process $\rightarrow$ Heat Diffusion Dynamics

Dynamics of each nodes

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Our Model:

\[ \text{argmin}_{W_*, b_*} \mathcal{L} = \int_0^T |X(t) - \hat{X}(t)| \, dt \]

subject to

\[ X_h(t) = \tanh \left( X(t) W_e + b_e \right) W_0 + b_0 \]

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

\[ X(t) = X_h(t) W_d + b_d \]

\[ \Phi = D^{-\frac{1}{2}} (D - A) D^{-\frac{1}{2}} \in \mathbb{R}^{n \times n} \]
Mechanism Discovery

- **Goals**: To find dynamical laws of complex systems

- **Graph Analysis tasks**
  - Density estimation vs. mechanism discovery
  - Data-driven discovery of differential equations

Image from [http://networksciencebook.com/chapter/4#hubs](http://networksciencebook.com/chapter/4#hubs)
A theorem constructing dynamic systems described by Differential Equations which generate the observed distribution.
Some Practical Tips

- **Data preprocessing**
  - Padding null atoms, augmenting null edges

- **Normalization matters**
  - Graphnorm, batchnorm, actnorm

- **Stable flows with less reconstruction error**
  - 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**
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)
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