Data Type 2: temporal change model

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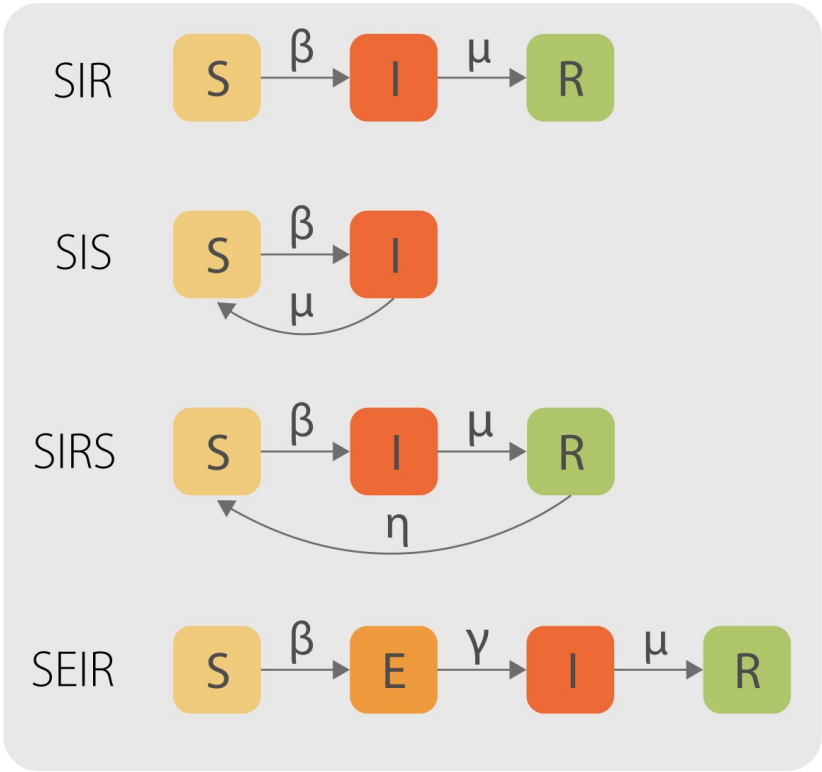
Agenda - temporal change model

- Traditional Methods in Epidemiology
  - Susceptible-Infected-Recovered (SIR) – like models
- Graph Neural Networks for Epidemiology
  - Basics of GNN
  - Spatio-Temporal GNN
  - Forward problem: forecast
  - Inverse problem: zero-patient
- GNN, SIR and PDE
- Open Problems

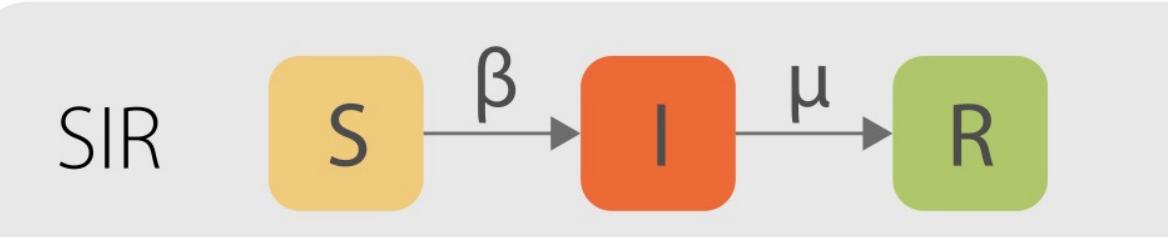
Epidemiology Models

- S: Susceptible
- I: Infectious
- R: Recovered
- E: Exposed



Pastor-Satorras, Romualdo, Claudio Castellano, Piet Van Mieghem, and Alessandro Vespignani. "Epidemic processes in complex networks." *Reviews of modern physics* 87, no. 3 (2015): 925.

Traditional Methods in Epidemiology



$$\frac{d\rho^I}{dt} = \beta\rho^I\rho^S - \mu\rho^I,$$

$$\frac{d\rho^S}{dt} = -\beta\rho^I\rho^S + \chi\rho^I,$$

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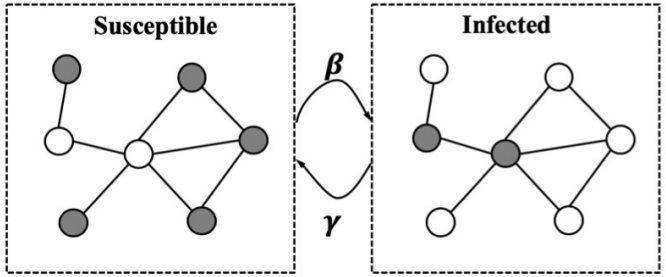
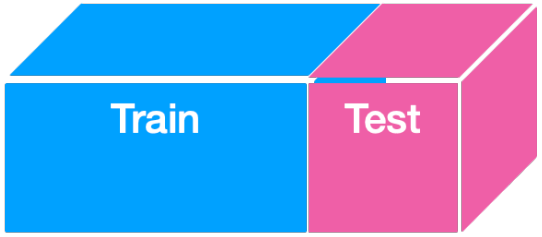
Graph Neural Networks for Epidemiology

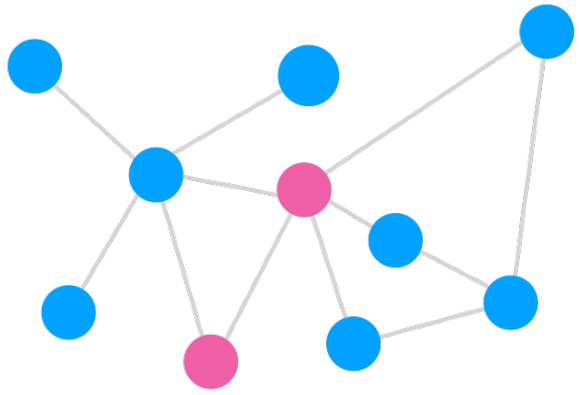
- SIR-like models
  - [+] temporal diffusion
  - [-] Ignore connectivity
- Graph neural networks (GNN)
  - [+] Characterize connectivity
  - [-] Lack temporal diffusion
- GNN + RNN
  - Connectivity + Temporal



Basics of GNN



Machine Learning
Block Split



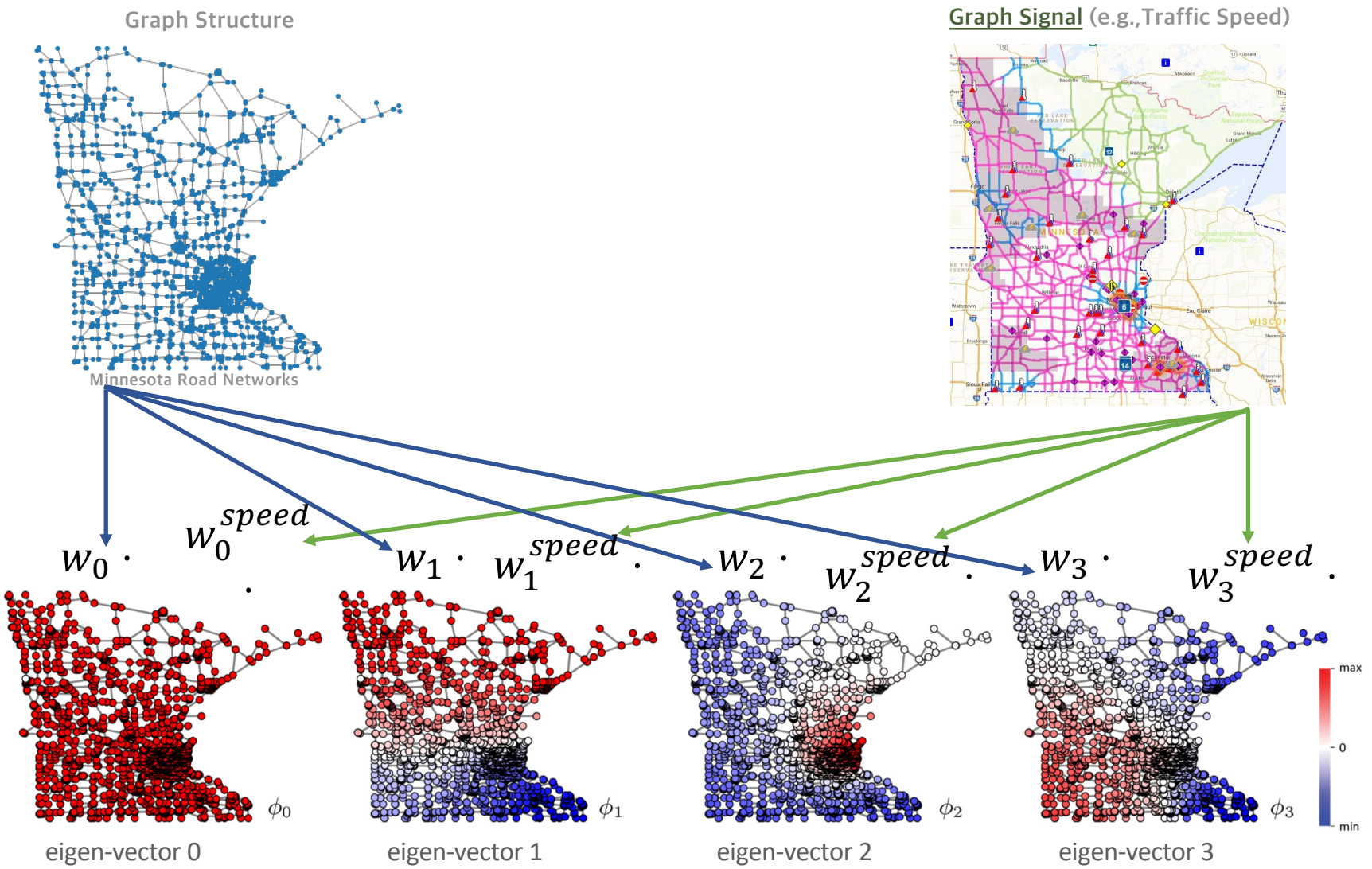
Graph Machine Learning
Geometric Split

Basics of GNN

- Spectral Decomposition

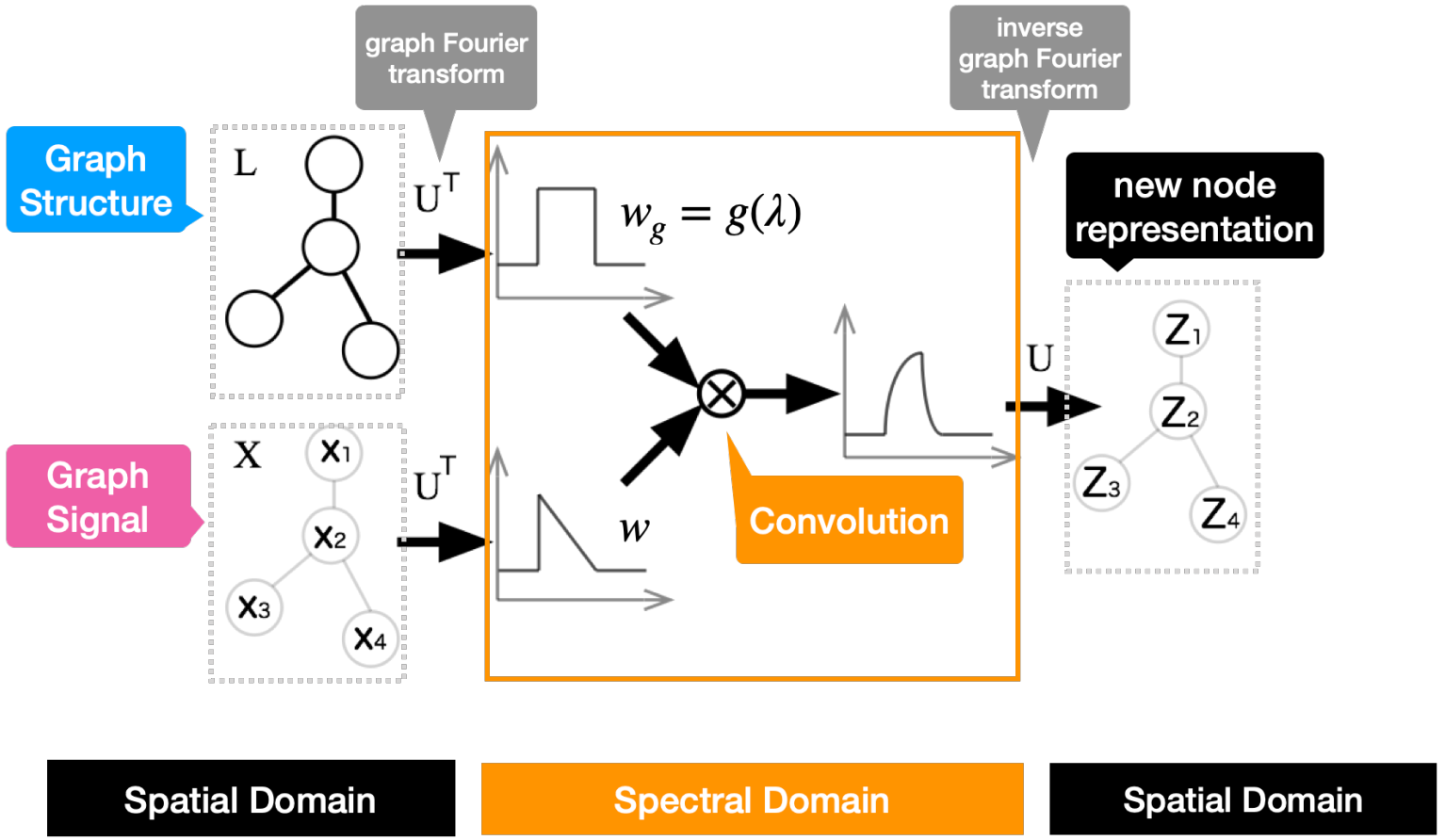
Img Source

Basics of GNN

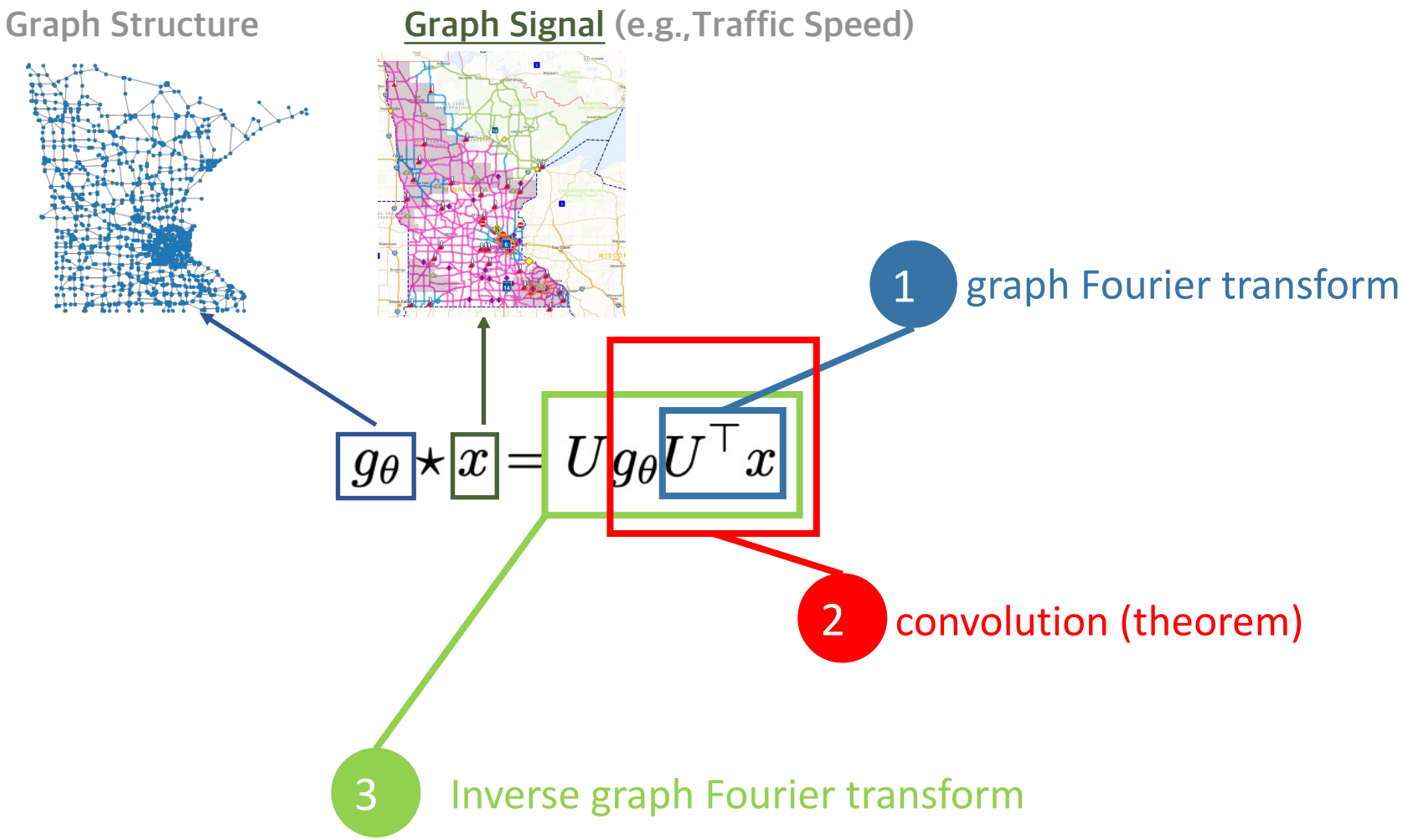


Graph Fourier Transform (Spectral Decomposition)

Basics of GNN

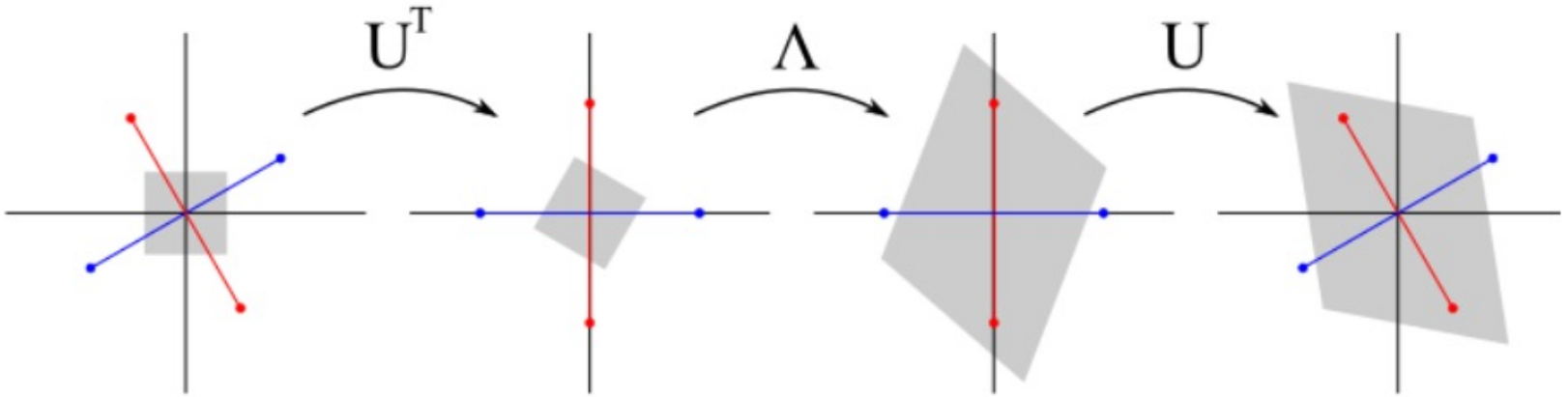


Basics of GNN



Basics of GNN

- Geometric Interpretation of Graph Fourier Transform



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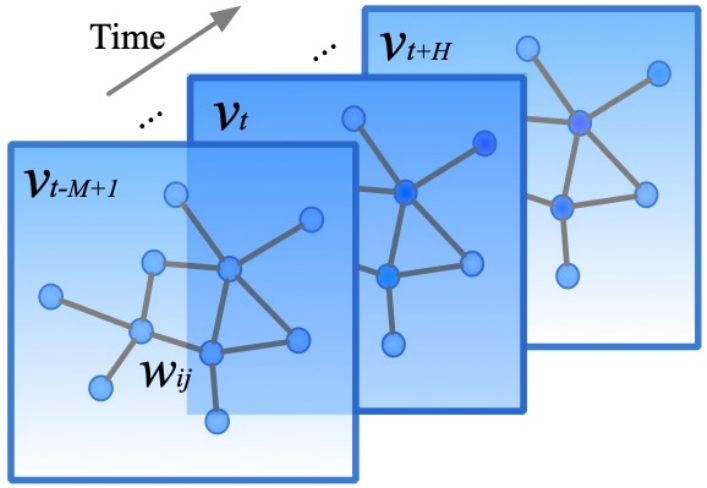
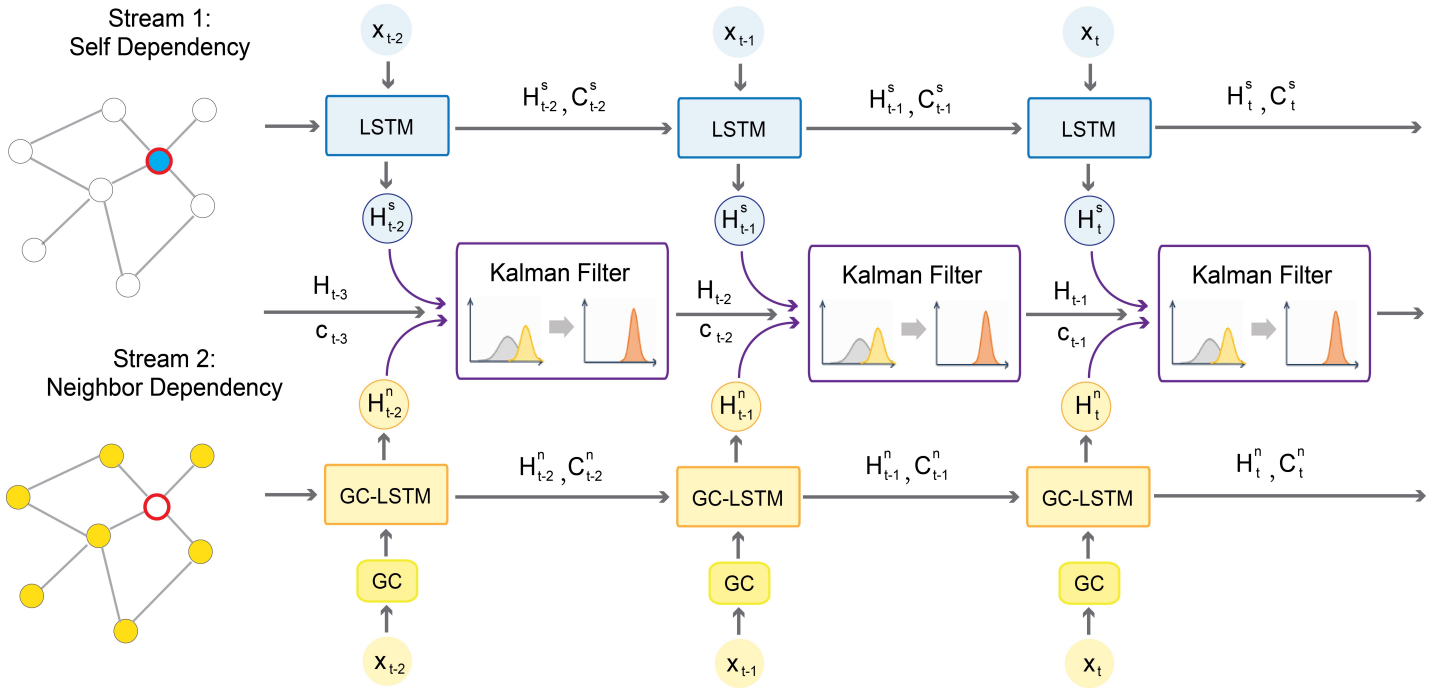
Spatio-Temporal GNN



- GNN for spatial neighbors
- RNN for temporal neighbors (itself)
- Options:
  - GNN + RNN
  - RNN + GNN

Yu, Bing, Haoteng Yin, and Zhanxing Zhu. "Spatio-temporal graph convolutional networks: A deep learning framework for traffic forecasting." arXiv preprint arXiv:1709.04875 (2017).

Spatio-Temporal GNN



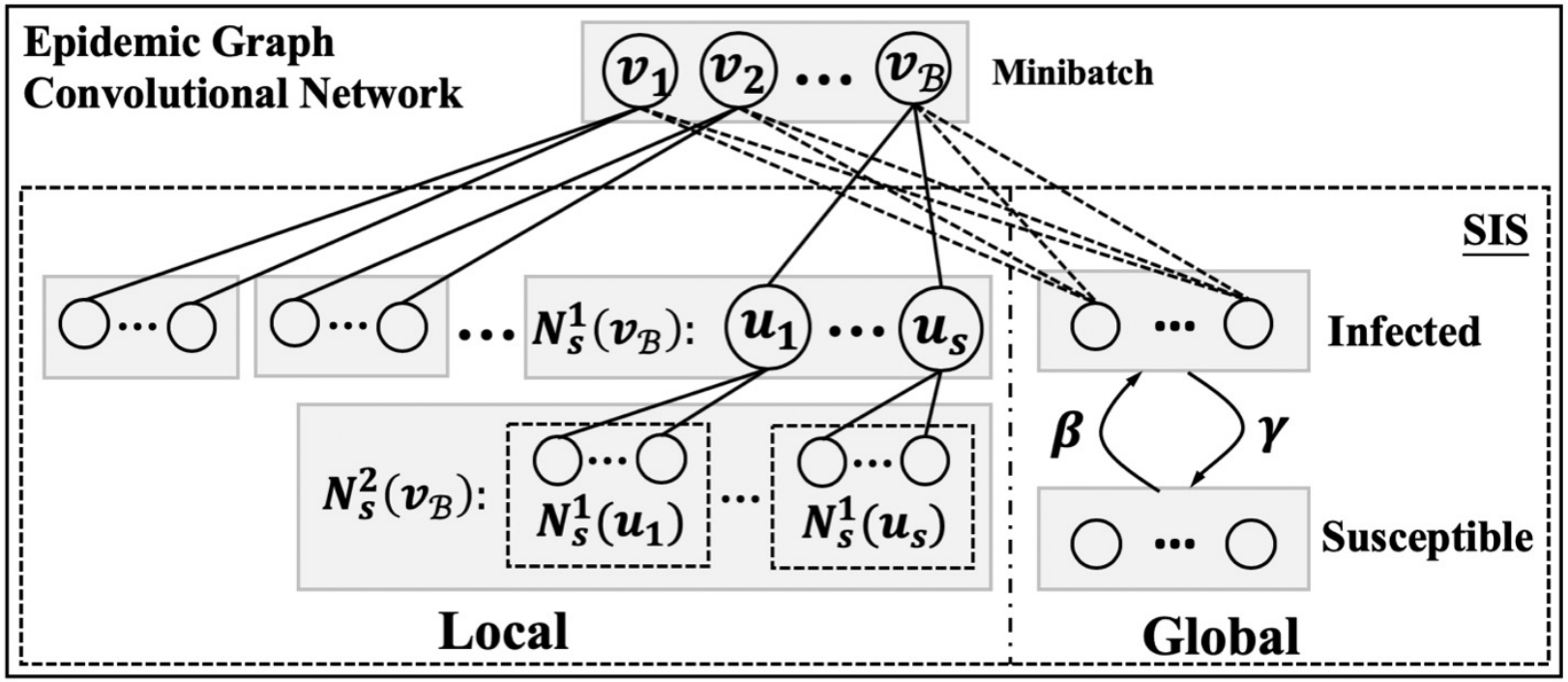
Learn weights by their variances: balance information with variance

Chen, Fanglan, Zhiqian Chen, Subhodip Biswas, Shuo Lei, Naren Ramakrishnan, and Chang-Tien Lu. "Graph Convolutional Networks with Kalman Filtering for Traffic Prediction." In *Proceedings of the 28th International Conference on Advances in Geographic Information Systems*, pp. 135-138. 2020.

Jiang, Weiwei, and Jiayun Luo. "Graph Neural Network for Traffic Forecasting: A Survey." *arXiv preprint arXiv:2101.11174*(2021).

GNN for Epidemiology

- Forecast



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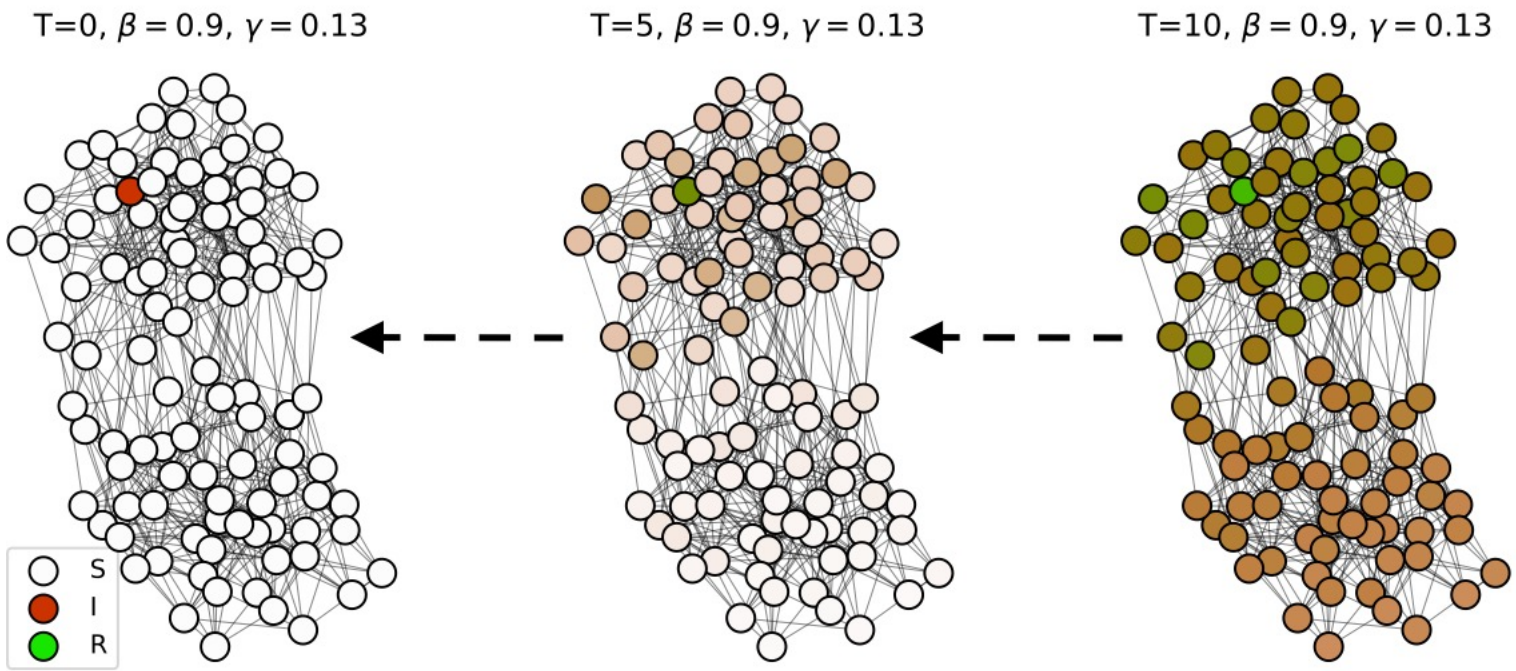
GNN for Epidemiology

- Finding Patient Zero
  - Use GNN to learn Reaction-Diffusion (RD)

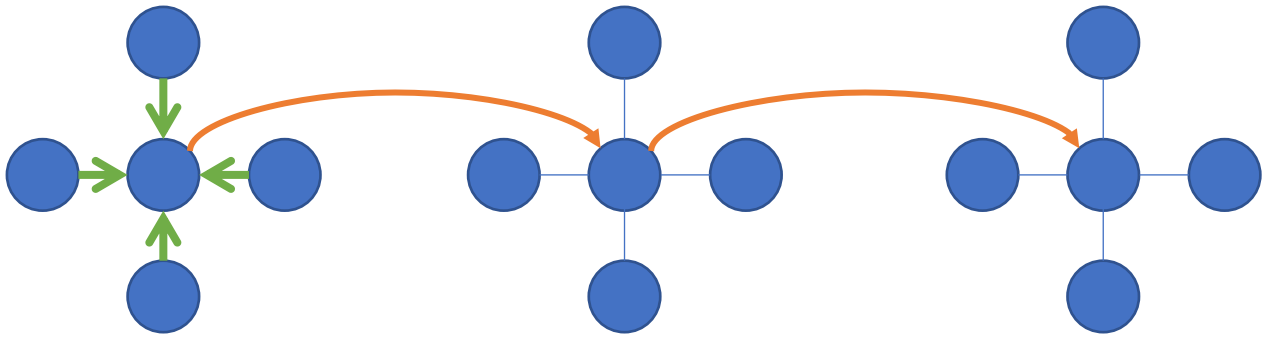


Shah, Chintan, Nima Dehmamy, Nicola Perra, Matteo Chinazzi, Albert-László Barabási, Alessandro Vespignani, and Rose Yu. "Finding Patient Zero: Learning Contagion Source with Graph Neural Networks." *arXiv preprint arXiv:2006.11913*(2020).

GNN, RNN, SIR and PDE

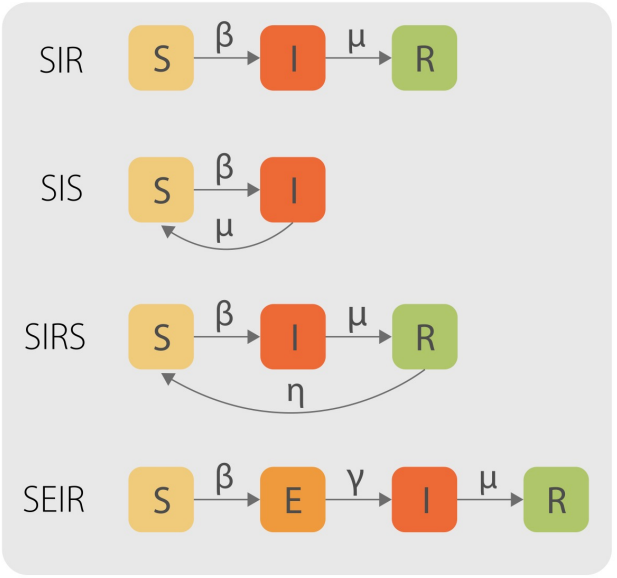
- RNN: $h_t = f(h_{t-1}, x)$
  - h_{t-1} denotes previous state
- GNN: $h_t = g(N_{t-1}, x)$
  - N_{t-1} denotes neighbors of x at time $t-1$

- If attributes are neighbor-dependent
  - RNN is equivalent to GNN on self-node
- Else
  - Combining RNN and GNN to get collect more information



GNN, RNN, SIR and PDE

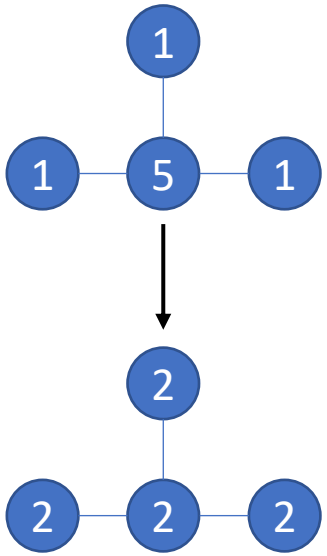
- SIR(-like) is a special case of GNN
  - Susceptible
    - $\frac{dS}{dt} = -\beta \frac{SI}{N}$
    - $h_S = g_1(h_S, h_I)$
  - Infectious
    - $\frac{dI}{dt} = \beta \frac{SI}{N} - \gamma I$
    - $h_I = g_2(h_S, h_I)$
  - Recovered
    - $\frac{dR}{dt} = \gamma I$
    - $h_R = g_3\,(h_I)$



- GNN:
  - $h_t = g(h_{t-1}, N_{t-1})$ where N_{t-1} are neighbors distribution in S, I, R

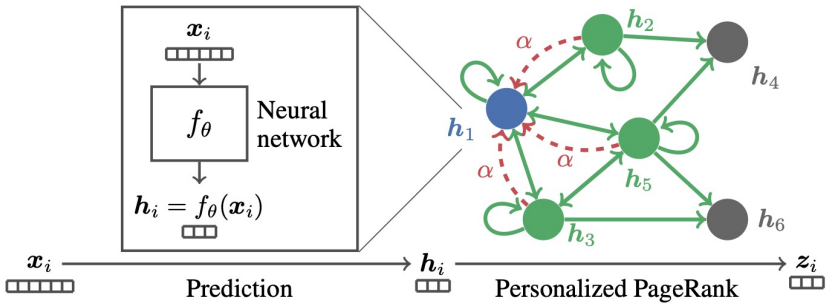
GNN, RNN, SIR and PDE

- GNN is a discretized PDE
  - $h_t = g(h_{t-1}, A) = h_{t-1}A = h_{t-1} + \sum_{i\sim N} h(i)_{t-1}$
  - Neighbor-smoothing
- Example:
  - 5 with neighbors 1, 1, 1 -> 2 for all
- Drawback
  - Propagation without fine control



GNN, RNN, SIR and PDE

- ResNet and PDE
  - $h_t = h_{t-1} + F(h_t)$
- GNN (PPNP)
  - $h_t = \alpha h_{t-1} + (1-\alpha)F(h_t)$
  - Where $F(h_t) = Ah_t$ (graph conv.)
- Rational function
  - $h_t = \frac{P(h_t)}{Q(h_t)}$
  - Where P & Q are polynomials
  - Rational approximation is more accurate than polynomial or linear function

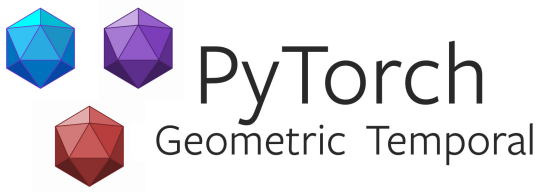


Klicpera, Johannes, Aleksandar Bojchevski, and Stephan Günnemann. "Predict then propagate: Graph neural networks meet personalized pagerank." *arXiv preprint arXiv:1810.05997*(2018).

Bianchi, Filippo Maria, Daniele Grattarola, Lorenzo Livi, and Cesare Alippi. "Graph neural networks with convolutional arma filters." IEEE Transactions on Pattern Analysis and Machine Intelligence (2021).

Implementation

- Diffusion of Epidemics
  - Independent cascade
  - Linear threshold
  - SIR, SIS, SEIR etc.
- PyTorch Geometric Temporal
  - STGCN
  - T-GCN
  - GC-LSTM
  - DCRNN



Open Problems

- Over-smoothing v.s. Long-term dynamics
  - Information disappears after several GNN layers
  - GNN w/ RNN models at most long-short term
- Continuous and discretized propagation
  - One GNN layer conduct one discretized propagation
- Temporal Networks
  - Topology changes along the time
- Digraph or DAG
  - Most of GNN focus on undirected graph

Reference

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Q&A

5 minutes break