Temporal Graph Neural Networks for Irregular Data

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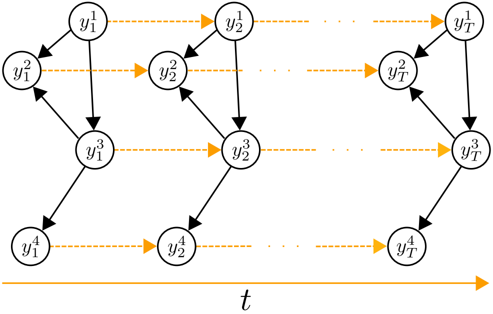
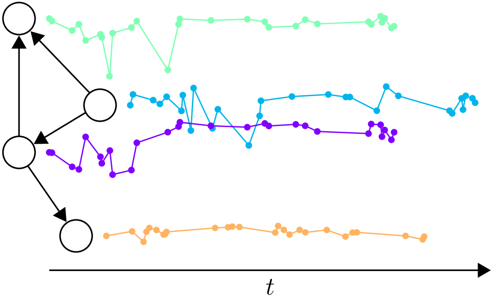
Background: Temporal Graph Neural Networks



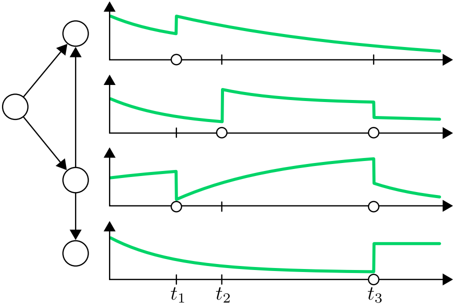
- Time series data with underlying graph structure
- Graph Neural Networks (GNNs) are deep learning models for graph-structured data
- Temporal GNNs include a time dimension

TGNN4I: Forecasting Irregular Graph-Structured Time Series



- One time series at each node
- Irregular observations
  - Irregular time steps
  - Observing subset of nodes
- Forecasting problems

Time-Continuous Latent States



- Time-continuous latent state in each node
- State defined by:
  - State dynamics in-between observations
  - State update when node is observed

Latent Dynamics: In-Between Observations

- State in node n

$$\boldsymbol{h}^n(t) = \bar{\boldsymbol{h}}_i^n + \tilde{\boldsymbol{h}}^n(t) \tag{1}$$

  - Static component $\bar{\boldsymbol{h}}_i^n$
  - Dynamic component $\tilde{\boldsymbol{h}}^n(t)$

Latent Dynamics: In-Between Observations

- State in node n

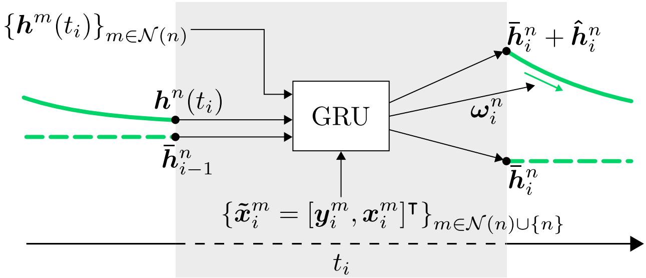
$$\boldsymbol{h}^n(t) = \bar{\boldsymbol{h}}_i^n + \tilde{\boldsymbol{h}}^n(t) \tag{1}$$

  - Static component $\bar{\boldsymbol{h}}_i^n$
  - Dynamic component $\tilde{\boldsymbol{h}}^n(t)$
- Define $\tilde{\boldsymbol{h}}^n(t)$ over $]t_i, t_j]$ as solution to the ODE

$$d\tilde{\boldsymbol{h}}^n(t) = A\tilde{\boldsymbol{h}}^n(t)\ dt \tag{2}$$

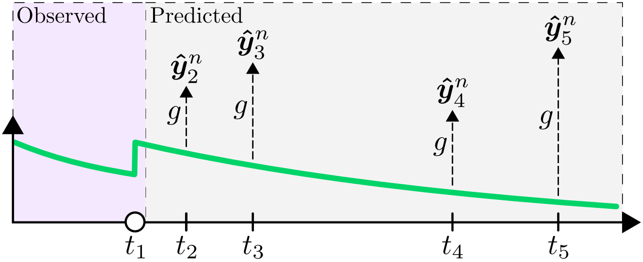
  with initial condition $\tilde{\boldsymbol{h}}^n(t_i) = \hat{\boldsymbol{h}}_i^n$.
- Closed form solution:
  - Exponential decay
  - Periodic dynamics

Latent Dynamics: Observation Update



- Gated Recurrent Unit (GRU) update
- GRU cell outputs
  - New state $\bar{\boldsymbol{h}}_i^n + \hat{\boldsymbol{h}}_i^n$
  - New static component $\bar{\boldsymbol{h}}_i^n$
  - Parameters $\boldsymbol{\omega}_i^n$ defining latent dynamics
- Extended with GNN layers

Making Predictions



- Predictive model g maps latent state $\rightarrow$ prediction

$$\hat{\boldsymbol{y}}_j^n = g(\boldsymbol{h}^n(t_j)) \tag{3}$$

  - GNN layers in g
- Predictions for arbitrary future time points!
  - Custom loss function

Experiments

Datasets

- Traffic (PEMS-BAY, METR-LA)
- Climate (USHCN)
- Synthetic periodic

Models

- TGNN4I with alternative dynamics
- Baseline models
  - All nodes (joint)ly
  - Independent (node)s

	PEMS-BAY (25% Obs.)	USHCN (T_{min})
Predict Previous	26.32	16.88
GRU-D (joint)	18.79	8.03
GRU-D (node)	8.79	13.12
Transformer (joint)	12.05	7.36
Transformer (node)	16.49	15.68
LG-ODE	27.00	-
TGNN4I (static)	7.41	6.97
TGNN4I (exponential)	**7.10**	**6.72**
TGNN4I (periodic)	**7.10**	**6.72**

Summary

- TGNN4I: A temporal GNN for forecasting irregular data
  - Time-continuous latent states to handle irregularity
  - GNN components to utilize graph structure
  - Predictions for arbitrary future time points
- Code available: `github.com/joeloskarsson/tgnn4i`

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