

Graph Deep Learning for Time Series and Spatiotemporal Data

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Module

Missing-Data Handling

Dealing with missing data

The problem of missing data

So far, we assumed to deal with **complete sequences**.

- i.e., to have valid observations associated with each node (sensor) and time step.

However, time series collected by real-world sensor networks often have **missing data**, due to:

- **faults**, of either transient or permanent nature;
- **asynchronicity** among the time series;
- **communication errors**...

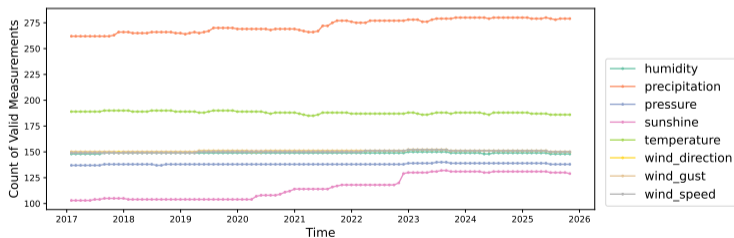
Most forecasting methods operate on complete sequences.

→ We need a way to **impute**, i.e., *reconstruct*, missing data.

Example: Data availability in PeakWeather

	Temp.	Humidity	Precip.	Sunshine	Pressure	Wind speed	Wind gusts	Wind dir.
Rain gauges	41/38	0/0	124/141	0/0	0/0	0/0	0/0	0/0
Meteo stations	148/148	148/148	138/138	103/129	137/138	149/150	150/150	150/150
Missing values	1.94%	0.96%	3.51%	13.02%	1.39%	1.46%	1.08%	1.10%

Number of stations per variable (# in Jan 2017 / # in Oct 2025). Missing data prc only for stations with that variable.



Missing data types

We can categorize missing data patterns according to the **conditional distribution** $p(\mathbf{m}_t^i | \mathbf{M}_{\leq t})$.

- **Point missing**

$p(\mathbf{m}_t^i = 0)$ is **the same** across nodes and time steps, i.e., RVs associated to each \mathbf{m}_t^i are iid.

$$p(\mathbf{m}_t^i) = \mathcal{B}(\eta) \quad \forall i, t$$

- **Block missing**

$p(\mathbf{m}_t^i = 0)$ is not independent from missing data **at other nodes and/or time steps**.

Temporal block missing $p(\mathbf{m}_t^i | \mathbf{m}_{t-1}^i) \neq p(\mathbf{m}_t^i)$

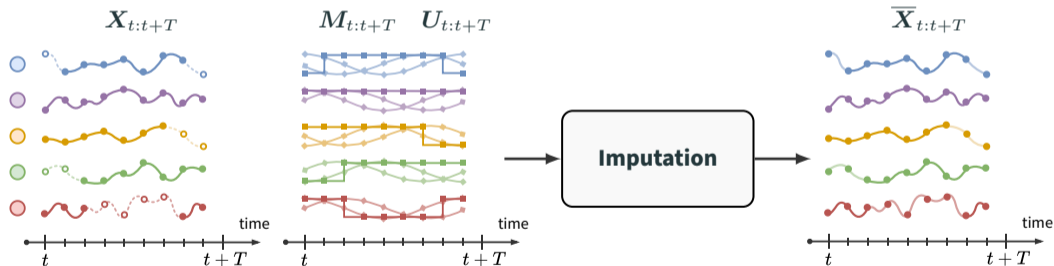
Spatial block missing $p(\mathbf{m}_t^i | \{\mathbf{m}_t^j\}^{j \neq i}) \neq p(\mathbf{m}_t^i)$

Spatiotemporal block missing $p(\mathbf{m}_t^i | \mathbf{m}_{t-1}^i, \{\mathbf{m}_t^j\}^{j \neq i}) \neq p(\mathbf{m}_t^i)$

Time series imputation

Time series imputation (TSI)

Given a window of observations $\mathbf{X}_{t:t+T}$, mask $\mathbf{M}_{t:t+T}$, and covariates $\mathbf{U}_{t:t+T}$, the goal is to estimate the missing observations in the sequence $\bar{\mathbf{X}}_{t:t+T}$.



→ We use a **mask** $m_t^i \in \{0, 1\}$ to distinguish between missing (0) and valid (1) observations.

Optimization

Parameters θ can be learned by **minimizing a loss function** $\ell(\cdot, \cdot)$ on **valid observations** in a training set:

$$\hat{\theta} = \arg \min_{\theta} \sum_{t=1}^T \sum_{i=1}^N \frac{\|\mathbf{m}_t^i \odot \ell(\hat{\mathbf{x}}_t^i, \mathbf{x}_t^i)\|_1}{\|\mathbf{m}_t^i\|_1}. \quad \leftarrow \quad \text{e.g., } \ell = (\hat{\mathbf{x}}_t^i - \mathbf{x}_t^i)^2$$

For imputation, we **mark** some valid observations **as missing** with mask $\overline{\mathbf{m}}_t^i$ to obtain ground-truth labels:

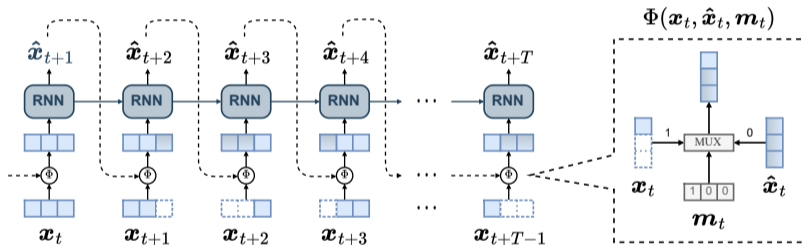
$$\hat{\theta} = \arg \min_{\theta} \sum_{t=1}^T \sum_{i=1}^N \frac{\|\overline{\mathbf{m}}_t^i \odot \ell(\overline{\mathbf{x}}_t^i, \mathbf{x}_t^i)\|_1}{\|\overline{\mathbf{m}}_t^i\|_1}.$$

 Data where $\overline{\mathbf{m}}_t^i = \mathbf{1}$ must **not be used** in the model to obtain the imputations.

Deep learning for TSI

Besides standard statistical methods, deep learning approaches have become a popular alternative.

- In particular, **autoregressive models** (e.g., RNNs).

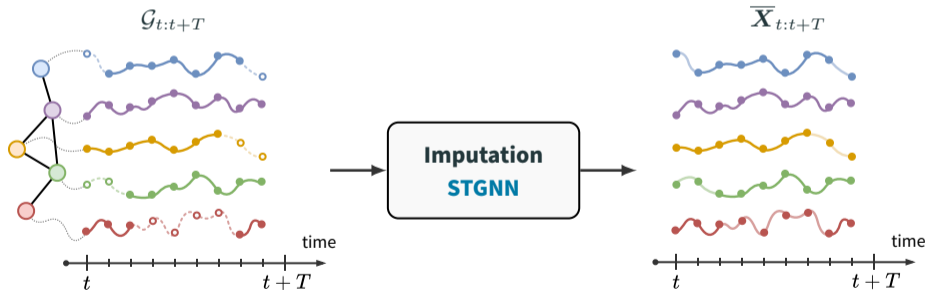


- 😊 Effective in exploiting past (and future, with bidirectional models) **node** observations.
- 😞 Struggle in capturing **nonlinear space-time dependencies**.

Time series imputation + relational inductive biases

Again, we can use the available relational information to condition the model, i.e.,

$$\mathbf{x}_{t+k}^i \sim p\left(\mathbf{x}_{t+k}^i \mid \mathbf{X}_{t:t+T} \odot \mathbf{M}_{t:t+T}, \mathbf{A}\right) \quad k \in [0, T)$$



Graph Recurrent Imputation Network (GRIN)

Similarly to GCRNN for forecasting, we can integrate graph processing into the autoregressive approach for imputation [3].

In these approaches, the distribution $p(\mathbf{x}_t^i | \mathbf{X}_{0:\infty} \odot \mathbf{M}_{0:\infty})$ is modeled into **three separate steps**:

Information from
previous observations.

$$p(\mathbf{x}_t^i | \mathbf{X}_{<t} \odot \mathbf{M}_{<t})$$

Typically modeled by bidirectional autoregressive models.

Information from
subsequent observations.

$$p(\mathbf{x}_t^i | \mathbf{X}_{>t} \odot \mathbf{M}_{>t})$$

Information from related
concurrent observations.

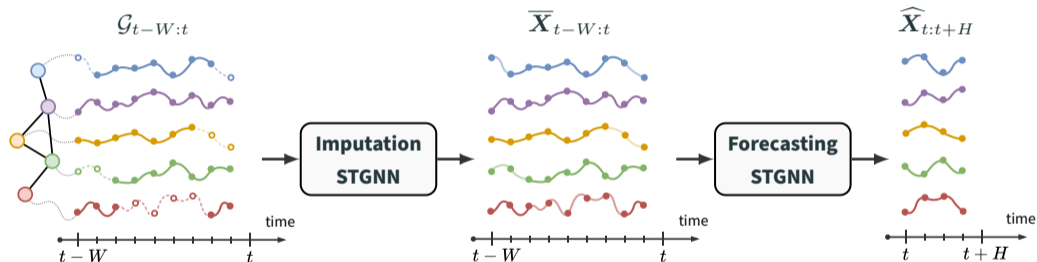
$$p(\mathbf{x}_t^i | \{\mathbf{x}_t^j \odot \mathbf{m}_t^j\}^{j \neq i})$$

Enabled by message passing.

[3] Cini, Marisca, and Alippi, "Filling the G_ap_s: Multivariate Time Series Imputation by Graph Neural Networks", ICLR 2022.

Imputation *before* forecasting

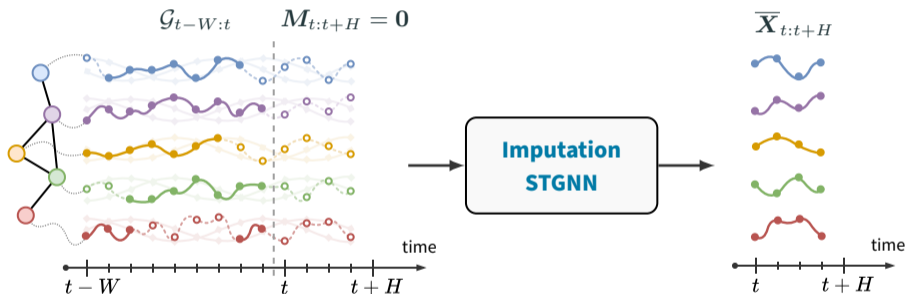
TSI can be used as a **preprocessing step** for a downstream task, e.g., forecasting.



- ☹️ Often necessary to use standard forecasting methods with irregular time series.
- ☹️ Might introduce **biases** due to errors in estimated values.

Imputation *in place of* forecasting

Imputation methods can also be adapted to perform forecasting.



- ☹ It is a **workaround** (this is not their purpose).
- ☹ Might perform poorly due to the absence of values in the forecasting horizon.

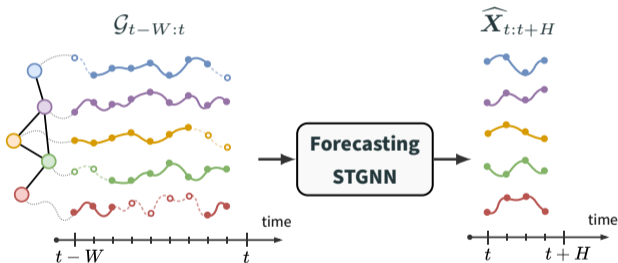
Forecasting from partial observations

A more direct approach: **avoid the reconstruction step!**

→ Design forecasting architecture to **directly deal with irregular observations.**

Benefits

- 😊 Learn how to leverage **only valid observations** specifically for the task at hand.
- 😊 Avoid the computational burden of **imputing missing values.**



[4] Zhang *et al.*, “Graph-guided network for irregularly sampled multivariate time series”, ICLR 2022.

[5] Zhong *et al.*, “Heterogeneous spatio-temporal graph convolution network for traffic forecasting with missing values”, IEEE ICDCS 2021.

[6] Marisca, Alippi, and Bianchi, “Graph-based Forecasting with Missing Data through Spatiotemporal Downsampling”, ICML 2024.

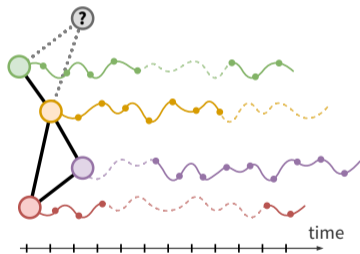
[7] Gravina, Zambon, Bacciu, and Alippi, “Temporal Graph ODEs for Irregularly-Sampled Time Series” 2024.

Virtual sensing

The practice of estimating unmeasured states using models and existing observations.

The power of graphs:

- 😊 The **relational** processing allows us to condition estimates on data **close in space**.
- 😊 The **inductive** property of MP allows us to handle **new nodes and edges**.
- 😊 Useful in applications where sensing has a cost.



[8] Wu *et al.*, “Inductive Graph Neural Networks for Spatiotemporal Kriging”, AAAI 2021.

[9] De Felice, Cini, Zambon, Gusev, *et al.*, “Graph-Based Virtual Sensing from Sparse and Partial Multivariate Observations”, ICLR 2024.

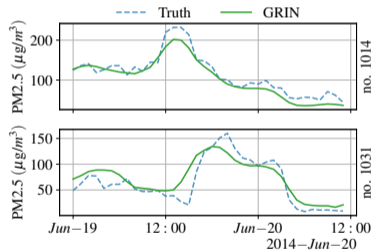
Graph imputation for virtual sensing

💡 Add a **fictitious node** with **no data** and let the model **infer** the corresponding time series.

Clearly, several assumptions are needed

- high degree of homogeneity of sensors,
- capability to reconstruct from observations at neighboring sensors,
- and many more...

Two virtual sensors for air quality. (from [3])



[3] Cini *et al.*, “Filling the G_ap_s: Multivariate Time Series Imputation by Graph Neural Networks”, ICLR 2022.

[10] Marisca *et al.*, “Learning to Reconstruct Missing Data from Spatiotemporal Graphs with Sparse Observations”, NeurIPS 2022.

Module

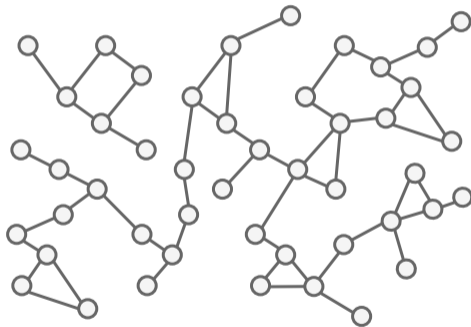
Scalability

Scalability

😊 The scalability feature

Graph-based processing allows us to

- 😊 learn a single inductive (**global**) model...
- 😊 ...while conditioning on related time series in a **sparse** fashion.
- 😊 The cost of this operation reduces from $\mathcal{O}(N^2)$ to $\mathcal{O}(|\mathcal{E}_t|)$





The scalability issue

Spatiotemporal data span – as the name suggests – **two dimensions**:

- the **spatial** dimension – the number of time series.
- the **time** dimension – the number of time steps per time series.

In the real world, dealing with **high-frequency, large-scale time series data** is quite common.

– E.g., smart cities, environmental monitoring, finance

-  A large amount of data needs to be **processed at once**.
-  In particular, to account for **long-range spatiotemporal dependencies**.

Computational complexity of STGNNs

W : length of time series · N : number of nodes · $|\mathcal{E}_t|$: number of edges · L : number of MP layers

The computational complexity of T&S models is given by:

- node-wise temporal processing – $\mathcal{O}(WN)$; $\rightarrow \mathcal{O}(W(N + L|\mathcal{E}_t|))$
- L MP layers **for each time step** – $\mathcal{O}(WL|\mathcal{E}_t|)$.

A first step toward improving scalability is represented by TTS models, which perform:

- node-wise temporal processing – $\mathcal{O}(WN)$; $\rightarrow \mathcal{O}(WN + L|\mathcal{E}_t|)$
- L MP layers **at the last time step** – $\mathcal{O}(L|\mathcal{E}_t|)$.

STT models, instead, do not have computational advantages over T&S models.

Graph subsampling

Computations can be reduced by training on **subgraphs** of the full network.

- sampling the **K -th order neighborhood** of a subset of nodes;
- **rewiring** the graph to reduce the total number of edges.



Mostly adapted from methods developed in **static graph processing** (e.g., [12], [13]).

- ☹ Subsampling might break long-range spatiotemporal dependencies.
- ☹ The learning signal may be noisy.

[11] Gandhi *et al.*, “Spatio-Temporal Multi-graph Networks for Demand Forecasting in Online Marketplaces”, ECML-PKDD 2021.

[12] Hamilton *et al.*, “Inductive representation learning on large graphs”, NeurIPS 2017.

[13] Rong *et al.*, “DropEdge: Towards Deep Graph Convolutional Networks on Node Classification”, ICLR 2020.

Pre-computation

Pre-processing methods (e.g., [14]) enable scalability to large graphs by:

- **precomputing** a representation for each **node's neighborhood ahead of training**;
- processing the obtained node representations as if they were **i.i.d. samples**.

An extension to spatiotemporal data is given by **SGP** [16], which acts in 2 steps:

1. obtain a temporal encoding at each time step with a deep **echo state network**¹;
2. propagate such encodings through the graph using powers of a **graph shift operator**.

[14] Frasca *et al.*, “SIGN: Scalable inception graph neural networks” 2020.

[15] Zambon *et al.*, “Graph Random Neural Features for Distance-Preserving Graph Representations”, ICML 2020.

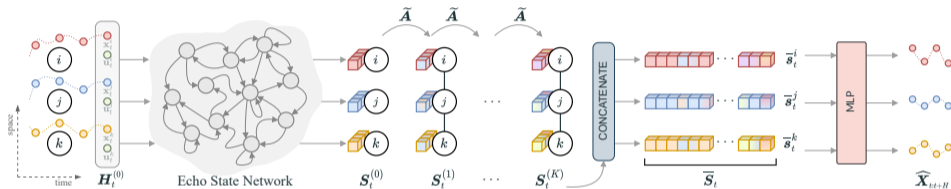
[16] Cini *et al.*, “Scalable Spatiotemporal Graph Neural Networks”, AAAI 2023.

[17] Liu *et al.*, “Do we really need graph neural networks for traffic forecasting?” Preprint 2023.

¹A randomized recurrent neural networks

SGP: Scalable Graph Predictor [16]

Extracted representations can be sampled uniformly across time and space during training.



- 😊 The cost of a training step is independent of W , N and $|\mathcal{E}_t|$.
- 😊 Performance matches state of the art.
- 😞 More storage space is required – the number of extracted features is $\gg d_x$.
- 😞 More reliant on hyperparameter selection than end-to-end approaches.

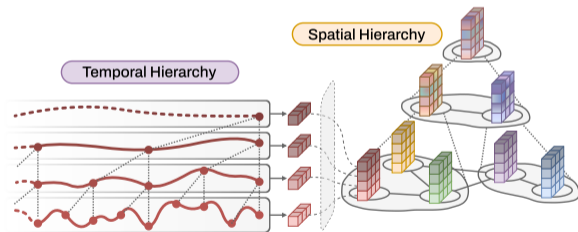
[16] Cini, Marisca, Bianchi, and Alippi, “Scalable Spatiotemporal Graph Neural Networks”, AAI 2023.

Hierarchical processing

We can reduce computational complexity by using **coarser-grained representations** of the input.

In space, this can be achieved through **graph pooling** [18].

- 😊 Reduced number of operations to reach the same receptive field.
- 😞 Introduce bottlenecks in information propagation.



[18] Grattarola, Zambon, Bianchi, and Alippi, "Understanding Pooling in Graph Neural Networks" 2024.

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