

Graph Deep Learning for Spatiotemporal Time Series

Forecasting, Reconstruction and Analysis

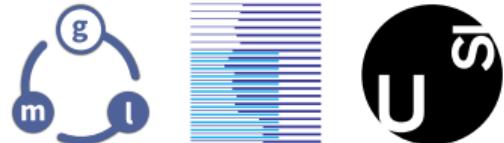
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ECML/PKDD, Turin · September 22, 2023

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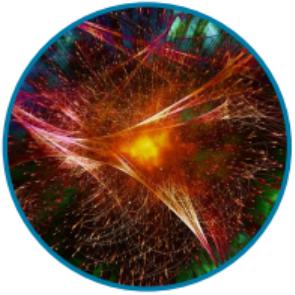
Traffic monitoring



Smart cities



Energy analitics

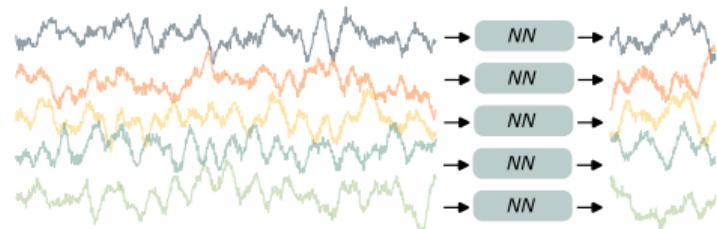


Physics



Stock markets

Deep learning for time series forecasting



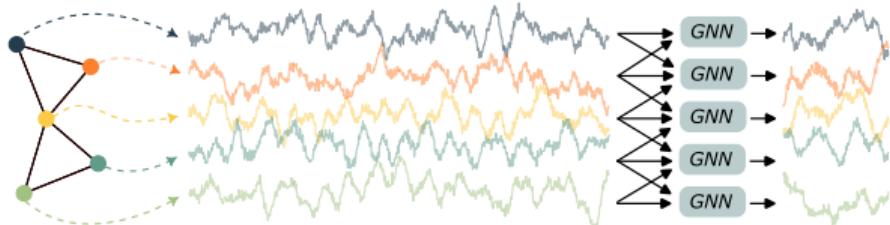
The standard deep learning approach to time series forecasting consists in training a **single neural network** on a collection of **time series**.

- Each time series is treated **independently** from the others.
- A single set of **shared learnable parameters** is used to predict each time series.
- Resulting models are **effective** and **efficient**.

⚠ Dependencies across time series are often **discarded**.

[1] K. Benidis *et al.*, “Deep Learning for Time Series Forecasting: Tutorial and Literature Survey”, ACM CS 2022.

Relational inductive biases



One way out is to embed such **relational structure** as an **architectural bias** into the processing.

Graph neural networks provide appropriate neural operators.

- **Message-passing** blocks allow for **localizing the predictions**
→ conditioning on observations at related time series (neighboring nodes).
- **Parameters** are **shared** and the model can operate on arbitrary sets of time series.

[2] D. Bacciu *et al.*, “A gentle introduction to deep learning for graphs”, NN 2020.

[3] M. M. Bronstein *et al.*, “Geometric deep learning: Grids, groups, graphs, geodesics, and gauges” 2021.

What this tutorial is about

This tutorial aims at merging two active and prominent research **fields**:

1. deep learning for time series and
2. deep learning on graphs.

- We provide a unified exposition of the recent advancements in graph-based time series processing, highlighting challenges and pitfalls.
- We offer researchers and practitioners a complete toolset of methodological guidelines, best practices, and software to exploit such framework in real-world problems.

A reference paper and Python notebook complement this presentation.

[4] A. Cini *et al.*, “Graph Deep Learning for Time Series Forecasting: A Comprehensive Methodological Framework” 2023.

Tutorial outline

Part 1

- 1.1)** Spatiotemporal time series
- 1.2)** Spatiotemporal GNNs
- 1.3)** Global and local models
- 1.4)** Model quality assessment

 Software demo

 Conclusions

Part 2

- 2.1)** Latent graph learning
- 2.2)** Learning in non-stationary environments
- 2.3)** Scalability
- 2.4)** Dealing with missing data

Part 1

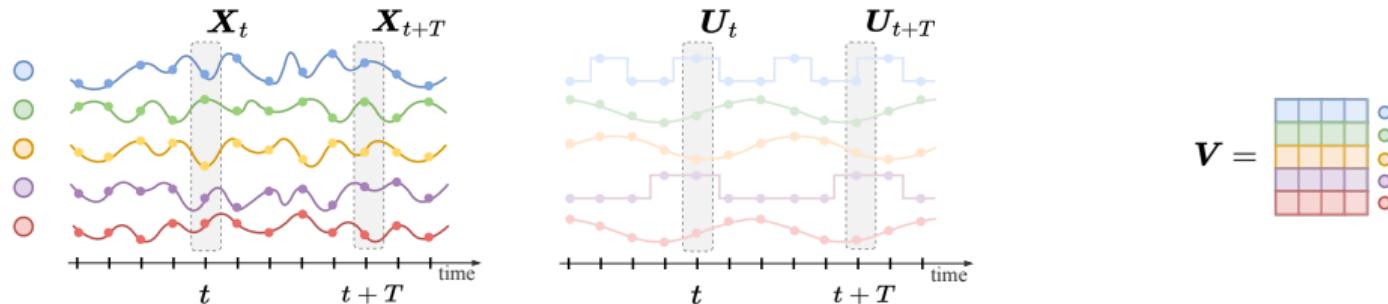
Graph-based Processing of Spatiotemporal Time series

Spatiotemporal time series

Collections of time series

We consider a set of N **correlated time series**, where each i -th time series is associated with:

- an **observation vector** $\mathbf{x}_t^i \in \mathbb{R}^{d_x}$ at each time step t ;
- a vector of **exogenous variable** $\mathbf{u}_t^i \in \mathbb{R}^{d_u}$ at each time step t ;
- a vector of **static (time-independent) attributes** $\mathbf{v}^i \in \mathbb{R}^{d_v}$.



Capital letters denote the stacked representations encompassing the N time series in the collection, e.g., $\mathbf{X}_t \in \mathbb{R}^{N \times d_x}$, $\mathbf{U}_t \in \mathbb{R}^{N \times d_u}$.

Correlated time series

We assume a **time-invariant** stochastic process

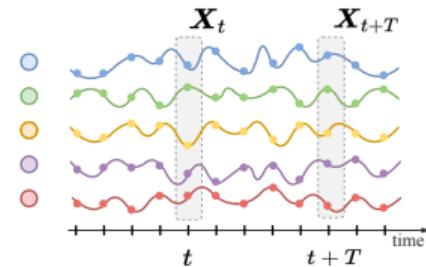
$$\boldsymbol{x}_t^i \sim p^i(\boldsymbol{x}_t^i | \boldsymbol{X}_{<t}, \boldsymbol{U}_{\leq t}, \boldsymbol{V})$$

generating the data \boldsymbol{x}_t^i for all $i = 1 \dots N$ and $t \in \mathbb{N}$.

Note that the time series:

- can be generated by **different processes**,
- can **depend on each other**,
- are assumed
homogenous, synchronous, regularly sampled.

→ These assumptions can be **relaxed**, as we will discuss in the 2nd part.



Notation:

$$\boldsymbol{X}_{t:t+T} = [\boldsymbol{X}_t, \dots, \boldsymbol{X}_{t+T-1}]$$

$$\boldsymbol{X}_{<t} = [\boldsymbol{X}_0, \dots, \boldsymbol{X}_{t-2}, \boldsymbol{X}_{t-1}]$$

Relational information

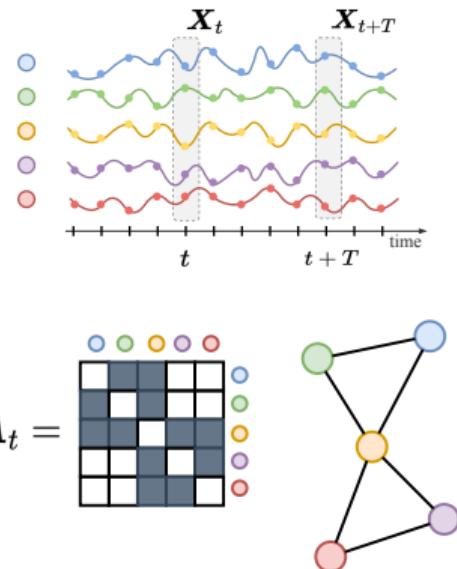
We assume the existence of **functional dependencies** between the time series.

- e.g., forecasts for one time series can be improved by accounting for the past values of other time series.

We model pairwise relationships existing at time step t with **adjacency matrix** $A_t \in \{0, 1\}^{N \times N}$.

- A_t can be **asymmetric** and **dynamic** (can vary with t).

- We call **spatial** the dimension spanning the time series collection.

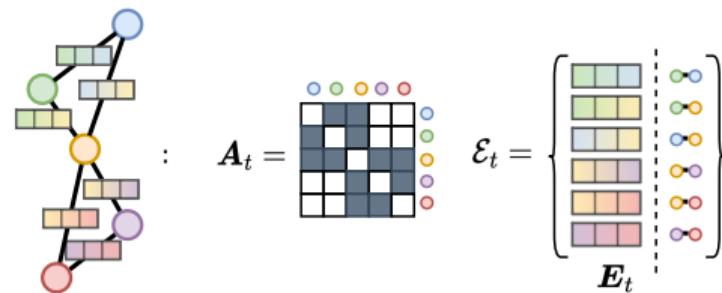


Relational information with attributes

Optional **edge attributes** $e_t^{ij} \in \mathbb{R}^{d_e}$ can be associated to each non-zero entry of A_t .

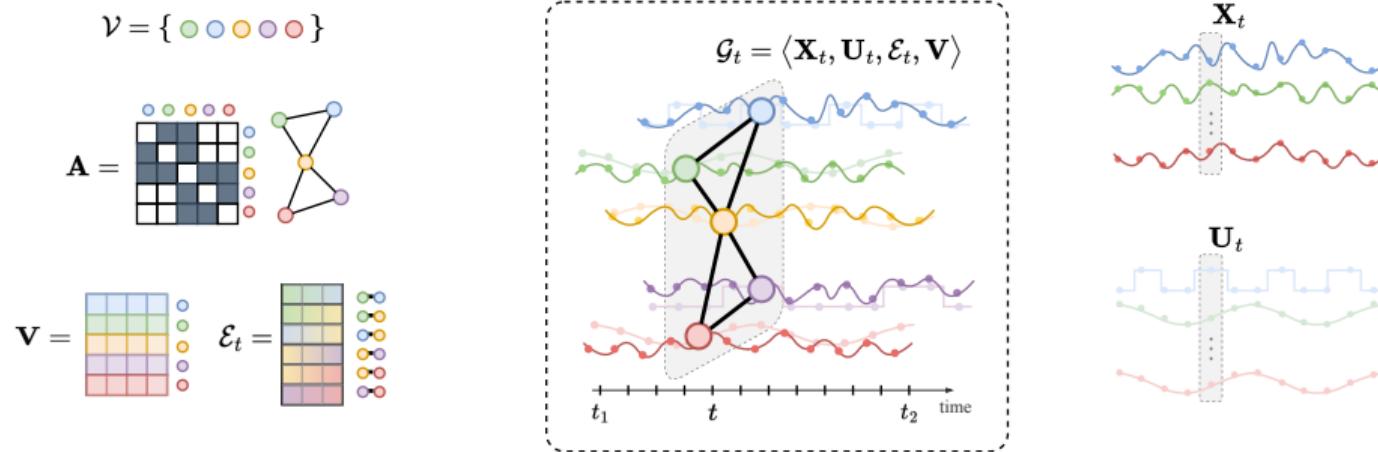
The **set of attributed edges** encoding all the available relational information is denoted by

$$\mathcal{E}_t \doteq \{\langle (i, j), e_t^{ij} \rangle \mid \forall i, j : A_t[i, j] \neq 0\}.$$



→ For many applications, A_t changes slowly over time and can be considered as **constant** within a short window of observations.

Spatiotemporal time series



We use the terms **node** and **sensor** to indicate the N entities generating the time series.

→ We refer to the node set together with the relational information as **sensor network**.

The tuple $\mathcal{G}_t \doteq \langle \mathbf{X}_t, \mathbf{U}_t, \mathcal{E}_t, \mathbf{V} \rangle$ contain all the available information associated with time step t .

Example: Traffic monitoring system

Consider a sensor network monitoring the speed of vehicles at crossroads.



- $X_{<t}$ collects past traffic speed measurements.
- U_t stores identifiers for time-of-the-day and day-of-the-week.
- V collects static sensor's features, e.g., type or number of lanes of the monitored road.
- \mathcal{E} can be obtained by considering the road network.
 - Road closures and traffic diversions can be accounted for with a dynamic topology \mathcal{E}_t .

Time series forecasting

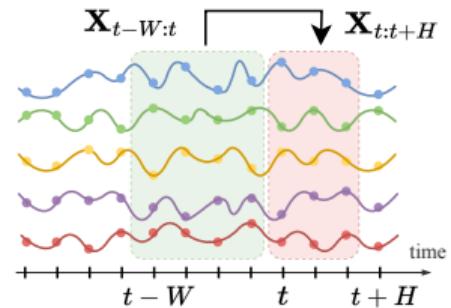
Multi-step time-series forecasting

Given a window of $W \geq 1$ past observations

$$\mathbf{X}_{t-W:t} = [\mathbf{X}_{t-W}, \dots, \mathbf{X}_{t-1}],$$

predict $H \geq 1$ future observations

$$\mathbf{x}_{t+h}^i, \quad i = 1 \cdots N, h = 1 \cdots H.$$



In particular, we are interested in learning a parametric model p_θ approximating the unknown data distribution p

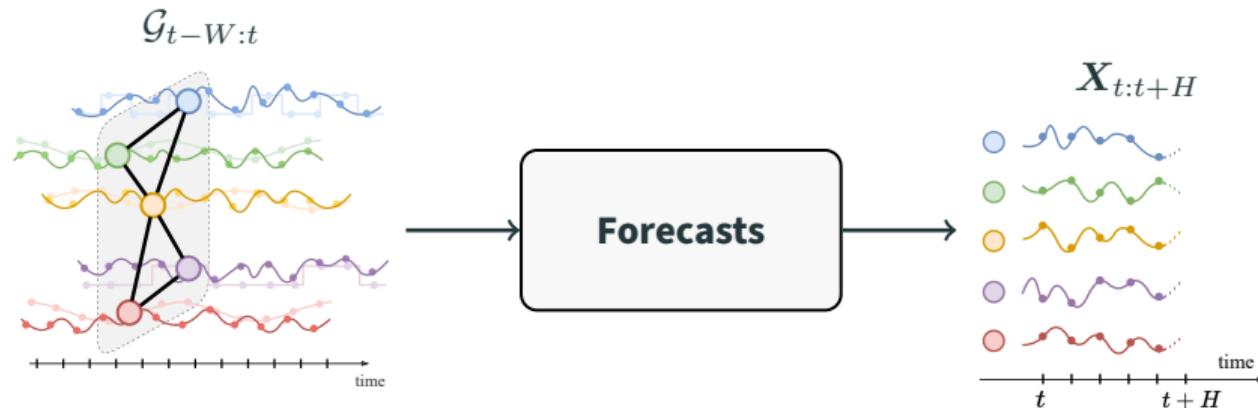
$$p_\theta (\mathbf{x}_{t+h}^i | \mathbf{X}_{t-W:t}, \mathbf{U}_{t-W:t+h}, \mathbf{V}) \approx p^i (\mathbf{x}_{t+h}^i | \mathbf{X}_{<t}, \mathbf{U}_{\leq t+h}, \mathbf{V}).$$

- θ is the model parameter vector.

Time series forecasting + relational inductive biases

Condition the model on the **relational** information $\mathcal{E}_{t-W:t}$

$$p_{\theta} (\mathbf{x}_{t+h}^i | \mathcal{G}_{t-W:t}, \mathbf{U}_{t-W:t+h}, \mathbf{V})$$



- ⚡ The conditioning on the sequence of attributed graphs acts as a **regularization** to localize predictions w.r.t. the **neighborhood of each node**.

Point forecasts

For simplicity, we focus here on **point forecasts**, rather than the modeling of full data distributions p , and consider predictive model

$$\hat{\mathbf{x}}_{t+h}^i = \mathcal{F}(\mathcal{G}_{t-W:t}, \mathbf{U}_{t:t+h}; \boldsymbol{\theta})$$

where $\hat{\mathbf{x}}_{t+h}^i$ approximates, e.g., $\mathbb{E}_p [\mathbf{x}_{t+h}^i]$.

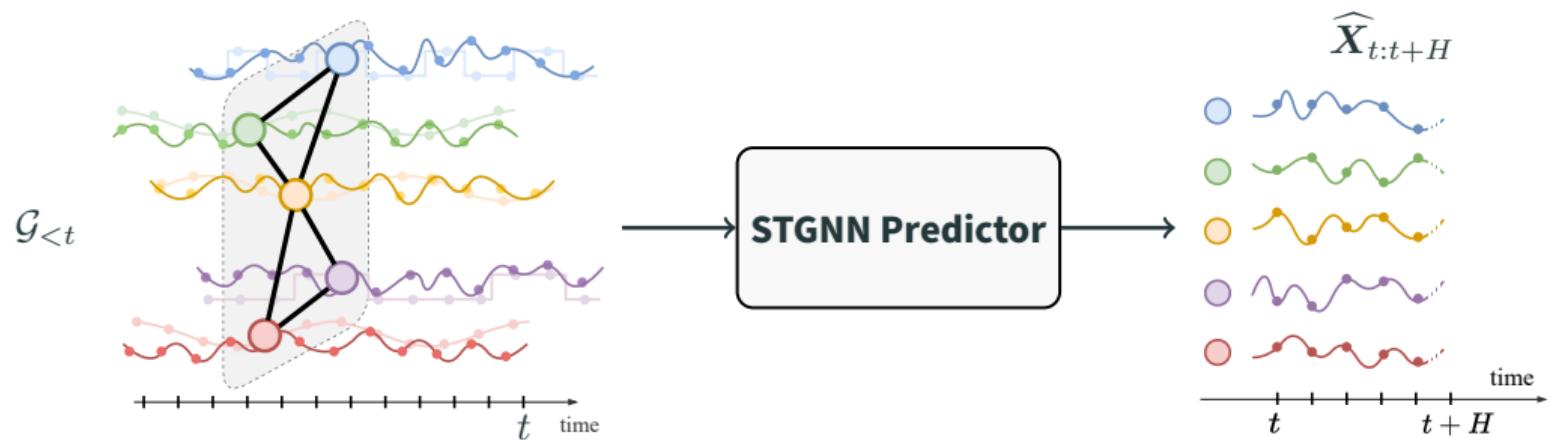
Parameters $\boldsymbol{\theta}$ can be learned by **minimizing a cost function** $\ell(\cdot, \cdot)$ (e.g., MSE) on a training set

$$\begin{aligned}\hat{\boldsymbol{\theta}} &= \arg \min_{\boldsymbol{\theta}} \frac{1}{NT} \sum_{t=1}^T \ell\left(\widehat{\mathbf{X}}_{t:t+H}, \mathbf{X}_{t:t+H}\right) \\ &= \arg \min_{\boldsymbol{\theta}} \frac{1}{NT} \sum_{t=1}^T \left\| \mathbf{X}_{t:t+H} - \widehat{\mathbf{X}}_{t:t+H} \right\|_2^2.\end{aligned}$$

Spatiotemporal Graph Neural Networks

Spatiotemporal Graph Neural Networks

We call **Spatiotemporal Graph Neural Network (STGNN)** a neural network exploiting both temporal and spatial relations of the input spatiotemporal time series.



We focus on models based on **message passing**.

Message-passing neural networks

To process the spatial dimension, we rely on the **message-passing (MP)** framework

$$\mathbf{h}^{i,l+1} = \text{UP}^l \left(\mathbf{h}^{i,l}, \underset{j \in \mathcal{N}(i)}{\text{AGGR}} \left\{ \text{MSG}^l \left(\mathbf{h}^{i,l}, \mathbf{h}^{j,l}, e^{ji} \right) \right\} \right), \quad (1)$$

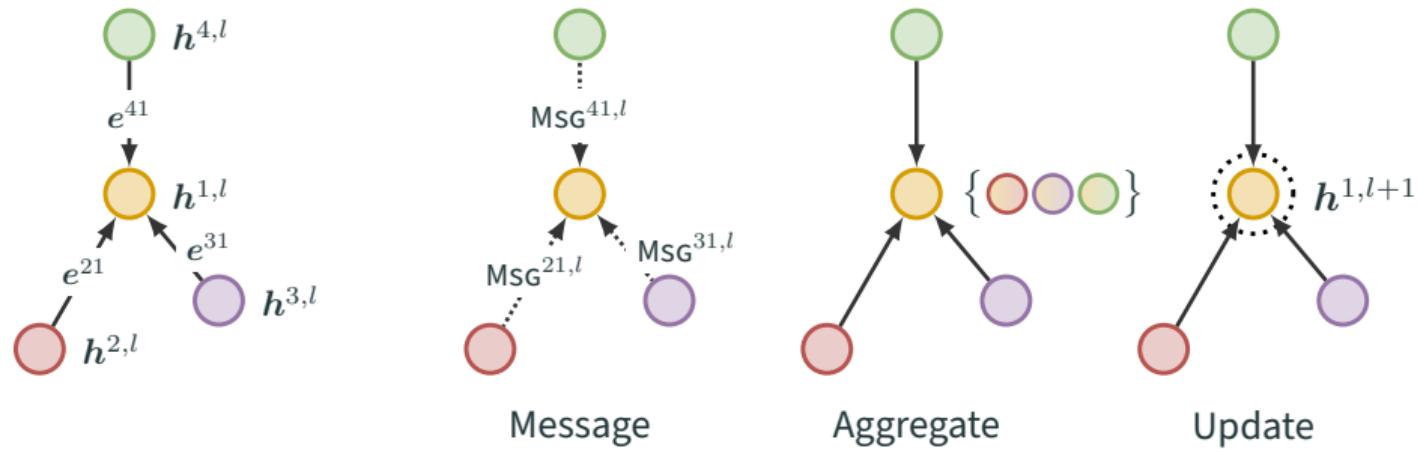
Where:

- $\text{MSG}^l(\cdot)$ is the **message function**, e.g., implemented by an multilayer perceptron (MLP).
- $\text{AGGR}\{\cdot\}$ is the permutation invariant **aggregation function**.
- $\text{UP}^l(\cdot)$ is the **update function**, e.g., implemented by an MLP.

Aggregation is performed over $\mathcal{N}(i)$, i.e., the set of neighbors of node i .

[5] J. Gilmer *et al.*, “Neural message passing for quantum chemistry”, ICML 2017.

Message passing in action



Spatiotemporal message passing

Starting from the MP framework, we can define a general scheme for **spatiotemporal message-passing (STMP)** networks:

$$\mathbf{h}_t^{i,l+1} = \text{UP}^l \left(\mathbf{h}_{\leq t}^{i,l}, \underset{j \in \mathcal{N}_t(i)}{\text{AGGR}} \left\{ \text{MSG}^l \left(\mathbf{h}_{\leq t}^{i,l}, \mathbf{h}_{\leq t}^{j,l}, e_{\leq t}^{ji} \right) \right\} \right)$$

Rather than vectors, STMP blocks process **sequences**.

→ STMP blocks must be implemented with operators that work on sequences!

We will look at **different implementations** of STMP blocks in the following.

[4] A. Cini *et al.*, “Graph Deep Learning for Time Series Forecasting: A Comprehensive Methodological Framework” 2023.

A general recipe

We consider STGNNs can be expressed as a sequence of three operations:

$$\mathbf{h}_{t-1}^{i,0} = \text{ENCODER}(\mathbf{x}_{t-1}^i, \mathbf{u}_{t-1}^i, \mathbf{v}^i), \quad (2)$$

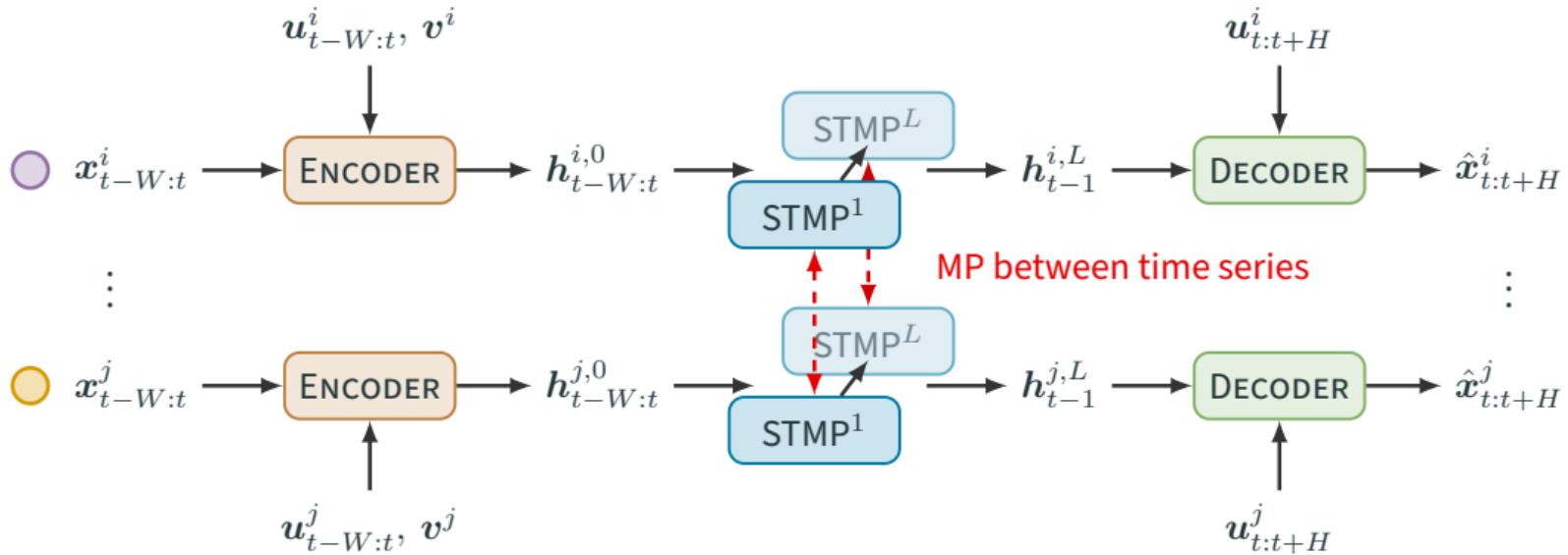
$$\mathbf{H}_{t-1}^{l+1} = \text{STMP}^l\left(\mathbf{H}_{\leq t-1}^l, \mathcal{E}_{\leq t-1}\right), \quad l = 0, \dots, L-1 \quad (3)$$

$$\hat{\mathbf{x}}_{t:t+H}^i = \text{DECODER}\left(\mathbf{h}_{t-1}^{i,L}, \mathbf{u}_{t:t+H}^i\right). \quad (4)$$

Where:

- $\text{ENCODER}(\cdot)$ is the encoding layer, e.g., implemented by an MLP.
- STMP is a stack of STMP layers.
- $\text{DECODER}(\cdot)$ is the readout layer, e.g., implemented by an MLP.

Framework overview



Design paradigms for STGNNs

Depending on the implementation of the STMP blocks, we categorize STGNNs into:

- **Time-and-Space (T&S)**

Temporal and spatial processing cannot be factorized in two separate steps.

- **Time-then-Space (TTS)**

Embed each time series in a vector, which is then propagated over the graph.

- **Space-then-Time (STT)**

Propagate nodes features at first and then process the resulting time series.



Time-and-Space

In T&S models, representations at every node and time step are the results of a **joint temporal and spatial encoding**

$$\mathbf{H}_{t-1}^{l+1} = \text{STMP}^l\left(\mathbf{H}_{\leq t-1}^l, \mathcal{E}_{\leq t-1}\right)$$

Several options exist.

- Integrate MP into neural operators for sequential data.
 - **Graph recurrent architectures, spatiotemporal convolutions, spatiotemporal attention, ...**
- Use temporal operators to compute messages.
 - **Temporal graph convolutions, spatiotemporal cross-attention, ...**
- Product graph representations.

Example 1: From Recurrent Neural Networks...

Consider a standard GRU [6] cell.

$$\mathbf{r}_t^i = \sigma(\Theta_r [\mathbf{x}_t^i || \mathbf{h}_{t-1}^i] + \mathbf{b}_r) \quad (5)$$

$$\mathbf{u}_t^i = \sigma(\Theta_u [\mathbf{x}_t^i || \mathbf{h}_{t-1}^i] + \mathbf{b}_u) \quad (6)$$

$$\mathbf{c}_t^i = \tanh(\Theta_c [\mathbf{x}_t^i || \mathbf{r}_t^i \odot \mathbf{h}_{t-1}^i] + \mathbf{b}_c) \quad (7)$$

$$\mathbf{h}_t^i = (1 - \mathbf{u}_t^i) \odot \mathbf{c}_t^i + \mathbf{u}_t^i \odot \mathbf{h}_{t-1}^i \quad (8)$$

Time series can be processed **independently** for each node or as a **single multivariate** time series.

[6] J. Chung *et al.*, “Empirical evaluation of gated recurrent neural networks on sequence modeling” 2014.

...to Graph Convolutional Recurrent Neural Networks

We can obtain a T&S model by implementing the gates of the GRU with MP blocks:

$$\mathbf{Z}_t^l = \mathbf{H}_t^{l-1} \quad (9)$$

$$\mathbf{R}_t^l = \sigma(\text{MP}_r^l([\mathbf{Z}_t^l || \mathbf{H}_{t-1}^l], \mathcal{E}_t)), \quad (10)$$

$$\mathbf{O}_t^l = \sigma(\text{MP}_o^l([\mathbf{Z}_t^l || \mathbf{H}_{t-1}^l], \mathcal{E}_t)), \quad (11)$$

$$\mathbf{C}_t^l = \tanh(\text{MP}_c^l([\mathbf{Z}_t^l || \mathbf{R}_t^l \odot \mathbf{H}_{t-1}^l], \mathcal{E}_t)), \quad (12)$$

$$\mathbf{H}_t^l = \mathbf{O}_t^l \odot \mathbf{H}_{t-1}^l + (1 - \mathbf{O}_t^l) \odot \mathbf{C}_t^l, \quad (13)$$

These T&S models are known as **graph convolutional recurrent neural networks (GCRNNs)** [7].

[7] Y. Seo *et al.*, “Structured sequence modeling with graph convolutional recurrent networks”, ICONIP 2018.

Popular GCRNNs

The first GCRNN has been introduced in [7], with MP blocks implemented as polynomial graph convolutional filters.

GCRNNs have become popular in the traffic forecasting context with the [Diffusion Convolutional Recurrent Neural Network \(DCRNN\)](#) architecture [8].

In DCRNN, MP is performed through [bidirectional diffusion convolution](#):

$$\mathbf{H}'_t = \sum_{k=0}^K \left(\mathbf{D}_{t,\text{out}}^{-1} \mathbf{A}_t \right)^k \mathbf{H}_t \Theta_1^{(k)} + \left(\mathbf{D}_{t,\text{in}}^{-1} \mathbf{A}_t^\top \right)^k \mathbf{H}_t \Theta_2^{(k)} \quad (14)$$

[7] Y. Seo *et al.*, “Structured sequence modeling with graph convolutional recurrent networks”, ICONIP 2018.

[8] Y. Li *et al.*, “Diffusion Convolutional Recurrent Neural Network: Data-Driven Traffic Forecasting”, ICLR 2018.

Example 2: Spatiotemporal convolutional networks (i)

A completely different approach is that of **spatiotemporal convolutional networks (STCNs)**, that **alternate spatial and temporal convolutional filters**:

- Compute intermediate representations by using a **node-wise temporal convolutional layer**:

$$\mathbf{z}_{t-W:t}^{i,l} = \text{TCN}^l \left(\mathbf{h}_{t-W:t}^{i,l-1} \right) \quad \forall i$$

where TCN^l indicates a temporal convolutional network layer.

- Then, compute the updated representation by using a **time-wise graph convolution**:

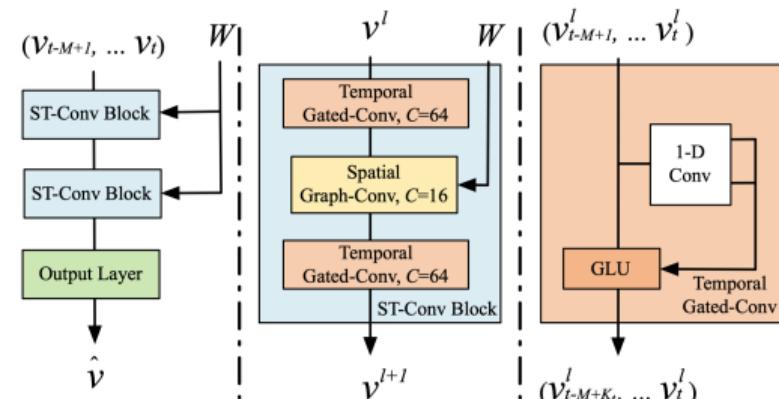
$$\mathbf{H}_t^l = \text{MP}^l \left(\mathbf{Z}_t^l, \mathcal{E}_t \right) \quad \forall t$$

Spatiotemporal convolutional networks (ii)

The first example of such architecture is the [STGCN](#) by Yu et al. [9].

The model is obtained by stacking STMP blocks consisting of

- a (gated) temporal convolution;
- a polynomial graph convolution;
- a second (gated) temporal convolution.



Courtesy of [9].

[9] B. Yu et al., “Spatio-temporal graph convolutional networks: a deep learning framework for traffic forecasting”, IJCAI 2018.

Example 3: Temporal Graph Convolution

A more integrated approach instead consists of using temporal operators to compute messages. For example, we can design STMP layers s.t.

$$\mathbf{h}_{t-W:t}^{i,l} = \text{TCN}_1^l \left(\mathbf{h}_{t-W:t}^{i,l-1}, \underset{j \in \mathcal{N}_t(i)}{\text{AGGR}} \left\{ \text{TCN}_2^l \left(\mathbf{h}_{t-W:t}^{i,l-1}, \mathbf{h}_{t-W:t}^{j,l-1}, \mathbf{e}_{t-W:t}^{ji} \right) \right\} \right).$$

Analogous models can be built by exploiting attention-based operators [10], [11].

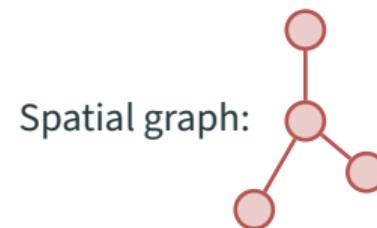
[10] I. Marisca *et al.*, “Learning to Reconstruct Missing Data from Spatiotemporal Graphs with Sparse Observations”, NeurIPS 2022.

[11] Z. Wu *et al.*, “TraverseNet: Unifying Space and Time in Message Passing for Traffic Forecasting”, TNNLS 2022.

Example 4: Product graph representations

Finally, an orthogonal option to those seen so far is to consider $\mathcal{G}_{t-W:t}$ as a single spatiotemporal graph \mathcal{S}_t .

Such **product graph** can be obtained by combining **temporal** and **spatial graphs**.



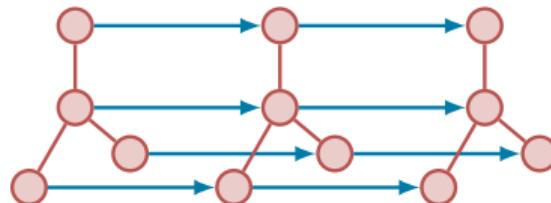
The resulting graph can be processed by any MP neural network.

[12] M. Sabbaqi *et al.*, “Graph-time convolutional neural networks: Architecture and theoretical analysis” 2022.

Building product graph representations

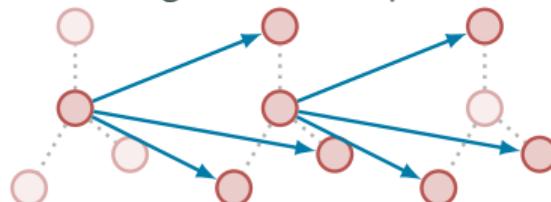
- **Cartesian product**

Spatial graphs are kept and each node is connected to itself in the previous time instant.



- **Kronecker product**

Each node is connected **only** to its neighbors in the previous time instant.

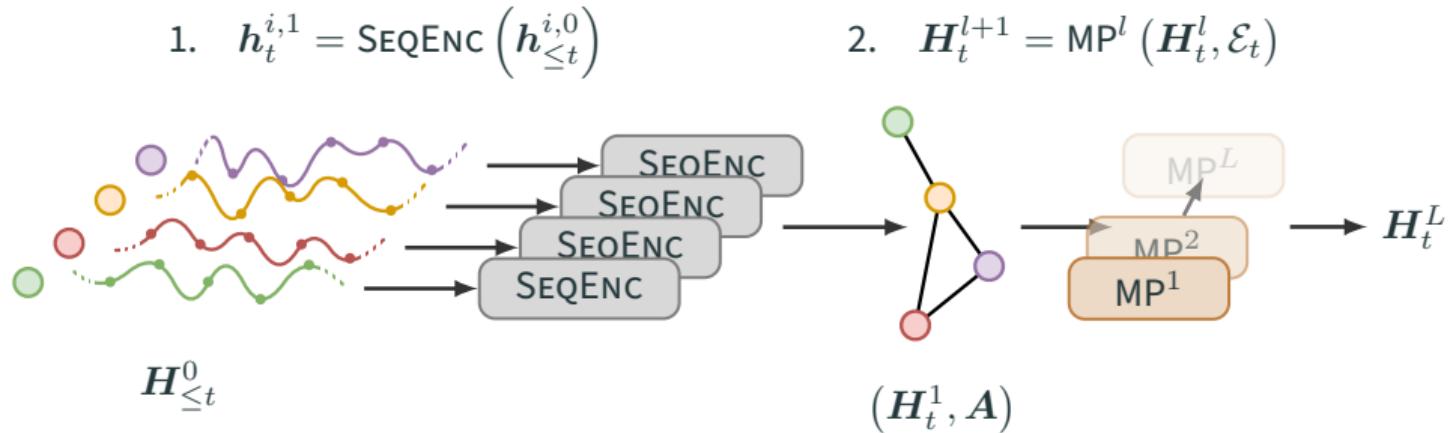


- ...

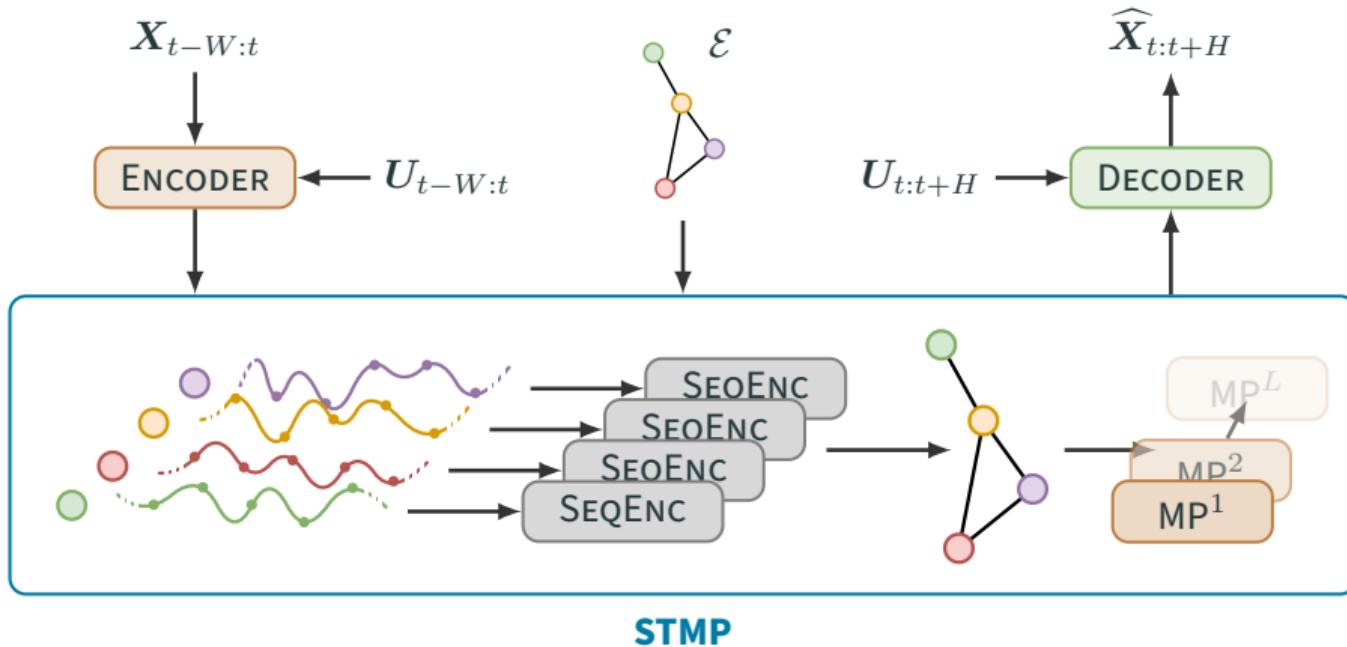
Time-then-Space models

The general recipe for a TTS model consists in:

1. **Embedding** each node-level time series in a vector.
2. **Propagating** obtained encodings throughout the graph with a stack of MP layers.



Full TTS model



Pros & Cons of TTS models

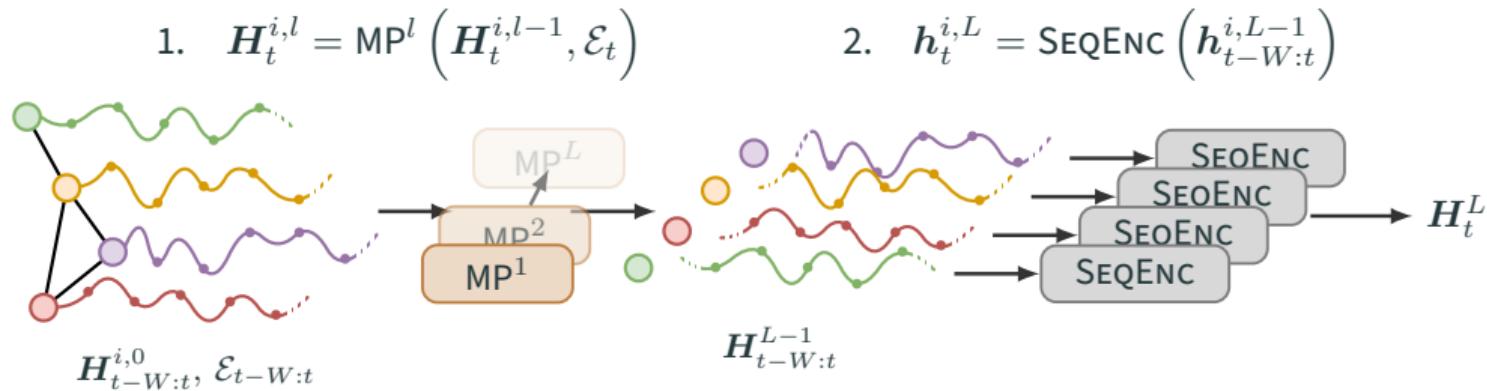
- Pros:**  Easy to implement and **computationally efficient**.
 We can **reuse operators** we already know.

- Cons:**  The 2-step encoding might introduce **information bottlenecks**.
 Accounting for **changes in topology** and **dynamic edge attributes** can be more problematic.

Space-then-Time

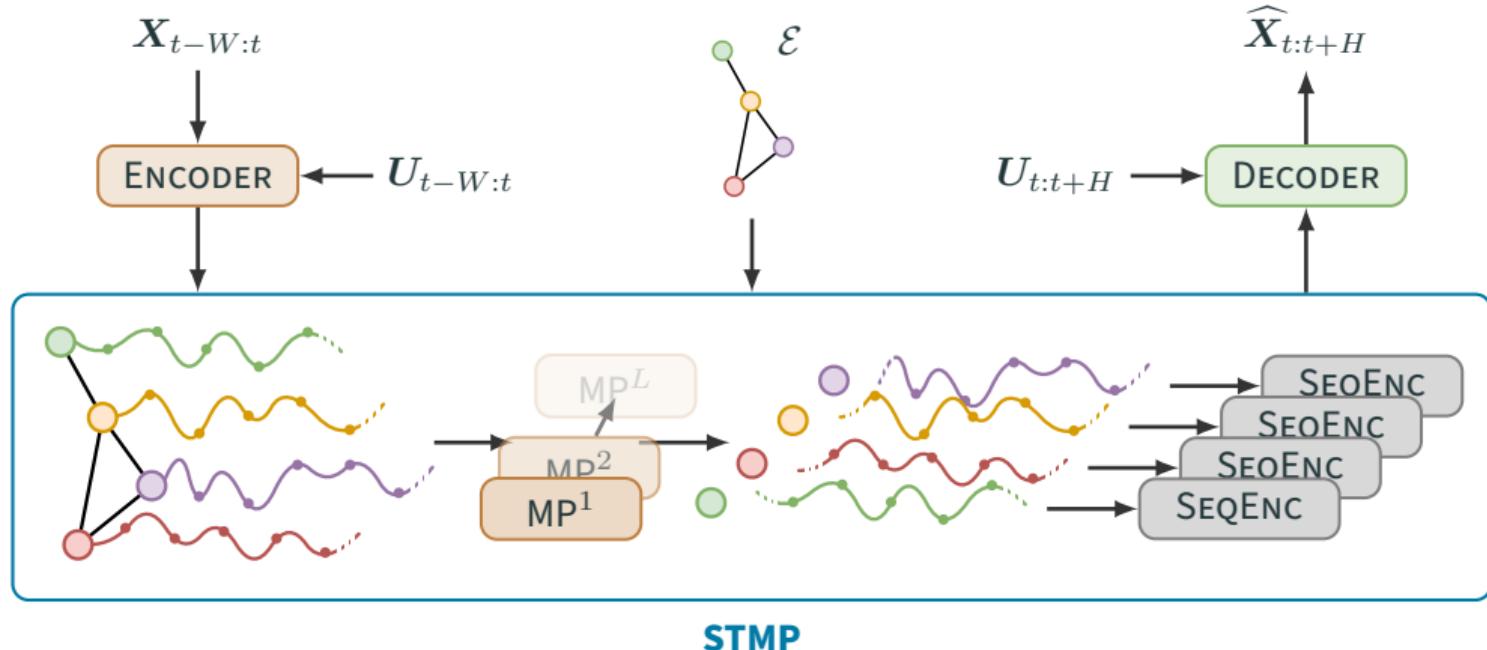
In STT approaches the two processing steps of TTS models are inverted:

1. Observations are **propagated among nodes** w.r.t. each time step using a stack of MP layers.
2. Each sequence of representations is processed by a **sequence encoder**.



⌚ They do not have the same computational advantages of TTS models.

Full STT model



Global and local models

Global vs local

A forecasting model is called **global** if its parameters are fitted to a group of time series
→ either univariate or multivariate.

Conversely, **local** models are **specific** to a single (possibly multivariate) time series.



A **global** model does not have any time-series-specific (local) parameters.

[13] P. Montero-Manso *et al.*, “Principles and algorithms for forecasting groups of time series: Locality and globality”, IJF 2021.

Trade-offs

Global models

- Just a **single model** needs to be trained and maintained.
- **Larger** amount of **data** available for training.
- Can be used in **inductive learning** scenarios (on unseen target time series).
- Theoretically, it can be **as expressive** as fitting a set of local models to each time series.

Local models

- Can more easily model **time-series-specific dynamics**.
- Often require **shorter input windows**.
- No problem in dealing with **heterogeneous/asynchronous** time series.

Globality and locality in STGNNs

STGNNs are typically **global** models: they do not rely upon node-specific parameters.

→ But they **condition** representations on each node's **neighborhood**, thus accounting for spatial dependencies.

Nonetheless, entirely global models might struggle to model **local effects**¹ and might require:

- :(impractically long observation windows;
- :(large model capacity.

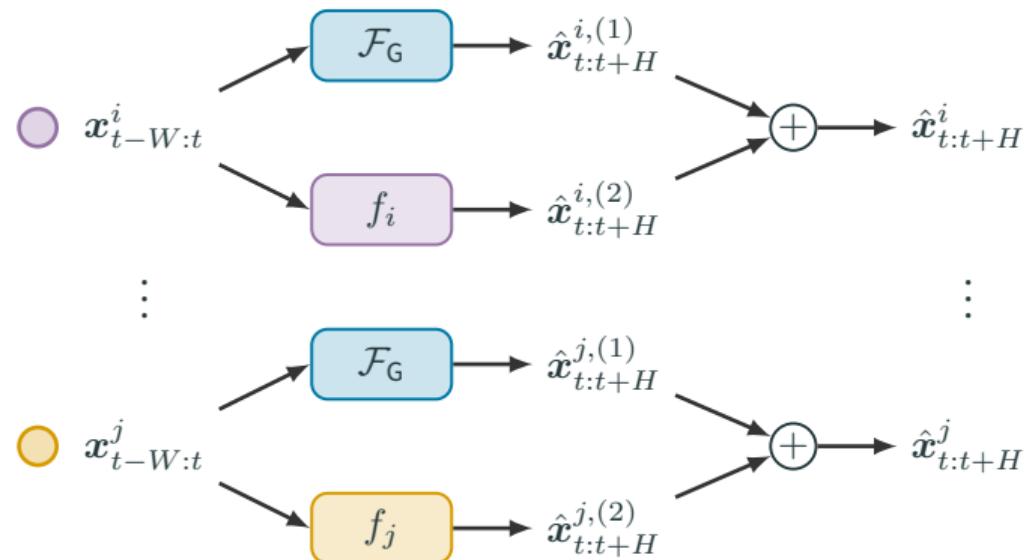
💡 We can use hybrid **global-local STGNNs** with specialized local components.

¹ Dynamics proper of each time series in the collection.

[14] A. Cini *et al.*, “Taming Local Effects in Graph-based Spatiotemporal Forecasting”, To appear in NeurIPS 2023.

Global-local STGNNs (Example 1)

A simple approach consists of combining a global model and a (simpler) local one:

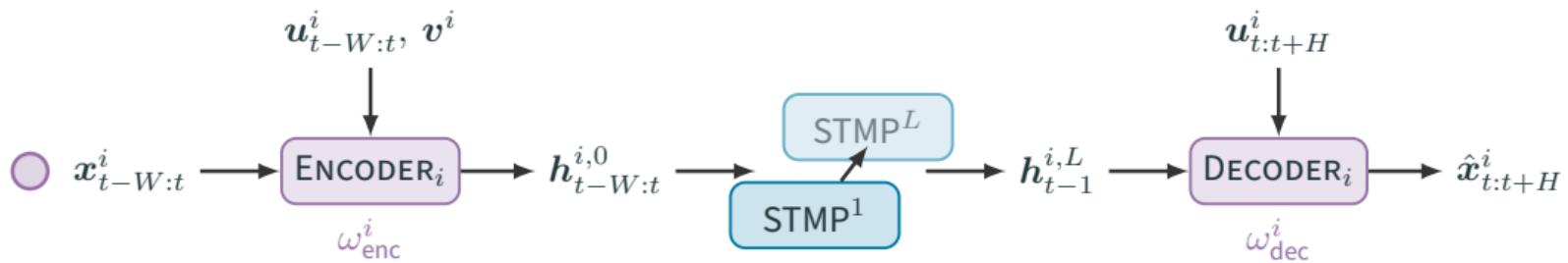


Global-local STGNNs (Example 2)

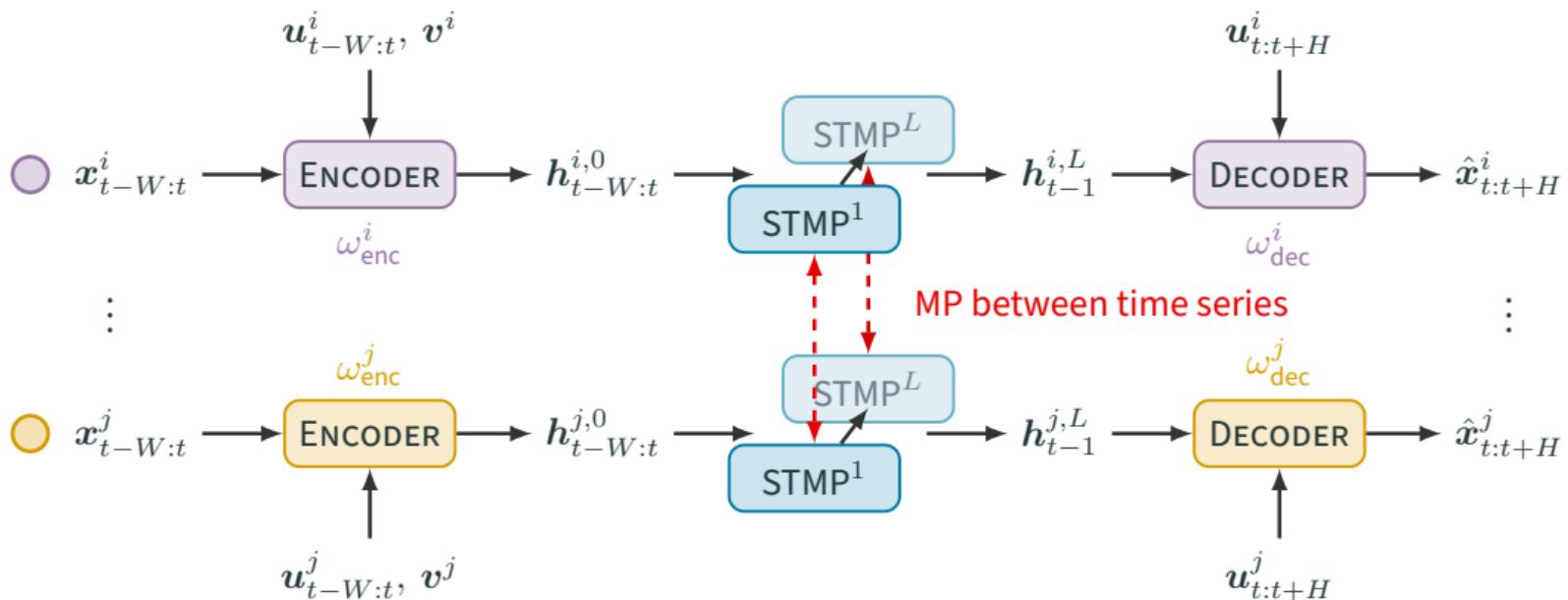
Another possibility is to use different weights for each time series at the encoding (ω_{enc}^i) and decoding (ω_{dec}^i) steps:

$$h_t^{i,0} = \text{ENCODER}_i(x_{t-W:t}^i, u_{t-W:t}^i, v^i; \omega_{\text{enc}}^i) \quad \hat{x}_{t:t+H}^i = \text{DECODER}_i(h_t^{i,L}, u_{t:t+H}^i; \omega_{\text{dec}}^i)$$

.....



Global-local STGNNs (Example 2)



Pros & Cons of global-local STGNNs

How to balance between the **global** and **local** modeling paradigms is problem-dependent.

Introducing **local** components specific to each time series in a global STGNN has several effects.

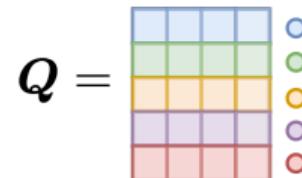
- 😊 Node-level effects are captured more efficiently than by fully global models.
 - 😊 Forecasting accuracy on the task is usually higher empirically.
 - 😢 The model's inductive capabilities are compromised (hard to handle unseen time series).
 - 😢 The number of learnable parameters can be much larger compared to fully global models.
- ⚡ We can mitigate these two drawbacks by associating each node with a learnable embedding.

Learnable node embeddings

Node embeddings are a table of learnable parameters

$Q \in \mathbb{R}^{N \times d_q}$ associated with each node.

They can be fed into modules of a global STGNN and learned end-to-end.



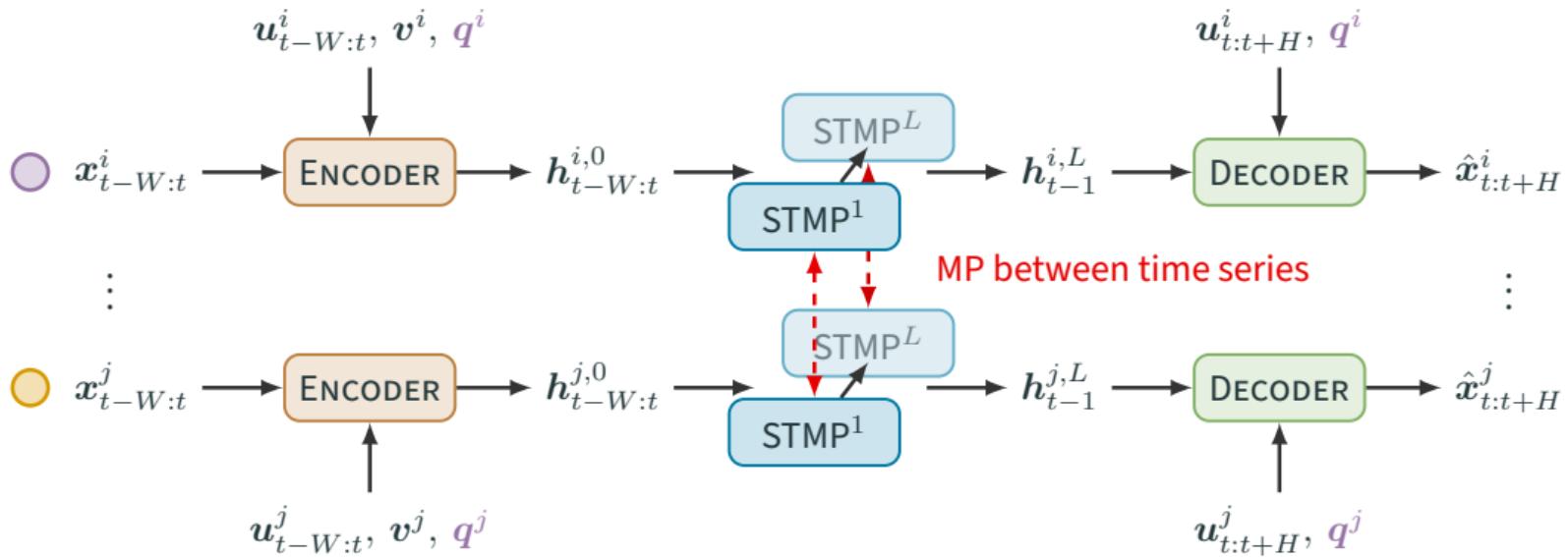
Example: node embeddings can be used to condition the encoding and decoding steps:

$$h_t^{i,0} = \text{ENCODER}(x_{t-1}^i, u_{t-1}^i, v^i, q^i) \quad \hat{x}_{t:t+H}^i = \text{DECODER}(h_t^{i,L}, u_{t:t+H}^i, q^i)$$

Note: all the weights of the ENCODER and DECODER modules can be shared among all the nodes.

[14] A. Cini *et al.*, “Taming Local Effects in Graph-based Spatiotemporal Forecasting”, To appear in NeurIPS 2023.

Node embeddings in action



Advantages of node embeddings

Using **node embeddings** to make an STGNN **global-local** allows us to:

1. **Amortize** the cost of **specializing** the model to each time series;
 - A **single** d_q -dimensional **vector** for each node is added to the model's parameters;
 - The same vector can be used **in multiple components** of the architecture.
2. **Transfer** the learned model to a **different** set of **time series** \mathcal{V}' more easily.
 - Only $|\mathcal{V}'|d_q$ parameters need to be tuned, while the **shared components** are **fixed**;
 - The embedding space can be **regularized** to better fit **embeddings** of new nodes [14].

[14] A. Cini *et al.*, “Taming Local Effects in Graph-based Spatiotemporal Forecasting”, To appear in NeurIPS 2023.

Example: global-local TTS

As an example, one can build a **global-local TTS model** by simply exploiting node embeddings and global RNN and MP layers as

$$\begin{aligned}\mathbf{h}_t^{i,0} &= \text{ENCODER}(\mathbf{x}_{t-1}^i, \mathbf{u}_{t-1}^i, \mathbf{v}^i, \mathbf{q}^i), \\ \mathbf{h}_t^{i,1} &= \text{RNN}(\mathbf{h}_{\leq t}^{i,0}), \\ \mathbf{H}_t^{l+1} &= \text{MP}^l(\mathbf{H}_{<t-1}^l, \mathcal{E}_{\leq t-1}), \quad l = 1, \dots, L-1 \\ \hat{\mathbf{x}}_{t:t+H}^i &= \text{DECODER}(\mathbf{h}_{t-1}^{i,L}, \mathbf{u}_{t:t+H}^i, \mathbf{v}^i, \mathbf{q}^i).\end{aligned}$$

Some empirical results

Models		GPVAR-Global (MAE)	GPVAR-Local (MAE)
Local	FC-RNN	.4393 _{± .0024}	.5978 _{± .0149}
	Local RNNs	.4047 _{± .0001}	.4610 _{± .0003}
Global	RNN	.3999 _{± .0000}	.5440 _{± .0003}
	RNN+MP	.3193 _{± .0000}	.3587 _{± .0049}
Global-local (w/ Emb.)	RNN	.3991 _{± .0001}	.4612 _{± .0003}
	RNN+MP	.3194 _{± .0001}	.3199 _{± .0001}
Optimal model		.3192	.3192

- **Global** models **can fall short** in certain scenarios.
- **Local** multivariate models can easily **overfit**.
- **Global-local** models can **strike** a good **compromise**.

Model quality assessment

Questions to answer

Consider a predictor \mathcal{F} trained to solve a time-series forecasting problem.

1. Is the predictor **optimal** for the problem at hand?
2. **Where** does the predictor appear sub-optimal?
3. **How** can we improve the predictor?

Remark: Multiple optimality criteria can be considered.



Relational inductive biases can help us here too.

Performance at task

Consider predictors $\mathcal{F}_a, \mathcal{F}_b$ from a set \mathbb{F} of models and performance metric M (e.g., MAE, MSE).

- we consider \mathcal{F}_a better than \mathcal{F}_b if $M(\mathcal{F}_a)$ is *statistically* better than $M(\mathcal{F}_b)$.
- we consider \mathcal{F}_a optimal if there is no $\mathcal{F}_b \in \mathbb{F}$ better than \mathcal{F}_a .

Can we further improve over the best model so far \mathcal{F}_a ?

- Either we find a new model \mathcal{F}_* better than \mathcal{F}_a
- or we need prior knowledge about the modeled system.

Model	M
\mathcal{F}_a	0.145 ± 0.002
\mathcal{F}_b	0.176 ± 0.005
\vdots	
\mathcal{F}_n	0.158 ± 0.004
\mathcal{F}_*	0.139 ± 0.001

Residual correlation analysis

Studying the correlation between prediction residuals $r_t^i \doteq x_{t:t+H}^i - \hat{x}_{t:t+H}^i$ allows for testing model optimality.

If residuals are **dependent**

⇒ there is **information** that the model **hasn't captured**

⇒ model predictions **can be improved**.

Serial correlation

Correlation between residuals at different time steps.

Spatial correlation

Correlation between residuals at different graph nodes.

Most of the research focused on either serial correlation [15]–[17] or spatial correlation [18], [19].

Statistical tests for residual correlation

Whiteness test

H_0 : residuals are uncorrelated H_1 : some residuals correlate

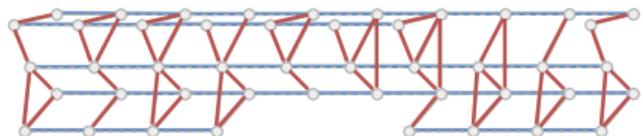
Define a test statistic $C(\{\mathbf{r}_t^i\}) = C(\mathcal{F}, \{\mathbf{x}_t^i\})$ and a threshold γ such that

If $|C(\{\mathbf{r}_t^i\})| > \gamma \implies \text{reject } H_0$.

Remarks: Residual correlation analysis

- 😊 Is independent of specific performance measures.
- 😢 Does not quantify how much a model can improve w.r.t. a specific performance metric.
- 😊 Does not rely on comparisons with other models.

AZ-Whiteness test: a spatio-temporal test



The test is defined by statistic

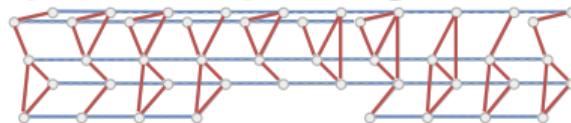
$$C(\{\mathbf{r}\}) = \underbrace{\sum_t \sum_{(i,j) \in \mathcal{E}_t} w_{ijt} \operatorname{sgn}(\langle \mathbf{r}_t^i, \mathbf{r}_t^j \rangle)}_{\text{spatial edge}} + \underbrace{\sum_t \sum_i w_{it} \operatorname{sgn}(\langle \mathbf{r}_t^i, \mathbf{r}_{t+1}^i \rangle)}_{\text{temporal edge}}$$

- distribution-free and residuals can be non-identically distributed.
- computation is linear in the number of edges and time steps.

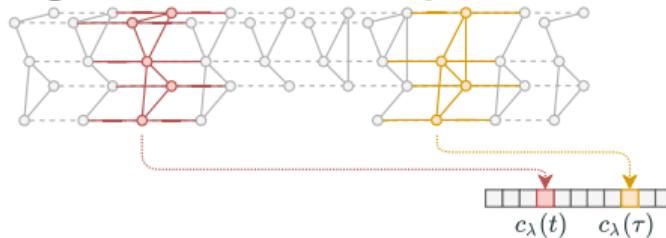
Where can we improve?

Analyzing the AZ-whiteness **test statistic** computed **on subgraphs** of the spatio-temporal graph allows for **discovering** insightful **correlation patterns**.

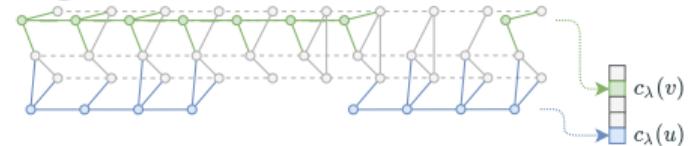
Spatial (or temporal) edges



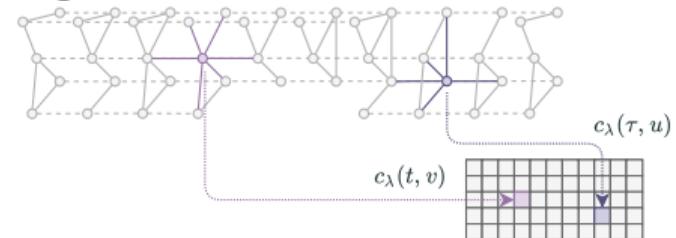
Edges related to a time step



Edges related to a node



Edges related to a node



Part 2

Challenges

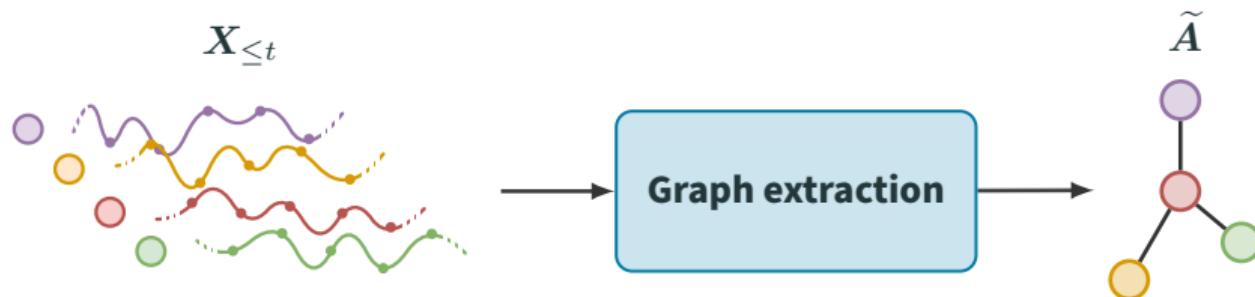
Challenges

- **Latent graph learning**
What to do when the underlying graph is not known?
- **Learning in non-stationary environments**
What to do when the environment changes?
- **Scalability**
How to deal with large collections of time series?
- **Dealing with missing data**
How to deal with missing observations within the time series?

Latent graph learning

Learning and adjacency matrix

- :(Relational information is **not** always **available**
- :(or might be **ineffective** in capturing spatial dynamics.
- : Relational architectural **biases** can nonetheless be exploited
 - **extract a graph** from the time series or node attributes

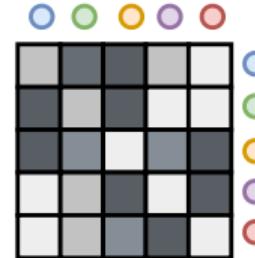


- It can be interpreted as **regularizing a spatial attention operator**.

Time-series similarities

Probably, the simplest approach to extract a graph from the time series is by computing [time series similarity scores](#).

- Pearson correlation
- Correntropy
- Granger causality
- Kernels for time series
- ...



→ Thresholding might be necessary to obtain binary and sparse graphs.

Latent graph learning

An integrated approach: learn the **relations** end-to-end with the downstream task

- as a function of the **input** data,
- as trainable **parameters** of the model,
- or **both**.

This problem is known as **latent graph learning** (or latent graph inference).

Two different approaches:

1. learning directly an **adjacency matrix** $\tilde{A} \in \mathbb{R}^{N \times N}$;
2. learning a **probability distribution over graphs** p_{Φ} generating \tilde{A} .

⚠ One key challenge is keeping both \tilde{A} and the subsequent computations **sparse**.
→ challenging with gradient-based optimization.

Direct approach

A direct approach consists in learning $\tilde{\mathbf{A}}$ as function $\xi(\cdot)$ of edge scores $\Phi \in \mathbb{R}^{N \times N}$ as

$$\tilde{\mathbf{A}} = \xi(\Phi)$$

Edge scores Φ

- can be a table of **learnable** model **parameters**,
- obtained as a **function** of the **inputs** and/or other parameters.

Function $\xi(\cdot)$ is a nonlinear activation

- it can be exploited to **make $\tilde{\mathbf{A}}$ sparse**.

$$\Phi = \begin{array}{c} \textcolor{blue}{\circ} \textcolor{green}{\circ} \textcolor{orange}{\circ} \textcolor{purple}{\circ} \textcolor{red}{\circ} \\ \textcolor{gray}{\square} \textcolor{darkgray}{\square} \textcolor{black}{\square} \textcolor{white}{\square} \textcolor{gray}{\square} \textcolor{darkgray}{\square} \\ \textcolor{darkgray}{\square} \textcolor{black}{\square} \textcolor{white}{\square} \textcolor{gray}{\square} \textcolor{darkgray}{\square} \textcolor{black}{\square} \\ \textcolor{white}{\square} \textcolor{gray}{\square} \textcolor{darkgray}{\square} \textcolor{black}{\square} \textcolor{white}{\square} \textcolor{gray}{\square} \\ \textcolor{gray}{\square} \textcolor{darkgray}{\square} \textcolor{black}{\square} \textcolor{white}{\square} \textcolor{gray}{\square} \textcolor{darkgray}{\square} \end{array} \quad \tilde{\mathbf{A}} = \begin{array}{c} \textcolor{blue}{\circ} \textcolor{green}{\circ} \textcolor{orange}{\circ} \textcolor{purple}{\circ} \textcolor{red}{\circ} \\ \textcolor{white}{\square} \textcolor{darkblue}{\square} \textcolor{white}{\square} \textcolor{white}{\square} \textcolor{darkblue}{\square} \\ \textcolor{darkblue}{\square} \textcolor{white}{\square} \textcolor{white}{\square} \textcolor{white}{\square} \textcolor{darkblue}{\square} \textcolor{white}{\square} \\ \textcolor{white}{\square} \textcolor{white}{\square} \textcolor{darkblue}{\square} \textcolor{white}{\square} \textcolor{white}{\square} \textcolor{darkblue}{\square} \\ \textcolor{white}{\square} \textcolor{white}{\square} \textcolor{darkblue}{\square} \textcolor{white}{\square} \textcolor{white}{\square} \textcolor{white}{\square} \end{array}$$

Direct approach: factorization methods

Many of the methods directly learning \tilde{A} , learn a **factorization** of the former to amortize the cost of the inference:

$$\tilde{A} = \xi(\Phi) \qquad \Phi = Z_s Z_t^\top$$

with

- $Z_s \in \mathbb{R}^{N \times d}$ **source** node embeddings
- $Z_t \in \mathbb{R}^{N \times d}$ **target** node embeddings

Z_s and Z_t can be learned as tables of (local) parameters or **as a function of the input window**.

[23] Z. Wu *et al.*, “Graph wavenet for deep spatial-temporal graph modeling”, IJCAI 2019.

Pro & Cons of the direct approach

- 😊 Easy to implement.
- 😊 Many possible parametrizations.
- 😊 Edge scores are usually easy to learn end-to-end.

- 😢 It often results in **dense computations** with $\mathcal{O}(N^2)$ complexity.
- 😢 Sparsifying $\tilde{\mathbf{A}}$ results in **sparse gradients**.
- 😢 Encoding prior structural information requires **smart parametrizations**.

Probabilistic methods

In this context, probabilistic methods aim at learning a parametric distribution p_{Φ} for $\tilde{\mathbf{A}}$ by minimizing

$$\mathcal{L}(\Phi) = \mathbb{E}_{\tilde{\mathbf{A}} \sim p_{\Phi}} \left[\ell \left(\widehat{\mathbf{X}}_{t:t+H}, \mathbf{X}_{t:t+H} \right) \right]. \quad (15)$$

- Again, we can factorize Φ and make p_{Φ} input dependent, e.g.,

$$\Phi = \xi (\mathbf{Z}_s \mathbf{Z}_t^\top) \qquad \qquad \tilde{\mathbf{A}} \sim p_{\Phi} (\mathbf{A} | \mathbf{X}_{<t}, \mathbf{U}_{<t}, \mathbf{V})$$

- Different parametrizations of p_{Φ} allow for embedding **sparsity priors** on the sampled graphs [22].



Gradient-based optimization requires $\nabla_{\Phi} \mathcal{L}(\Phi)$
→ it can be **challenging** and **computationally expensive**.

[22] A. Cini *et al.*, “Sparse graph learning from spatiotemporal time series”, JMLR 2023.

Monte Carlo gradient estimators

💡 One approach is to **reparametrize** $\tilde{\mathbf{A}} \sim p_{\Phi}(\mathbf{A})$ as: $\tilde{\mathbf{A}} = g(\Phi, \varepsilon)$, $\varepsilon \sim p(\varepsilon)$ decoupling parameters Φ from the random component ε : $\nabla_{\Phi} \mathcal{L}(\Phi) = \mathbb{E}_{\varepsilon} \left[\nabla_{\Phi} \ell(\widehat{\mathbf{X}}, \mathbf{X}) \right]$.

- 😊 Practical and **easy** to implement,
- 😢 rely on **continuous relaxations** and make subsequent computations scale with $\mathcal{O}(N^2)$.

💡 Conversely, **score-function** (SF) gradient estimators rely on the relation

$$\nabla_{\Phi} \mathbb{E}_{p_{\Phi}} \left[\ell(\widehat{\mathbf{X}}, \mathbf{X}) \right] = \mathbb{E}_{p_{\Phi}} \left[\ell(\widehat{\mathbf{X}}, \mathbf{X}) \nabla_{\Phi} \log p_{\Phi} \right]$$

- 😢 suffer from **high variance** (use variance reduction techniques),
- 😊 allow to **keep computations sparse**.

→ we can use **Monte Carlo** estimator.

[24] T. Kipf *et al.*, “Neural relational inference for interacting systems”, ICML 2018.

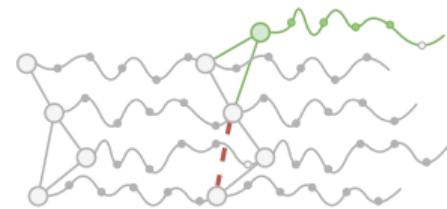
[22] A. Cini *et al.*, “Sparse graph learning from spatiotemporal time series”, JMLR 2023.

Learning in Non-Stationary Environments

Inductive learning

In real-world applications, one often needs to

- operate under **changes** in the network **connectivity**
- make predictions for **newly added nodes**
- **transfer** the model to **different** sensor **networks** (collections of time series)



Useful in **several tasks**, like, forecasting, missing data imputation, and virtual sensing.

⚠ **Performance** can easily **degrade** if the **data distribution** of target nodes

- deviates from that at **training nodes**
- **changes over time**.

[25] G. Ditzler *et al.*, “Learning in Nonstationary Environments: A Survey”, IEEE CIM 2015.

[14] A. Cini *et al.*, “Taming Local Effects in Graph-based Spatiotemporal Forecasting”, To appear in NeurIPS 2023.

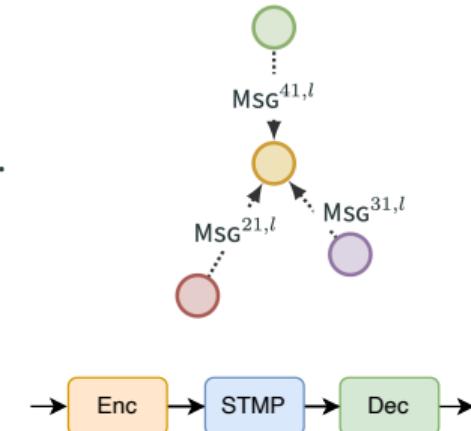
Transferability of STGNNs

Global STGNNs are **inductive** and can directly be used in the above settings, provided that the training and target data are similar enough.

- MP operates on **generic neighborhoods**
- MP **parameters** are **shared** across nodes

Otherwise, STGNNs **need** to be **adjusted**

- **fine-tuning** (a subset of) the weights of the model on the new data
- exploiting **transfer learning** strategies



⚠ Global-local STGNNs reduce the cost of transfer learning

- sharing most of the **parameters** and finetuning node-specific parameters only
- node **embeddings** can be **regularized** to facilitate the learning further.

[26] G. Panagopoulos *et al.*, “Transfer graph neural networks for pandemic forecasting”, AAAI 2021.

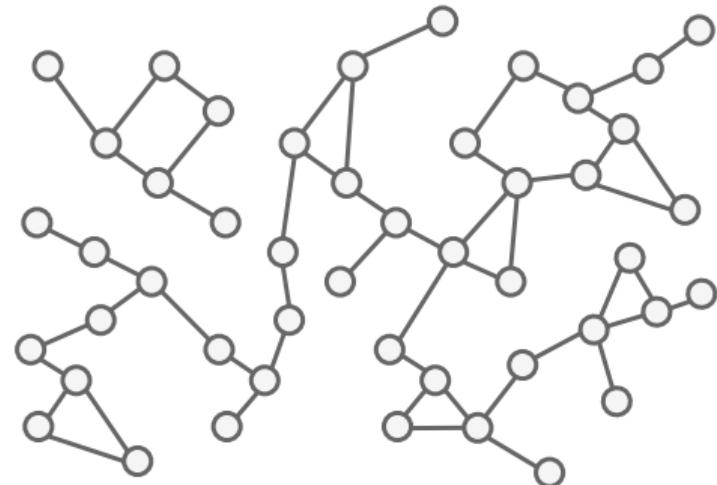
[27] T. Mallick *et al.*, “Transfer learning with graph neural networks for short-term highway traffic forecasting”, ICPR 2021.

[14] A. Cini *et al.*, “Taming Local Effects in Graph-based Spatiotemporal Forecasting”, To appear in NeurIPS 2023.

Scalability

The scalability feature

- 😊 **Graph-based processing** allows us to learn a single model...
- 😊 ...able to deal with a **large collection** of time series...
- 😊 ...while accounting for the most relevant **relational information**.



The scalability issue

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

- the **spatial** dimension, corresponding to the number of time series (sensors).
- the **time** dimension, corresponding to the number of time steps (number of observations acquired per sensor).

In the real world, dealing with **thousands of sensors** acquiring data at **high sampling rates** is quite common (e.g., smart cities).

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

Computational complexity of STGNNs

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:

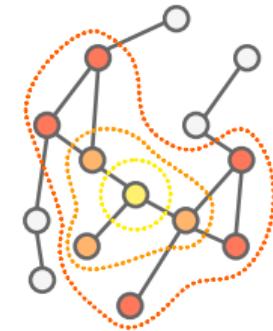
- node-wise temporal processing – $\mathcal{O}(WN)$; $\rightarrow \mathcal{O}(WN + L|\mathcal{E}_t|)$
- L MP layers **at the last time step** – $\mathcal{O}(L|\mathcal{E}_t|)$.

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, e.g., by

- 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., [28], [29]).

- :(sad face) Subsampling might break long-range spatiotemporal dependencies.
- :(sad face) The learning signal may be noisy.

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

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

Pre-computation

Pre-processing methods (e.g., [30]) 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** [31], which acts in 2 steps:

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

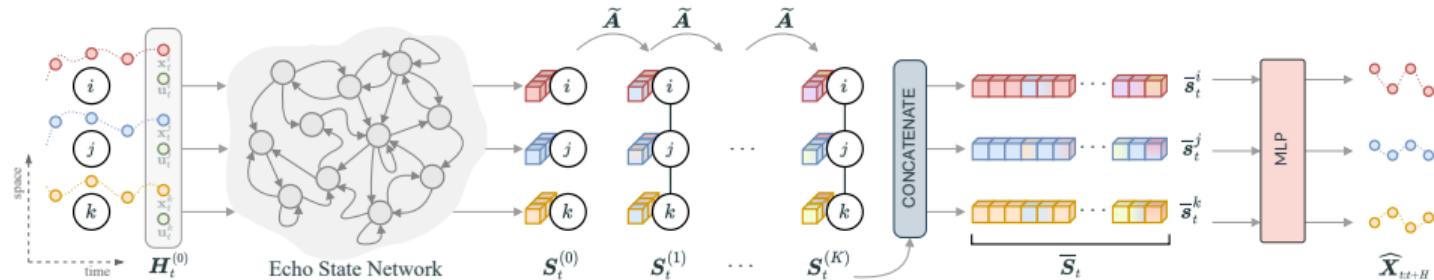
[30] F. Frasca *et al.*, “SIGN: Scalable inception graph neural networks” 2020.

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

² A randomized recurrent neural networks

SGP: Scalable Graph Predictor [31]

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, as the number of extracted features is much higher than d_x .
- 😢 More reliant on hyperparameter selection than end-to-end approaches.

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

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:

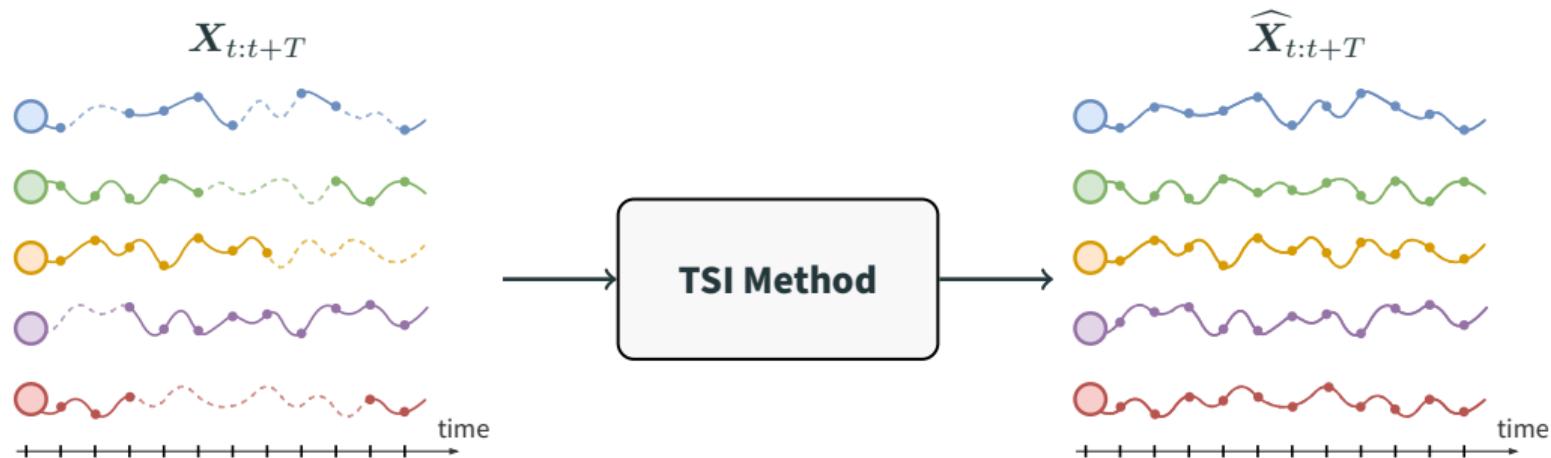
- faults, of either transient or permanent nature;
- asynchronicity among the time series;
- communication errors...

Most forecasting methods operate on complete sequences.

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

Time series imputation (i)

The problem of reconstructing missing values in a sequence of data is often referred to as **time series imputation** (TSI).



Time series imputation (ii)

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



Time series imputation

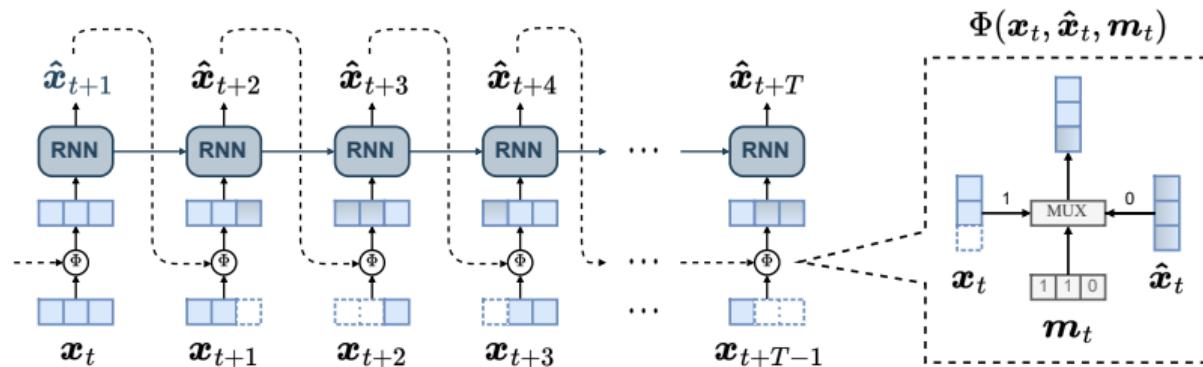
Given a window of $T \geq 1$ observations $\mathcal{X}_{<T}$ with missing values, the **time series imputation** problem consists in estimating the missing observations in the sequence

$$\mathbf{x}_t^i \sim p(\mathbf{x}_t^i | \mathcal{X}_{<T}) \quad \forall i, t \text{ such that } m_t^i = 0$$

with $\mathcal{X}_{<T} = \{\mathbf{x}_t^i \mid \mathbf{x}_t^i \in \mathcal{X}_{<T} \text{ and } m_t^i = 1\}$ being the **observed set**.

Deep learning for TSI

Besides standard statistical methods, deep learning approaches have become a popular alternative, in particular, **autoregressive models** (e.g., RNNs).



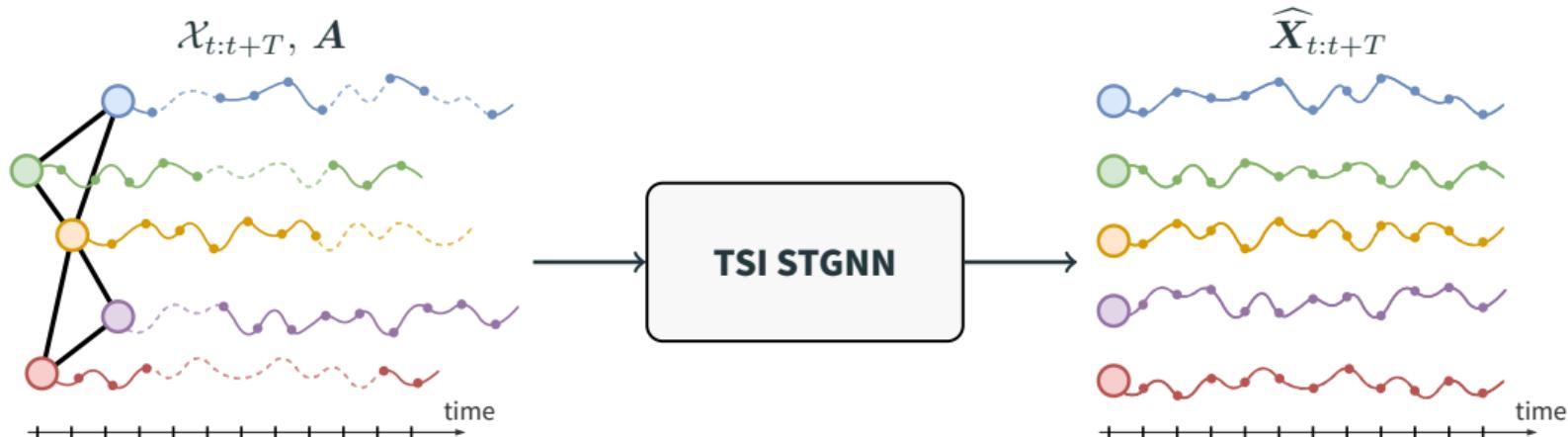
- 😊 Effective in exploiting past (and future, with bidirectional models) **node** observations...
- 😢 ...but struggle in capturing **nonlinear space-time dependencies**.

Time series imputation + relational inductive biases

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

$$\mathbf{x}_t^i \sim p(\mathbf{x}_t^i | \mathcal{X}_{<T}, \mathbf{A})$$

As done for the forecasting problem, we can use STGNNs to address the imputation task.



Graph Recurrent Imputation Network

Cini et al. [32] propose a GCRNN that builds upon the autoregressive approach for imputation:

- A (graph-based) RNN (i.e., a GCRNN cell) is used to **encode** the sequence of **only valid observations**:

$$\mathbf{Z}_t = \text{STMP}(\mathbf{H}_{<t} \odot \mathbf{M}_{<t}, \mathcal{E}_{<t}).$$

- An additional MP layer is used as **spatial decoder**, to account for **concurrent observations at neighbors**:

$$\hat{\mathbf{x}}_t^i = \text{DEC} \left(\mathbf{z}_t^i, \underset{j \in \mathcal{N}(i) \setminus \{i\}}{\text{AGGR}} \left\{ \text{MSG}(\mathbf{z}_t^j, \mathbf{x}_t^j) \right\} \right).$$

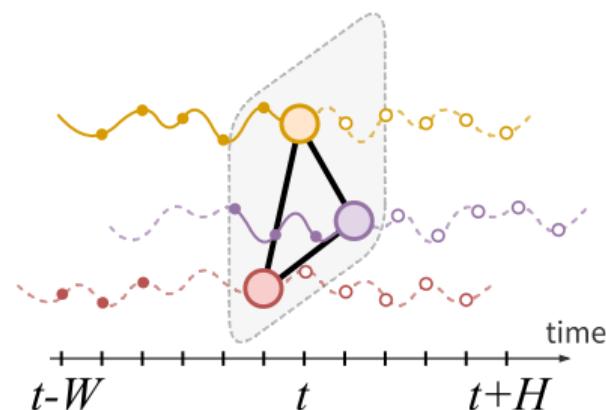
[32] A. Cini *et al.*, “Filling the G_ap_s: Multivariate Time Series Imputation by Graph Neural Networks”, ICLR 2022.

Forecasting from Partial Observations

A more direct approach to the problem is to **avoid the reconstruction step** and consider forecasting architecture that can **directly deal with irregular observations**.

The mechanisms used in imputation models
can be adapted to build forecasting
architectures.

- Such models can be used to **jointly impute** missing observations and **forecast** future values.

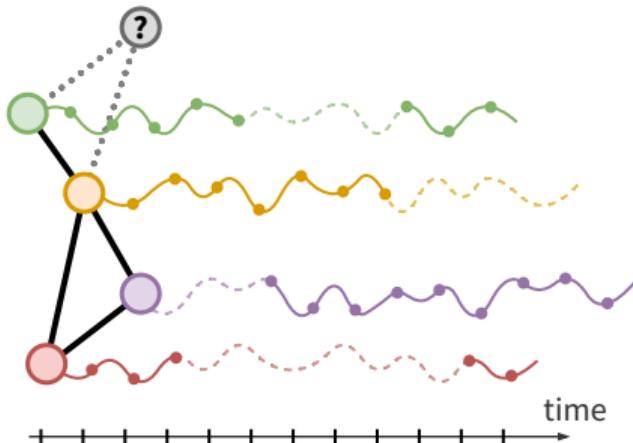


Beyond imputation

Graph-based imputation methods estimate missing values at an **existing node** by using available information at **neighboring nodes**.

Question:

Can we use the same approach to **infer** observations of **virtual sensors**, i.e., fictitious nodes **not** associated with an existing sensor?



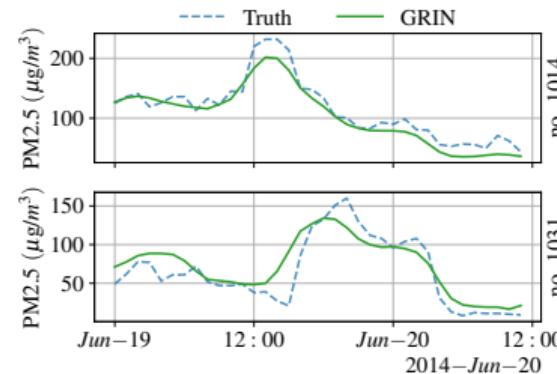
Virtual sensing

💡 Simulate the presence of a sensor by adding a node with **no data**, then 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...

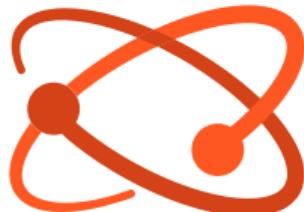
Two virtual sensors for air quality. (from [32])



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Coding Spatiotemporal GNNs

tsl: PyTorch Spatiotemporal Library



tsl (Torch Spatiotemporal) is a python library built upon [PyTorch](#) and [PyG](#) to accelerate research on neural spatiotemporal data processing methods, with a focus on **Graph Neural Networks**.



Notebook

Spatiotemporal Graph Neural Networks with tsl



[Open in Colab](#)

Conclusions

Some Takeaways



- 😊 Relational inductive biases allow for exploiting dependencies among the time series
- 😊 while sharing most of the model parameters
- 😊 Global-local STGNNs are a safe choice in non-inductive settings

Challenges

- 🔗 latent graph learning
- ➕ missing data imputation

- ↗ inductive learning
- 📶 scalability



Ivan Marisca



Andrea Cini

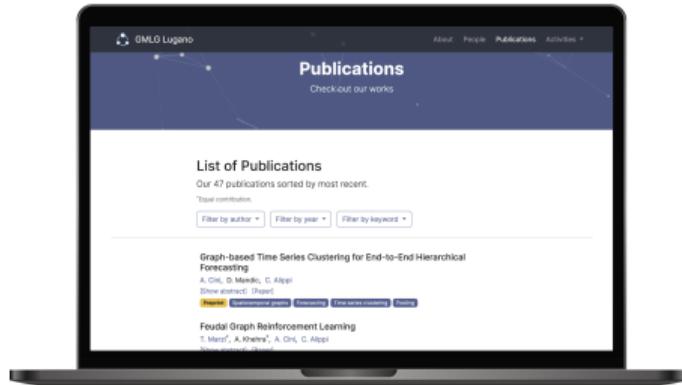


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THE END

Questions?

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