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Graph Deep Learning for Time Series Processing

Forecasting, Reconstruction and Analysis

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Introduction

Traffic monitoring

Smart cities

Energy analitics

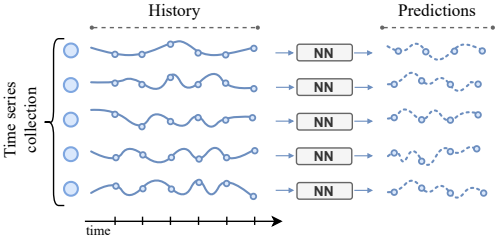
Physics

Stock markets

Deep learning for time series forecasting

Modern deep learning forecasting methods rely on a single neural network trained on a collection of related time series.

- ☺ Each time series is processed **independently**.
- ☺ Parameters are **shared**.
- ☺ Effective and **sample efficient**.
- ☹ **Dependencies are neglected**.

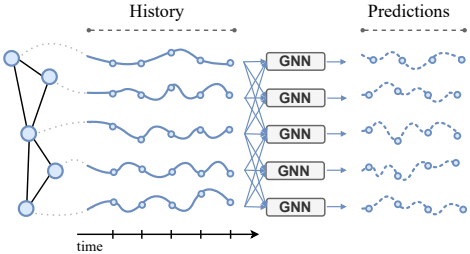


[1] Salinas *et al.*, “DeepAR: Probabilistic forecasting with autoregressive recurrent networks”, IJF 2020.
[2] Benidis *et al.*, “Deep Learning for Time Series Forecasting: Tutorial and Literature Survey”, ACM CS 2022.

Graph deep learning for time series forecasting

We will show graph deep learning (GDL) provides appropriate operators to go beyond these limitations.

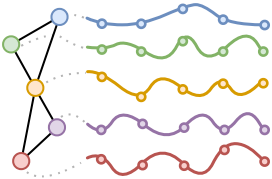
- ☺ **Dependencies** are **embedded into the processing** as inductive biases.
- ☺ Operate on **sets** of **correlated time series**.
- ☺ Parameters are **shared**.



☹ There are inherent **challenges** in applying this processing to data from the real world.

What this tutorial is about

This tutorial presents advances coming from the combination of



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

The objective of the tutorial is to provide:

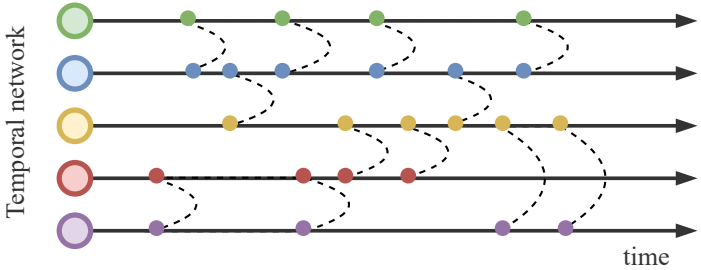
1. a comprehensive framework for graph-based time series processing models;
2. methods to address challenges and potential pitfalls;
3. tools and guidelines for real-world applications and developing new methods.

This presentation is complemented by a demo and a tutorial paper [3].

[3] Cini, Marisca, Zambon, and Alippi, “Graph Deep Learning for Time Series Forecasting”, Preprint 2023.

What this tutorial is <u>not</u> about

⚠ This tutorial is **<u>not</u>** about processing sequences of interactions in **temporal networks**.



→ Graphs will be a representation of the (dynamic) relationships among (possibly irregular) time series.

Tutorial outline

Part 1

1.1) Correlated time series

1.2) Graph-based representation

1.3) STGNN architectures

1.4) Global and local models

Software demo

Part 2

2.1) Scalability

2.2) Dealing with missing data

2.3) Latent graph learning

2.4) Model quality assessment

Conclusions

Part 1

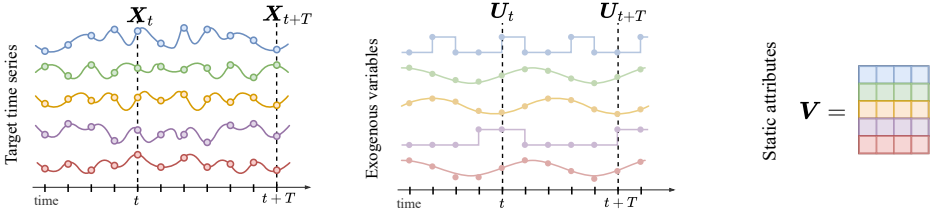
Graph-based Processing of Correlated Time series

Correlated time series

Collections of time series

We consider a set $\mathcal{D}$ of N correlated time series. Each i-th time series can be associated with:

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



Capital letters denote the stacked N time series, i.e., $\boldsymbol{X}_t \in \mathbb{R}^{N \times d_x}$, $\boldsymbol{U}_t \in \mathbb{R}^{N \times d_u}$.

$\rightarrow$ We call spatial the dimension spanning the collection.

[3] Cini *et al.*, "Graph Deep Learning for Time Series Forecasting", Preprint 2023.

Correlated time series

We consider a time-invariant stochastic process generating each time series as

$$\boldsymbol{x}_t^i \sim p^i\left(\boldsymbol{x}_t^i \middle| \boldsymbol{X}_{<t}, \boldsymbol{U}_{\leq t}, \boldsymbol{V}\right) \quad \text{for all } i = 1 \dots N, t = 0, \dots, T-1$$

and assume the existence of a causality à la Granger among time series.

Furthermore time series

- are assumed

  a) homogenous, b) synchronous, c) regularly sampled.

- can be generated by different processes.

Notation:

$$\mathcal{X}_t = \langle \boldsymbol{X}_t, \boldsymbol{U}_t, \boldsymbol{V} \rangle$$

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

❗ Assumptions a),b),c) can be relaxed as we will discuss in the 2nd part.

Example: Traffic monitoring system

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

- $\boldsymbol{X}_{<t}$ collects past traffic speed measurements.
- $\boldsymbol{U}_t$ stores identifiers for time-of-the-day and day-of-the-week.
- $\boldsymbol{V}$ collects static sensor's features, e.g., type or number of lanes of the monitored road.

$\rightarrow$ Strong dependencies among time series that reflect the road network.

Forecasting

Time series forecasting

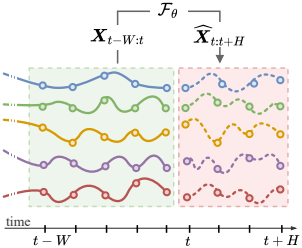
Multi-step time-series forecasting

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

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

predict $H \geq 1$ future observations

$$\boldsymbol{X}_{t+h} \qquad h = 1, \dots, H.$$



In particular, we are interested in learning a parametric model $\mathcal{F}(\,\cdot\,;\boldsymbol{\theta})$ s.t.

$$\mathcal{F}(\mathcal{X}_{t-W:t}, \boldsymbol{U}_{t:t+H}; \boldsymbol{\theta}) = \widehat{\boldsymbol{X}}_{t:t+H} \approx E_p\left[\boldsymbol{X}_{t:t+H}\right].$$

Probabilistic predictors can be considered as well, but we focus on point forecasts.

Training objective

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

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

❗ Choosing a different cost function allows for predicting other values.

→ **Example:** minimizing the MAE results in forecasts of the median.

Global and local predictors

Local models

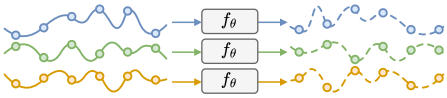
$$\hat{\boldsymbol{x}}^i_{t+h} = f\left(\boldsymbol{x}^i_{t-W:t}, \ldots; \boldsymbol{\theta}^i\right)$$

Example: Box-Jenkins method

☺ Tailored to each time series.

☹ Inefficient.

Global models



$$\hat{\boldsymbol{x}}^i_{t+h} = f\left(\boldsymbol{x}^i_{t-W:t}, \ldots; \boldsymbol{\theta}\right)$$

Example: DeepAR [1]

☺ Sample efficient.

☺ Allows for more complex models.

☹ Both approaches neglect dependencies among time series.

[1] Salinas *et al.*, “DeepAR: Probabilistic forecasting with autoregressive recurrent networks”, IJF 2020.
[4] Montero-Manso *et al.*, “Principles and algorithms for forecasting groups of time series: Locality and globality”, IJF 2021.

Accounting for spatial dependencies

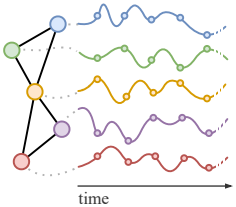
- One option is to consider the input as single multivariate time series
  - → Resulting predictors are **local**: $\widehat{\boldsymbol{X}}_{t+h} = f\left(\boldsymbol{X}_{t-W:t}, \ldots; \boldsymbol{\theta}\right).$
    - ☹ High sample complexity and poor scalability.
- Models operating on sets of time series would allow to keep parameters shared.
  - → Resulting predictors are **global**: $\widehat{\boldsymbol{X}}^{\mathcal{S}}_{t+h} = \mathcal{F}\left(\boldsymbol{X}^{\mathcal{S}}_{t-W:t}, \ldots; \boldsymbol{\theta}\right), \qquad \forall \mathcal{S} \subseteq \mathcal{D}$
    - ☺ Can be implemented by attention-based models (e.g, Transformers).
    - ☹ Does not exploit structural priors, high computational and sample complexity.
- Other methods (e.g., [5]) rely on dimensionality reduction to extract shared latent factors.
    - ☺ Might work well if data are low-rank.
    - ☹ Local and relational information are lost and can still suffer from, scalability issues.

[2] Benidis *et al.*, "Deep Learning for Time Series Forecasting: Tutorial and Literature Survey", ACM CS 2022.
[5] Sen *et al.*, "Think globally, act locally: A deep neural network approach to high-dimensional time series forecasting", NeurIPS 2019.

Graph-based representation

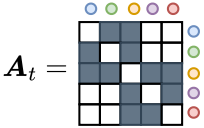
Relational information

Exploit functional dependencies as an inductive bias to improve the forecasts.



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

- $\boldsymbol{A}_t$ can be **asymmetric** and **dynamic** (can vary with t).

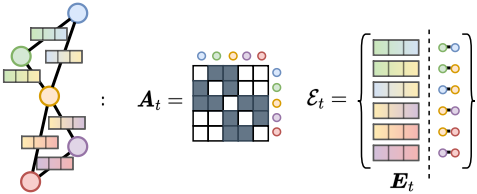


Relational information with attributes

Optional edge attributes $\boldsymbol{e}_t^{ij} \in \mathbb{R}^{d_e}$ can be associated to each non-zero entry of $\boldsymbol{A}_t$.

The set of attributed edges is denoted by

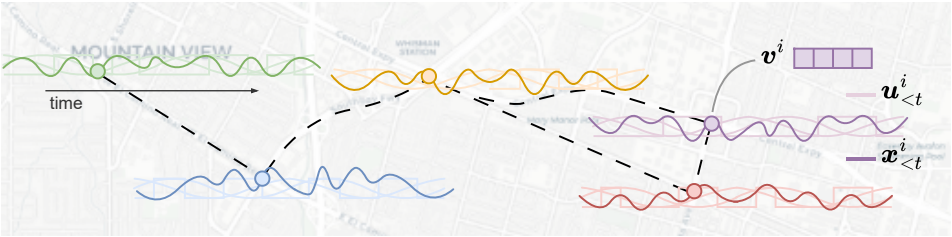
$$\mathcal{E}_t \doteq \{\langle (i,j), \boldsymbol{e}_t^{ij} \rangle \mid \forall i,j : \boldsymbol{A}_t[i,j] \neq 0\}.$$



$\rightarrow$ Edge attributes can be both **categorical** or **numerical**.

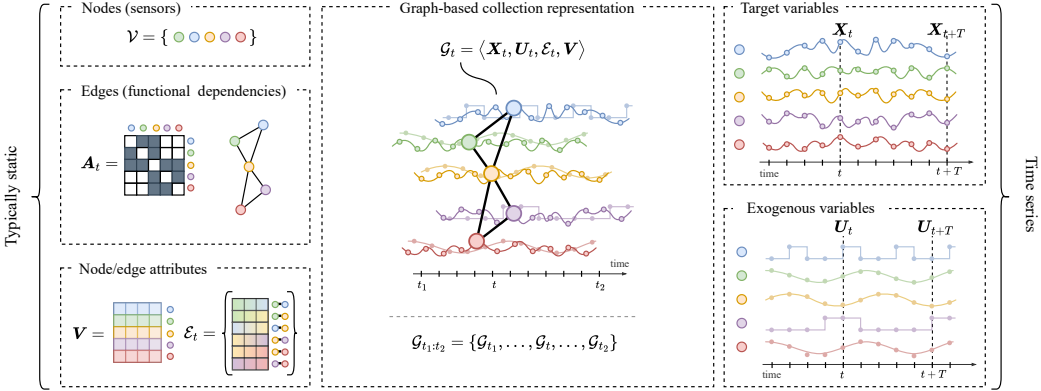
Example: Traffic monitoring system

Consider again the sensor network of the previous example.



- Edges in $\mathcal{E}$ can be obtained by considering the road network.
  - $\rightarrow$ Road closures and traffic diversions can be accounted for with a dynamic topology $\mathcal{E}_t$.

Graph-based representations for correlated time series



$\mathcal{G}_t \doteq \langle \boldsymbol{X}_t, \boldsymbol{U}_t, \mathcal{E}_t, \boldsymbol{V} \rangle$ contains the available information w.r.t. time step t.

[3] Cini *et al.*, “Graph Deep Learning for Time Series Forecasting”, Preprint 2023.

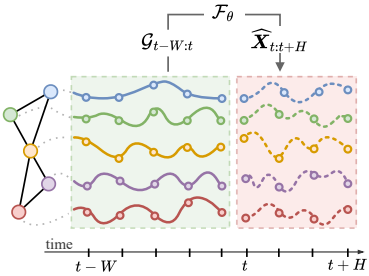
Relational inductive biases for time series forecasting

Forecasts can be conditioned on the available relational information $\mathcal{E}_{t-W:t}$

$$\widehat{\boldsymbol{X}}^{\mathcal{S}}_{t:T+H} = \mathcal{F}\left(\mathcal{G}^{\mathcal{S}}_{t-W:t}, \boldsymbol{U}^{\mathcal{S}}_{t:t+H}; \boldsymbol{\theta}\right) \qquad \forall \mathcal{S} \in \mathcal{D}$$

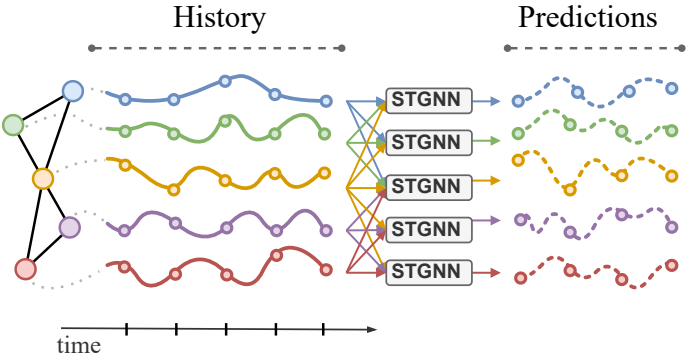
The conditioning can act as a regularization to localize predictions w.r.t. each node.

- ☺ Relational priors prune spurious correlations.
- ☺ More scalable than standard multivariate models.
- ☺ Can forecast any subset of correlated time series.



Spatiotemporal graph neural networks

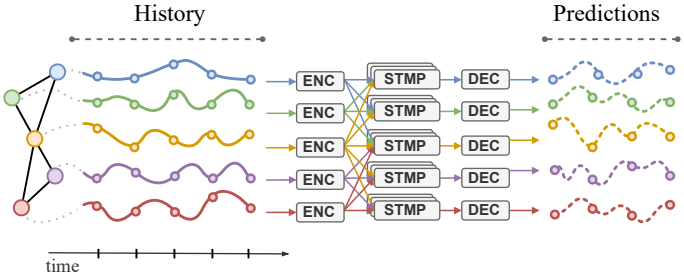
We call spatiotemporal graph neural networks (STGNNs) a neural network exploiting both temporal and spatial relations of the input spatiotemporal time series.



We focus on models based on message passing (MP).

A general recipe for building STGNNs

We consider STGNNs consisting of three main components



- $\textsc{Enc}(\cdot)$ is the **encoding** layer, e.g., implemented by an MLP.
- $\textsc{STMP}(\cdot)$ is a stack of **spatiotemporal message-passing (STMP)** layers.
- $\textsc{Dec}(\cdot)$ is the **readout** layer, e.g., implemented by an MLP.

[3] Cini *et al.*, “Graph Deep Learning for Time Series Forecasting”, Preprint 2023.

A closer look

Representations are updated as follows.

$$\boldsymbol{h}_{t-1}^{i,0} = \textsc{Encoder}\left(\boldsymbol{x}_{t-1}^{i}, \boldsymbol{u}_{t-1}^{i}, \boldsymbol{v}^{i}\right), \tag{1}$$

$$\boldsymbol{H}_{t-1}^{l+1} = \textsc{STMP}^{l}\left(\boldsymbol{H}_{\leq t-1}^{l}, \mathcal{E}_{\leq t-1}\right), \quad l = 0, \dots, L-1 \tag{2}$$

$$\hat{\boldsymbol{x}}_{t:t+H}^{i} = \textsc{Decoder}\left(\boldsymbol{h}_{t-1}^{i,L}, \boldsymbol{u}_{t:t+H}^{i}\right). \tag{3}$$

- $\textsc{Enc}(\cdot)$ process each observation independently.
- $\textsc{STMP}(\cdot)$ is where propagation through time and space happens.
- $\textsc{Dec}(\cdot)$ maps each representation to predictions.

[3] Cini *et al.*, “Graph Deep Learning for Time Series Forecasting”, Preprint 2023.

Spatiotemporal message-passing (STMP)

STMP blocks can be defined as:

$$\boldsymbol{h}_t^{i,l+1} = \textsc{Up}^l\left(\boldsymbol{h}_{\leq t}^{i,l}, \underset{j\in\mathcal{N}_t(i)}{\textsc{Aggr}}\left\{\textsc{Msg}^l\left(\boldsymbol{h}_{\leq t}^{i,l}, \boldsymbol{h}_{\leq t}^{j,l}, \boldsymbol{e}_{\leq t}^{ji}\right)\right\}\right)$$

Each block processes **sequences** while accounting for **relational dependencies**.

As in standard MP operators:

- $\textsc{Msg}^l(\,\cdot\,)$ is a **message function**, e.g., implemented by *temporal convolutional layers*.
- $\textsc{Aggr}\{\,\cdot\,\}$ is a permutation invariant **aggregation function**.
- $\textsc{Up}^l(\,\cdot\,)$ is an **update function**, e.g., implemented by an RNN.

❗ Blocks can be implemented by composing MP and sequence modeling operators.
→ Many possible designs exist.

[3] Cini *et al.*, "Graph Deep Learning for Time Series Forecasting", Preprint 2023.
[6] Gilmer *et al.*, "Neural message passing for quantum chemistry", ICML 2017.

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)**
  Each time series is embedded in a vector and then representations are propagated on the graph.
- **Space-then-Time (STT)**
  Spatial propagation is performed before processing the resulting time series.

Time-and-Space

In T&S models, representations at every node and time step are obtained by jointly propagating representation through time and space.

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

Several options exist.

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

Example 1: From Recurrent Neural Networks...

Consider a standard GRU cell [7].

$$\boldsymbol{r}_t^i = \sigma\left(\boldsymbol{\Theta}_r\left[\boldsymbol{x}_t^i || \boldsymbol{h}_{t-1}^i\right] + \boldsymbol{b}_r\right) \tag{4}$$

$$\boldsymbol{u}_t^i = \sigma\left(\boldsymbol{\Theta}_u\left[\boldsymbol{x}_t^i || \boldsymbol{h}_{t-1}^i\right] + \boldsymbol{b}_u\right) \tag{5}$$

$$\boldsymbol{c}_t^i = \tanh\left(\boldsymbol{\Theta}_c\left[\boldsymbol{x}_t^i || \boldsymbol{r}_t^i \odot \boldsymbol{h}_{t-1}^i\right] + \boldsymbol{b}_c\right) \tag{6}$$

$$\boldsymbol{h}_t^i = \left(1 - \boldsymbol{u}_t^i\right) \odot \boldsymbol{c}_t^i + \boldsymbol{u}_t^i \odot \boldsymbol{h}_{t-1}^i \tag{7}$$

Time series are processed independently for each node or as a single multivariate time series.

[7] 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:

$$\boldsymbol{Z}_t^l = \boldsymbol{H}_t^{l-1} \tag{8}$$

$$\boldsymbol{R}_t^l = \sigma\left(\mathsf{MP}_r^l\left(\left[\boldsymbol{Z}_t^l \| \boldsymbol{H}_{t-1}^l\right], \mathcal{E}_t\right)\right), \tag{9}$$

$$\boldsymbol{O}_t^l = \sigma\left(\mathsf{MP}_o^l\left(\left[\boldsymbol{Z}_t^l \| \boldsymbol{H}_{t-1}^l\right], \mathcal{E}_t\right)\right), \tag{10}$$

$$\boldsymbol{C}_t^l = \tanh\left(\mathsf{MP}_c^l\left(\left[\boldsymbol{Z}_t^l \| \boldsymbol{R}_t^l \odot \boldsymbol{H}_{t-1}^l\right], \mathcal{E}_t\right)\right), \tag{11}$$

$$\boldsymbol{H}_t^l = \boldsymbol{O}_t^l \odot \boldsymbol{H}_{t-1}^l + (1 - \boldsymbol{O}_t^l) \odot \boldsymbol{C}_t^l, \tag{12}$$

These T&S models are known as graph convolutional recurrent neural networks (GCRNNs) [8].

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

Popular GCRNNs

The first GCRNN has been introduced in [8], with message passing (MP) blocks implemented as polynomial graph convolutional filters.

GCRNNs have become popular in traffic forecasting with the Diffusion Convolutional Recurrent Neural Network (DCRNN) architecture [9].

DCRNN relies on a bidirectional diffusion convolution:

$$\boldsymbol{H}_t' = \sum_{k=0}^{K} \left(\boldsymbol{D}_{t,\text{out}}^{-1}\boldsymbol{A}_t\right)^k \boldsymbol{H}_t\boldsymbol{\Theta}_1^{(k)} + \left(\boldsymbol{D}_{t,\text{in}}^{-1}\boldsymbol{A}_t^\top\right)^k \boldsymbol{H}_t\boldsymbol{\Theta}_2^{(k)} \tag{13}$$

[8] Seo *et al.*, "Structured sequence modeling with graph convolutional recurrent networks", ICONIP 2018.
[9] Li *et al.*, "Diffusion Convolutional Recurrent Neural Network: Data-Driven Traffic Forecasting", ICLR 2018.

Example 2: Spatiotemporal convolutional networks (i)

Spatiotemporal convolutional networks (STCNs) instead **alternate spatial and temporal convolutions**:

1. Compute intermediate representations by using a temporal convolutional layer:

$$\boldsymbol{z}_{t-W:t}^{i,l} = \mathsf{TCN}^l \left(\boldsymbol{h}_{t-W:t}^{i,l-1} \right) \qquad \forall\, i$$

   where TCN^l indicates a temporal convolutional layer.

2. Compute the updated representation at each time step by using a graph convolution:

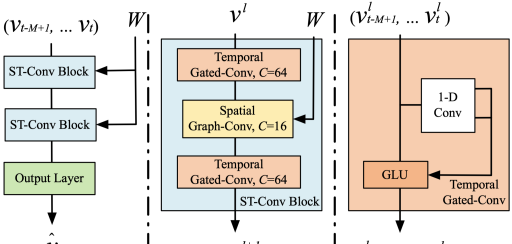
$$\boldsymbol{H}_t^l = \mathsf{MP}^l \left(\boldsymbol{Z}_t^l, \mathcal{E}_t \right) \qquad \forall\, t$$

Spatiotemporal convolutional networks (ii)

The first example of such architecture is the STGCN by Yu et al. [10].

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 [10].

More advanced implementations exist, e.g., see Graph Wavenet [11].

[10] Yu *et al.*, "Spatio-temporal graph convolutional networks: a deep learning framework for traffic forecasting", IJCAI 2018.
[11] Wu *et al.*, "Graph wavenet for deep spatial-temporal graph modeling", IJCAI 2019.

Example 3: Temporal Graph Convolution

A more integrated approach instead consists of implementing a temporal propagation mechanism in the message function.

For example, we can design STMP layers s.t.

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

Analogous models can be built with any sequence modeling architecture.

→ **Example:** many rely on attention-based operators [12][13].

[12] Marisca *et al.*, "Learning to Reconstruct Missing Data from Spatiotemporal Graphs with Sparse Observations", NeurIPS 2022.
[13] Wu *et al.*, "TraverseNet: Unifying Space and Time in Message Passing for Traffic Forecasting", TNNLS 2022.

Example 4: Product graph representations

An alternative option is to consider the sequence $\mathcal{G}_{t-W:t}$ as a **single graph** with temporal and spatial edges.

In particular, **product graph representations** can be obtained by combining the two edge sets.

Temporal graph:

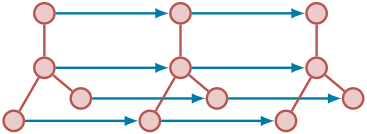
Spatial graph:

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

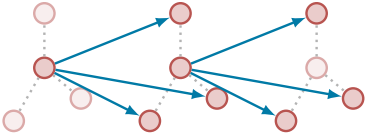
[14] Sabbaqi *et al.*, "Graph-time convolutional neural networks: Architecture and theoretical analysis", TPAMI 2023.

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.



- ...

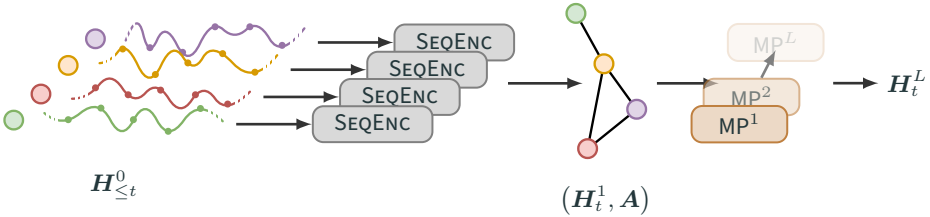
Time-then-Space models

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.

1. $\boldsymbol{h}_t^{i,1} = \textsc{SeqEnc}\left(\boldsymbol{h}_{\leq t}^{i,0}\right)$

2. $\boldsymbol{H}_t^{l+1} = \mathrm{MP}^l\left(\boldsymbol{H}_t^l, \mathcal{E}_t\right)$



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.

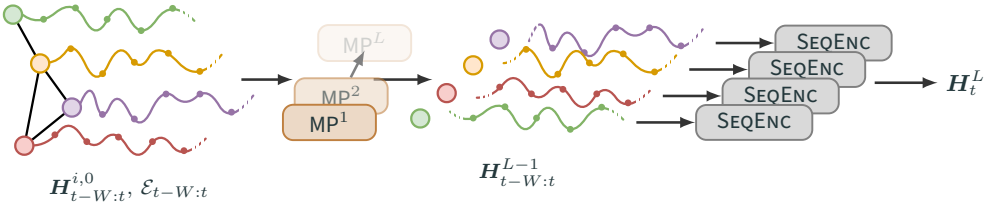
Space-then-Time

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.

1. $\boldsymbol{H}_t^{i,l} = \mathrm{MP}^l\left(\boldsymbol{H}_t^{i,l-1}, \mathcal{E}_t\right)$

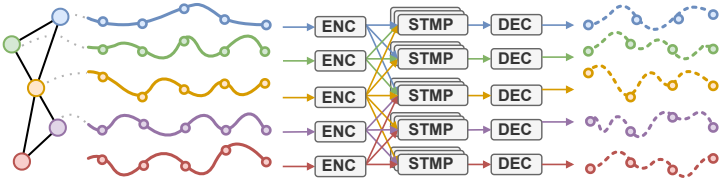
2. $\boldsymbol{h}_t^{i,L} = \textsc{SeqEnc}\left(\boldsymbol{h}_{t-W:t}^{i,L-1}\right)$



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

Global and local models

Globality and locality in STGNNs

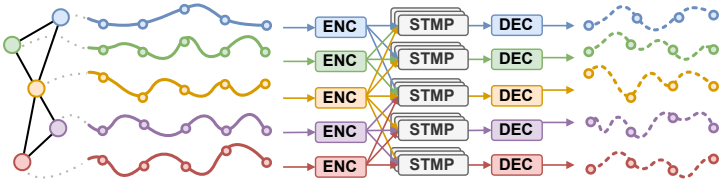


Standard STGNNs are **global** models.

- ☺ Can handle arbitrary node sets.
- ☺ Neighbors provide further conditioning on the predictions.
- ☹ Might struggle with local effects.
- ☹ Might need long windows and high model capacity.

💡 Use hybrid global-local STGNNs.

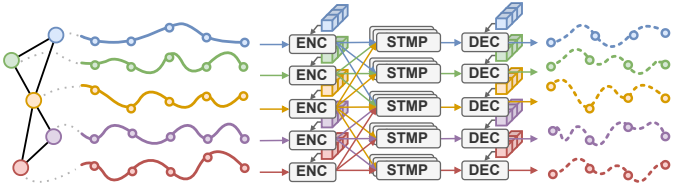
Global-local STGNNs



We can turn some global components of the architecture into local.

- ☺ Resulting models can capture local effects.
- ☹ Might require a large number of local parameters.

Global-local STGNNs with node embeddings



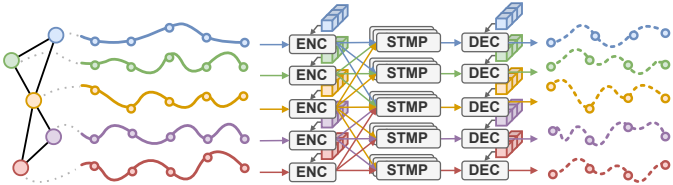
Node embeddings can amortize the learning of local components.

Node embeddings are a table of **learnable parameters** $Q \in \mathbb{R}^{N \times d_q}$ associated with **each node**.

- ☺ Fed into encoder/decoder, amortize the learning of local components.
- ☺ Most of the model's parameters remain shared.
- 😐 Number of parameters scales linearly with the number of time series . . .
  - → One might consider intermediate solutions, e.g., learning embeddings for clusters of time series.

[15] Cini *et al.*, "Taming Local Effects in Graph-based Spatiotemporal Forecasting", NeurIPS 2023.

Transferability



❗ Hybrid global-local STGNNs are not inductive models.

However, the cost of transfer learning can be reduced.

- ☺ Keep shared parameters fixed and finetune local parameters only.
- ☺ Node embeddings can be regularized to facilitate transfer further.

[15] Cini, Marisca, Zambon, and Alippi, "Taming Local Effects in Graph-based Spatiotemporal Forecasting", NeurIPS 2023.
[16] Butera, De Felice, Cini, and Alippi, "On the Regularization of Learnable Embeddings for Time Series Processing", Preprint 2024.

Some empirical results

MODELS	MetrLA	PemsBAY	CER-E	AQI	MetrLA	PemsBAY	CER-E	AQI
Reference arch.	Global models				+ Local node embeddings			
RNN	3.54 ± .00	1.77 ± .00	4.57 ± .01	14.02 ± .04	**3.15** ± .03	**1.59** ± .00	**4.22** ± .02	**13.73** ± .04
GCRNN-IMP	3.35 ± .01	1.70 ± .01	4.44 ± .01	12.87 ± .02	**3.10** ± .01	**1.59** ± .00	**4.18** ± .01	**12.48** ± .03
RNN+IMP	3.34 ± .01	1.72 ± .00	4.39 ± .01	12.74 ± .02	**3.08** ± .01	**1.58** ± .00	**4.12** ± .03	**12.33** ± .02
GCRNN-AMP	3.22 ± .02	1.65 ± .00	4.57 ± .04	12.29 ± .02	**3.07** ± .02	**1.59** ± .00	**4.17** ± .02	**12.17** ± .05
RNN+AMP	3.24 ± .01	1.66 ± .00	4.31 ± .01	12.30 ± .02	**3.06** ± .01	**1.58** ± .01	**4.13** ± .01	**12.15** ± .02
Baseline arch.	Original				+ Local node embeddings			
DCRNN	3.22 ± .01	1.64 ± .00	4.28 ± .01	12.96 ± .03	**3.07** ± .02	**1.60** ± .00	**4.13** ± .02	**12.53** ± .02
GraphWaveNet	3.05 ± .03	**1.56 ± .01**	**3.97 ± .01**	12.08 ± .11	**2.99** ± .02	1.58 ± .00	4.01 ± .01	**11.81** ± .04
AGCRN	3.16 ± .01	**1.61 ± .00**	4.45 ± .01	13.33 ± .02	**3.14** ± .00	1.62 ± .00	**4.37** ± .02	**13.28** ± .03

Table 1: MAE on benchmark datasets.

Transfer learning results

We consider datasets coming from four different traffic networks.

→ **One of the networks is left out** at training time and used for evaluating **transferability**.

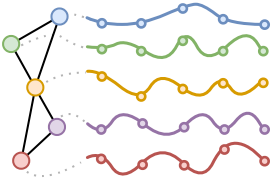
RNN+IMP		PEMS03	PEMS04	PEMS07	PEMS08
Fine-tuning	Global	15.30 ± 0.03	21.59 ± 0.11	23.82 ± 0.03	15.90 ± 0.07
	Embeddings	14.64 ± 0.05	20.27 ± 0.11	**22.23 ± 0.08**	**15.45 ± 0.06**
	– **Variational**	**14.56 ± 0.03**	20.19 ± 0.05	22.43 ± 0.02	**15.41 ± 0.06**
	– **Clustering**	**14.60 ± 0.02**	**19.91 ± 0.11**	**22.16 ± 0.07**	**15.41 ± 0.06**
Zero-shot		18.20 ± 0.09	23.88 ± 0.08	32.76 ± 0.69	20.41 ± 0.07

Table 2: Transfer learning results (MAE) after fine-tuning on a week of data.

[15] Cini *et al.*, "Taming Local Effects in Graph-based Spatiotemporal Forecasting", NeurIPS 2023.

End of Part 1: what we have so far

1. We formalized the problem of processing correlated time series.
2. Graph representations allows for modeling dependencies among them.
3. We discussed forecasting problem and global/local deep learning models for time series.
4. We saw approaches to building spatiotemporal graph neural networks and the associated trade-offs.



Before discussing challenges, we will look at software implementations of the above.

DEMO

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**.

- torch-spatiotemporal.readthedocs.io
- github.com/TorchSpatiotemporal/tsl

Notebook

Spatiotemporal Graph Neural Networks with tsl

Open in Colab

[17] Cini and Marisca, *Torch Spatiotemporal*, https://github.com/TorchSpatiotemporal/tsl 2022.

Part 2

Challenges

Challenges

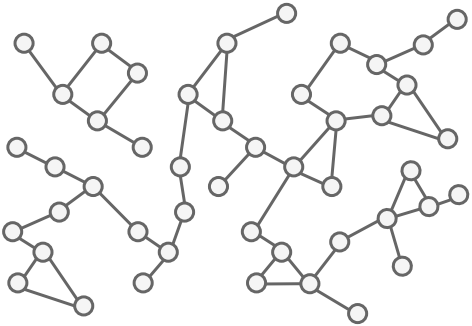
- **Scalability**
  How to deal with large collections of time series?
- **Dealing with missing data**
  How to deal with missing observations within the time series?
- **Latent graph learning**
  What to do when the underlying graph is not known?
- **Model quality assessment**
  How to evaluate our graph-based model?

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 – $\mathcal{O}(WN)$;
- L MP layers **for each time step** – $\mathcal{O}(WL|\mathcal{E}_t|)$.

$\rightarrow \mathcal{O}(W(N + L|\mathcal{E}_t|))$

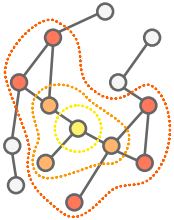
A first step toward improving scalability is represented by TTS models, which perform:

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

$\rightarrow \mathcal{O}(WN + L|\mathcal{E}_t|)$

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., [19], [20]).

☹ Subsampling might break long-range spatiotemporal dependencies.

☹ The learning signal may be noisy.

[18] Gandhi *et al.*, "Spatio-Temporal Multi-graph Networks for Demand Forecasting in Online Marketplaces", ECML-PKDD 2021.
[19] Hamilton *et al.*, "Inductive representation learning on large graphs", NeurIPS 2017.
[20] Rong *et al.*, "DropEdge: Towards Deep Graph Convolutional Networks on Node Classification", ICLR 2020.

Pre-computation

Pre-processing methods (e.g., [21]) 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 [22], which acts in 2 steps:

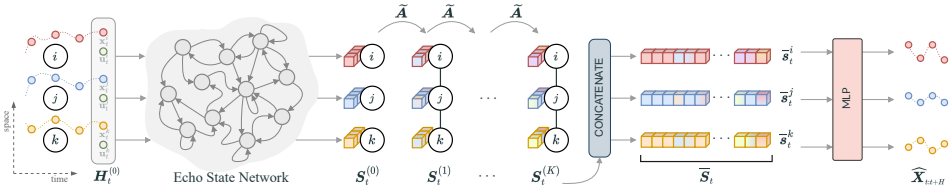
1. obtain a temporal encoding at each time step with a deep echo state network[1];
2. propagate such encodings through the graph using powers of a graph shift operator.

[21] Frasca *et al.*, "SIGN: Scalable inception graph neural networks" 2020.
[22] Cini *et al.*, "Scalable Spatiotemporal Graph Neural Networks", AAAI 2023.
[23] Liu *et al.*, "Do we really need graph neural networks for traffic forecasting?" Preprint 2023.

[1] A randomized recurrent neural networks

SGP: Scalable Graph Predictor [22]

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.

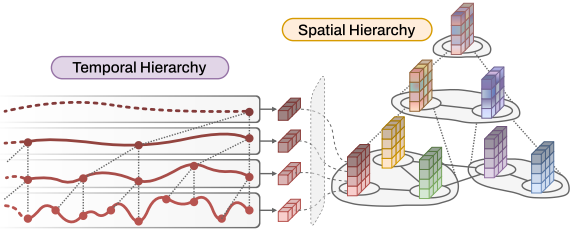
[22] Cini *et al.*, "Scalable Spatiotemporal Graph Neural Networks", AAAI 2023.

Hierarchical processing

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

In space, this can be achieved through graph pooling [24].

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



[24] Grattarola *et al.*, "Understanding Pooling in Graph Neural Networks" 2024.

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...

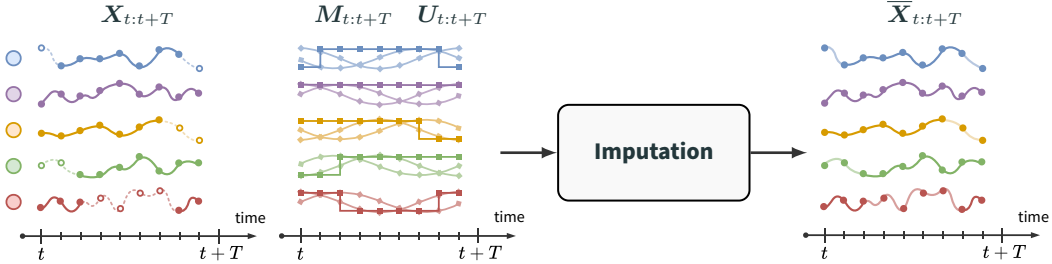
Most forecasting methods operate on complete sequences.

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

Time series imputation

Time series imputation (TSI)

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



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

Missing data types

We can categorize missing data patterns according to the conditional distribution $p\left(\boldsymbol{m}_t^i \mid \boldsymbol{M}_{\leq t}\right)$.

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

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

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

Temporal block missing $\quad p\left(\boldsymbol{m}_t^i \mid \boldsymbol{m}_{t-1}^i\right) \neq p\left(\boldsymbol{m}_t^i\right)$

Spatial block missing $\quad p\left(\boldsymbol{m}_t^i \mid \left\{\boldsymbol{m}_t^j\right\}^{j \neq i}\right) \neq p\left(\boldsymbol{m}_t^i\right)$

Spatiotemporal block missing $\quad p\left(\boldsymbol{m}_t^i \mid \boldsymbol{m}_{t-1}^i, \left\{\boldsymbol{m}_t^j\right\}^{j \neq i}\right) \neq p\left(\boldsymbol{m}_t^i\right)$

Optimization

Parameters $\boldsymbol{\theta}$ can be learned by minimizing a loss function $\ell(\,\cdot\,,\,\cdot\,)$ on valid observations in a training set:

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

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

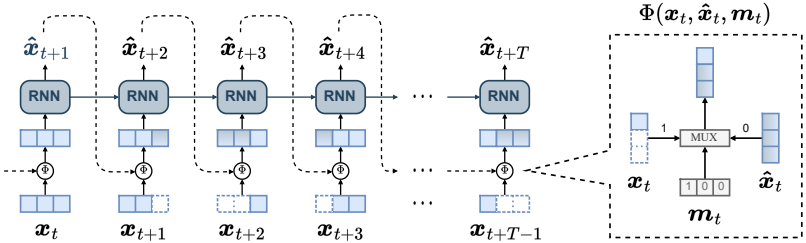
$$\widehat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \sum_{t=1}^{T} \sum_{i=1}^{N} \frac{\left\| \overline{\boldsymbol{m}}_t^i \odot \ell\left(\overline{\boldsymbol{x}}_t^i, \boldsymbol{x}_t^i\right) \right\|_1}{\left\| \overline{\boldsymbol{m}}_t^i \right\|_1}.$$

⚠ Data where $\overline{\boldsymbol{m}}_t^i = \mathbf{1}$ 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).



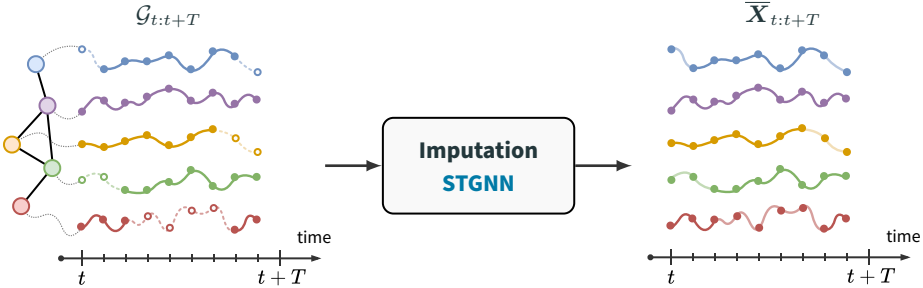
☺ Effective in exploiting past (and future, with bidirectional models) node observations.

☹ 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.,

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



Graph Recurrent Imputation Network (GRIN)

Similarly to GCRNN for forecasting, we can integrate graph processing into the autoregressive approach for imputation [25].

In these approaches, the distribution $p\left(\boldsymbol{x}_t^i \mid \boldsymbol{X}_{0:\infty} \odot \boldsymbol{M}_{0:\infty}\right)$ is modeled into three independent steps:

Information from previous observations.

$$p\left(\boldsymbol{x}_t^i \mid \boldsymbol{X}_{<t} \odot \boldsymbol{M}_{<t}\right)$$

Information from subsequent observations.

$$p\left(\boldsymbol{x}_t^i \mid \boldsymbol{X}_{>t} \odot \boldsymbol{M}_{>t}\right)$$

Information from related concurrent observations.

$$p\left(\boldsymbol{x}_t^i \mid \left\{\boldsymbol{x}_t^j \odot \boldsymbol{m}_t^j\right\}^{j \neq i}\right)$$

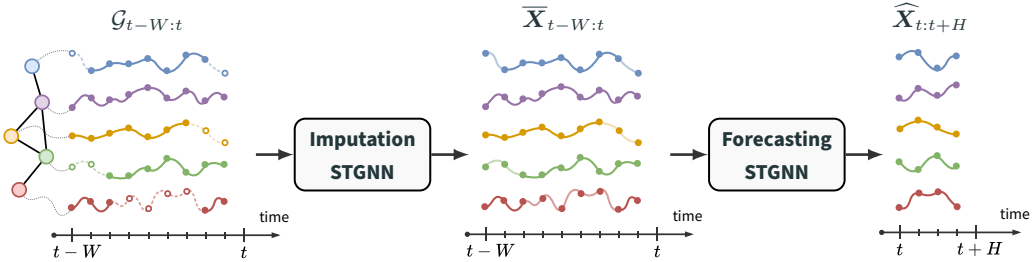
Typically modeled by bidirectional autoregressive models.

Enabled by message passing.

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

Imputation *before* forecasting

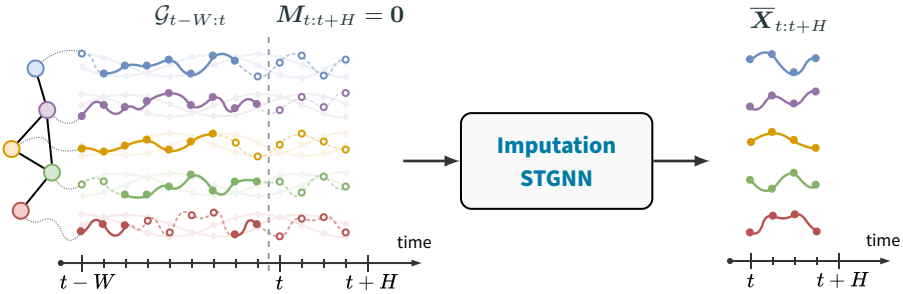
TSI is often used as a preprocessing step for a downstream task, e.g., forecasting.



- ☹ 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.



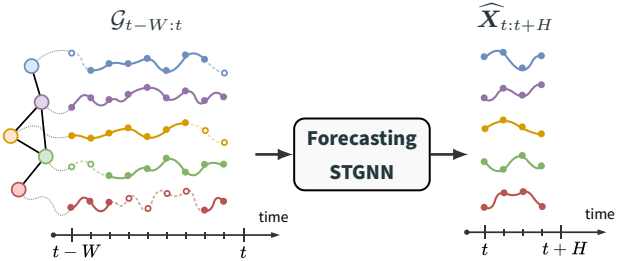
- ☹ It is a workaround (this is not their purpose).
- ☹ Might perform poorly due to the absence of values in the forecasting horizon.

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.



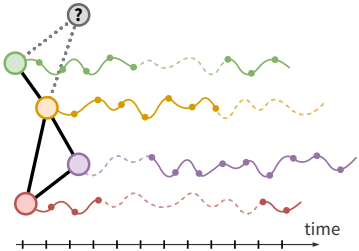
[26] Zhang *et al.*, "Graph-guided network for irregularly sampled multivariate time series", ICLR 2022.
[27] Zhong *et al.*, "Heterogeneous spatio-temporal graph convolution network for traffic forecasting with missing values", IEEE ICDCS 2021.
[28] Marisca *et al.*, "Graph-based Forecasting with Missing Data through Spatiotemporal Downsampling", ICML 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.



[29] Wu *et al.*, "Inductive Graph Neural Networks for Spatiotemporal Kriging", AAAI 2021.
[30] De Felice *et al.*, "Graph-Based Virtual Sensing from Sparse and Partial Multivariate Observations", ICLR 2024.

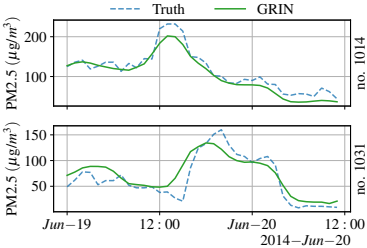
Graph imputation for virtual sensing

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 [25])



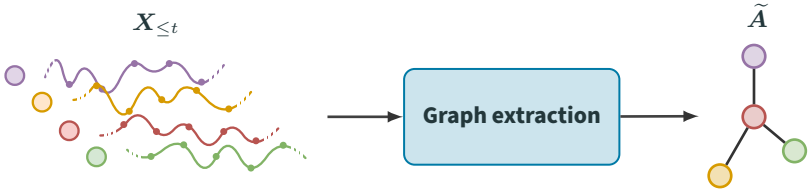
[12] Marisca *et al.*, "Learning to Reconstruct Missing Data from Spatiotemporal Graphs with Sparse Observations", NeurIPS 2022.
[25] Cini *et al.*, "Filling the G_ap_s: Multivariate Time Series Imputation by Graph Neural Networks", ICLR 2022.

Latent graph learning

Learning an adjacency matrix

☹ Relational information is not always (or only partially) 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

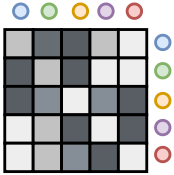


- When possible, the learned graph should be sparse.
- It can be interpreted as regularizing a spatial attention operator.
- This task is found under different names:
  graph structure learning, latent graph learning, graph inference...

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.

Inferring latent structures from time series

Model the graph as a latent variable determining the realizations of the time series.

- They rely on assumptions, such as of signal smoothness and of a diffusion process.

Dedicated loss functions are formulated and minimized, e.g.,

$$\text{trace}(\boldsymbol{X}^\top \boldsymbol{L} \boldsymbol{X}) = \frac{1}{2} \sum_{ij} \boldsymbol{A}_{i,j} \|\boldsymbol{X}_i - \boldsymbol{X}_j\|_2^2$$

constraining $\boldsymbol{L}$ (or $\boldsymbol{A}$) to be a Laplacian (adjacency matrix) and promoting sparsity.

$\rightarrow$ These approaches are commonly derived from a graph signal processing point of view.

[31] Dong *et al.*, "Learning Laplacian matrix in smooth graph signal representations", IEEE TSP 2016.
[32] Mateos *et al.*, "Connecting the dots: Identifying network structure via graph signal processing", IEEE SP Mag 2019.

Task-oriented latent graph learning

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

$\rightarrow$ e.g., by minimizing the forecasting error (MAE, MSE...).

Two different formulations:

1. learning directly an adjacency matrix $\boldsymbol{A} \in \mathbb{R}^{N \times N}$;
2. learning a probability distribution over graphs p_Φ generating $\boldsymbol{A}$ (often $\in \{0, 1\}^{N \times N}$).

⚠ One key challenge is keeping both $\boldsymbol{A}$ and the subsequent computations sparse.

$\rightarrow$ non-trivial with gradient-based optimization.

Direct approach

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

$$\widetilde{\boldsymbol{A}} = \xi\left(\Phi\right)$$

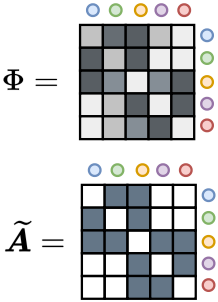
Edge scores Φ

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

$$\Phi = \Phi(\boldsymbol{X}, \widetilde{\Phi}).$$

Function $\xi(\,\cdot\,)$ can enforce structures on $\widetilde{\boldsymbol{A}}$, like,

$\rightarrow$ make $\widetilde{\boldsymbol{A}}$ binary, a k-NN graph, a tree...

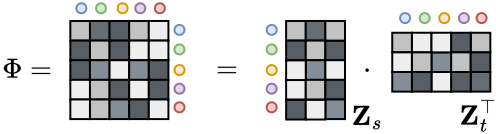


Edge score factorization

The number of possible edge scores is quadratic in the number of nodes ($\Phi \in \mathbb{R}^{N \times N}$)

$\rightarrow$ a common approach is to factorize Φ:

$$\widetilde{\boldsymbol{A}} = \xi\left(\Phi\right) \qquad \Phi = \boldsymbol{Z}_s \boldsymbol{Z}_t^\top$$



with

- $\boldsymbol{Z}_s \in \mathbb{R}^{N \times d}$ source node embeddings
- $\boldsymbol{Z}_t \in \mathbb{R}^{N \times d}$ target node embeddings

$\boldsymbol{Z}_s$ and $\boldsymbol{Z}_t$ can be learned as tables of (local) parameters or as a function of the input window.

[11] 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 $\boldsymbol{A}$ 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 $\boldsymbol{A}$.

- Different parametrizations of p_Φ allow for embedding graph structural priors on the sampled graphs, e.g., edge density, bound node degrees.

Graphs of independent edges

For every edge (i, j)

$$\boldsymbol{A}_{i,j} \sim \text{Bernoulli}(\sigma(\Phi_{i,j})).$$

Fixed-degree graphs

For each node i, sample w/o replacement k nodes from

$$\text{Categorical}\left(\text{SoftMax}(\Phi_{i,1}, \dots, \Phi_{i,N})\right).$$

- As seen before, Φ can be factorized and p_Φ made input dependent, e.g.,

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

[33] Kazi *et al.*, “Differentiable graph module (dgm) for graph convolutional networks”, IEEE TPAMI 2022.
[34] Cini *et al.*, “Sparse graph learning from spatiotemporal time series”, JMLR 2023.

Learning graph distributions

Training losses average over all graphs according to p_Φ, e.g., based on point predictions

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

where $\boldsymbol{X}_{t:t+H} = \mathcal{F}(\boldsymbol{X}_{t-W:t}, \boldsymbol{A}; \theta)$.

More generally, comparing predictive distributions by means of a divergence measure Δ

$$\mathcal{L}(\Phi) = \Delta\left(p_\Phi(\widehat{\boldsymbol{X}}_{t:t+H}), p(\boldsymbol{X}_{t:t+H})\right).$$

⚠ Gradient-based optimization requires computing $\nabla_\Phi \mathcal{L}(\Phi)$,
$\rightarrow$ i.e., differentiating w.r.t. the parameters of the integrated distribution.

- ☹ Analytical computations is often unfeasible;
- ☹ Monte Carlo approximations require care.

Monte Carlo gradient estimators

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

- ☺ 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

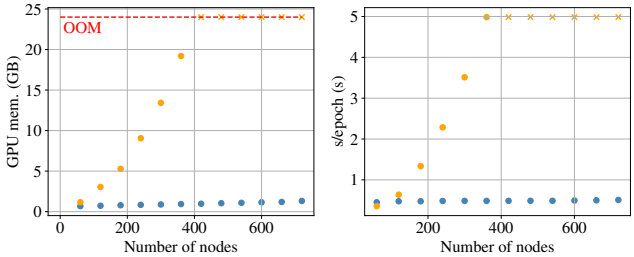
$$\nabla_\Phi \mathbb{E}_{p_\Phi}\left[\ell(\widehat{\boldsymbol{X}}, \boldsymbol{X})\right] = \mathbb{E}_{p_\Phi}\left[\ell(\widehat{\boldsymbol{X}}, \boldsymbol{X}) \nabla_\Phi \log p_\Phi\right]$$

- ☹ suffer from high variance (use variance reduction techniques),
- ☺ allow to keep computations sparse through the model.

$\rightarrow$ we can use Monte Carlo estimator.

[35] Kipf *et al.*, "Neural relational inference for interacting systems", ICML 2018.
[34] Cini *et al.*, "Sparse graph learning from spatiotemporal time series", JMLR 2023.

Computational efficiency



- Score-function
- Pathwise

With score-based gradient estimators $\nabla_\Phi \mathcal{L}(\Phi) = \mathbb{E}_{\boldsymbol{A}\sim p_\Phi}\left[\ell(\widehat{\boldsymbol{X}}, \boldsymbol{X})\nabla_\Phi \log p_\Phi(\boldsymbol{A})\right]$.

☺ They are computationally efficient as ∇_Φ is computed with respect to $\log p_\Phi(\boldsymbol{A})$.

- do not rely on continuous relaxation of discrete random variables;
- allow for sparse message passing to compute $\widehat{\boldsymbol{X}}$ (and, in turn, of $\ell(\widehat{\boldsymbol{X}}, \boldsymbol{X})$) by rely on sparse matrices $\boldsymbol{A}$.

☹ They can be sample inefficient due to the high variance of the gradient estimates.

Uncertainty quantification

While probabilistic models have been used to enable learning of discrete variables (graph edges), the associated edge probabilities can carry information about the relevance of the associated connections.

→ It enables some degree of explainability and better informed decision-making.

Assessing the calibration of latent variables is hard on real data.

→ This is due to their latent nature, for which observations are not available.

Studies provide some learning guarantees, e.g.,

> Minimizing appropriate divergence measures $\Delta\left(p(\boldsymbol{X}), p_\Phi(\widehat{\boldsymbol{X}})\right)$ of the data and predictive distributions $p(\boldsymbol{X}), p_\Phi(\widehat{\boldsymbol{X}})$, respectively, enables calibration of the $p_\Phi(\boldsymbol{A})$.

[36] Gray *et al.*, "Bayesian inference of network structure from information cascades", IEEE TSIPN 2020.
[37] Manenti *et al.*, *Learning Latent Graph Structures and Their Uncertainty*, Preprint 2024.

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

Given two predictors $\mathcal{F}_a, \mathcal{F}_b$ 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 other model $\mathcal{F}_b$ better than $\mathcal{F}_a$.

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

$\rightarrow$ Either we find a new model $\mathcal{F}_*$ better than $\mathcal{F}_a$

$\rightarrow$ or we need prior knowledge about the modeled system.

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

Residual correlation analysis

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

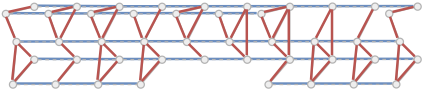
If residuals are dependent
$\implies$ there is information that the model hasn't captured
$\implies$ model predictions can be improved.

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.

Research focused mainly on either serial correlation [38]–[40] or spatial correlation [41], [42].

AZ-Whiteness test: a spatio-temporal test



The test is defined by statistic

$$C(\{\boldsymbol{r}\}) = \underbrace{\sum_t \sum_{(i,j)\in\mathcal{E}_t} w_{ijt}\,\mathrm{sgn}(\langle \boldsymbol{r}_t^i, \boldsymbol{r}_t^j\rangle)}_{\text{spatial edge}} + \underbrace{\sum_t \sum_i w_{it}\,\mathrm{sgn}(\langle \boldsymbol{r}_t^i, \boldsymbol{r}_{t+1}^i\rangle)}_{\text{temporal edge}} \qquad \to \mathcal{N}(0,1)$$

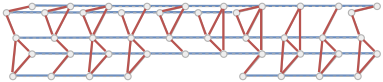
- ☺ distribution-free and residuals can be non-identically distributed.
- ☺ computation is linear in the number of edges and time steps.

[43] Zambon *et al.*, "AZ-whiteness Test: A Test for Signal Uncorrelation on Spatio-Temporal Graphs", NeurIPS 2022.

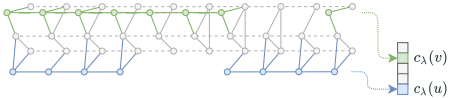
Where can we improve?

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

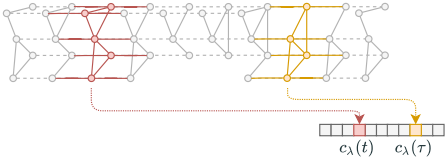
Spatial (or temporal) edges



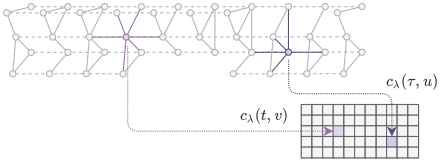
Edges related to a node



Edges related to a time step



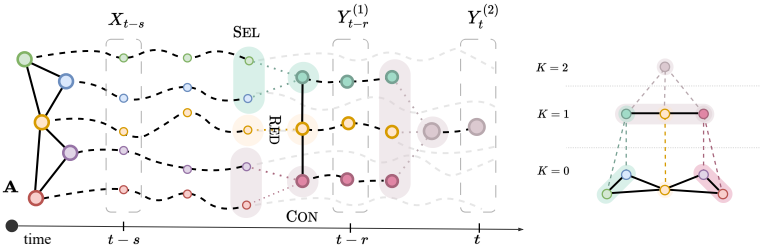
Edges related to a node



[44] Zambon *et al.*, "Where and How to Improve Graph-based Spatio-temporal Predictors" 2023.

Future directions

Hierarchical processing



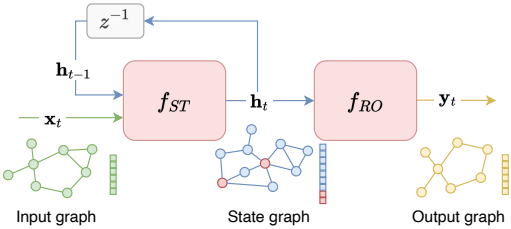
- Standard STGNNs operate at a fixed spatiotemporal scale.
- Combine hierarchical and graph-based representations.
- Exploit higher-order dependencies by operating on hierarchical representations of the input.
- Can also be used for hierarchical forecasting and to obtain reconciled predictions.

[45] Yu *et al.*, "ST-Unet: A spatio-temporal U-network for graph-structured time series modeling" 2019.
[46] Cini *et al.*, "Graph-based Time Series Clustering for End-to-End Hierarchical Forecasting", ICML 2024.
[28] Marisca *et al.*, "Graph-based Forecasting with Missing Data through Spatiotemporal Downsampling", ICML 2024.

State-space models

$$\begin{cases} \mathbf{h}_t = f_{\mathsf{ST}}(\mathbf{h}_{t-1}, \mathbf{x}_{t-1}, \boldsymbol{\eta}_{t-1}) \\ \mathbf{y}_t = f_{\mathsf{RO}}(\mathbf{h}_t, \boldsymbol{\nu}_t) \end{cases}$$

- Inputs $\mathbf{x}_t$, states $\mathbf{h}_t$, and outputs $\mathbf{y}_t$ are different attributed graphs.
- $\boldsymbol{\eta}_t, \boldsymbol{\nu}_t$ are noise terms at the node/edge level.



[47] Rangapuram *et al.*, "Deep State Space Models for Time Series Forecasting", NeurIPS 2018.
[48] Zambon *et al.*, *Graph State-Space Models*, Preprint 2023.
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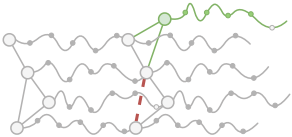
[50] Buchnik *et al.*, "GSP-kalmannet: Tracking graph signals via neural-aided Kalman filtering", IEEE TSP 2024.
[51] Chouzenoux *et al.*, "Sparse graphical linear dynamical systems", JMLR 2024.

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.

[15] Cini *et al.*, "Taming Local Effects in Graph-based Spatiotemporal Forecasting", NeurIPS 2023.
[52] Yin *et al.*, "Nodetrans: A graph transfer learning approach for traffic prediction", Preprint 2022.
[53] Prabowo *et al.*, "Traffic forecasting on new roads using spatial contrastive pre-training (SCPT)" 2024.

Benchmarks

Open datasets

In line with OGB [54], TGB [55], TGB 2.0 [56].

- Energy analytics (CER-E, PV-US) [22]
- Traffic flow (LargeST) [57]
- ...

Software

Standard model evaluation platforms

- Torch SpatioTemporal [17]
- BasicTS [58]
- ...

[22] Cini *et al.*, "Scalable Spatiotemporal Graph Neural Networks", AAAI 2023.
[57] Liu *et al.*, "Largest: A benchmark dataset for large-scale traffic forecasting", NeurIPS (D&B) 2024.
[17] Cini *et al.*, *Torch Spatiotemporal*, https://github.com/TorchSpatiotemporal/tsl 2022.
[58] Shao *et al.*, "Exploring Progress in Multivariate Time Series Forecasting: Comprehensive Benchmarking and Heterogeneity Analysis", IEEE TKDE 2024.

Conclusions

Some Takeaways

Deep Learning for **time series** + Deep Learning on **graphs**

- Relational inductive biases allow for exploiting dependencies among the time series,
- ...while sharing most of the model parameters,
- ...and overcoming limits due to irregularities in time and space.
- Whenever possible, global-local models are a safe starting point.

Challenges. Scalability • Missing data • Latent graph learning • Model quality assessment

Resources. Tutorial paper [3] • Open-source library [17]

[3] Cini, Marisca, Zambon, and Alippi, "Graph Deep Learning for Time Series Forecasting", Preprint 2023.
[17] Cini and Marisca, *Torch Spatiotemporal*, https://github.com/TorchSpatiotemporal/tsl 2022.

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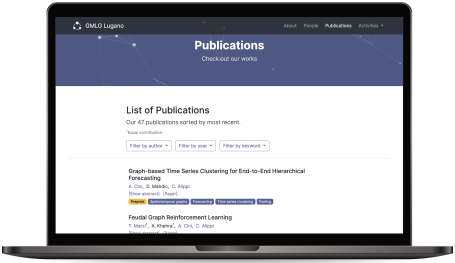

THE END

Questions?

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