Modeling Spatio-Temporal Systems with Graph-based Machine Learning

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Department of Computer and Information Science

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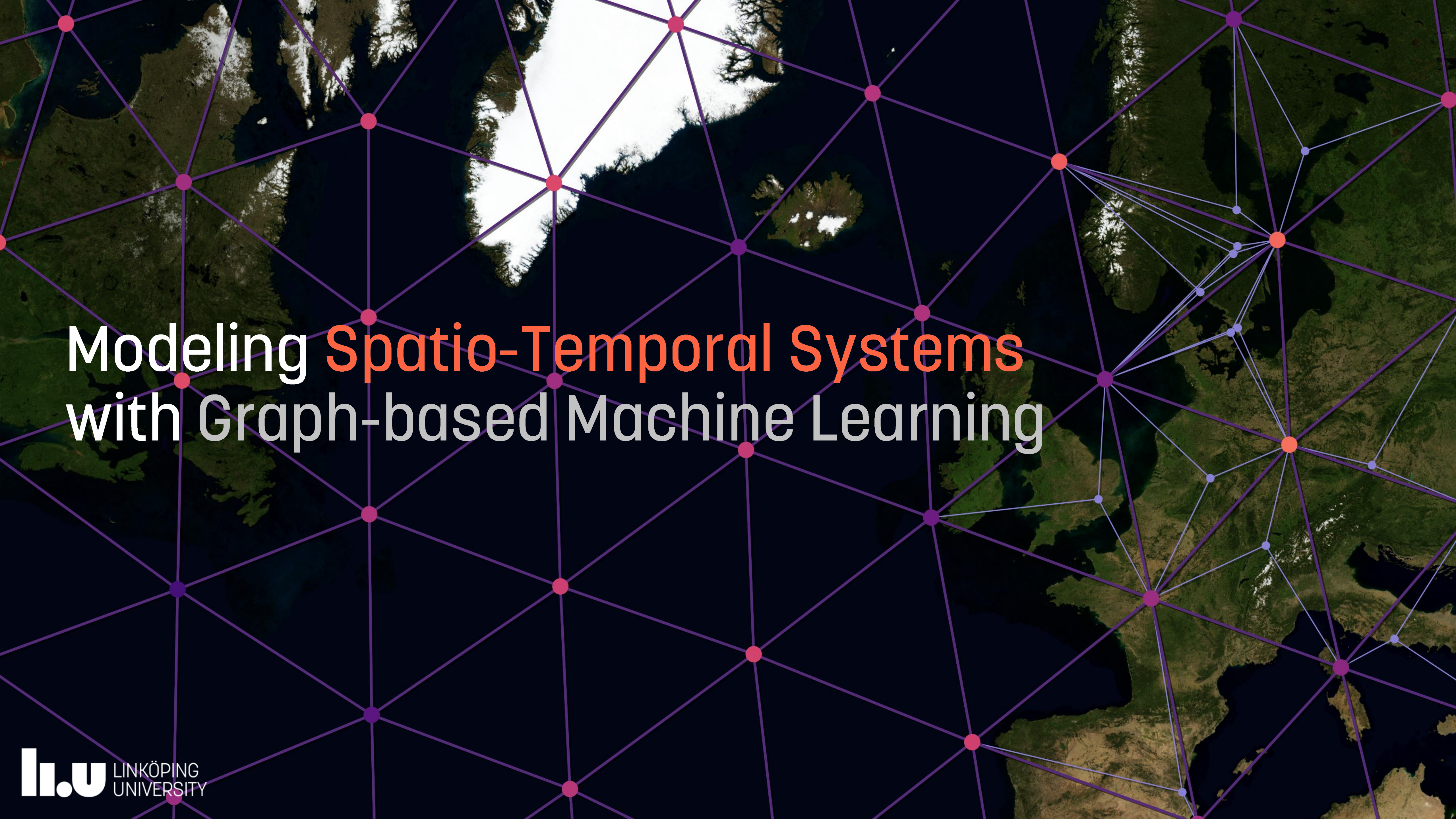

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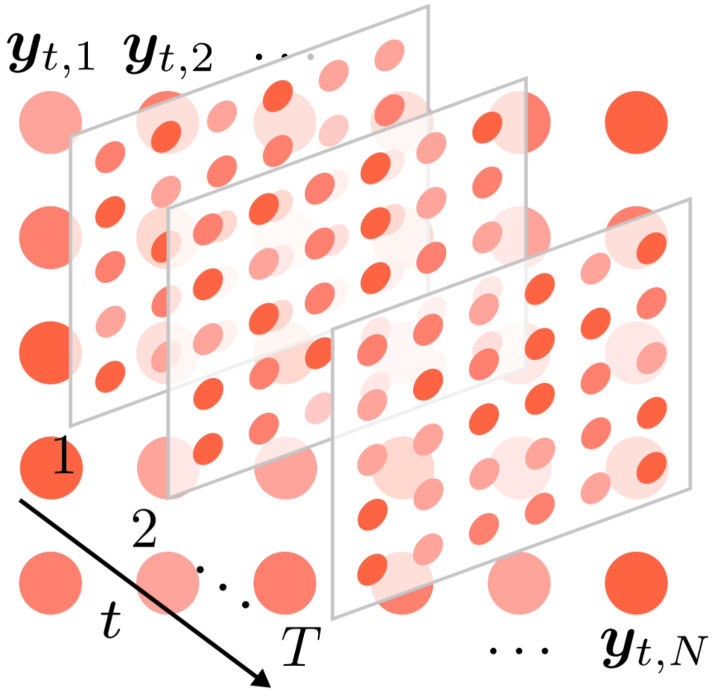
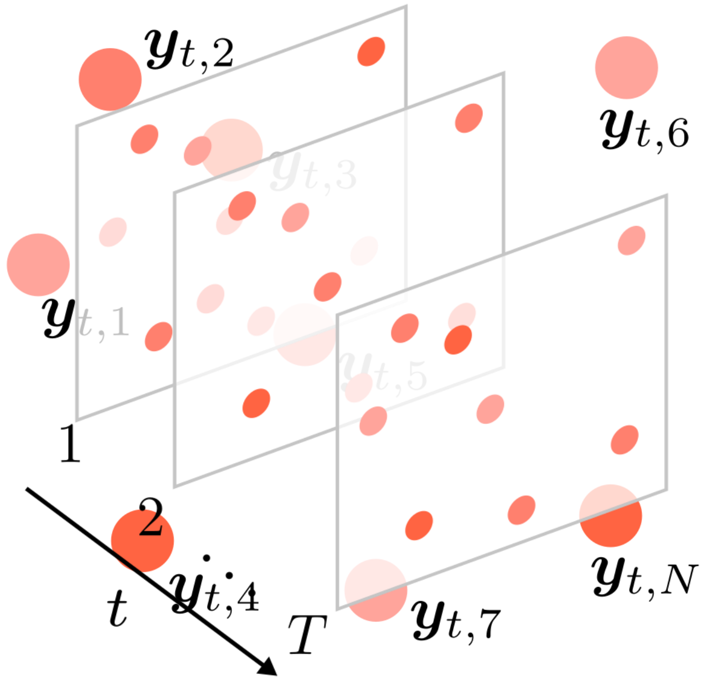
Spatio-temporal systems

Spatio-temporal data

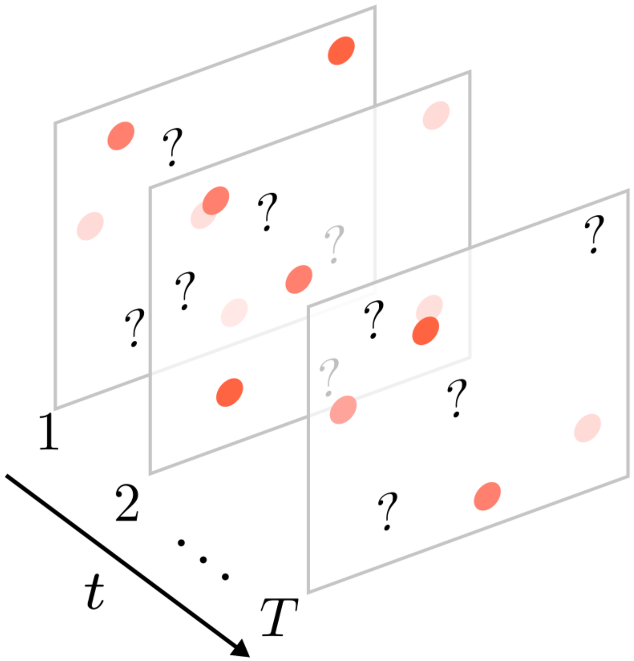


Regular grid

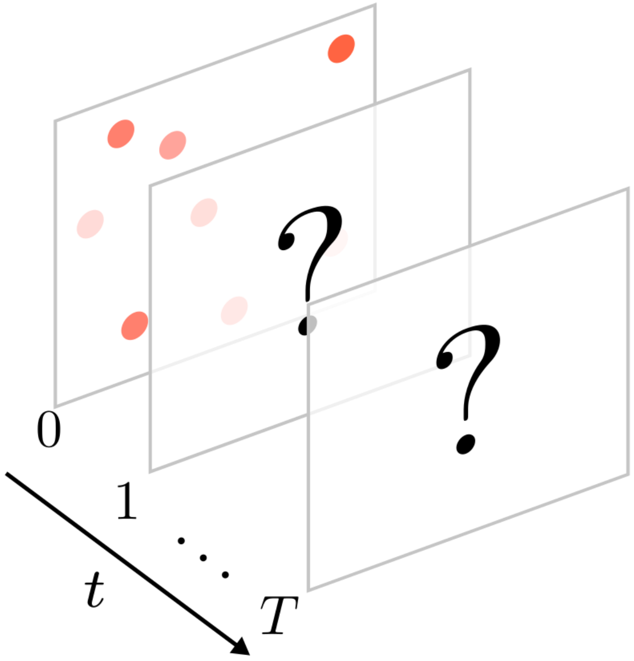


Irregular grid

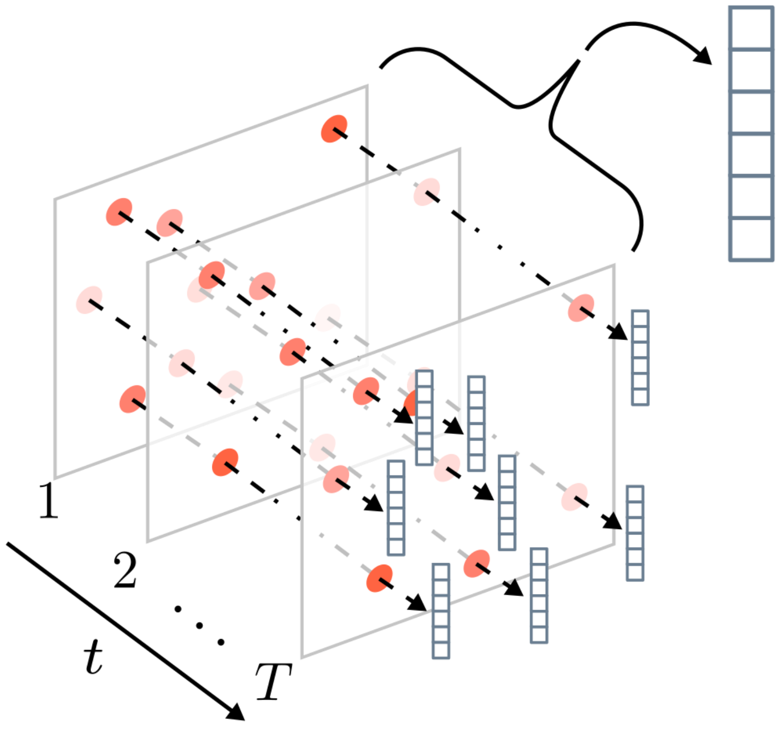
Machine learning problems



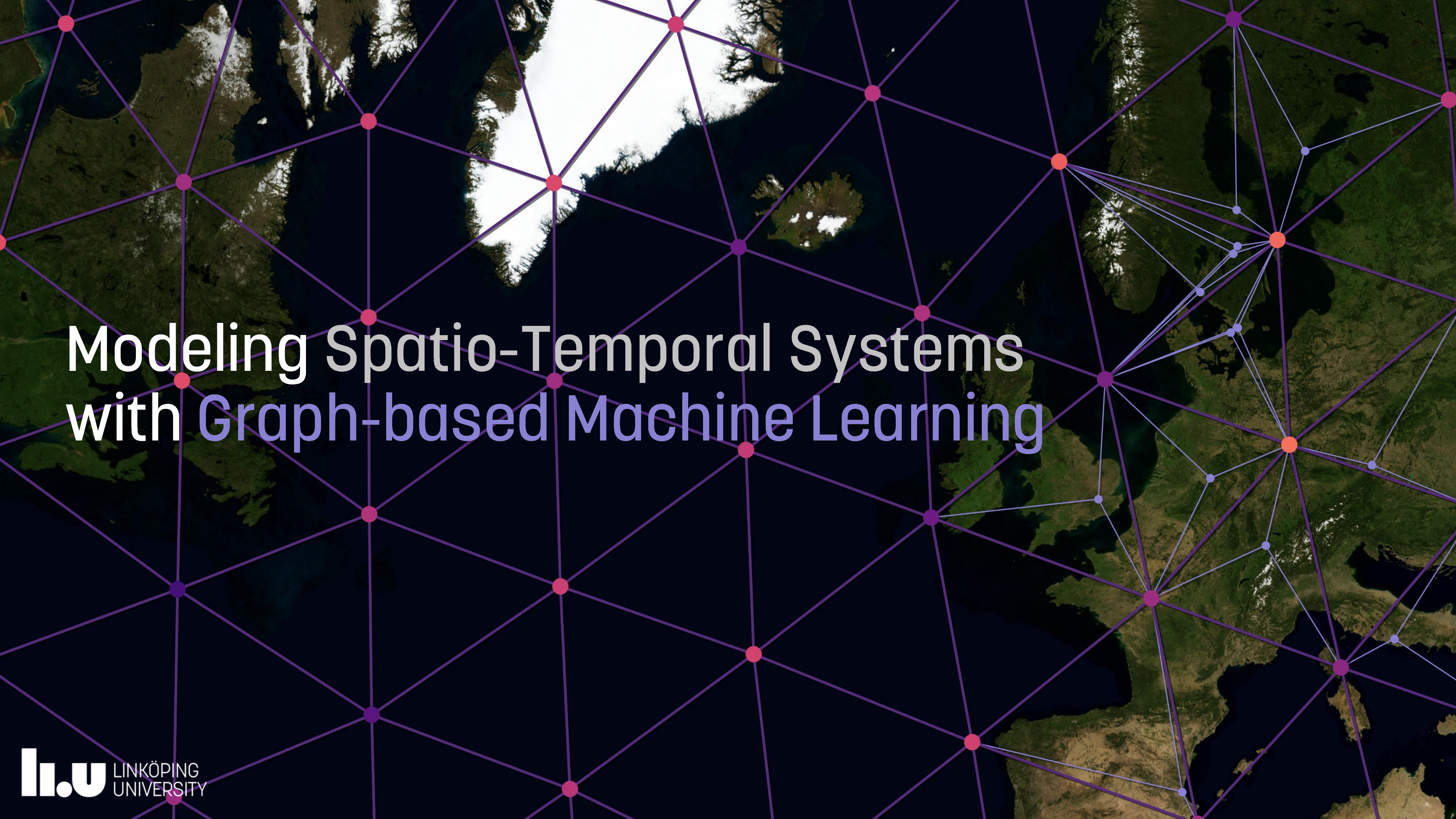
Prediction at new times and locations



Forecasting



Representation learning



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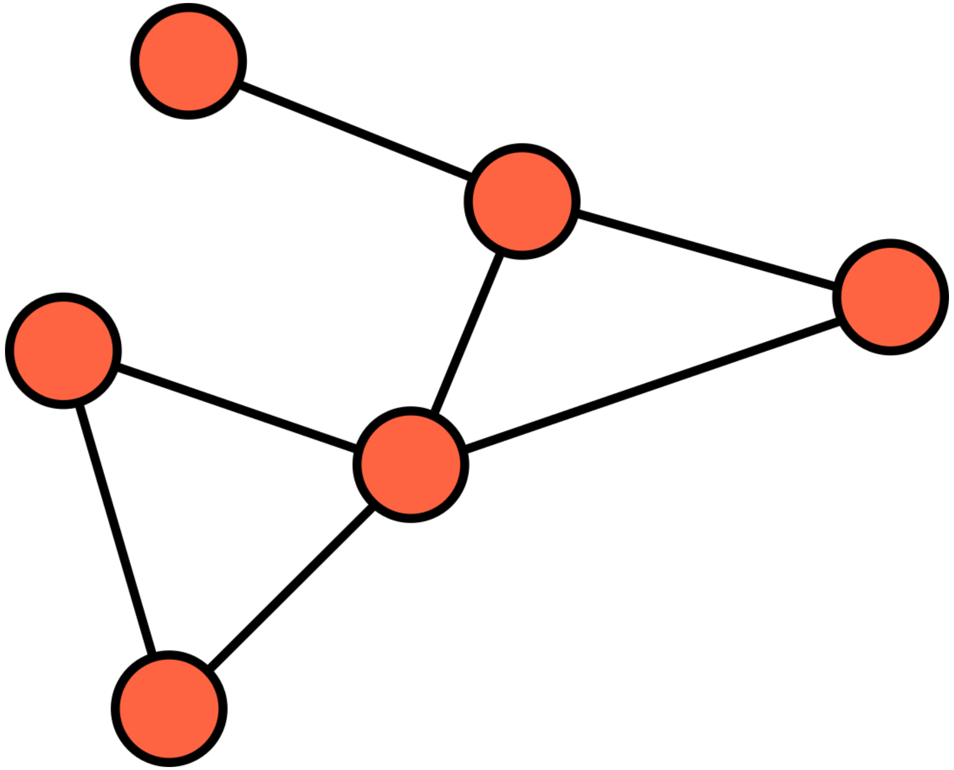
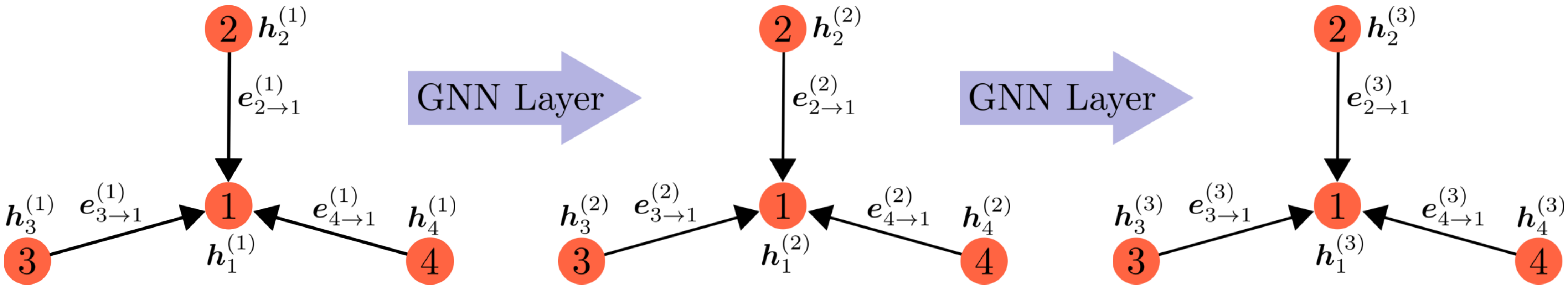
Graph-based machine learning

- Graph $\mathcal{G} = (V, E)$
  - Nodes V
  - Edges E
  - Encoding spatial relationships

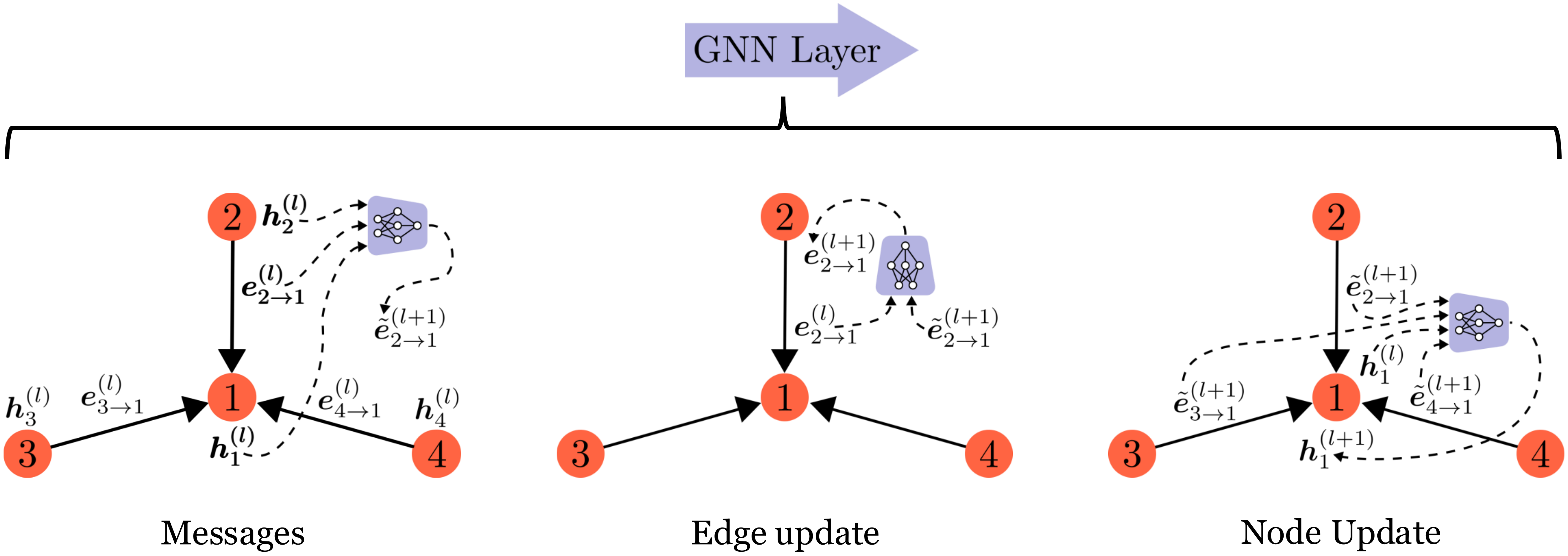
- Probabilistic graphical models
- Graph Neural Networks (GNNs)



Graph Neural Networks (GNNs)

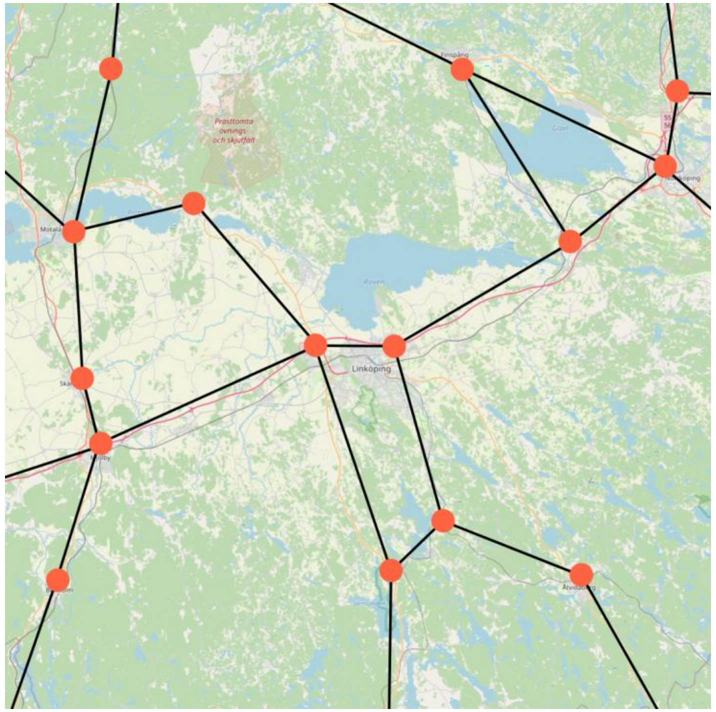


GNN Layer[1]

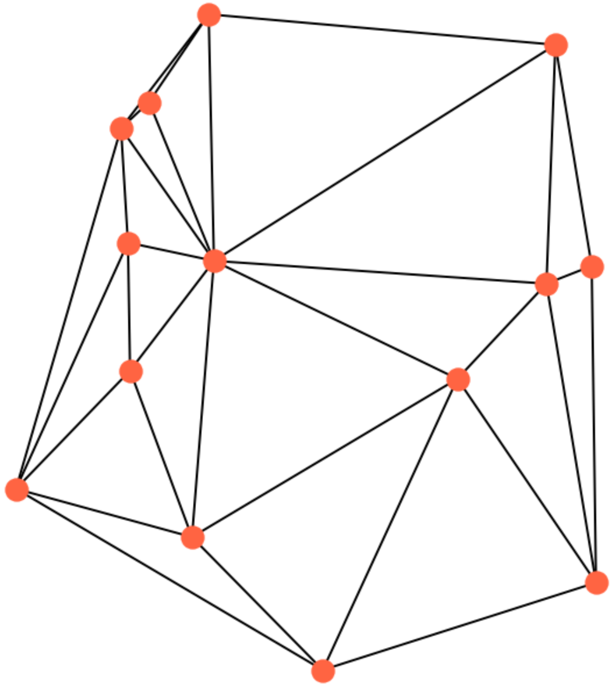


[1] J. Gilmer, et al. (2017). *Neural Message Passing for Quantum Chemistry*. ICML.,
P. Battaglia, et al. (2018). *Relational inductive biases, deep learning, and graph networks.* Preprint.

Spatial graphs



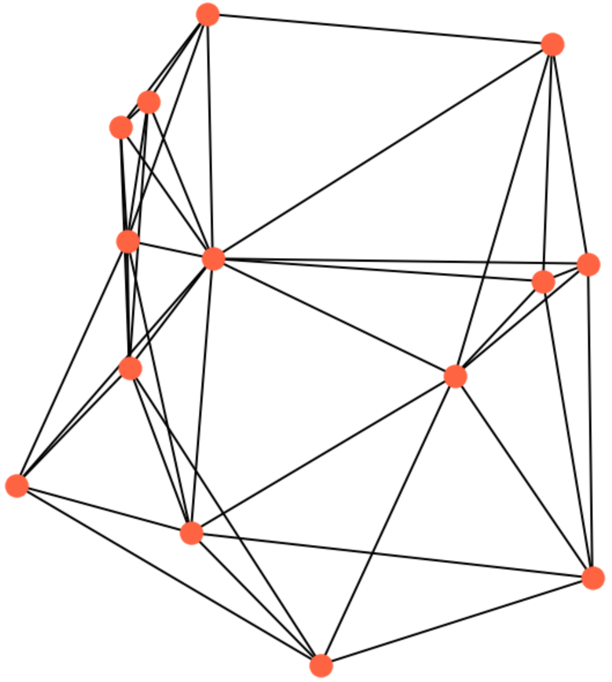
Existing spatial networks[1]



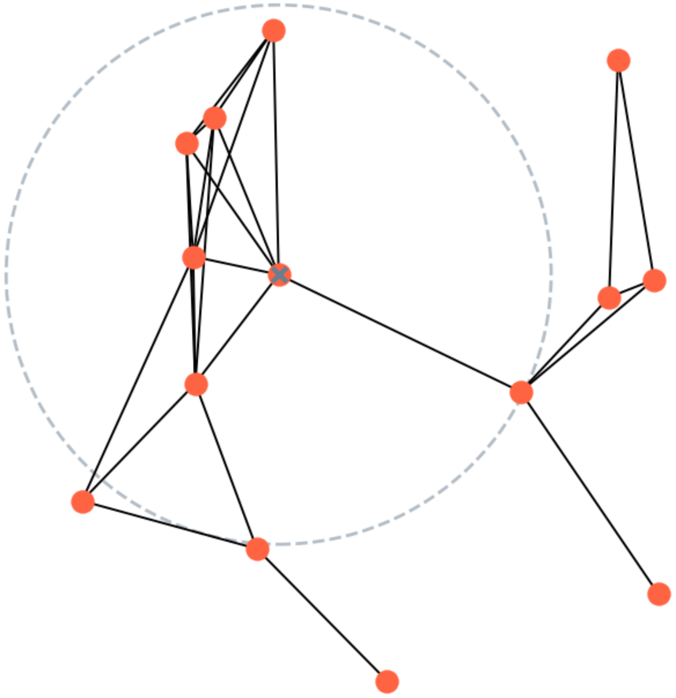
Sets of spatial points

[1] © OpenStreetMap Contributors

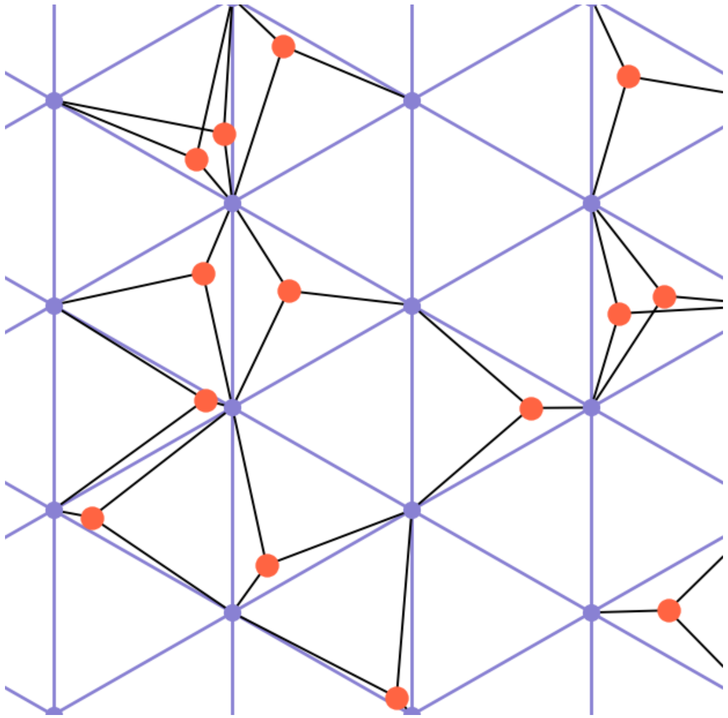
Spatial graph connectivity



k-nearest neighbors graph

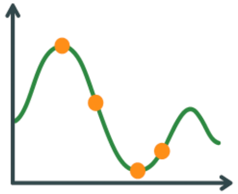


Radius graph



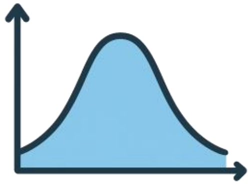
Connect to mesh graph

Papers



Paper 1
AISTATS 2023

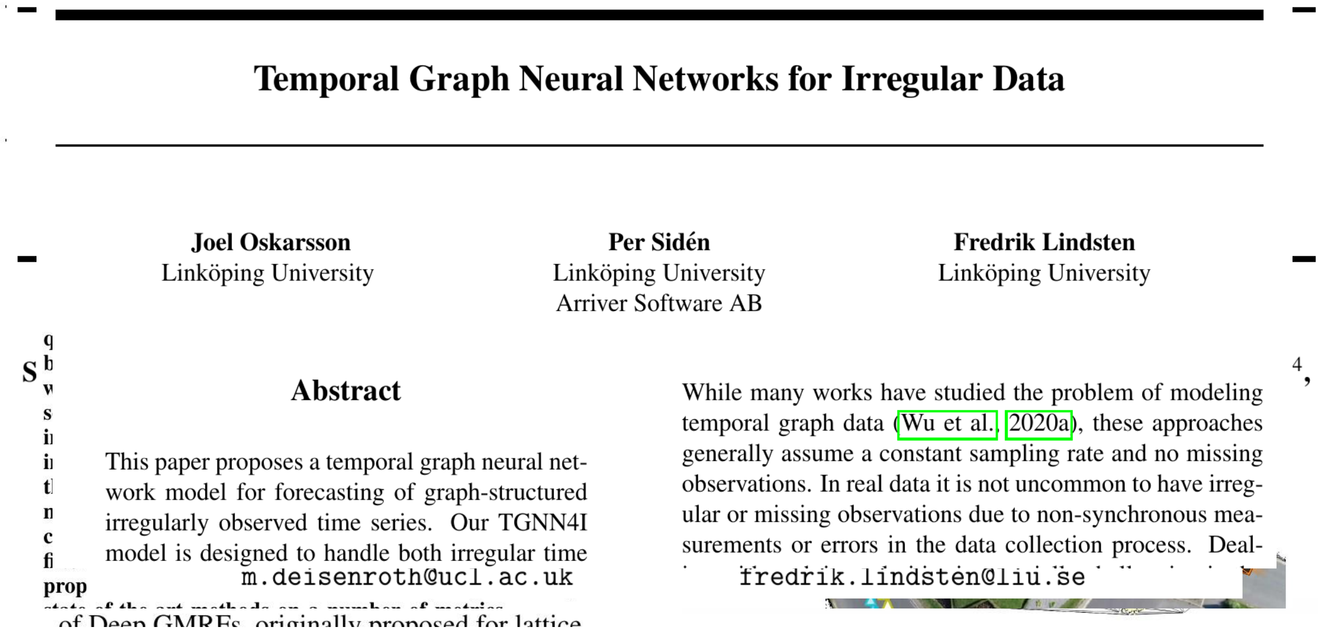
Paper 2
IEEE IV 2023



Paper 3
ICML 2022

Paper 4
NeurIPS 2024

Paper 5
Preprint, under review



Temporal Graph Neural Networks for Irregular Data

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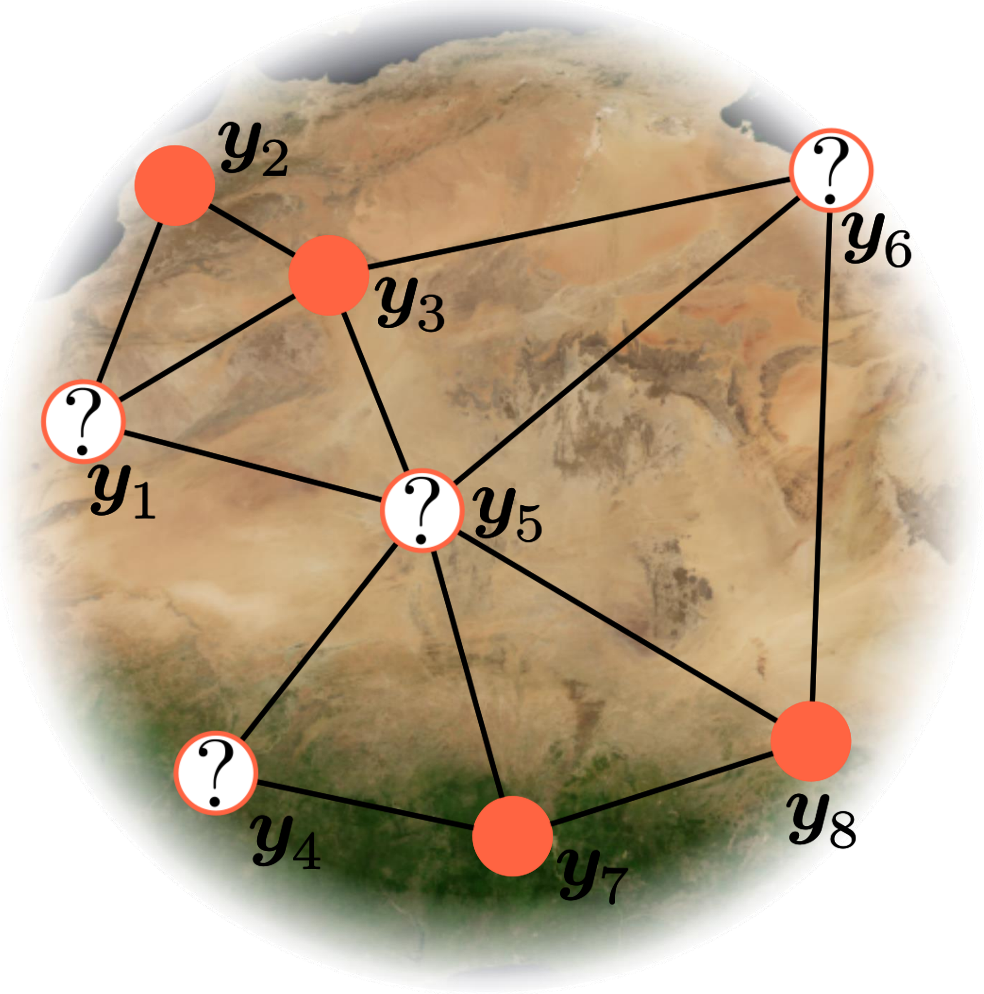
Abstract

This paper proposes a temporal graph neural network model for forecasting of graph-structured irregularly observed time series. Our TGNN4I model is designed to handle both irregular time

While many works have studied the problem of modeling temporal graph data (Wu et al., 2020a), these approaches generally assume a constant sampling rate and no missing observations. In real data it is not uncommon to have irregular or missing observations due to non-synchronous measurements or errors in the data collection process. Deal-

* Equal contribution

Prediction at unobserved locations



- Example applications:
  - Climate monitoring
  - Social networks

- Gaussian models 

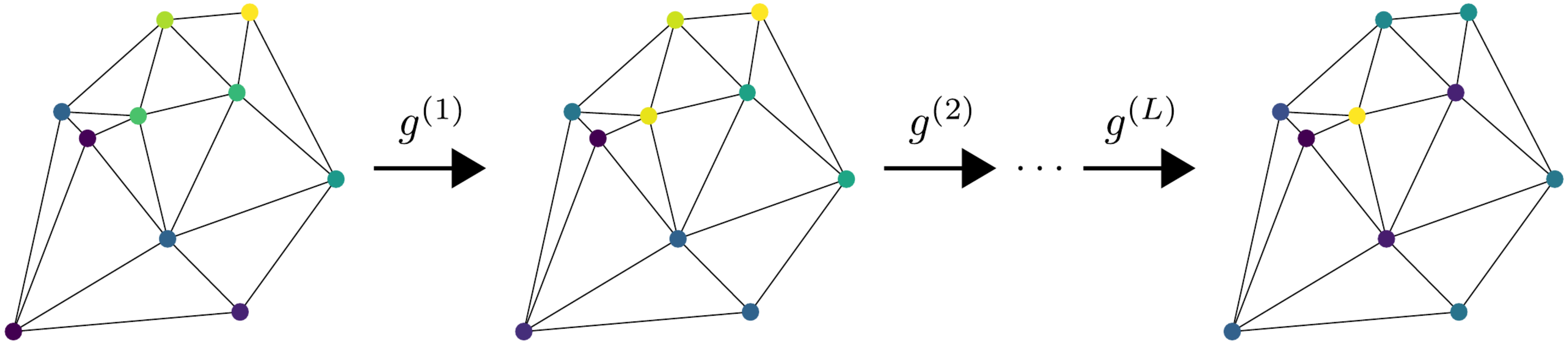
$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} = (z + \epsilon) \sim \mathcal{N}\left(\mu, Q^{-1} + \sigma^2 I\right)$$

$$\epsilon \sim \mathcal{N}\left(\mathbf{0}, \sigma^2 I\right)$$

Deep Gaussian Markov random fields

$$\boldsymbol{z} \sim \mathcal{N}\left(\boldsymbol{\mu}, Q^{-1}\right) \qquad\qquad g(\boldsymbol{z}) \sim \mathcal{N}(\mathbf{0}, I)$$

$$g = g^{(L)} \circ g^{(L-1)} \circ \cdots \circ g^{(1)}$$

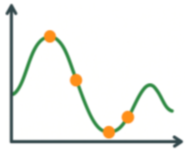


$\boldsymbol{z} \sim \mathcal{N}\left(\boldsymbol{\mu}, Q^{-1}\right)$ $\qquad$ $\mathcal{N}(\mathbf{0}, I)$

- Previous work[1]: Regular grids $\Longrightarrow$  Paper 3: General graphs

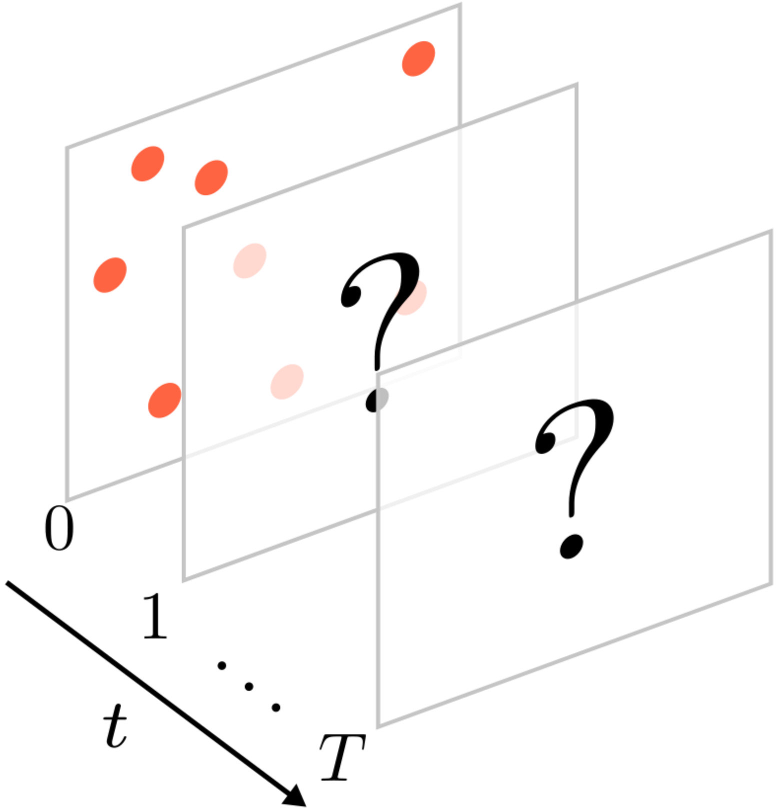
[1] P. Sidén & F. Lindsten (2020). *Deep Gaussian Markov random fields*. ICML.

Spatio-temporal forecasting

- Deterministic forecasting  

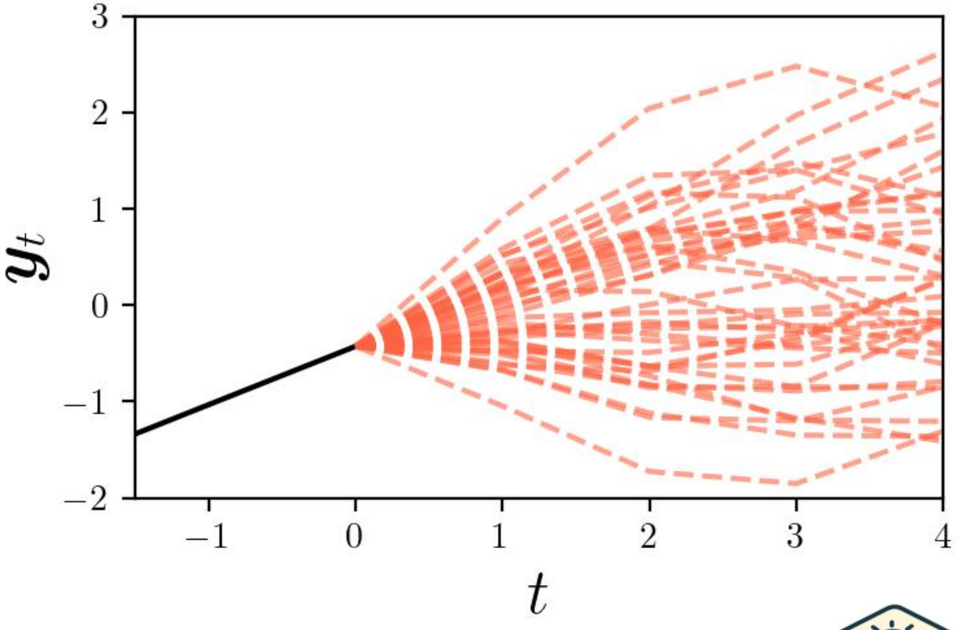
$$\left(\hat{Y}_t\right)_{t=1}^{T} = f(Y_0)$$

$$Y_t = \begin{bmatrix} — & \boldsymbol{y}_{t,1}^{\top} & — \\ — & \boldsymbol{y}_{t,2}^{\top} & — \\ & \vdots & \\ — & \boldsymbol{y}_{t,N}^{\top} & — \end{bmatrix}$$

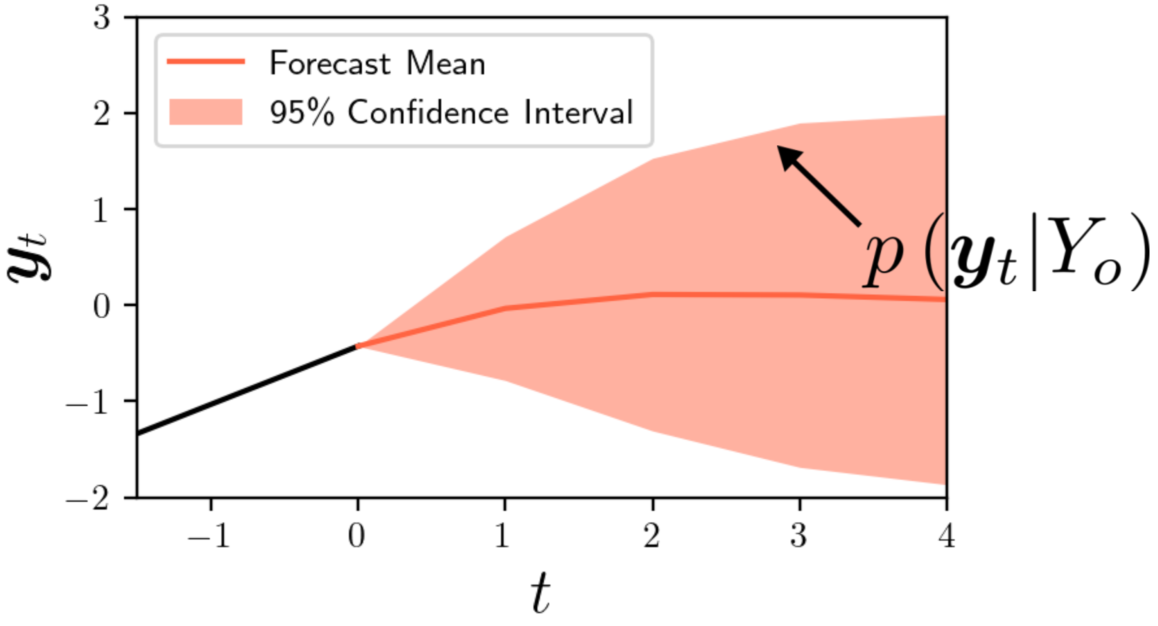


Probabilistic forecasting

$$p\Big((Y_t)_{t=1}^{T}\Big|Y_0\Big)$$

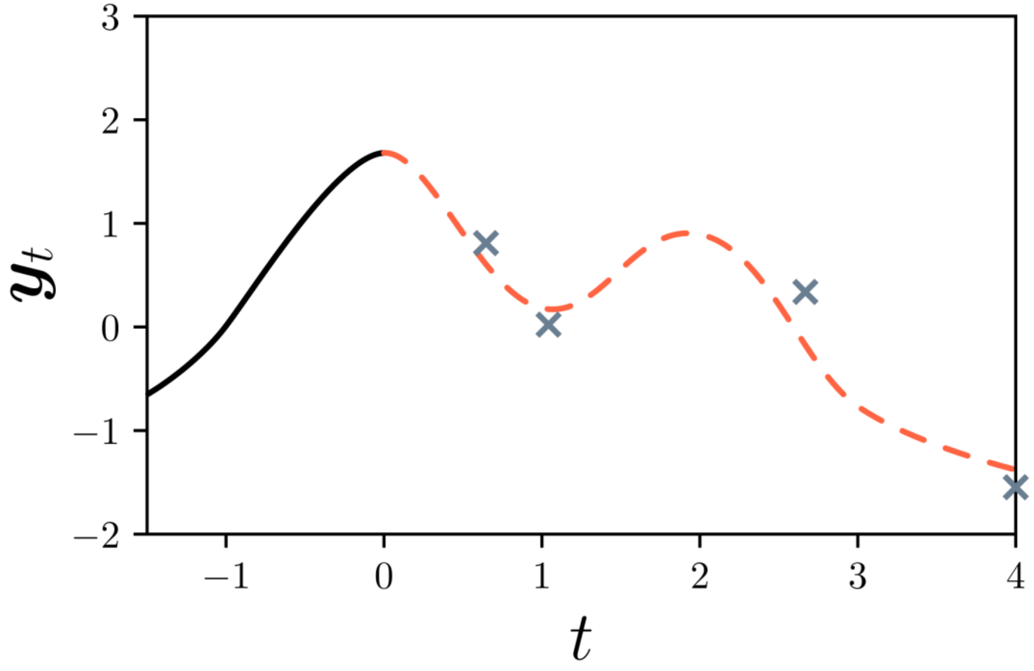


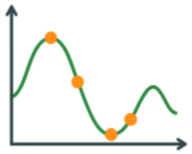
Sample-based
(Ensemble forecasting)



Explicit distribution

Continuous time



- Irregular observations 
  - Paper 1: In spatio-temporal forecasting with GNNs

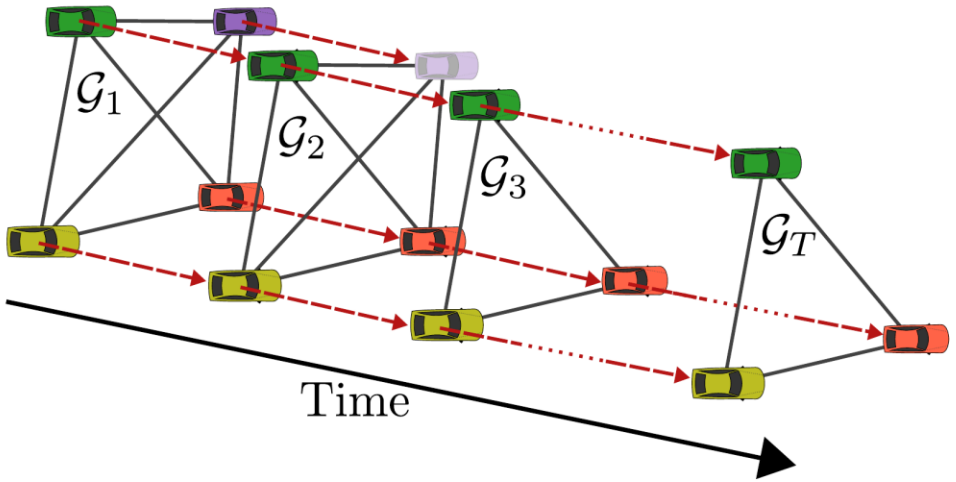
- Constraining dynamics 
  - Neural Ordinary Differential Equations[1]

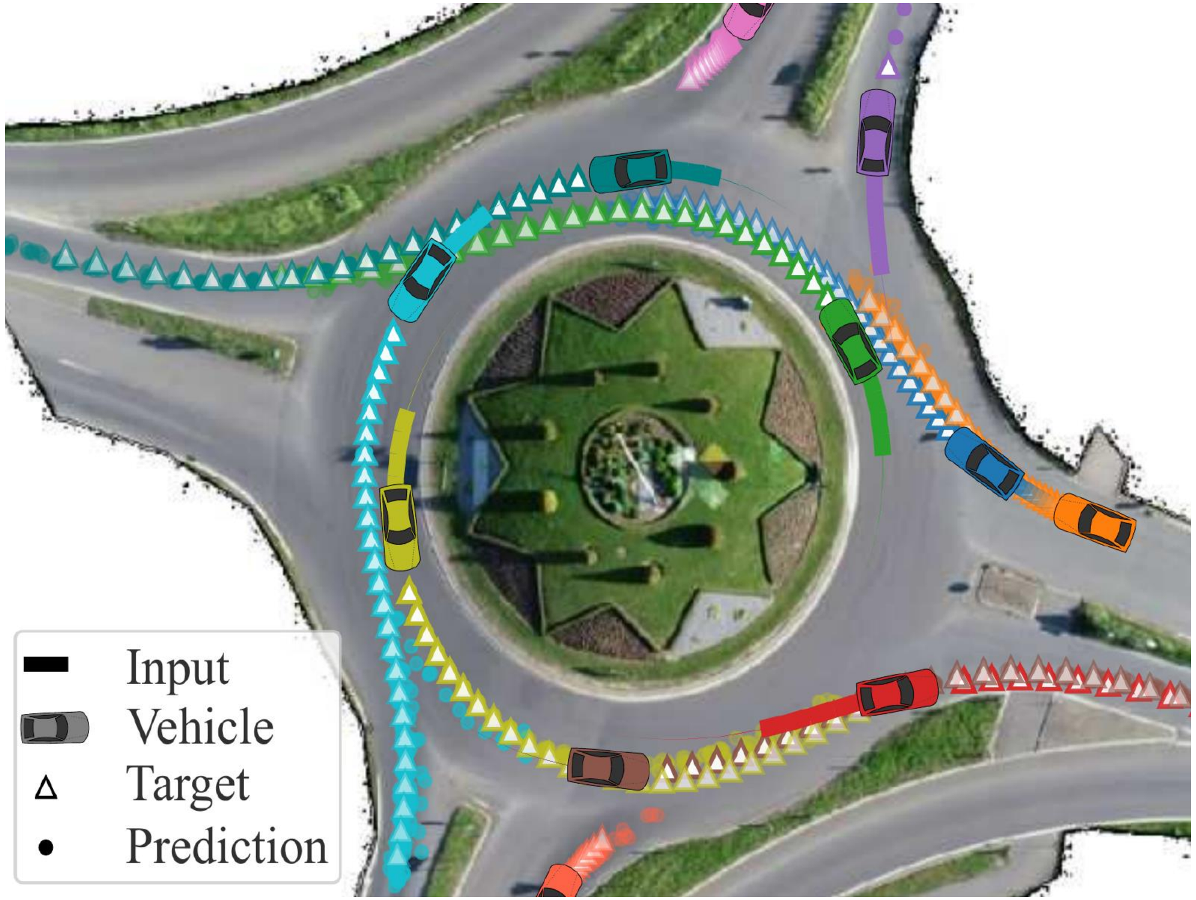
$$\frac{d}{d\tau}\boldsymbol{y}(\tau) = f_\theta(\boldsymbol{y}(\tau), \dots)$$

[1] R.T. Chen, et al. (2018). *Neural ordinary differential equations*. NeurIPS.

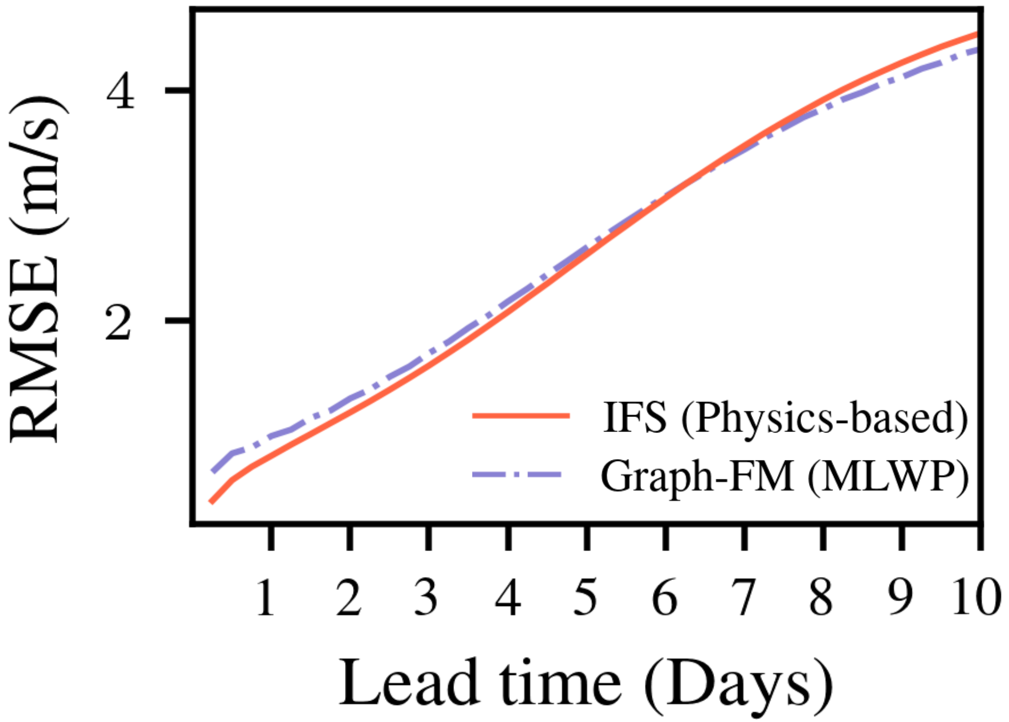
Trajectory forecasting 🚗

- Forecasted values are locations
- Multi-agent





Machine Learning Weather Prediction (MLWP)



RMSE of 10 m zonal wind

Graph-based MLWP[1]

$$\hat{Y}_t = f_\theta(Y_{t-1})$$

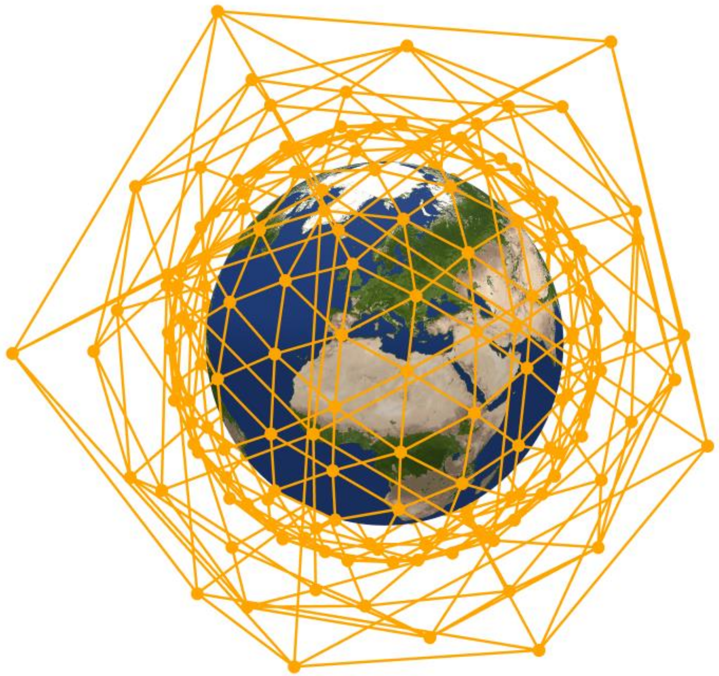
Encode

Mesh graph
Process

Decode

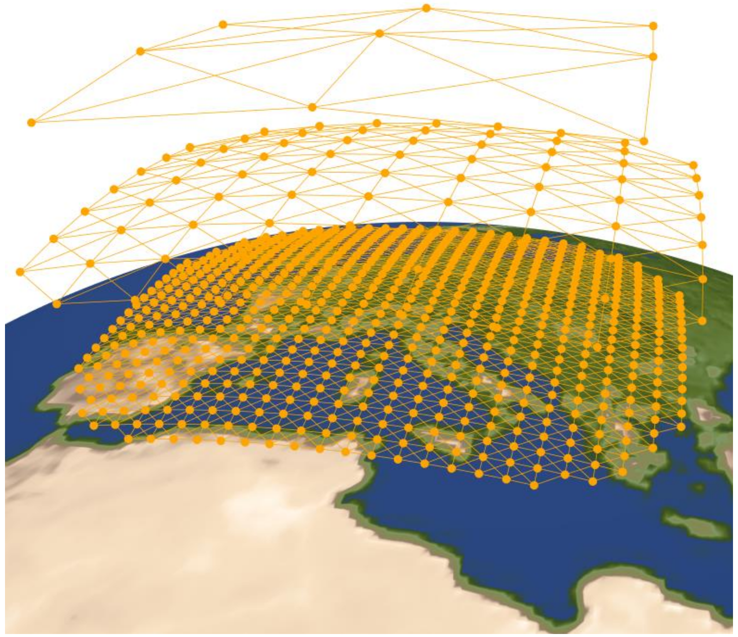
[1] R. Keisler (2022). *Forecasting global weather with graph neural networks*. Preprint.,
R. Lam, et al. (2023). *Learning skillful medium-range global weather forecasting*. Science.,

Global and regional forecasting



Global model 

Hierarchical mesh graph



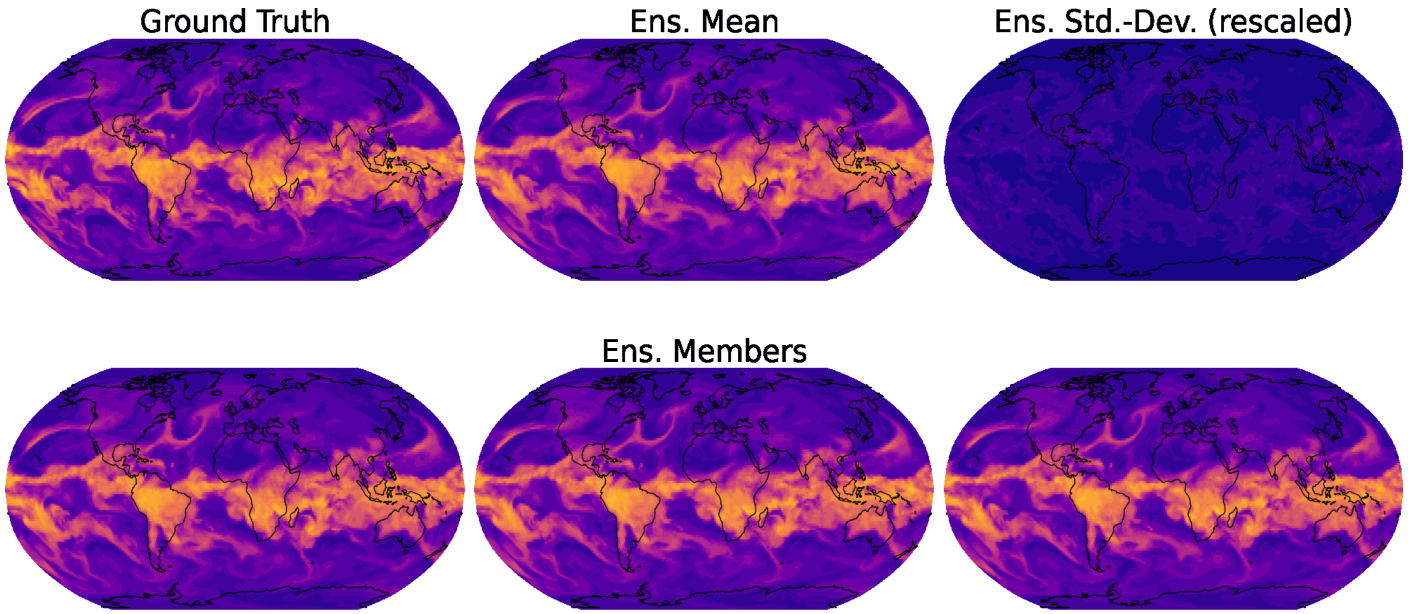
Limited area model  

Hierarchical mesh graph

MLWP ensemble forecasting

$$p\Big((Y_t)_{t=1}^{T}\Big|Y_0\Big) = \prod_{t=1}^{T} p(Y_t|Y_{t-1})$$

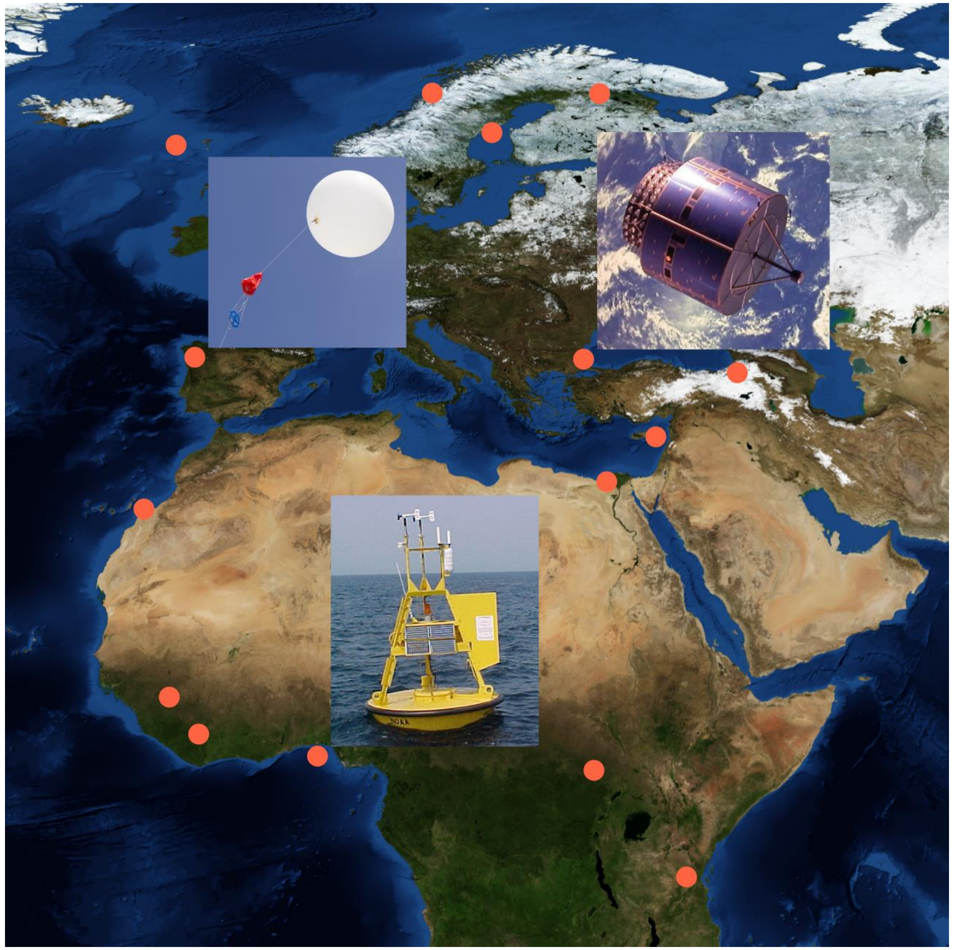
- Latent variable models[1]
- Diffusion models[2]



Specific humidity

[1] Y. Hu, et al. (2023). *SwinVRNN: A data-driven ensemble forecasting model via learned distribution perturbation*. JAMES
[2] I. Price, et al. (2025). *Probabilistic weather forecasting with machine learning*. Nature.,
M. Andrae, et al. (2025). *Continuous Ensemble Weather Forecasting with Diffusion Models*. ICLR.,
E. Larsson, et al. (2025). *Diffusion-LAM: Probabilistic Limited Area Weather Forecasting with Diffusion*. CCAI Workshop @ ICLR.

Outlook



- Irregular observations
- Probabilistic forecasting
- MLWP directly using observations

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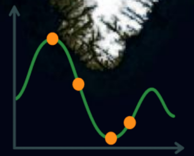


Paper 1: **J. Oskarsson**, P. Sidén, and F. Lindsten. *Temporal graph neural networks for irregular data.* AISTATS, 2023

Paper 2: T. Westny, **J. Oskarsson**, B. Olofsson, and E. Frisk. *MTP-GO: Graph-based probabilistic multi-agent trajectory prediction with neural ODEs.* IEEE IV, 2023

Paper 3: **J. Oskarsson**, P. Sidén, and F. Lindsten. *Scalable deep Gaussian Markov random fields for general graphs.* ICML, 2022

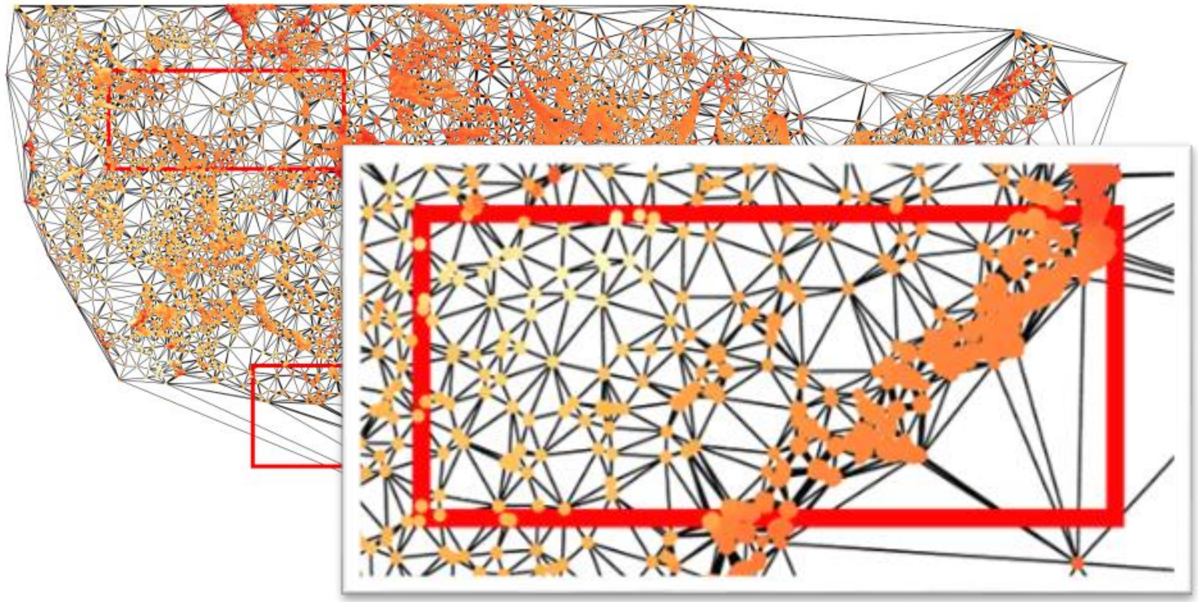
Paper 4: **J. Oskarsson**, T. Landelius, M. P. Deisenroth, and F. Lindsten. *Probabilistic weather forecasting with hierarchical graph neural networks.* NeurIPS, 2024

Paper 5: S. Adamov*, **J. Oskarsson***, et al. *Building machine learning limited area models: Kilometer-scale weather forecasting in realistic settings.* Preprint, under review, 2025

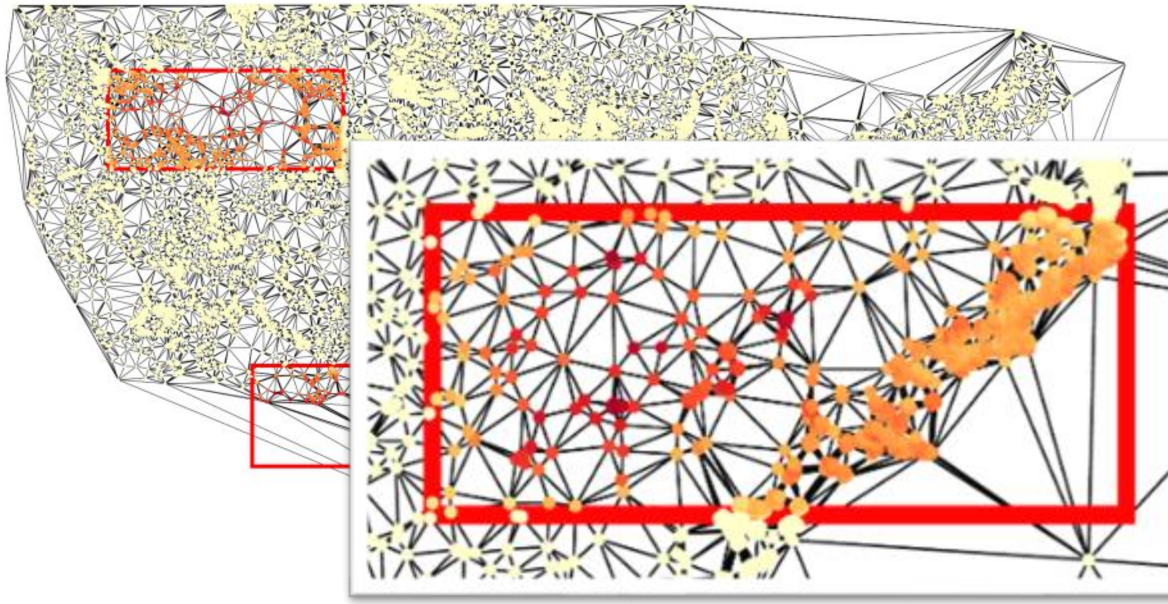
* Equal contribution

Example: Wind speeds

- Nodes in red boxes unobserved



Mean



Standard deviation