

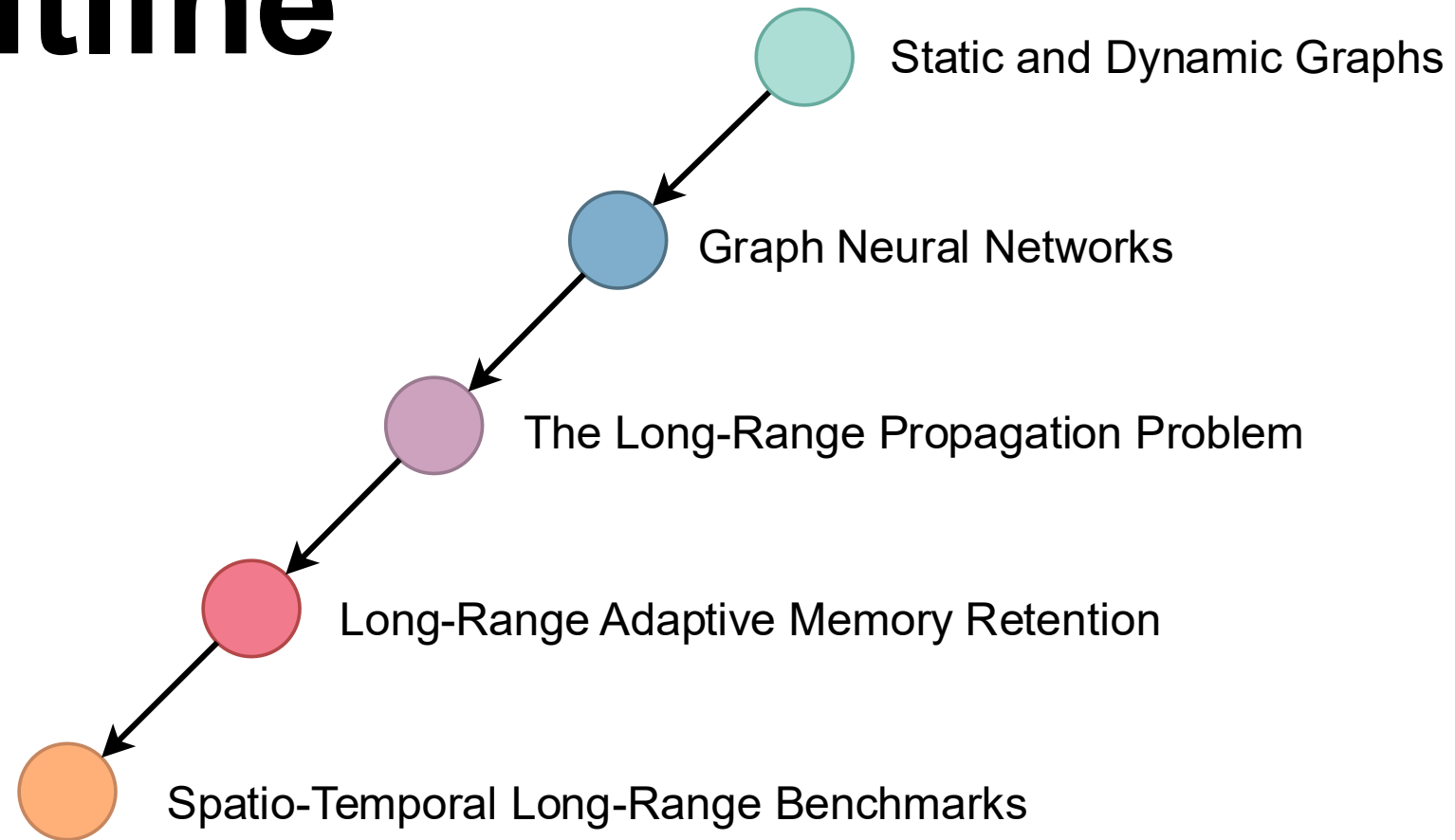


UNIVERSITÀ DI PISA

Dynamic Graphs: The Long-Range Challenge

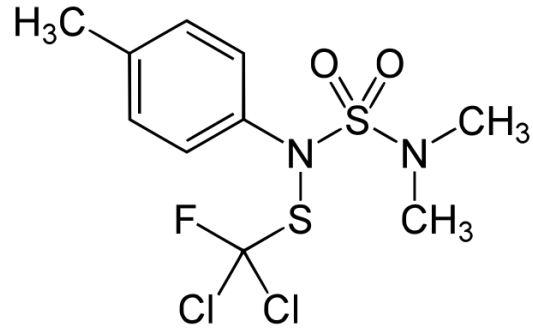
Mauriana Pesaresi Seminar Series

Outline



Static and Dynamic Graphs

Graphs are everywhere!



Molecules



Social Networks

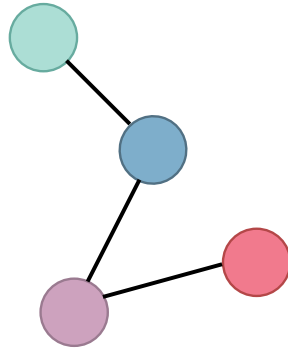


Transportation Networks

And many others...

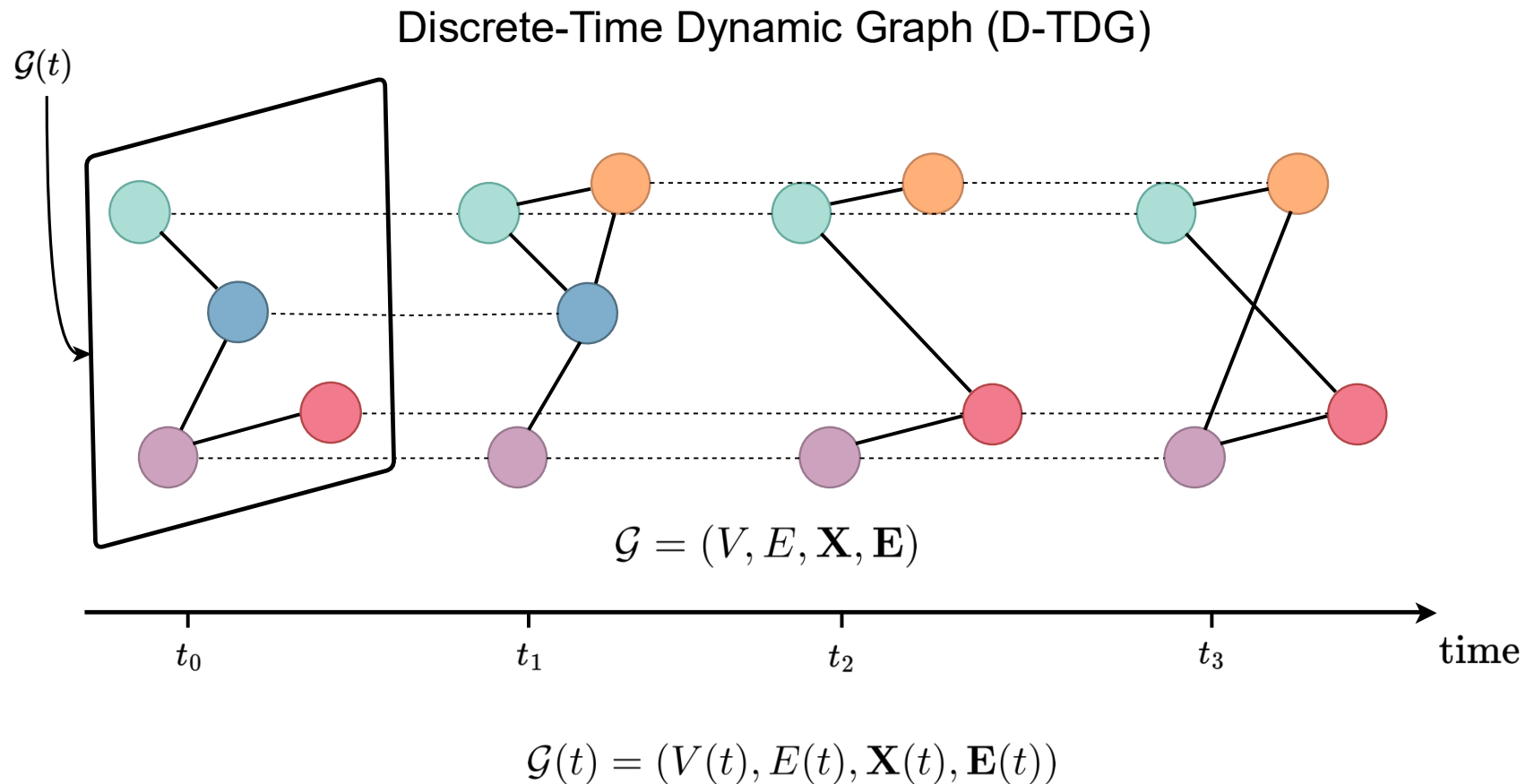
From Static to Dynamic Graphs

Static Graph



$$\mathcal{G} = (V, E, \mathbf{X}, \mathbf{E})$$

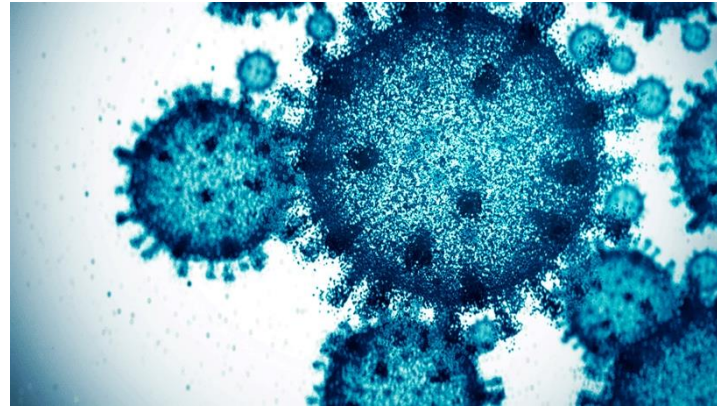
From Static to Dynamic Graphs



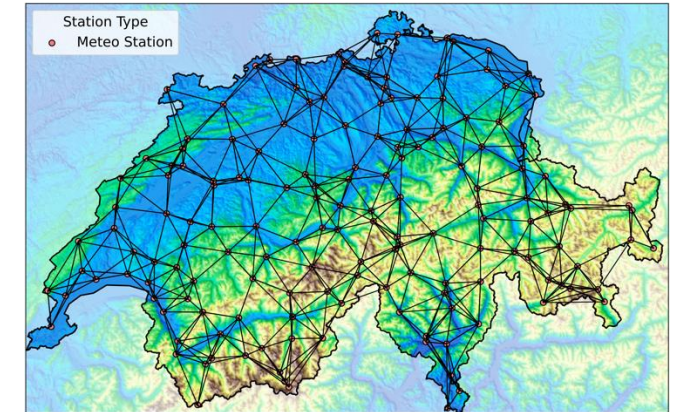
The World is Dynamic



Transportation Networks
“Will a road be congested?”



Infections
“Who will get infected?”



Climate Forecasting
“Will it be windy?”

Research Questions

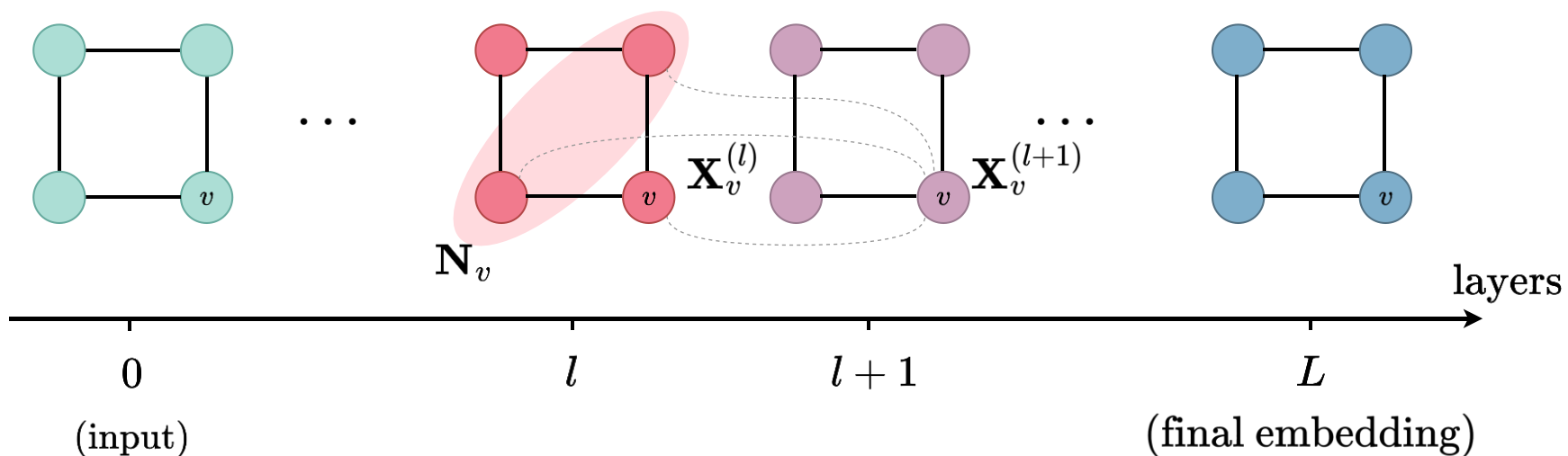
- How do we handle time to learn good graph representations?
- Can we predict when and how the graph will change in the future?

Graph Neural Networks

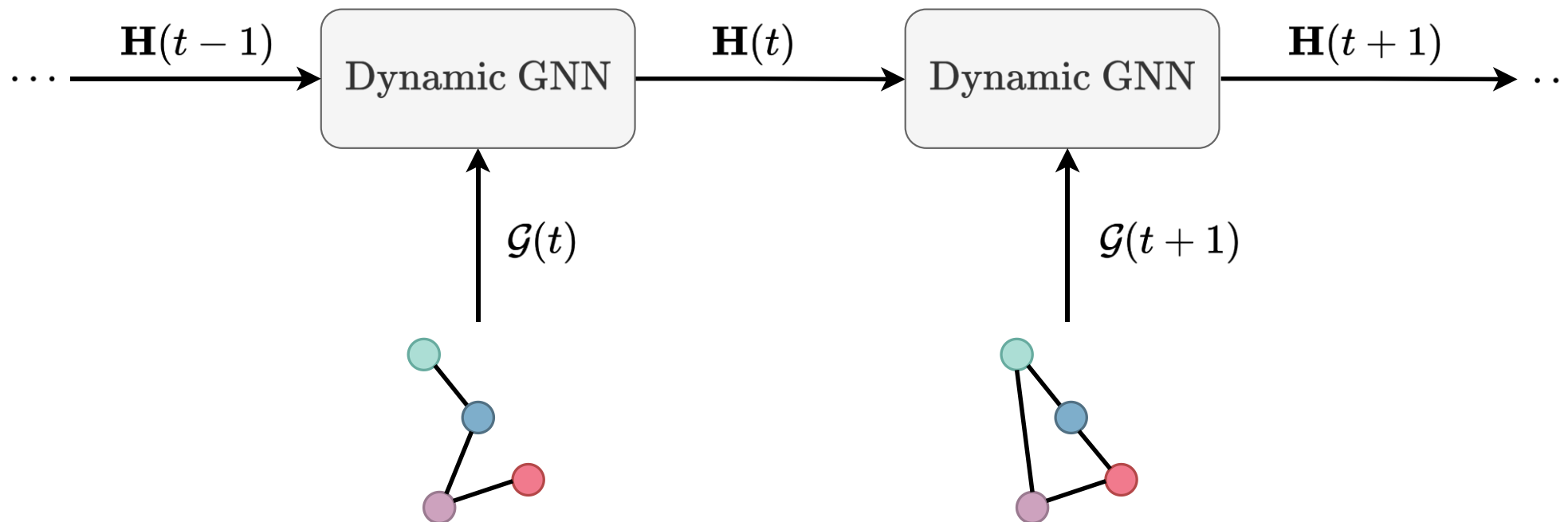
Graph Neural Networks (GNNs)

Neural Message Passing Framework

Update the representation of a node aggregating neighbors' messages



Dynamic Graph Neural Networks



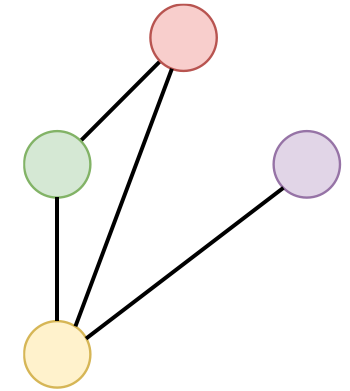
Possible implementations

- **Time and space (T&S)**
- **Time then space (TTS)**

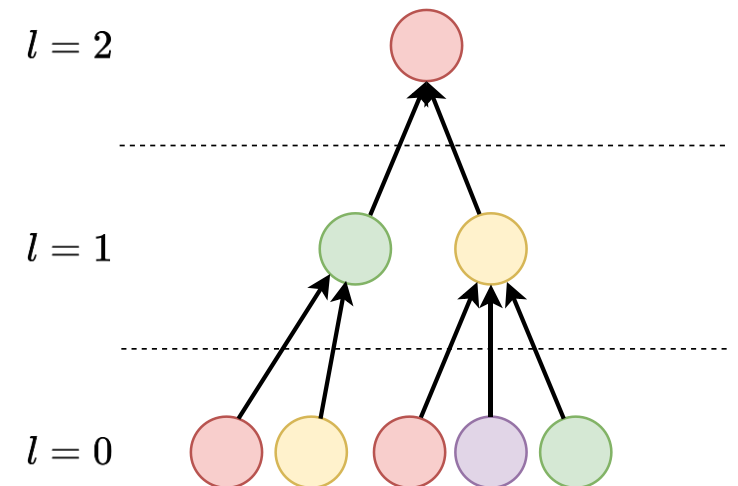
Long-Range Propagation

Long-Range Propagation

- **Problem:** learning on graphs typically needs to consider a specific range of node interactions
 - Multiple rounds of message passing widens the receptive field
 - But... The number of involved node representations **grows exponentially** with rounds (layers)
- For temporal graphs, this issue repeats in the sequence



Computational Graph



Towards Adaptive Memory Retention

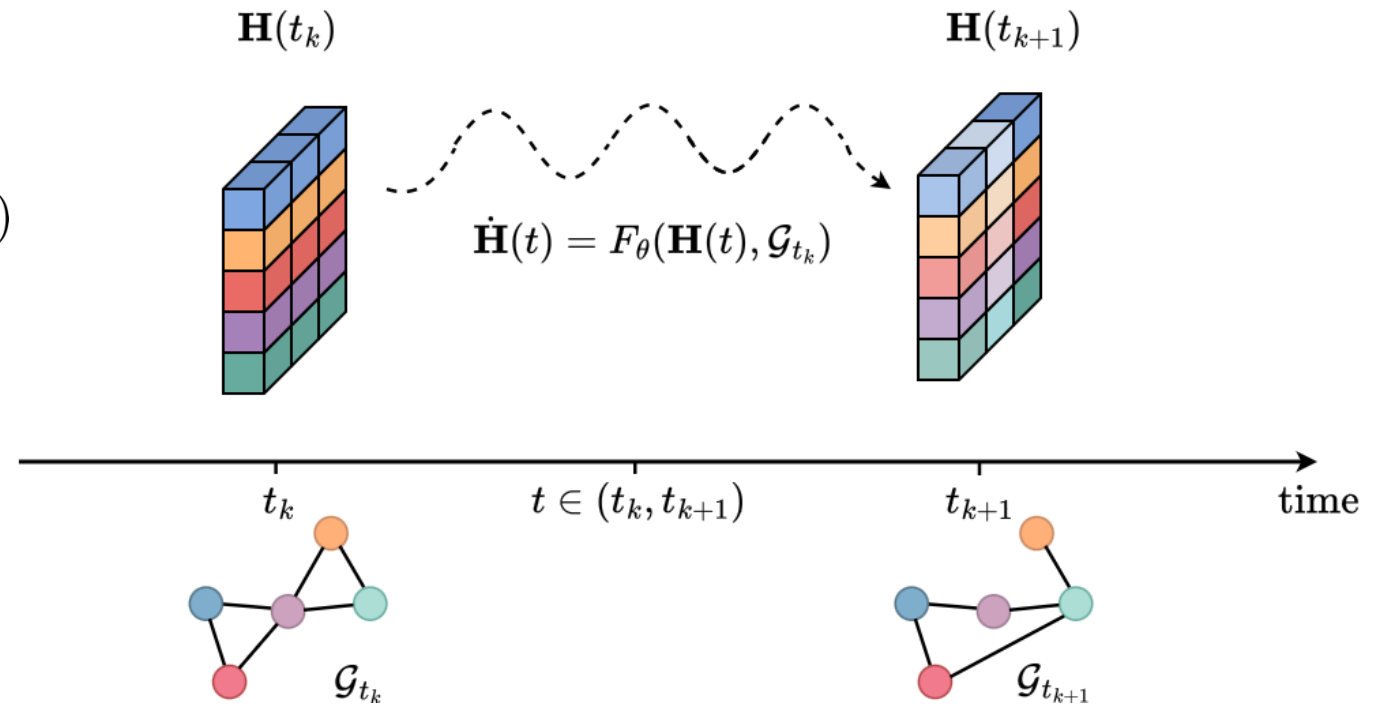
- **Problem**
 - Dissipative models forget knowledge
 - Non-dissipative models keep building up information without discarding irrelevant signals
- Long-range modeling requires **filtering irrelevant data**, especially on sequences
- **Solution**
 - Take a non-dissipative architecture
 - Given the input sequence, **learn the optimal degree of dissipation**

Long-Range Adaptive Memory Retention

The Dynamical System Perspective

GNNs \equiv discretization of a continuous process

$$\begin{cases} \dot{\mathbf{H}}(t) = F_{\theta}(\mathbf{H}(t); \mathcal{G}_{t_k}) & t \in (t_k, t_{k+1}) \\ \mathbf{H}(t^+) = G_{\phi}(\mathbf{H}(t^-), \mathbf{X}(t)) & t \in \mathcal{T} \\ \mathbf{H}(0) = \mathbf{H}_0 & t = t_0 \end{cases}$$



Long-range Adaptive Memory Retention

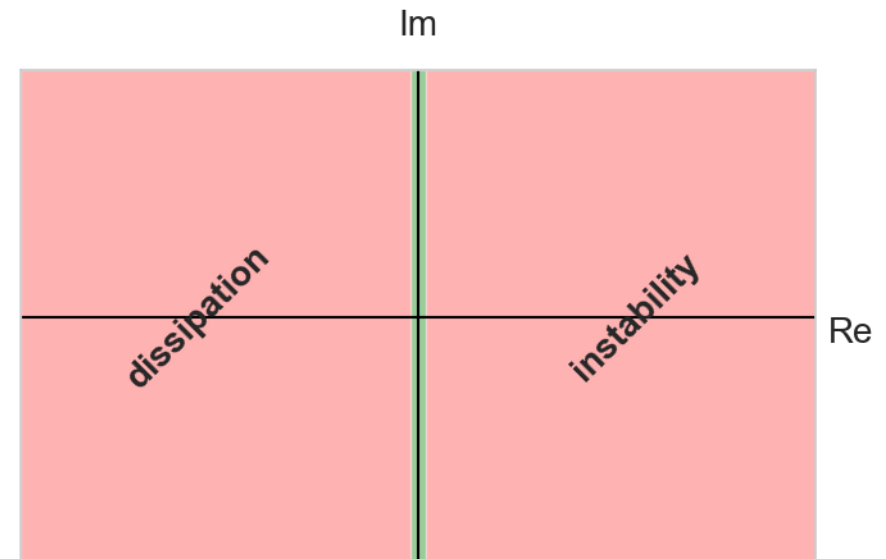
Notation

- For any **square** matrix M
 - Subtracting its transpose yields an **antisymmetric** matrix $M_{\text{sk}} = M - M^T$
 - Summing its transpose yields a symmetric matrix $M_{\text{sym}} = M + M^T$
- **Idea**
 - Parametrize the model's space diffusion with **antisymmetric** weight matrices
 - **Relax** the antisymmetry via a learned diagonal damping term
 - Integrate external inputs in the system with a **controlled** linear combination

The importance of the Parametrization

Relaxed antisymmetry ensures **stability** and **controlled dissipation**

- $Re(\lambda_i(\mathbf{J}(t))) > 0$ \longrightarrow unstable system
- $Re(\lambda_i(\mathbf{J}(t))) \ll 0$ \longrightarrow long-range dependencies are forgotten
- $Re(\lambda_i(\mathbf{J}(t))) \approx 0$ \longrightarrow **non-dissipative** system
 - No gradient vanishing/explosion during training



Long-range Adaptive Memory Propagation

- **Space:** information diffusion via message passing and adaptive dissipativity

$$F_{\theta} = \sigma \left(\mathbf{H}(t) \left(\mathbf{W}_{\text{sk}} - \mathbf{\Gamma} \right) + \mathcal{S}(\mathbf{A}(t_k), \mathbf{H}(t); \mathbf{V}_{\text{sk}}) + \mathcal{K}(\mathbf{A}(t_k), \mathbf{H}(t); \mathbf{Z}_{\text{sym}}) \right)$$

Adaptive memory retention

Example of a 3x3 matrix

$$\begin{pmatrix} 0 & w_{12} & w_{13} \\ -w_{12} & 0 & w_{23} \\ -w_{13} & -w_{23} & 0 \end{pmatrix} - \begin{pmatrix} s(\gamma_1) & 0 & 0 \\ 0 & s(\gamma_2) & 0 \\ 0 & 0 & s(\gamma_3) \end{pmatrix} = \begin{pmatrix} -s(\gamma_1) & w_{12} & w_{13} \\ -w_{12} & -s(\gamma_2) & w_{23} \\ -w_{13} & -w_{23} & -s(\gamma_3) \end{pmatrix}$$

θ : Model Parameters

Long-range Adaptive Memory Propagation

- **Space:** information diffusion via message passing and adaptive dissipativity

$$F_{\theta} = \sigma \left(\mathbf{H}(t) (\mathbf{W}_{\text{sk}} - \mathbf{\Gamma}) + \underbrace{\mathcal{S}(\mathbf{A}(t_k), \mathbf{H}(t); \mathbf{V}_{\text{sk}})}_{\text{Weight-antisymmetric neighborhood aggregation}} + \underbrace{\mathcal{K}(\mathbf{A}(t_k), \mathbf{H}(t); \mathbf{Z}_{\text{sym}})}_{\text{Space-antisymmetric neighborhood aggregation}} \right)$$

Weight-antisymmetric
neighborhood aggregation

Space-antisymmetric
neighborhood aggregation

- **Time:** external impulses (inputs) integration in the system

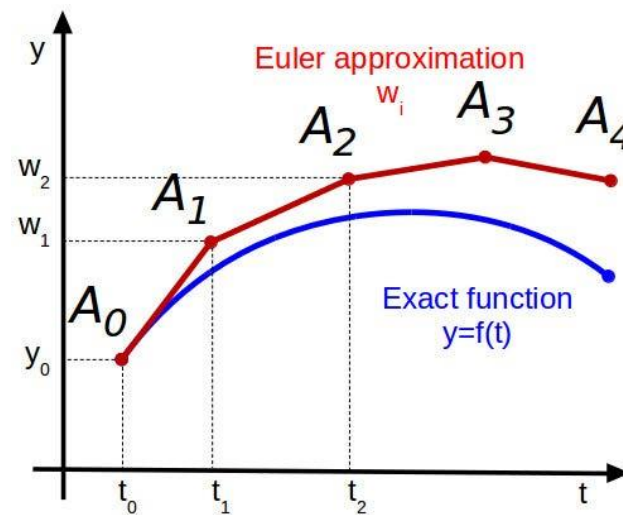
$$G_{\phi} = \frac{1}{\xi} \left(\mathbf{H}(t_k^-) + \mu \mathbf{X}(t_k) \mathbf{U} \right),$$

θ, ϕ : Model Parameters

Practical Implementation

- **Space:** Forward Euler discretization of the ODE for L steps, with step size ϵ

$$\mathbf{H}^{(l+1)}(t) = \mathbf{H}^{(l)}(t) + \epsilon F_{\theta}(\mathbf{H}^{(l)}(t); \mathcal{G}_t)$$



Practical Implementation

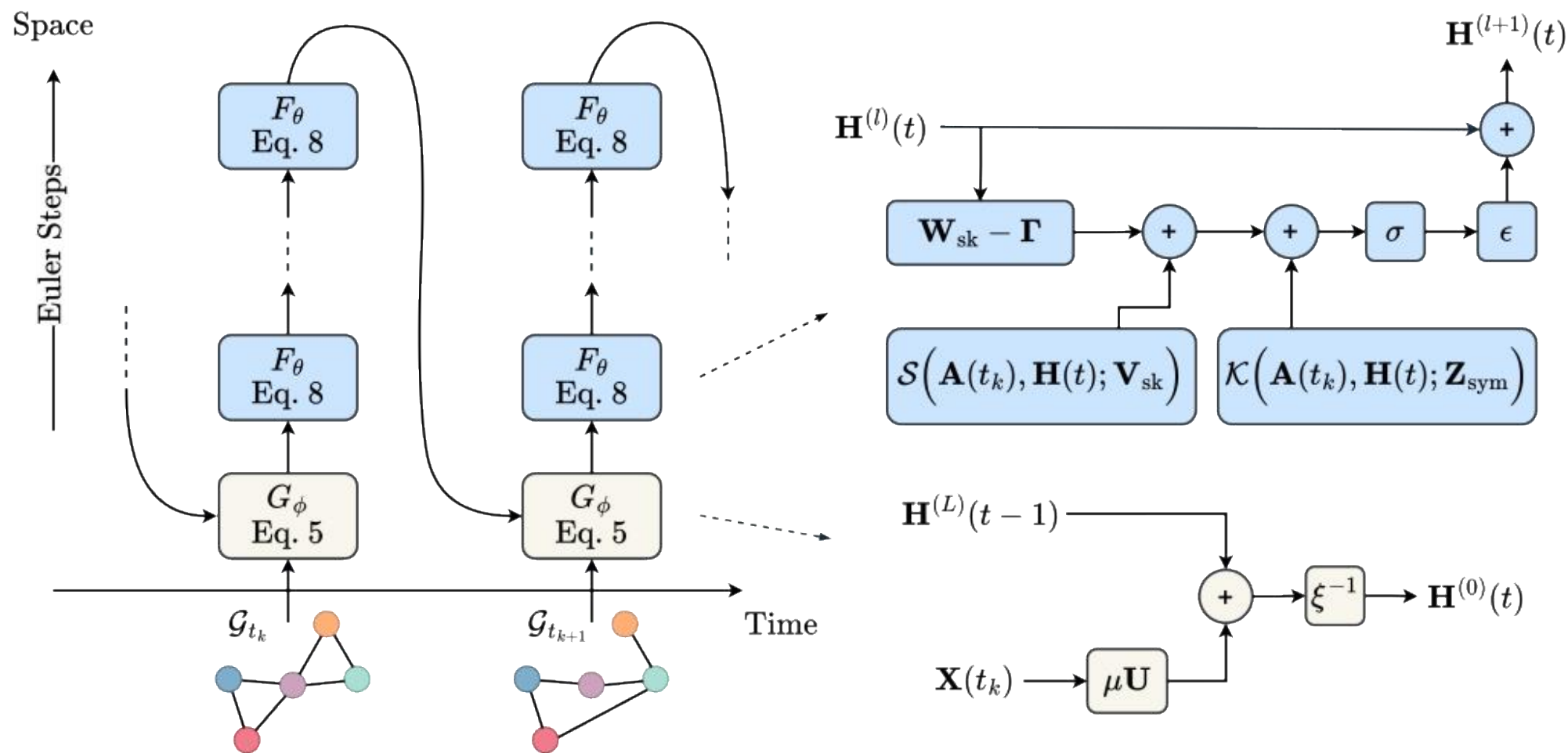
- **Space:** Forward Euler discretization of the ODE for L steps, with step size ϵ

$$\mathbf{H}^{(l+1)}(t) = \mathbf{H}^{(l)}(t) + \epsilon F_{\theta}(\mathbf{H}^{(l)}(t); \mathcal{G}_t)$$

- **Time:** Take last Forward Euler step and combine it with the input

$$\mathbf{H}^{(0)}(t+1) = \frac{1}{\xi} \left(\mathbf{H}^{(L)}(t) + \mu \mathbf{X}(t_k) \mathbf{U} \right),$$

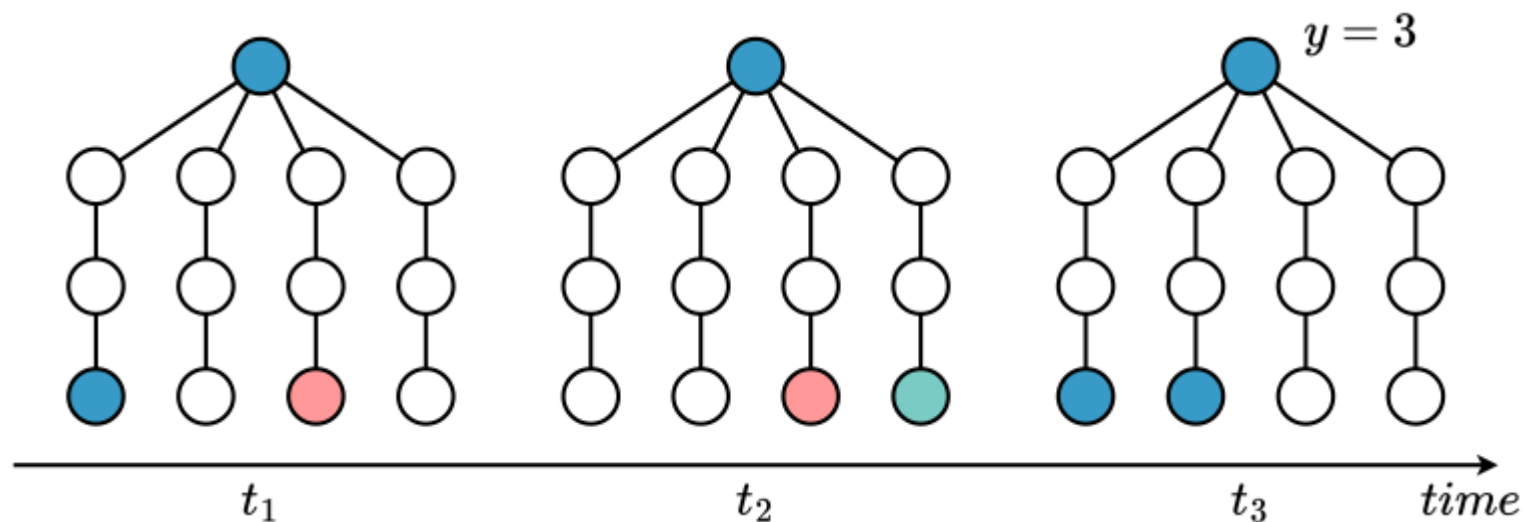
LAMP Architecture



Spatio-Temporal Long-Range Benchmark

Colored Leaf Counting

- **Input:** N sequences of length T , number of colors K , spider graph topology
- **Target:** Count how many times leaves emitted the same color of the root



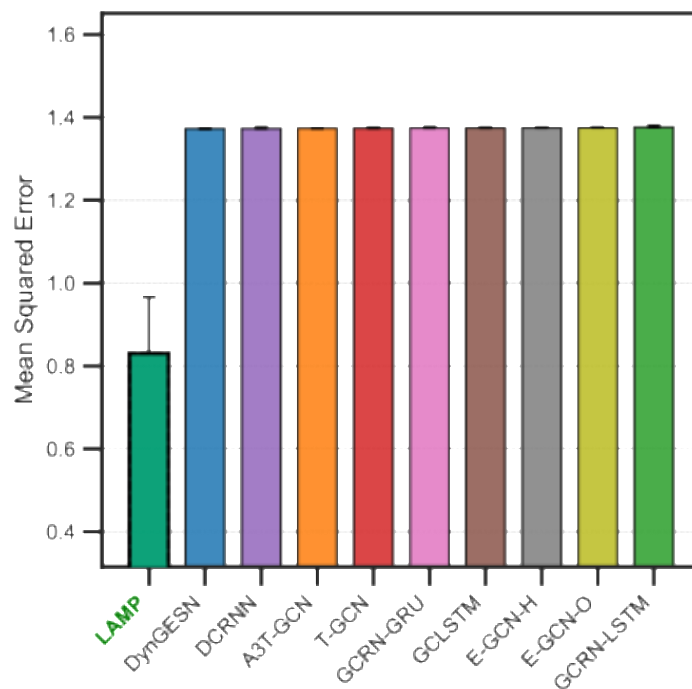
Colored Leaf Counting – Single Color

Can the model propagate and accumulate sparse temporal signals between distant nodes?

Ours DynGESN A3T-GCN GCRN-LSTM T-GCN DCRNN GCLSTM GCRN-GRU E-GCN-H E-GCN-O

$T = 600$

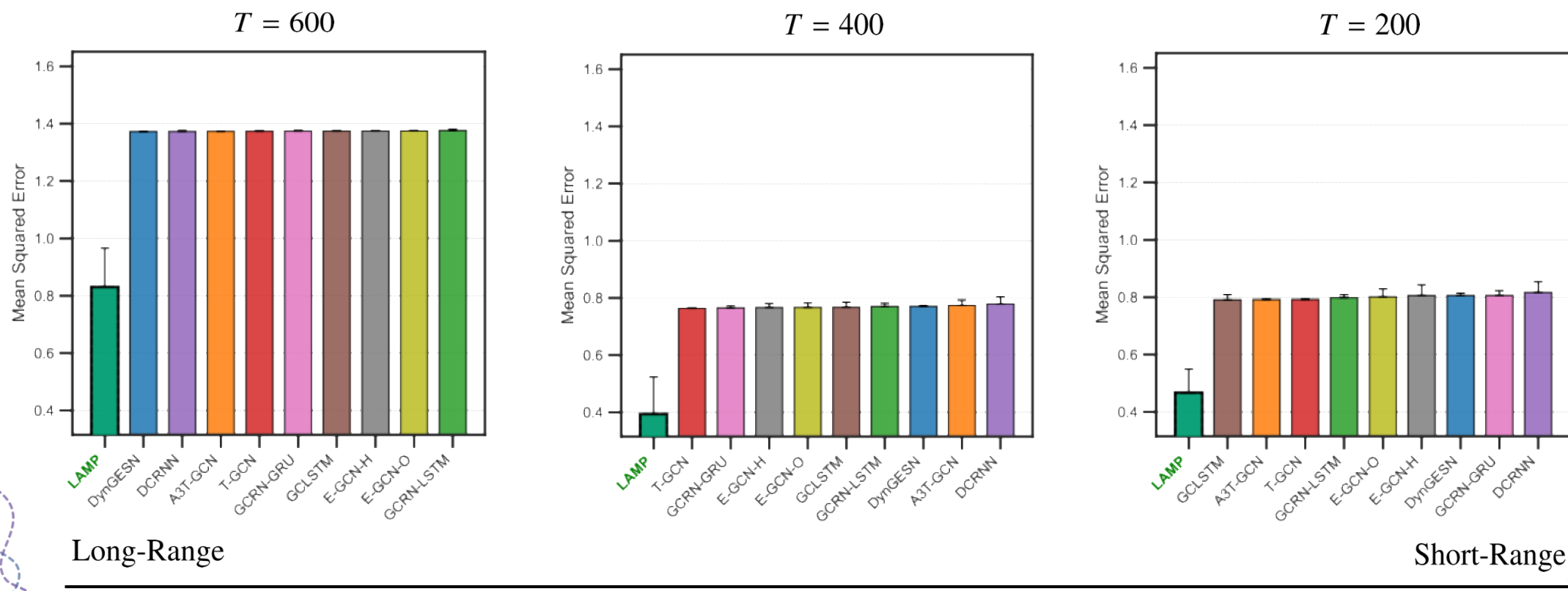
**The lower,
the better** (↓)



Colored Leaf Counting – Single Color

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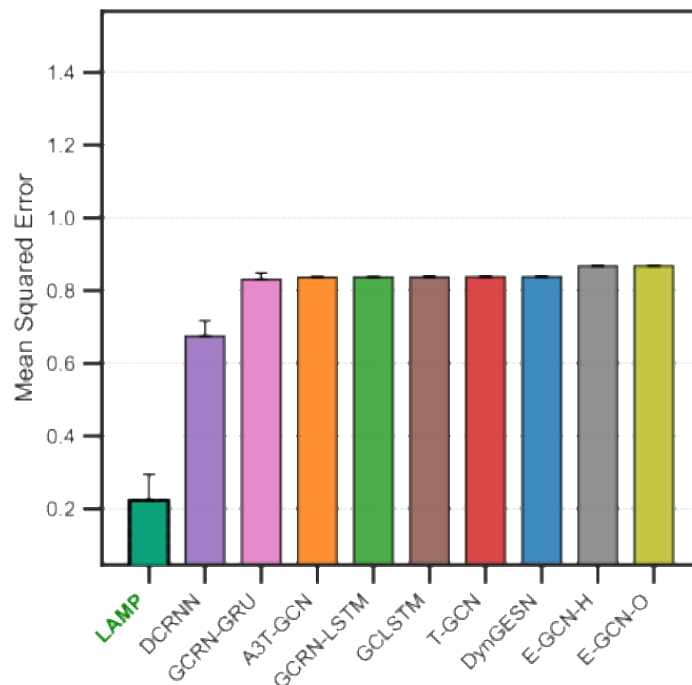
Colored Leaf Counting – Three Colors

Can the model propagate and accumulate sparse temporal signals between distant nodes?

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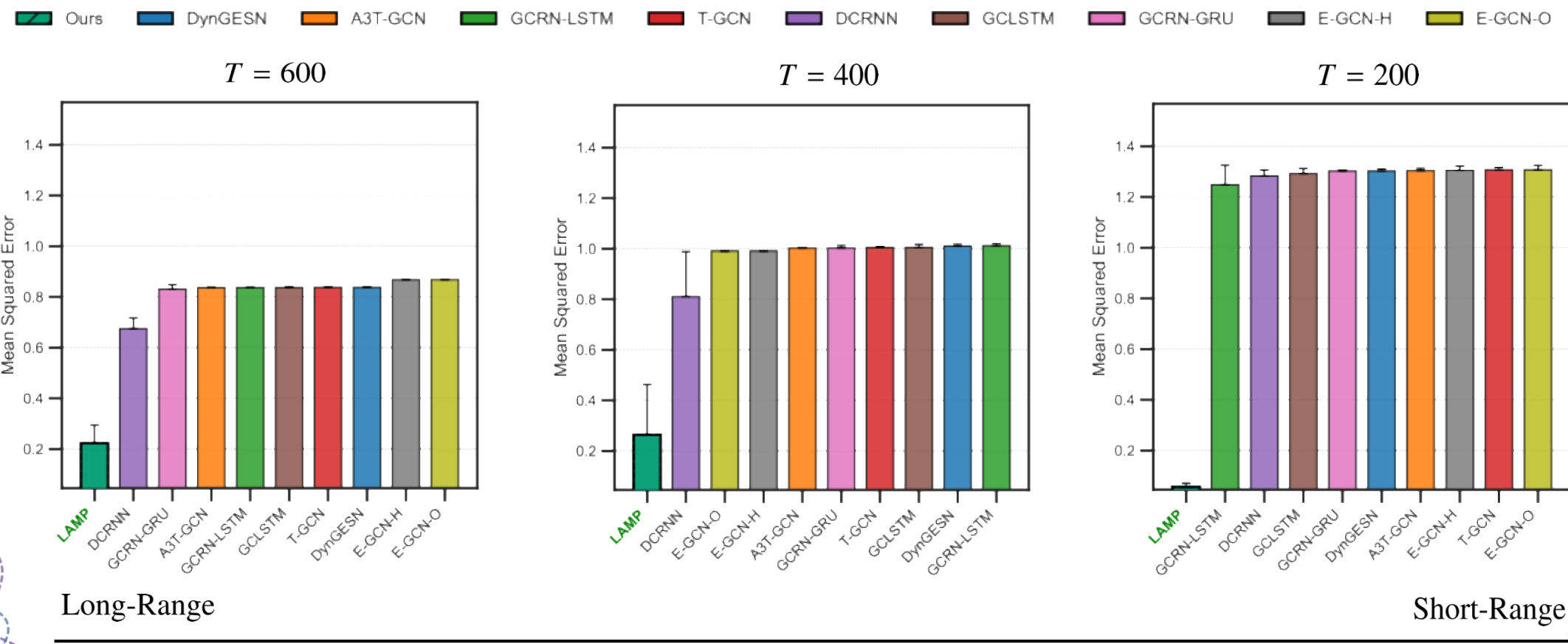
$T = 600$

**The lower,
the better** (↓)



Colored Leaf Counting – Three Colors

Can the model propagate and accumulate sparse temporal signals between distant nodes?



Conclusions

- Long-Range Propagation is an **open problem**
- A clever architectural design helps limiting this problem
- **Questions**
 - What happens if the set of nodes **changes** over time?
 - How to ensure a **node-level** adaptive dissipation rate?
 - Is there a way of having instantaneous propagation between snapshots?