Generalization and Robustness of Graph Neural ODEs for Dynamical Systems on Graphs

Moritz Laber, Brennan Klein

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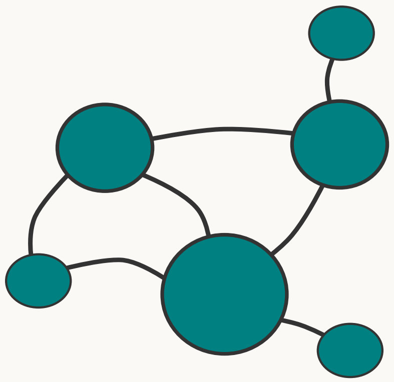
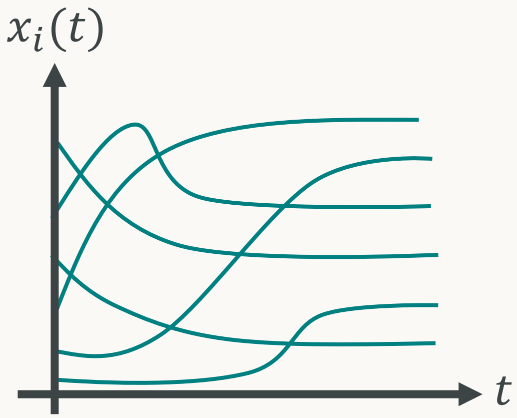
Dynamics from Data



graph A



node-wise timeseries $x_i(t)$

Dynamics from Data

Classical ODEs:
Handcraft differential equations using domain knowledge.

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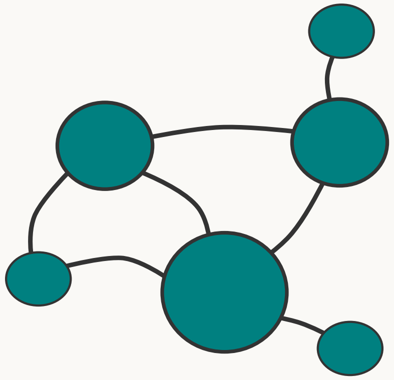

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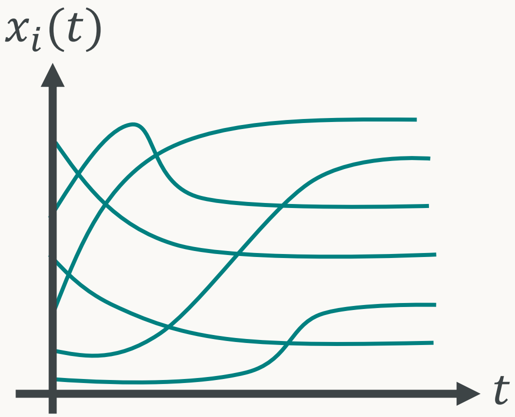

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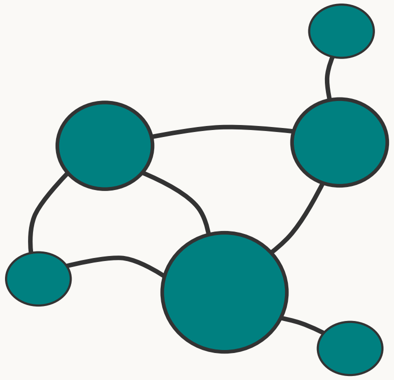

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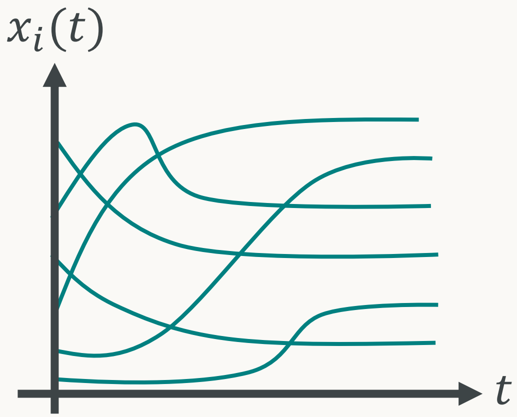

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Learn differential equations from timeseries data.

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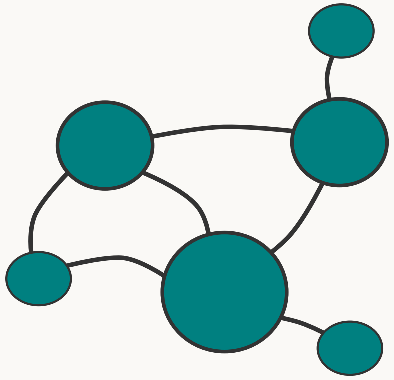

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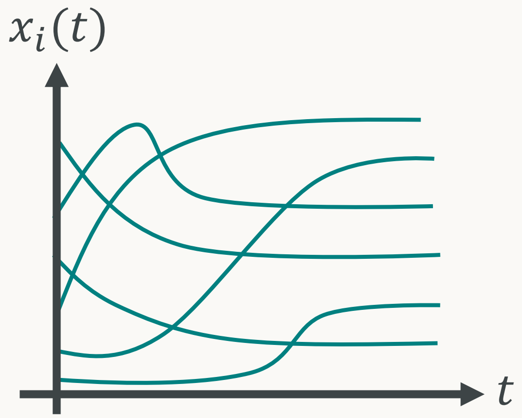

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Questions: How do the performance and robustness of neural ODEs depend on the network? [4]

[1] *Chen et al.* NeurIPS (2018), [2] *Poli et al.* AAAI (2022), [3] *Kidger* PhD Thesis (2022)

[4] *Vasiliauskaite & Antulov-Fantulin* Comms Phys. 7 1 (2024)

Contributions

We train neural ODEs on **different dynamical systems** and **graphs from the $\mathbb{S}^1$ model** with different structural characteristics

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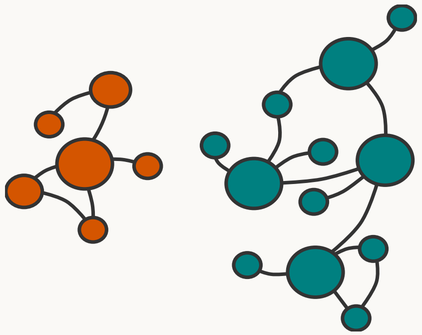
We evaluate their **performance and robustness** in terms of four criteria:

Generalization:
Graph Size



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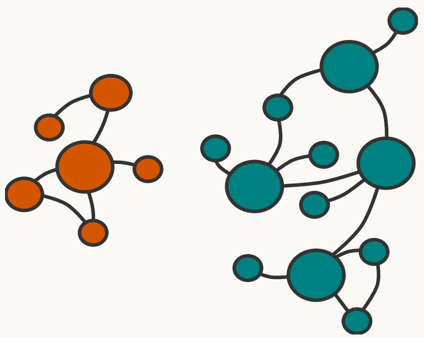

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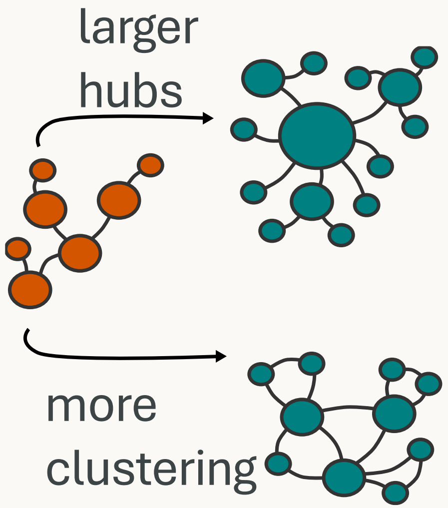
Generalization: Graph Properties



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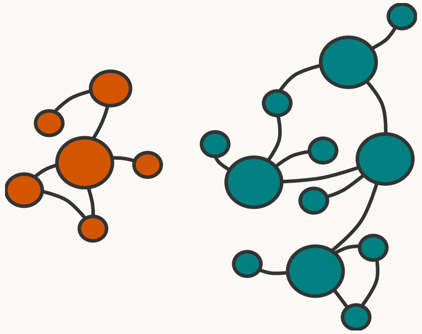

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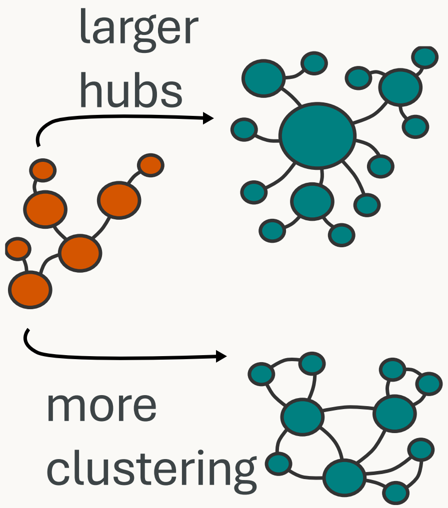
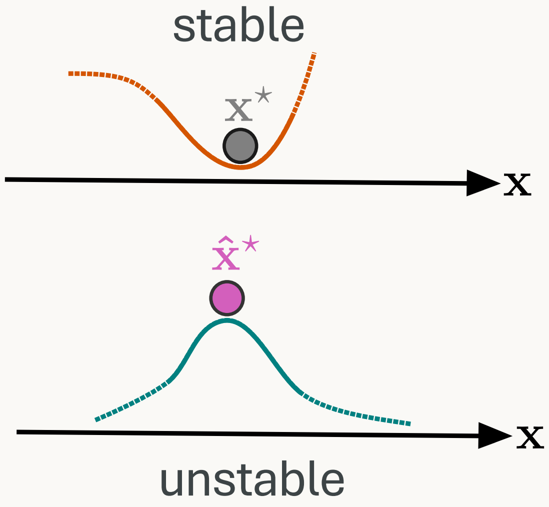


Robustness: Local Stability



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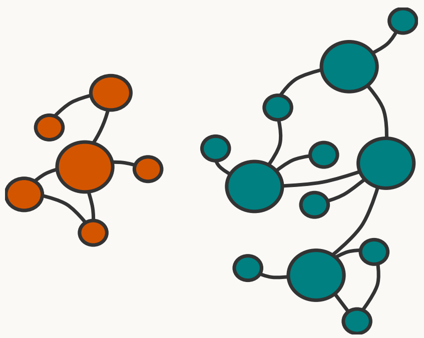

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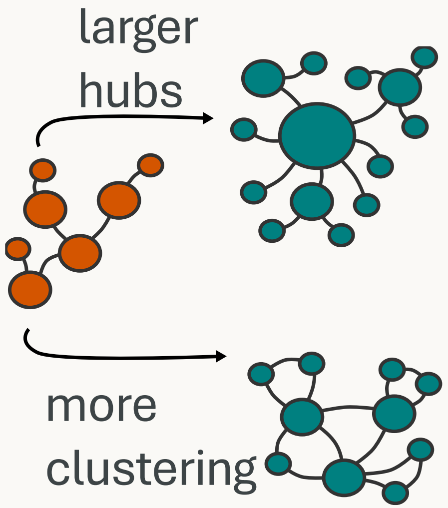

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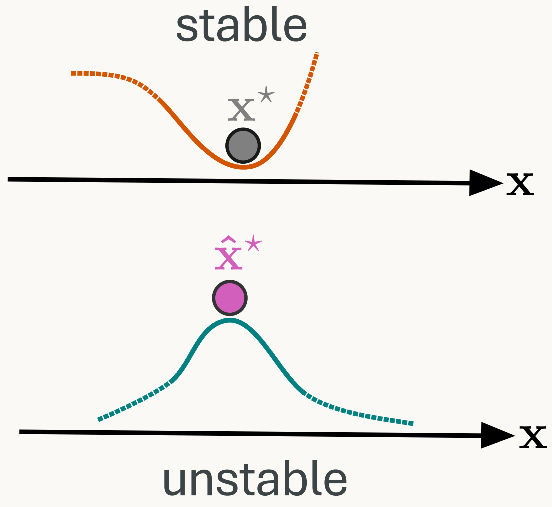
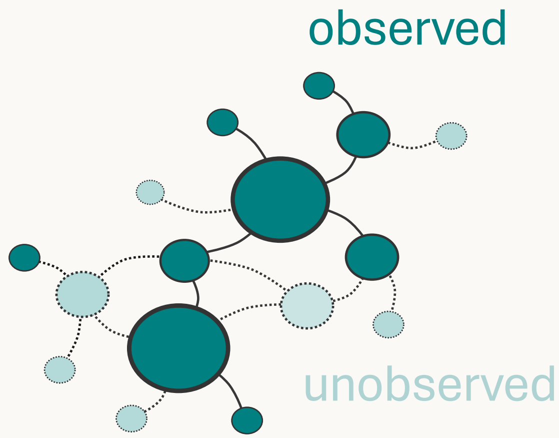


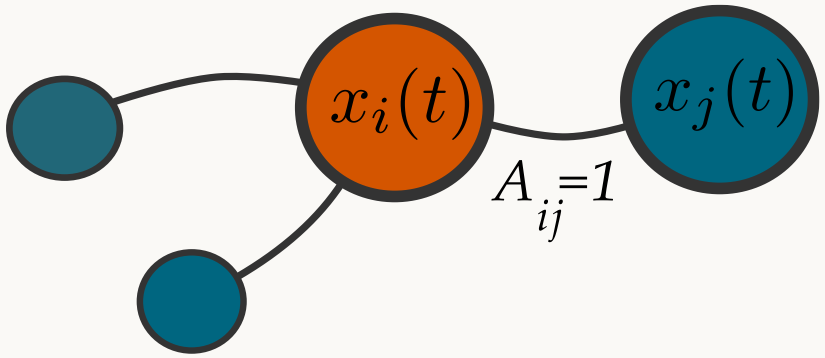
Robustness: Missing Nodes



(Neural) ODEs on Graphs

Many dynamical systems on graphs are well described by [1]

$$\frac{dx_i}{dt} = f\big(x_i(t)\big) + \sum_{j \in \mathcal{V}} A_{ij} h^{\text{ego}}\big(x_i(t)\big) h^{\text{alt}}\big(x_j(t)\big)$$



[1] *Barzel & Barabási* Nat. Phys. 9 673-681 (2013)

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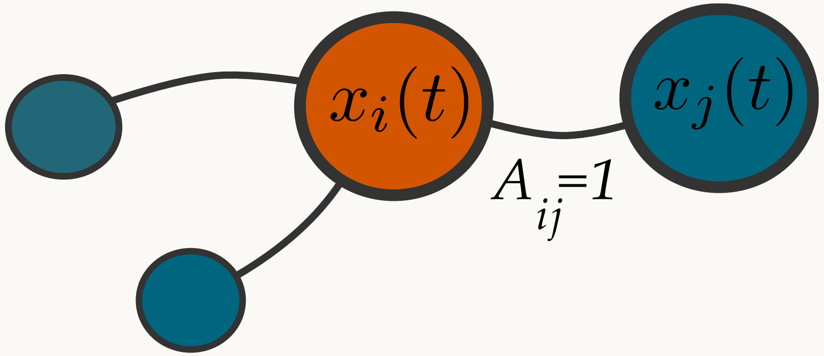

These equations form also the basis for our neural ODE architecture

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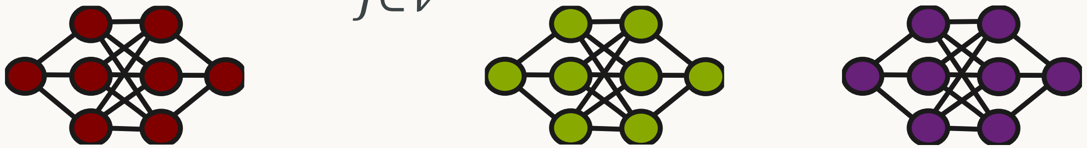

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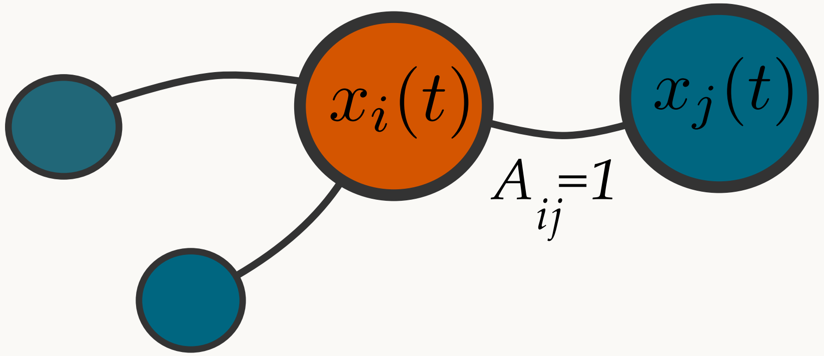

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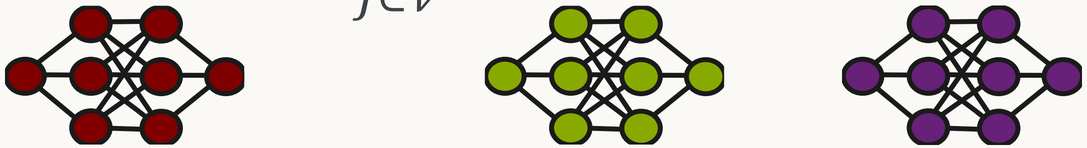

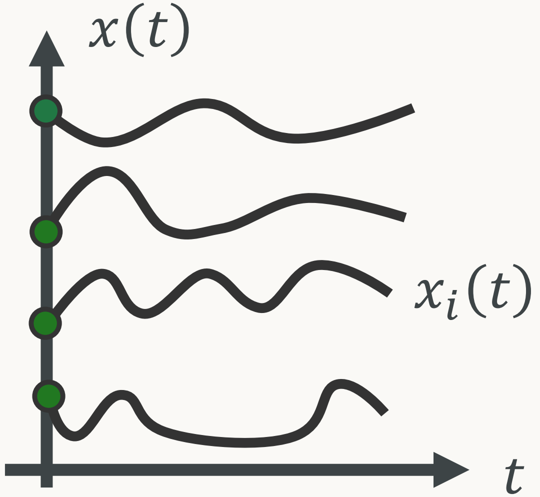

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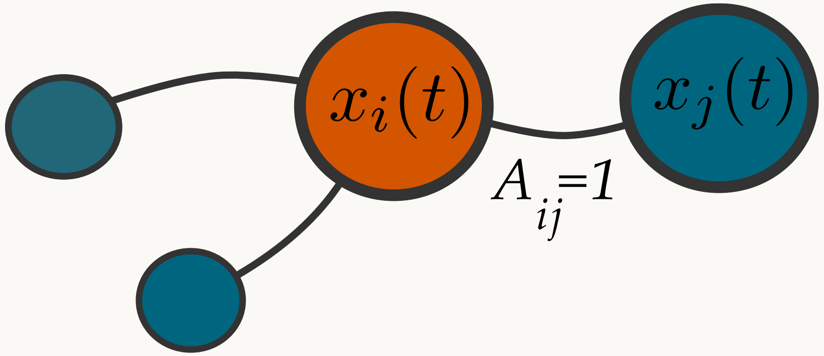

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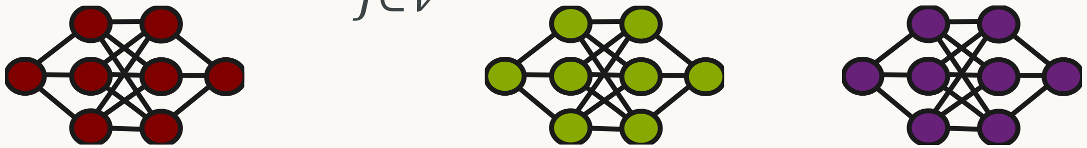

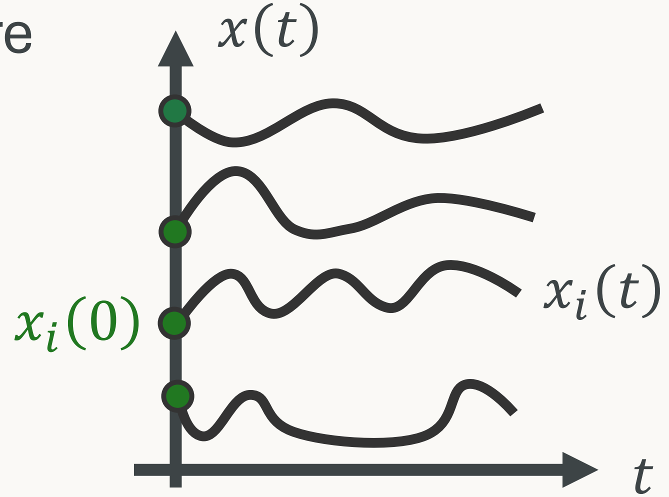

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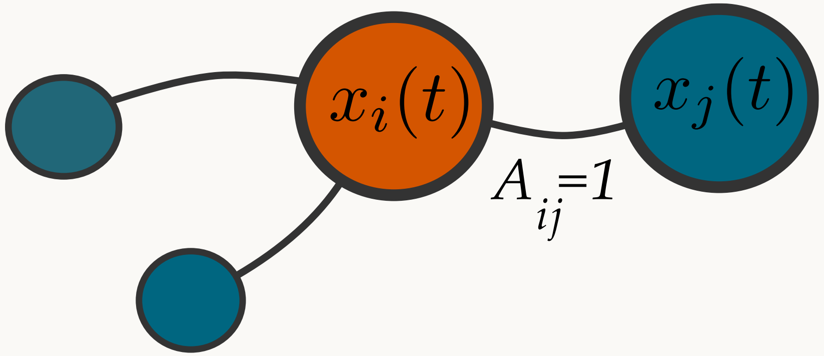

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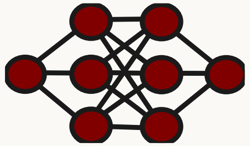

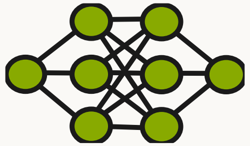

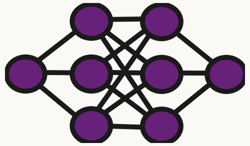

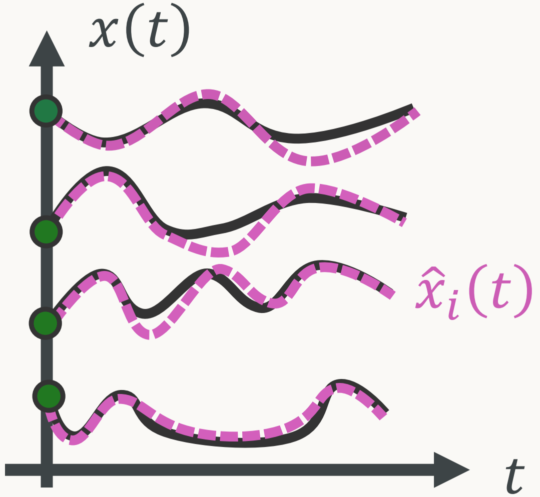

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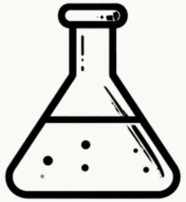
Setup: Dynamics

We use synthetic data from **five dynamical systems** from different domains [1,2].

Susceptible-Infected-Susceptible (SIS)



Mass-Action Kinetics (MAK)

Michaelis-Menten Model (MM)

Birth-Death Process (BD)

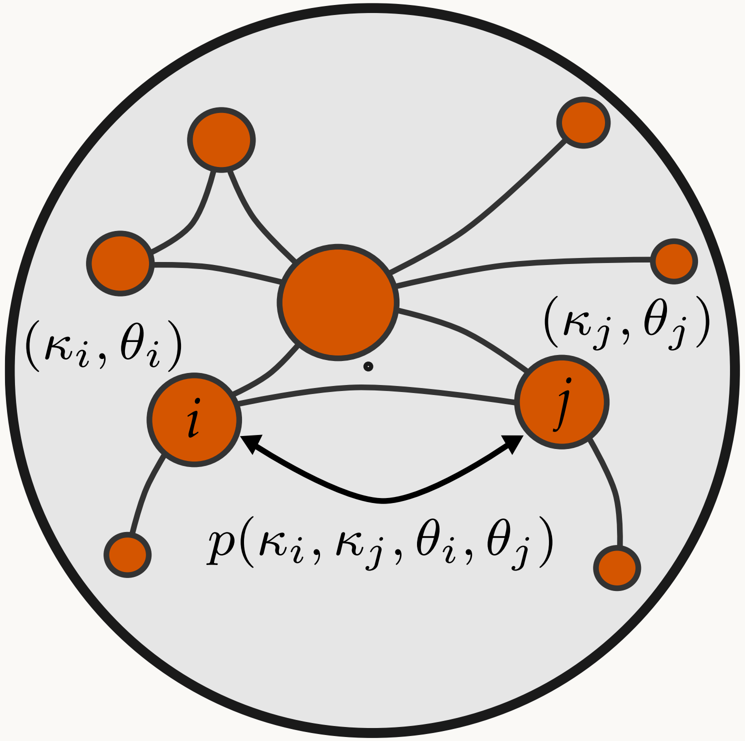
Neuronal Dynamics (ND)

[1] *Meena* et al. Nat. Phys. 19 1033 (2023) [2] *Hens et al.* Nat. Phys. 15 403-412 (2019)

Setup: Graphs

We use the $\mathbb{S}^1$ model [1,2] to generate graphs with different properties:

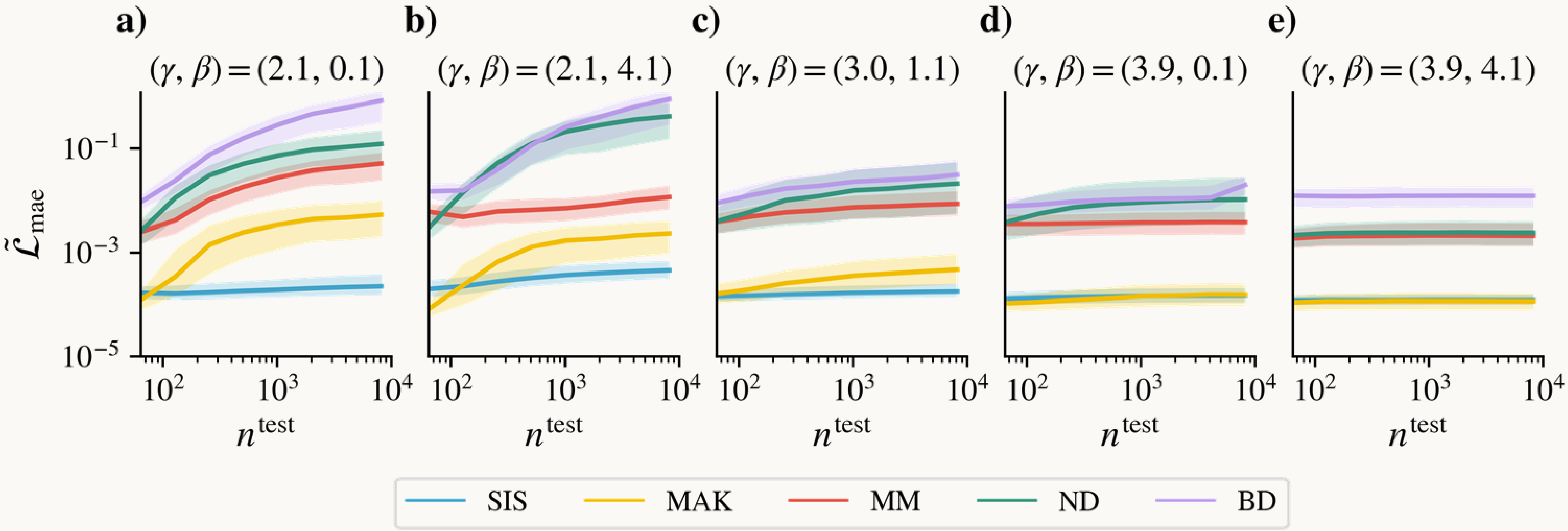
- number of nodes: $n \in \{64, \dots, 8192\}$
- average degree $\bar{k} = 10$
- exponent of the degree distribution $\gamma \in [2.1, \dots, 3.9]$.
  - **lower γ ➔ larger hubs.**
- inverse temperature $\beta \in [0.1, \dots, 4.1]$.
  - **larger β ➔ more clustering.**



[1] *Serrano* et al. PRL 100, 078701 (2008) [2] *Krioukov* et al. PRE 82 036106 (2010)

Generalization: Larger graphs

Generalization to larger graphs is **possible for low degree heterogeneity.**
Clustering has limited influence on size generalization.



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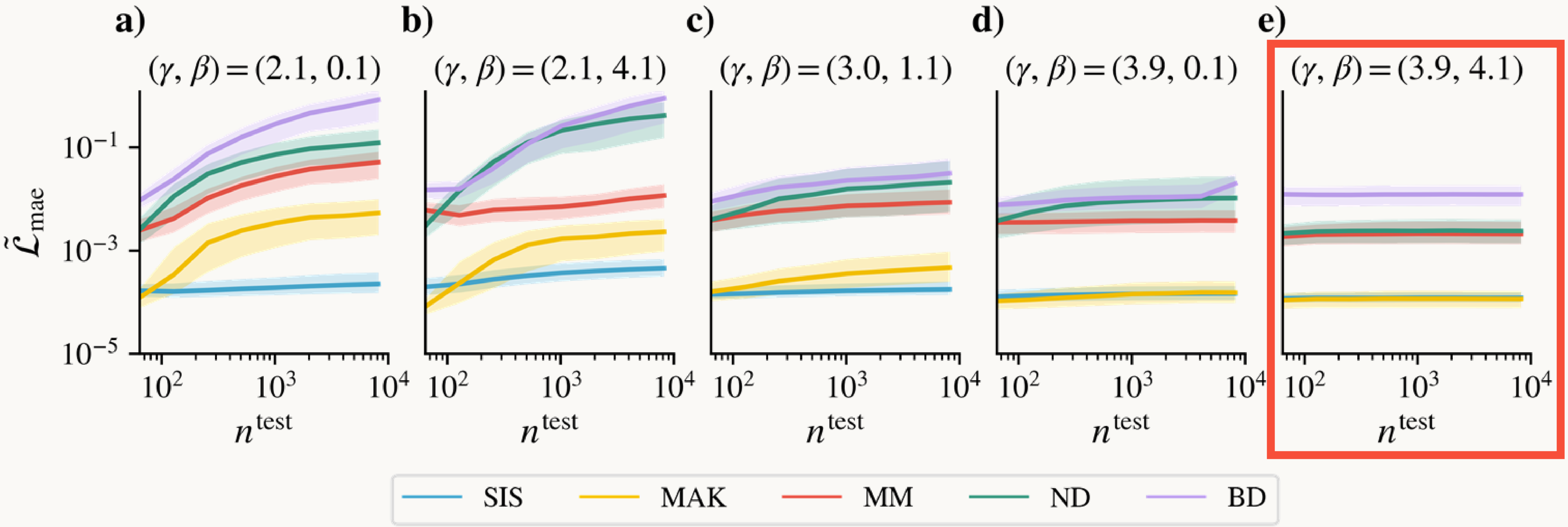

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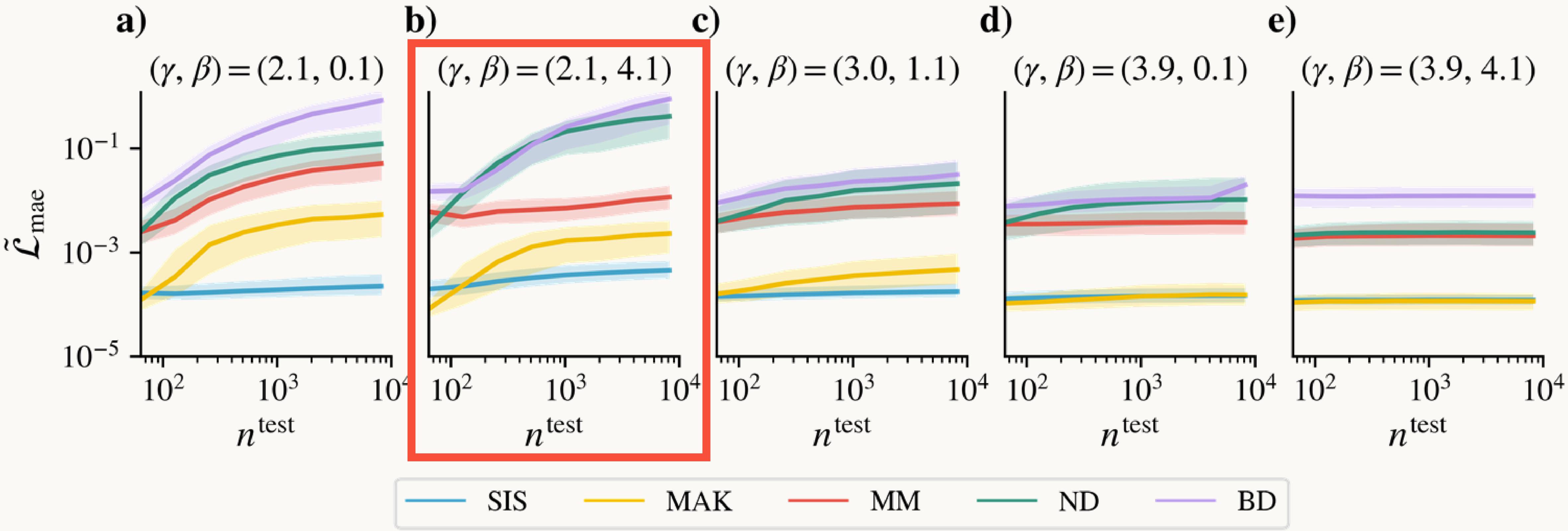

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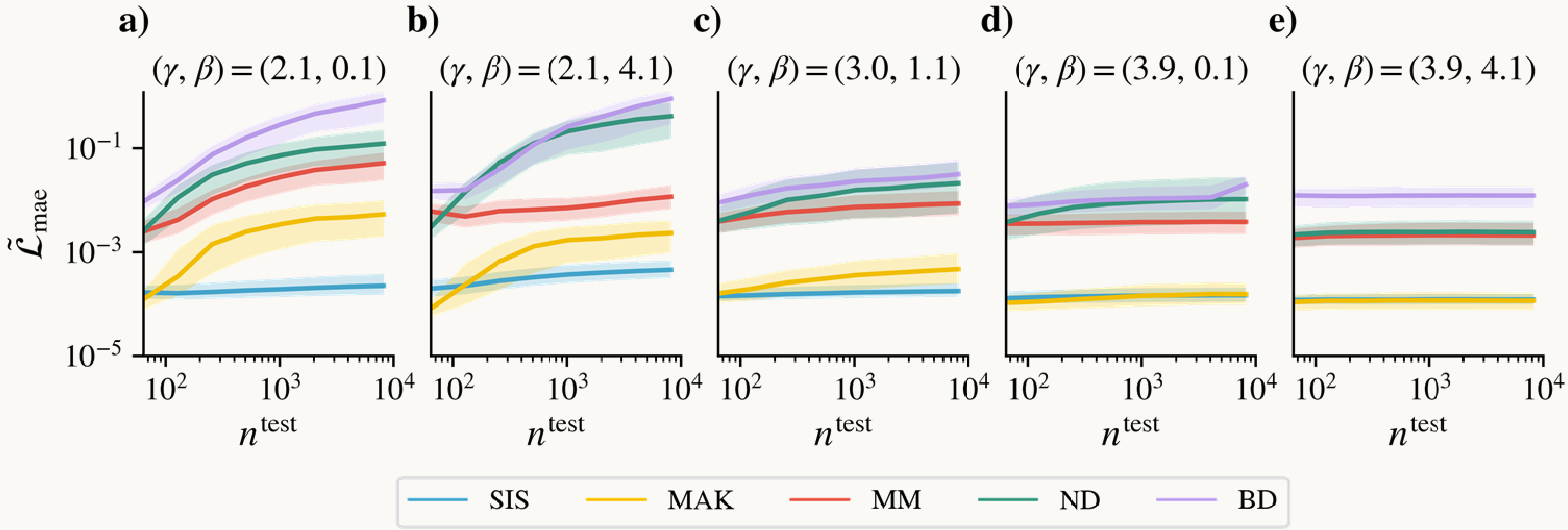
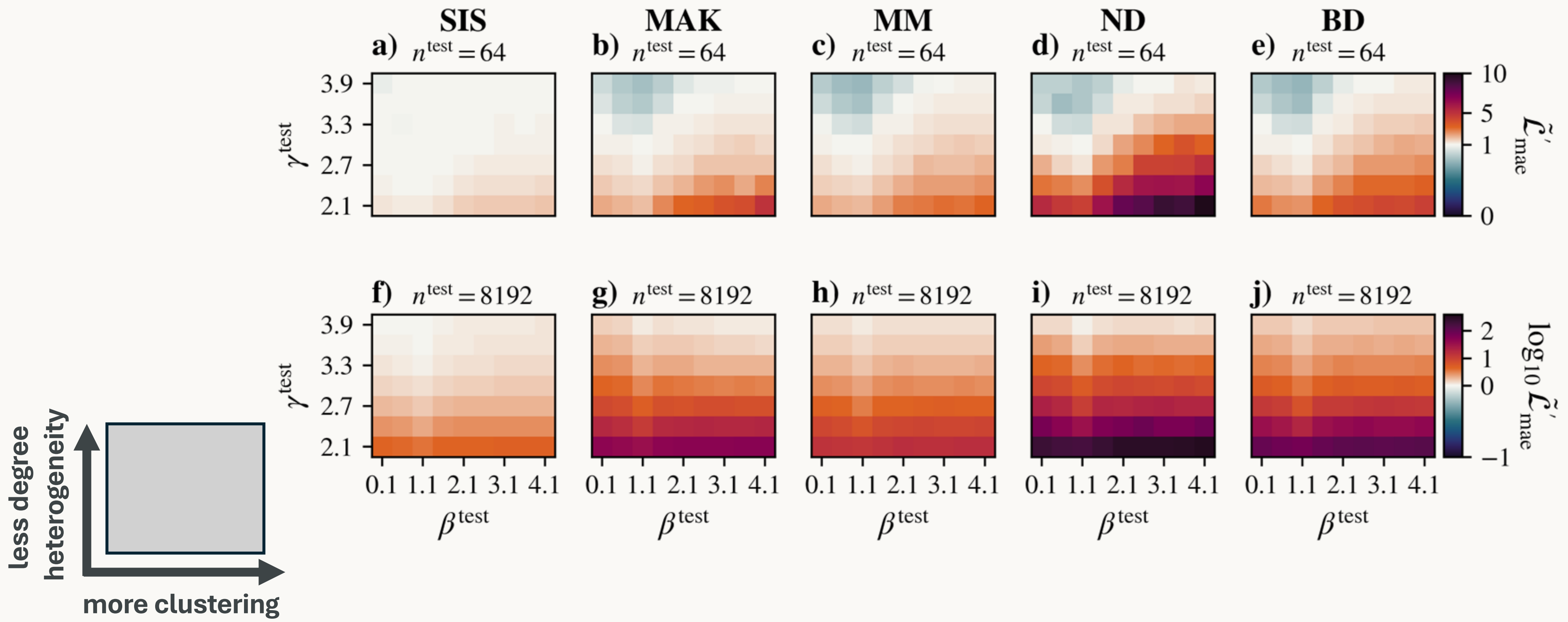


Generalization: Structurally different graphs

Performance is **good on less clustered**, and **less degree heterogeneous graphs**, but degrades with larger degree heterogeneity.



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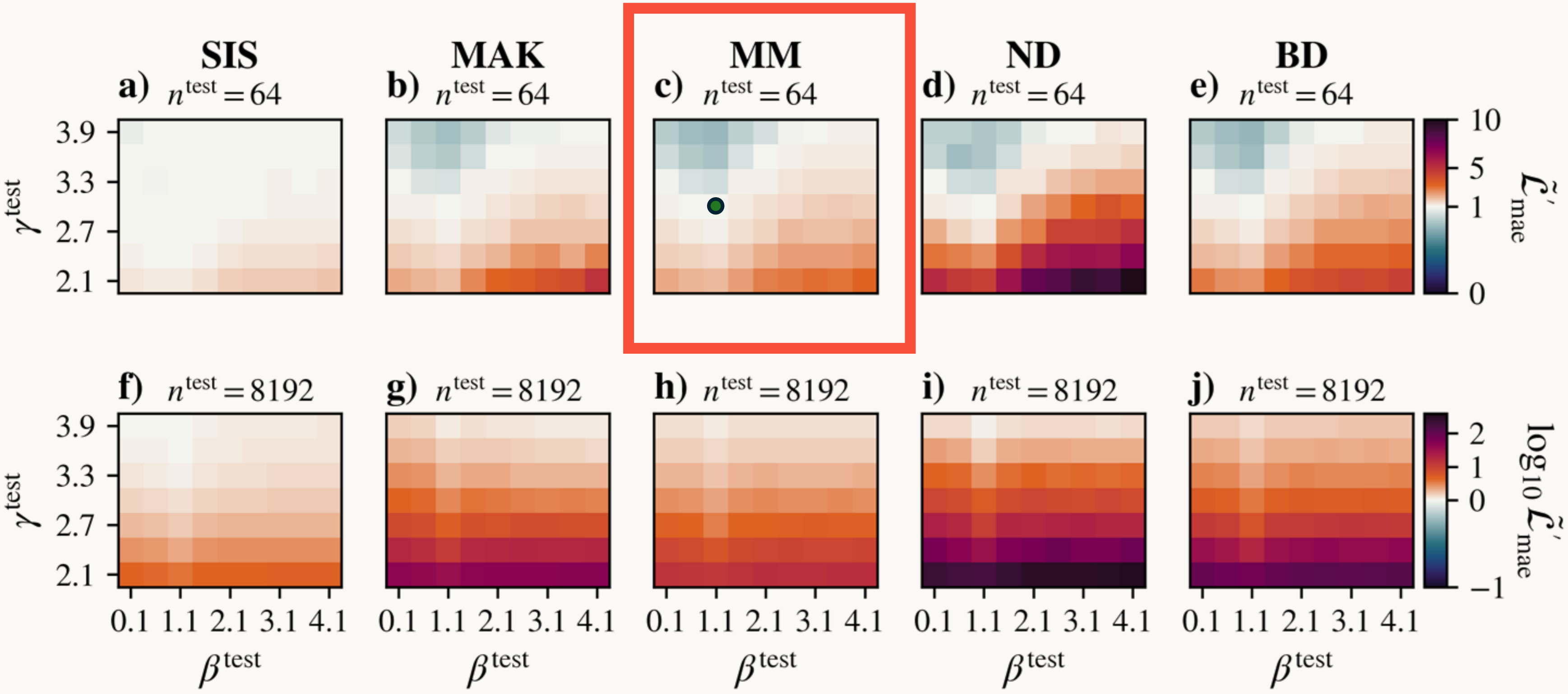

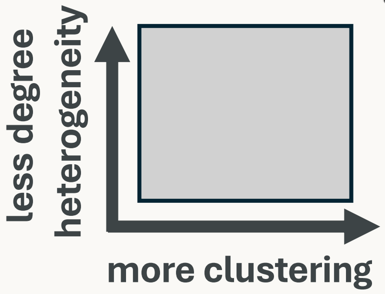

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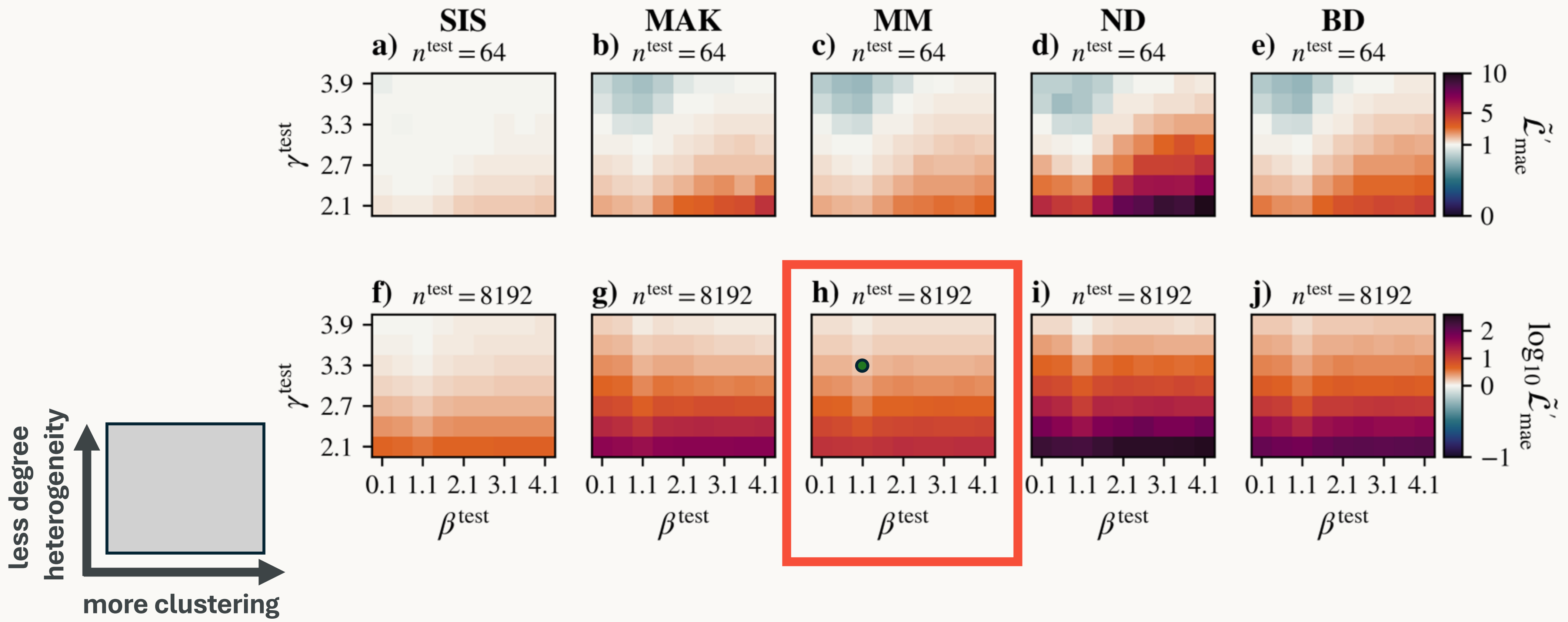

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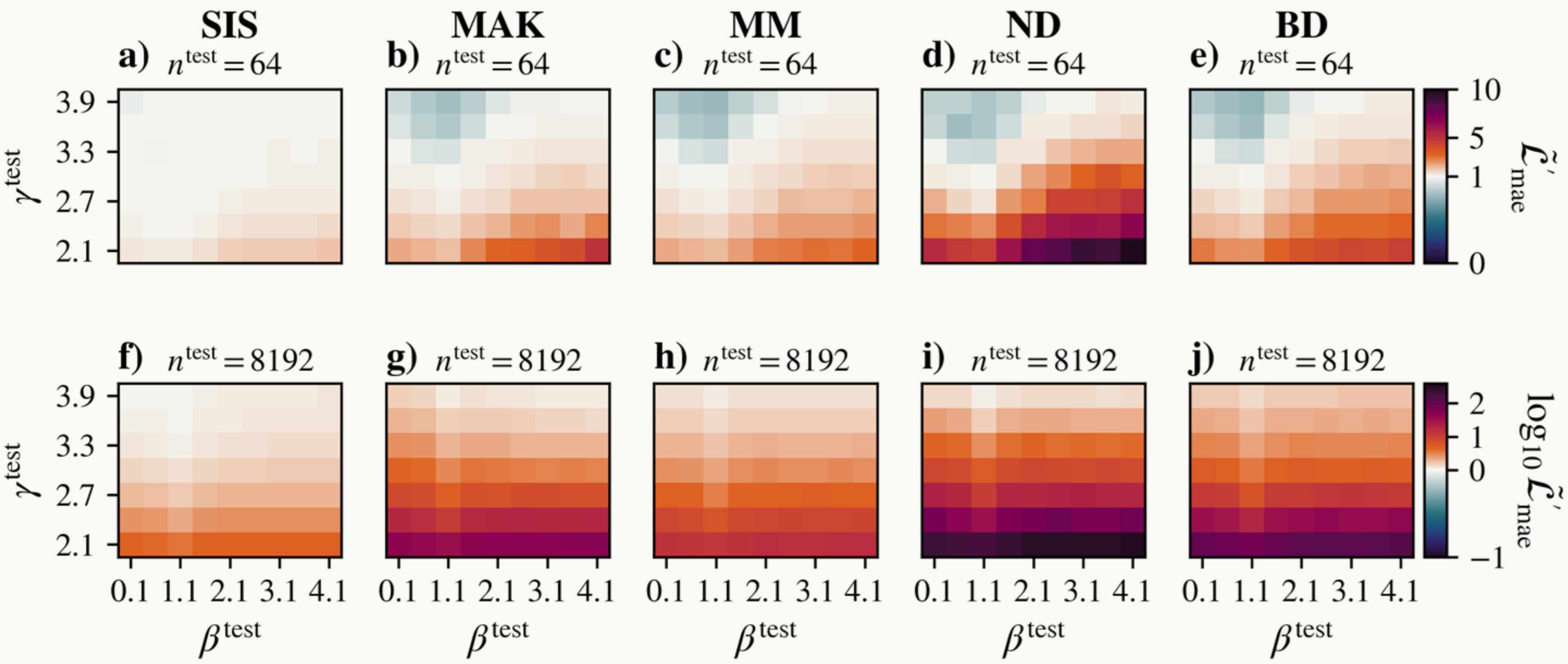
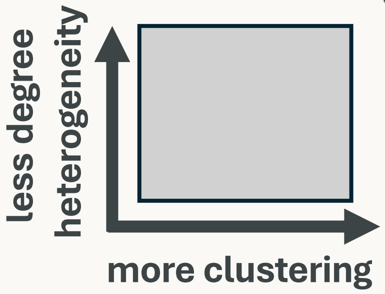
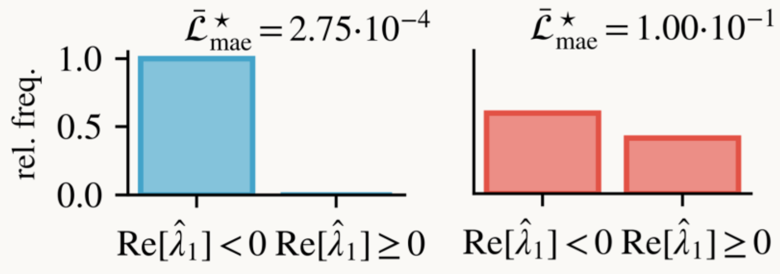




Robustness

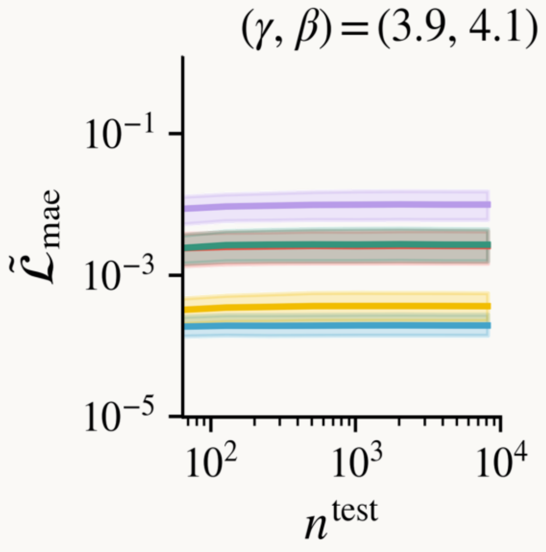
Local Stability

Well performing models **also capture stability**. Models that don't do well find wrong or even unstable fixed points.



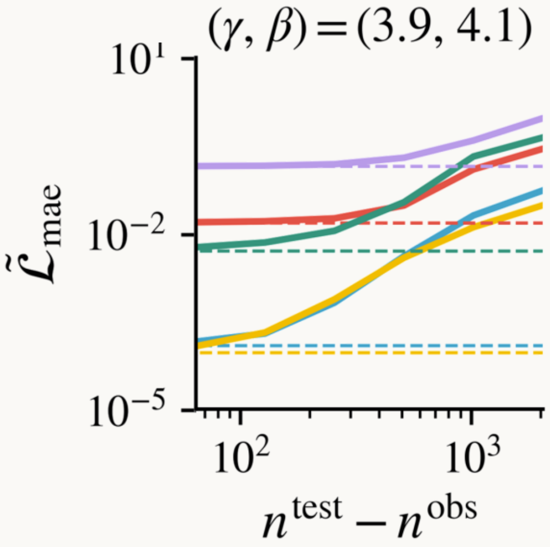
Noisy Training Data

Size generalization results are **robust to moderate noise** in the training data.



Missing Nodes

Performance degrades fast with missing nodes, even only a few are non-observed at prediction time.



Conclusion

Neural ODEs can exhibit excellent size generalization for some dynamical systems and if graphs are not too degree heterogeneous.

However, they struggle to generalize to graphs that are more degree heterogeneous than the training graph and are brittle to missing nodes at time of deployment.

Paper will appear soon!

Thanks to Melanie Weber and Tina Eliassi-Rad.

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Copyright

Laber M., Klein B., Eliassi-Rad T. *When do neural ordinary differential equations generalize on complex networks?* arXiv:2602.08980 (2026)