When do Neural ODEs Generalize on Complex Networks?

Moritz Laber, Tina Eliassi-Rad, Brennan Klein



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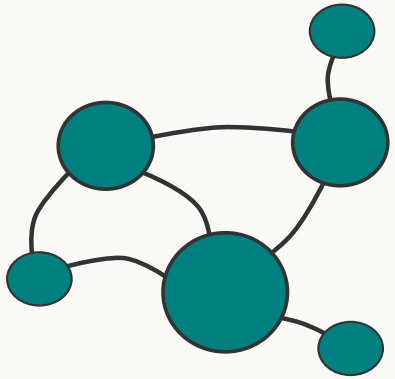
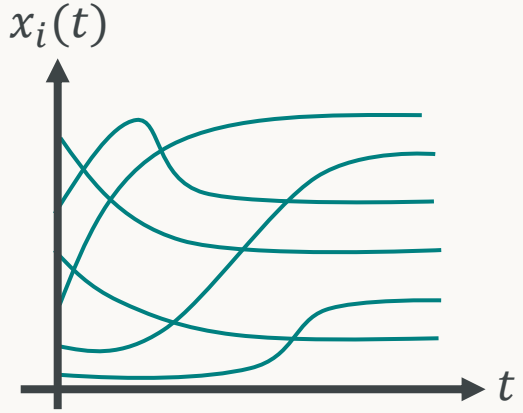
Network Science Student Research Symposium, Boston, US, 2026-02-19

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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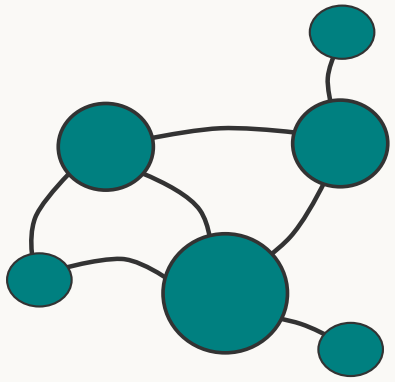

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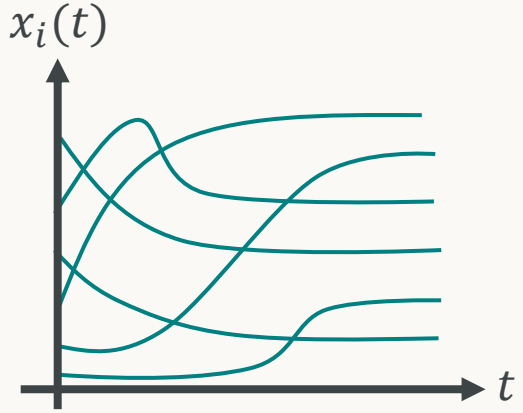

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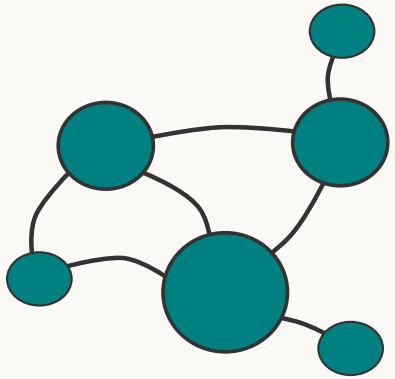

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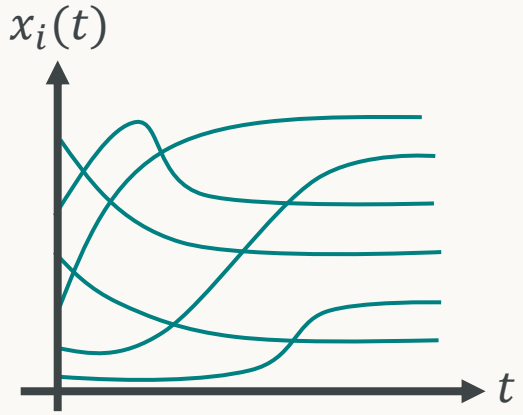

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Learn differential equations from timeseries data.

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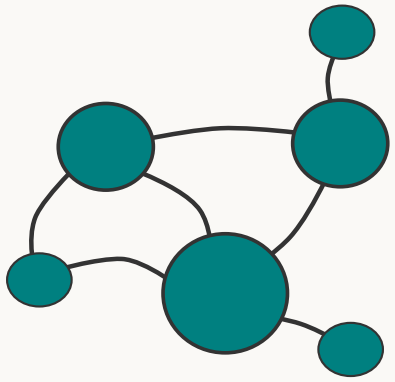

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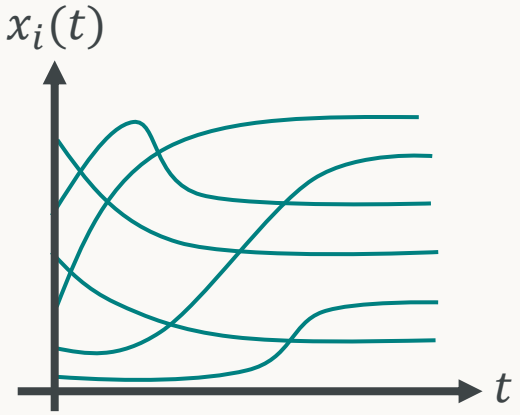

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Questions: How do the performance and robustness of neural ODEs depend on the network? [4]

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

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

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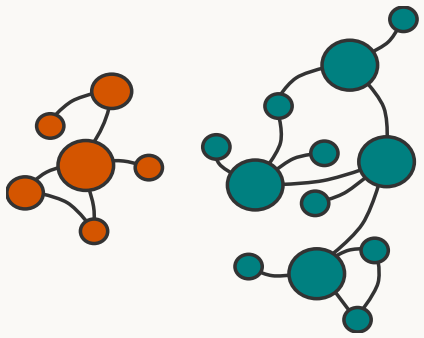
We evaluate their **performance and robustness** in terms of four criteria:

Generalization:

Graph Size



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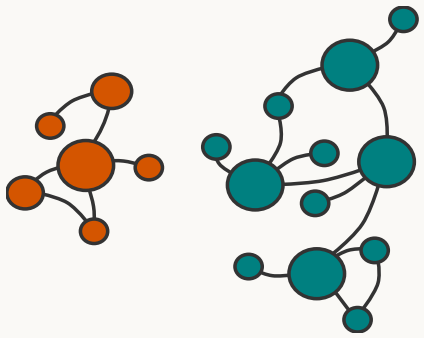

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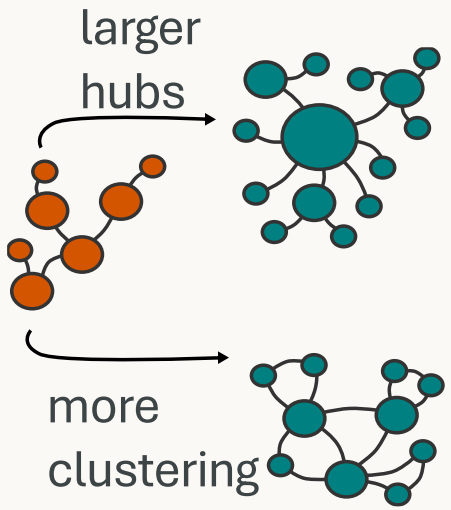

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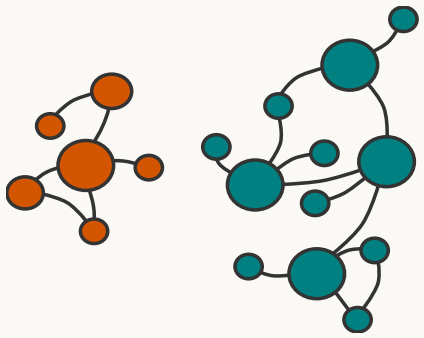

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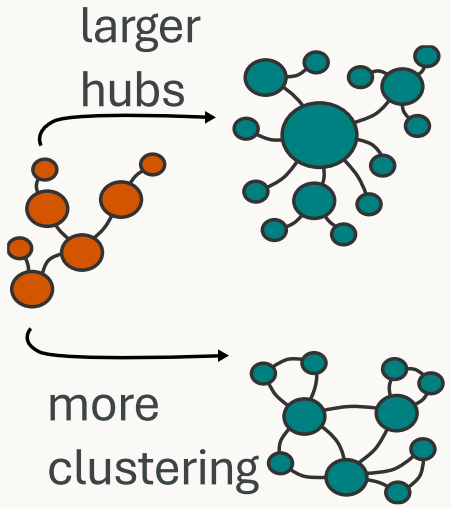
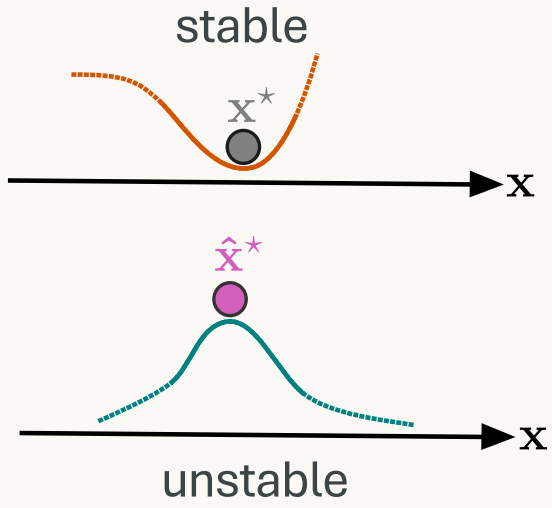


Robustness: Local Stability



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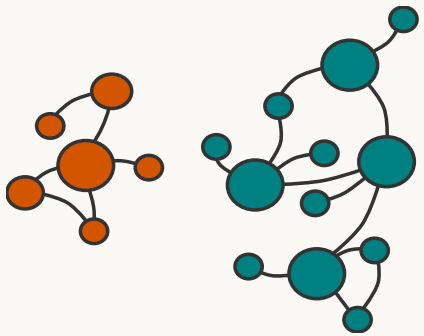

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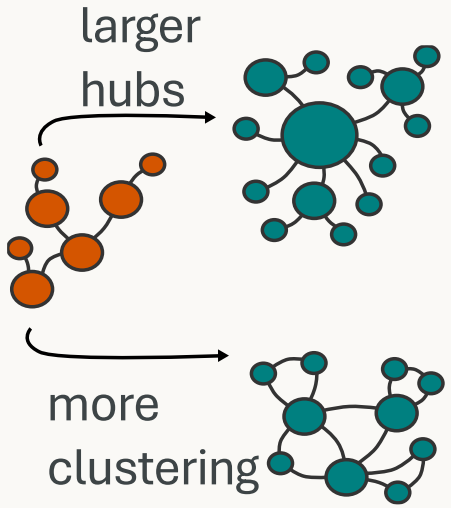

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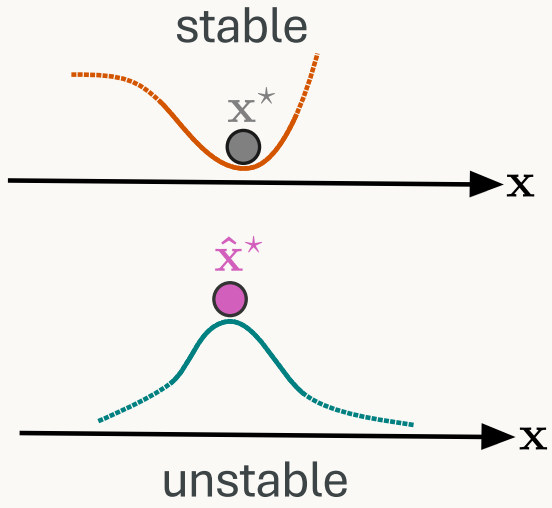

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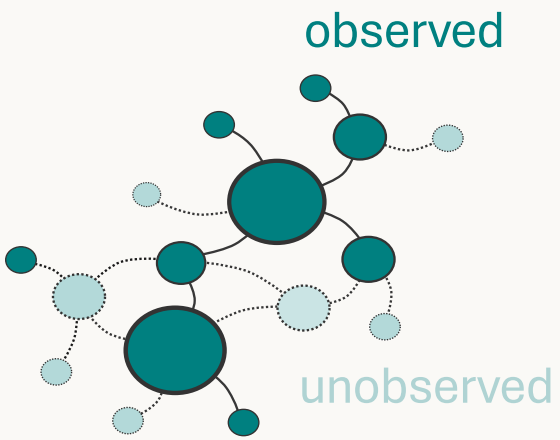

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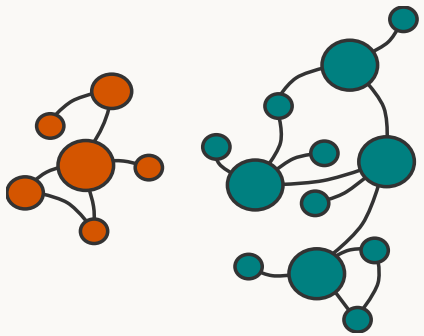

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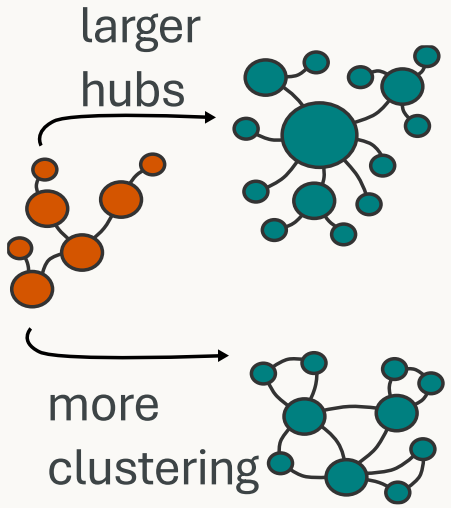

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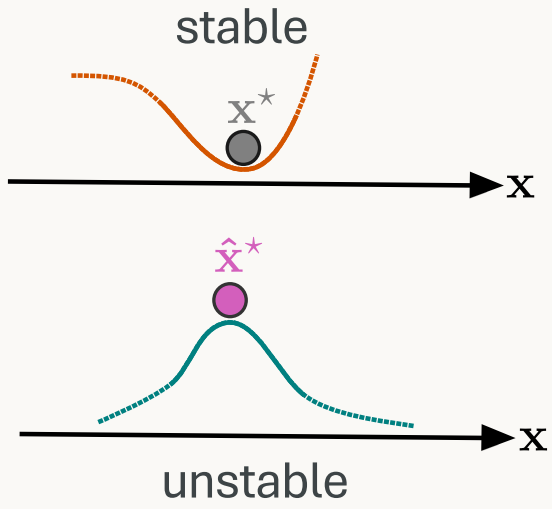

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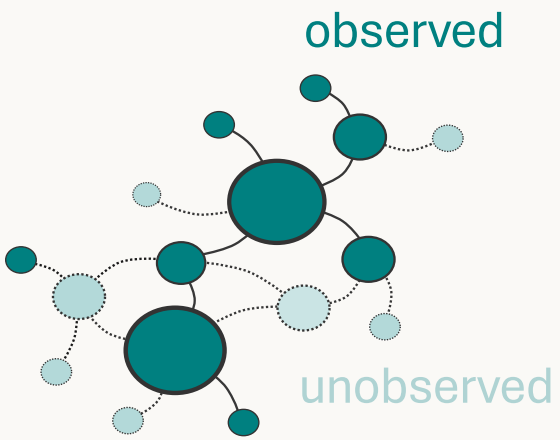

Background: Neural ODEs

Neural ODEs are ordinary differential equations in which the vector field is parameterized by a neural network.

$$\frac{dx_i}{dt} = f_\omega(t, x_1(t), \dots, x_n(t)) \qquad x_i(t=0) = \tilde{x}_i$$

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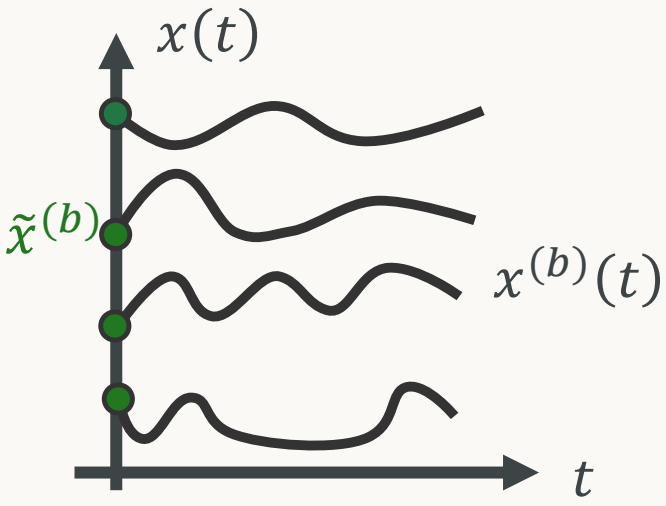

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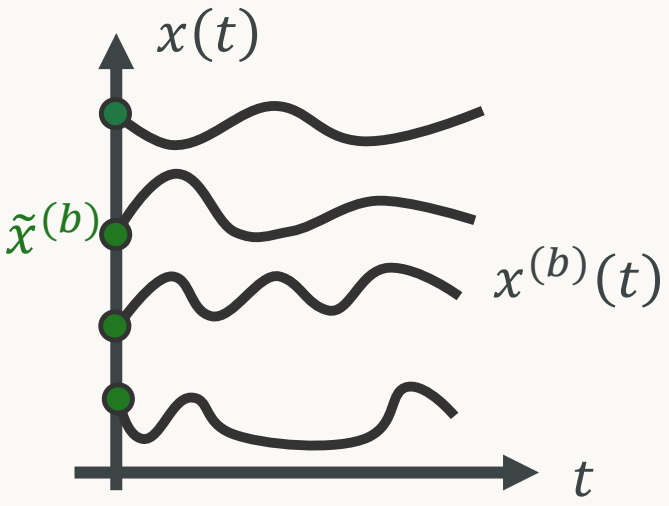

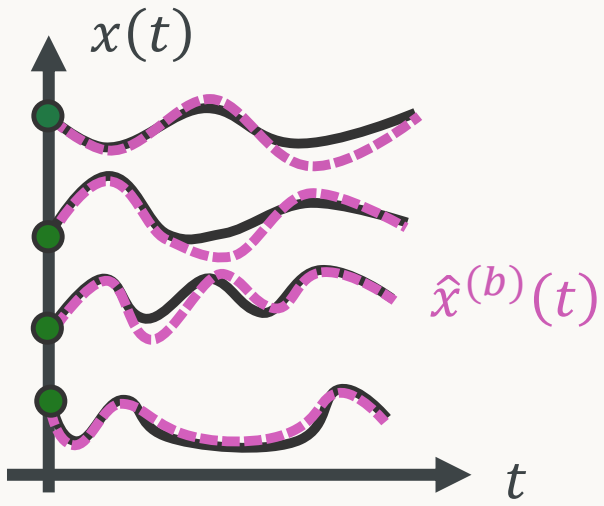

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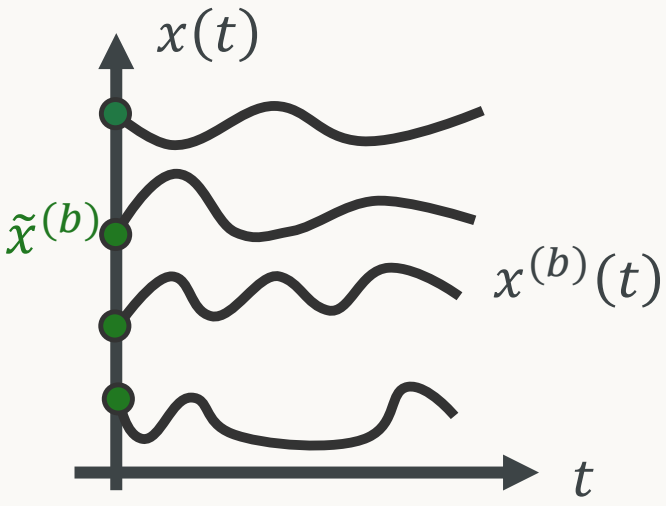

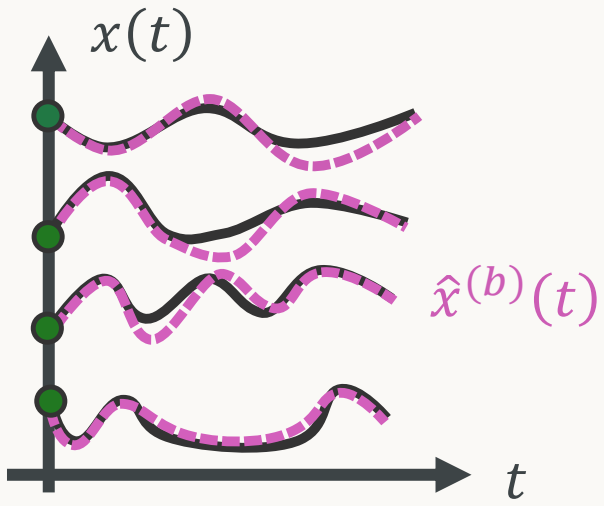

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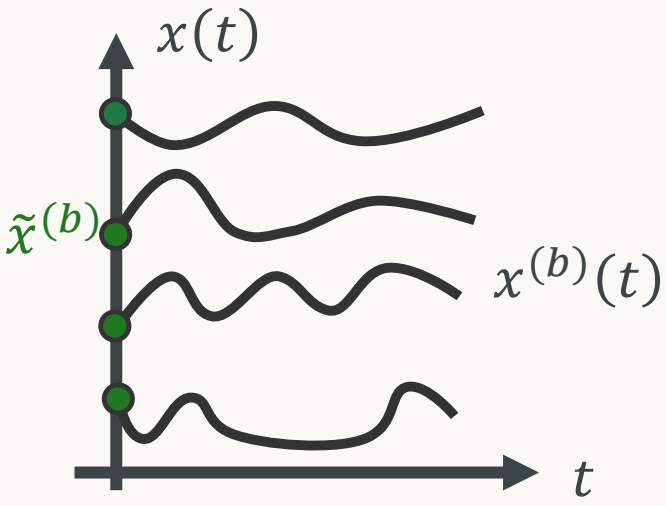

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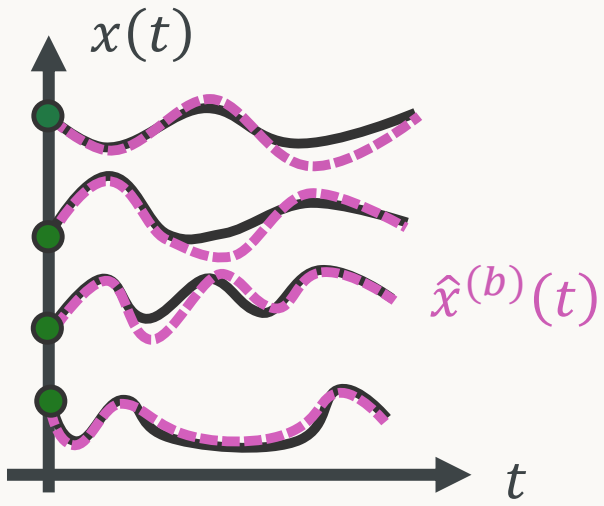

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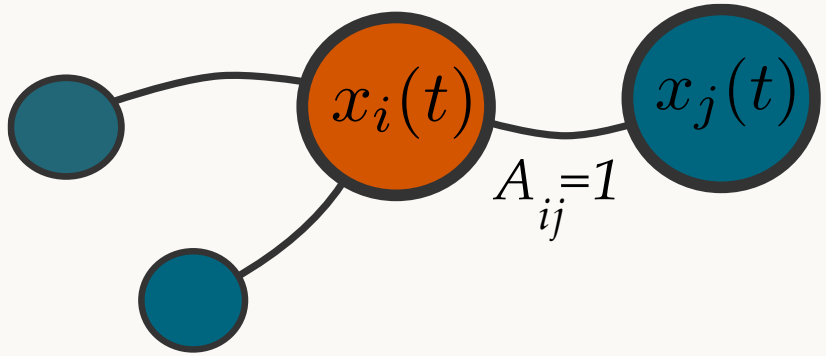
There are several ways to compute this term, some of them still actively researched [1].

[1] *Kidger* PhD Thesis (2022)

Background: ODEs on Graphs

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

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



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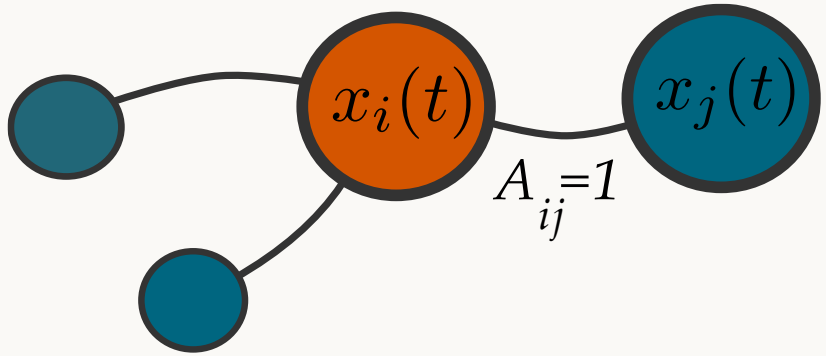

Example: SIS-Model

$$\frac{dx_i}{dt} = -\mu x_i(t) + \sum_{j \in \mathcal{V}} A_{ij}\, \beta\left(1 - x_i(t)\right) x_j(t)$$

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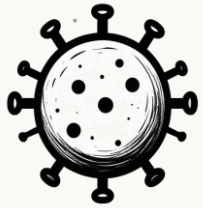
Setup: Dynamics

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)

Neural ODEs on Graphs

Replace f, h^{ego}, h^{alt} by separate neural networks f_ω, h_ω^{ego}, h_ω^{alt} to obtain a Neural ODE:

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

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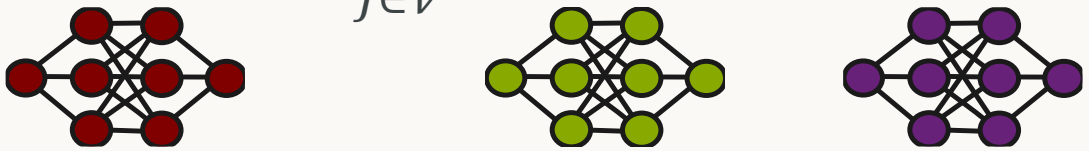

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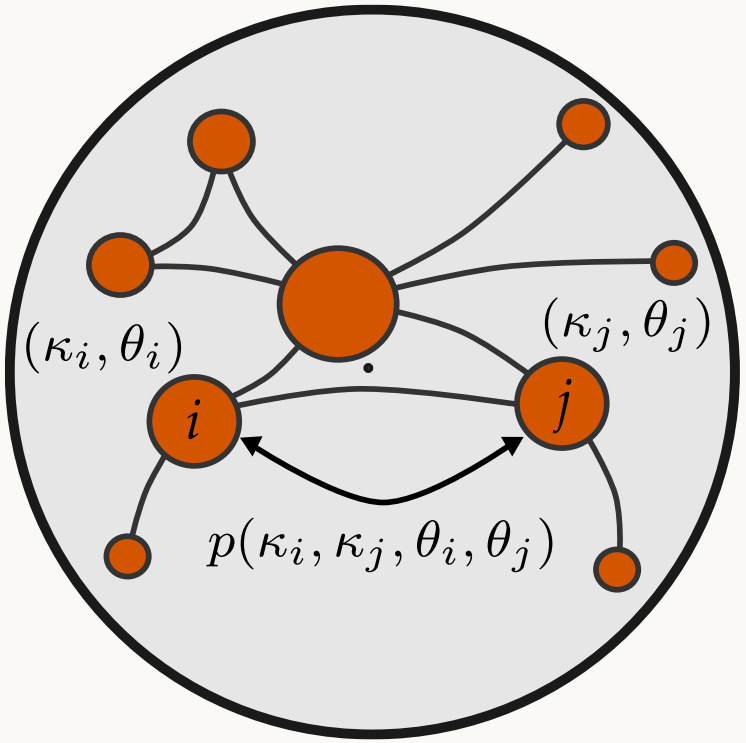
Background: $\mathbb{S}^1$ model

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

The model has **four parameters**:

- the *number of nodes* n
- the *average degree* $\bar{k}$
- the *exponent* γ of the degree distribution
  → controls degree heterogeneity
- The *inverse temperature* β
  → controls the clustering coefficient



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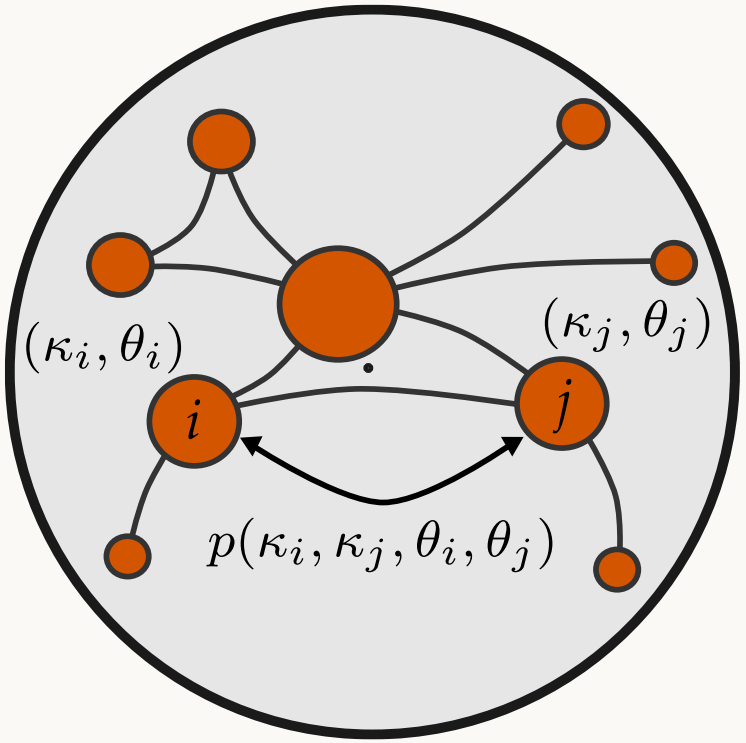
  → controls degree heterogeneity: **small γ → large hubs**
- The *inverse temperature* β
  → controls the clustering coefficient: **large β → strong clustering**



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Setup

Graphs

- number of nodes: $n \in \{64, \dots, 8192\}$
- average degree $\bar{k} = 10$
- exponent $\gamma \in [2.1, \dots, 3.9]$
- inverse temperature $\beta \in [0.1, \dots, 4.1]$

Dynamics

- SIS-Model (SIS),
- Mass-Action Kinetics (MAK)
- Birth-Death Process (BD)
- Neural Dynamics (ND)
- Michaelis-Menten (MM) model

Model

- 3 MLPs with layers 3 with 64 neurons.
- Dormand-Prince 4(5) ODE solver

Evaluation

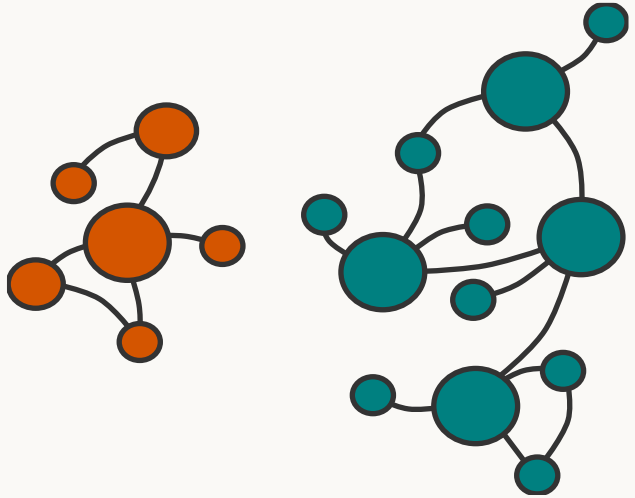
- mean absolute error $\mathcal{L}_{\text{mae}}$
- 100 test graphs

Generalization: Larger Graphs

Question: Can Neural ODEs, trained on small graphs, generalize to larger ones?

Motivation

- Size generalization is highly desirable for efficiency.
- Theoretical and empirical evidence for size generalization in (graph) machine learning is mixed [1,2].

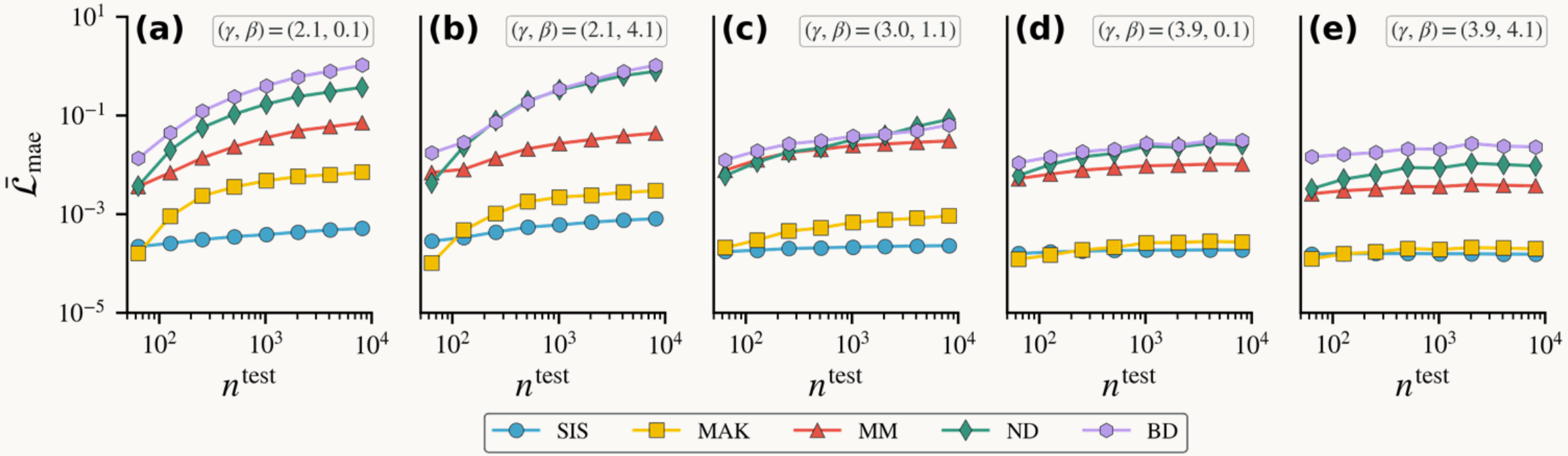


$n^{\text{train}} \ll n^{\text{test}}$

[1] *Yehudai et al.* ICML (2021) [2] *Anil et al.* NeurIPS (2022)

Generalization: Larger Graphs

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



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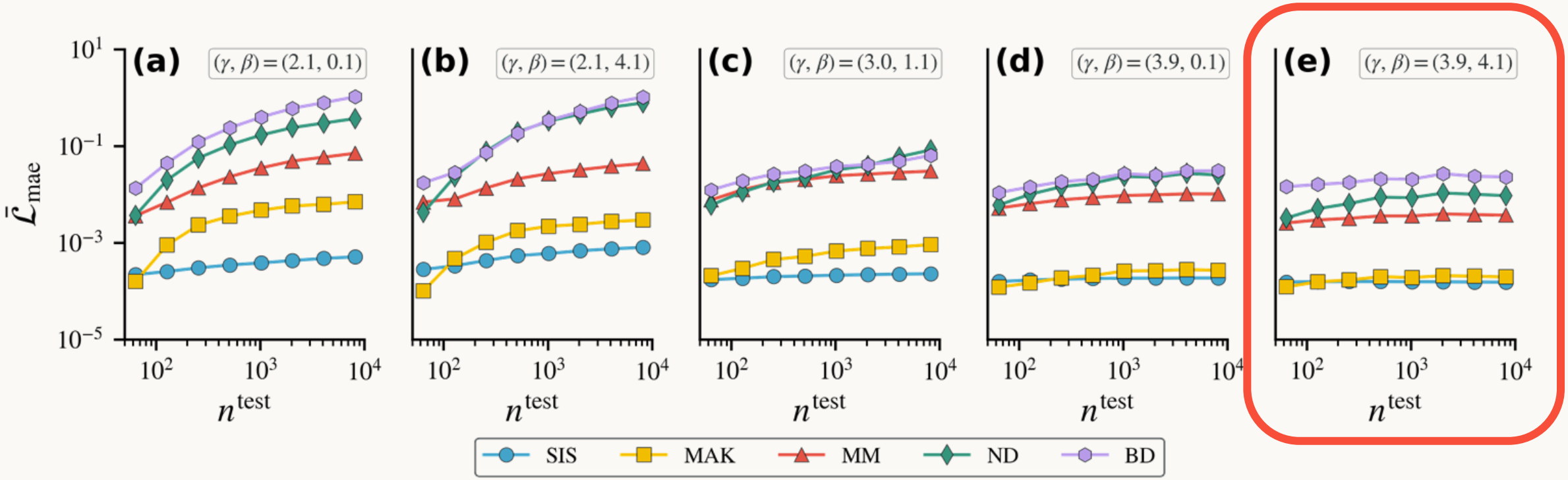

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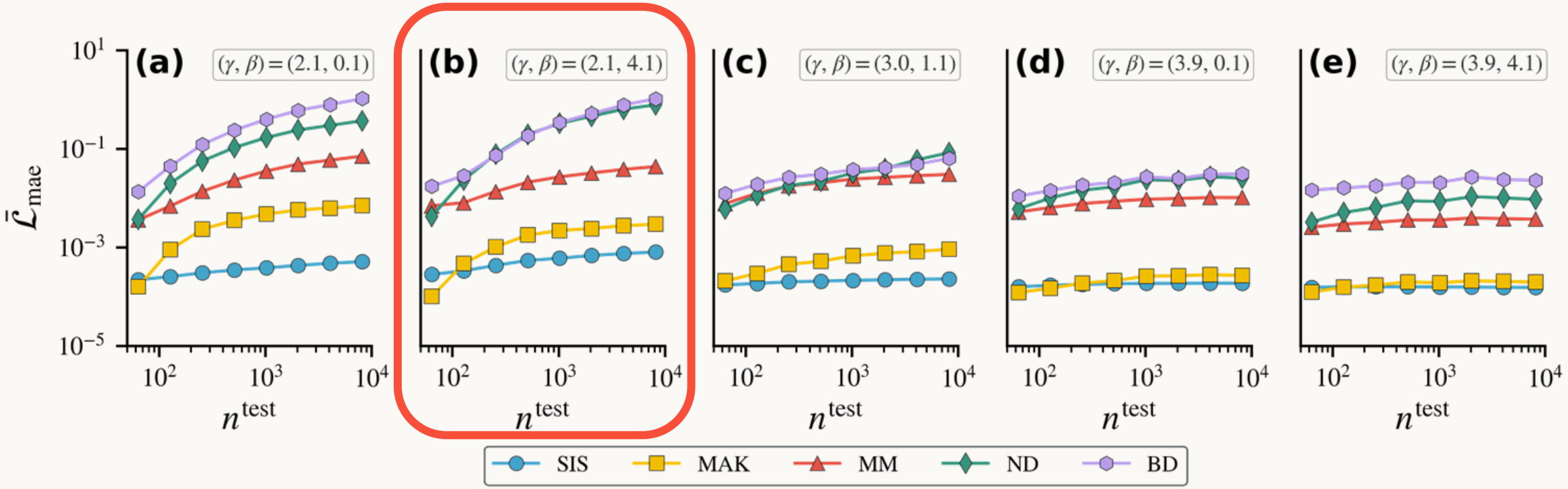

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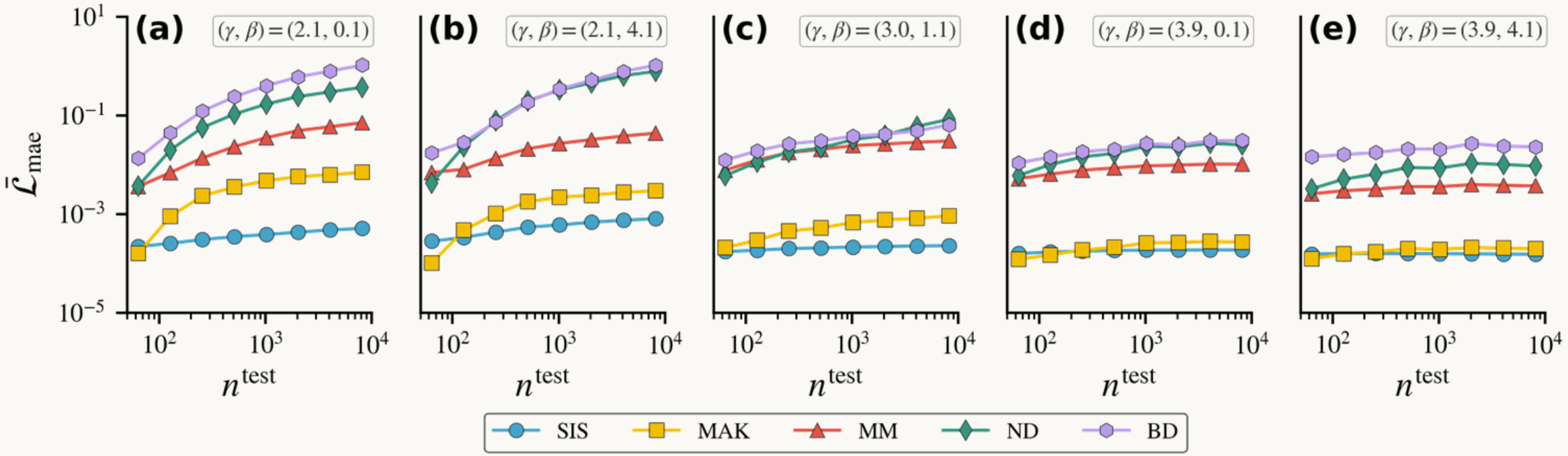


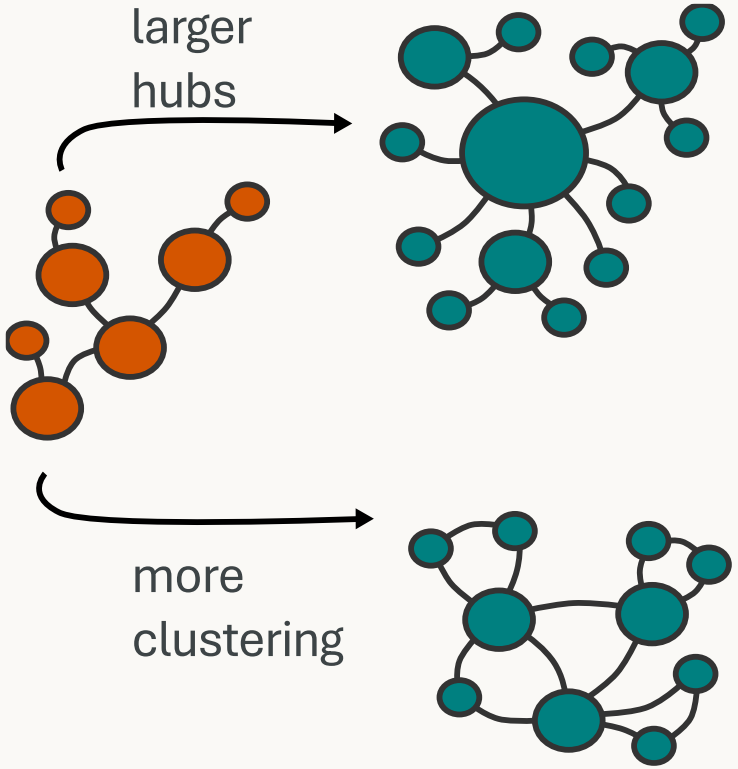
Generalization: Structurally Different Graphs

Question: Can Neural ODEs generalize to networks with different properties?

Motivation

- Many complex systems constantly evolve, causing potential mismatch between graph properties at training and test time.

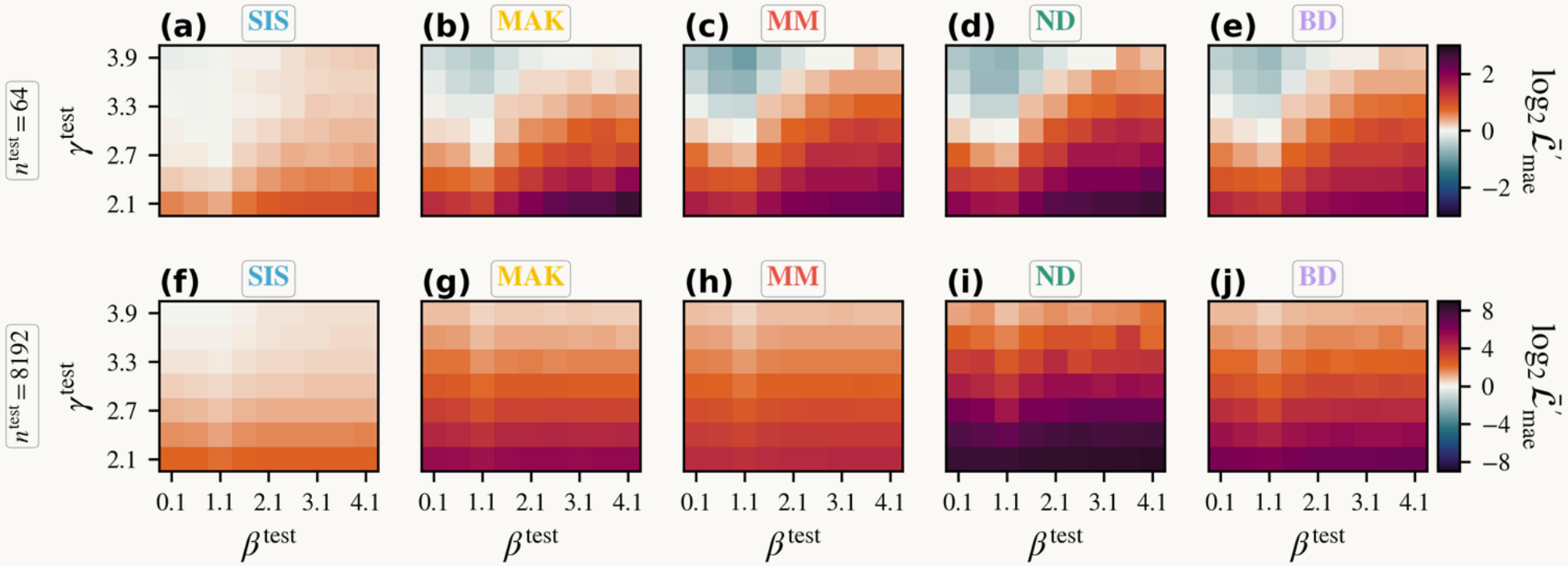
- Graph machine learning models are usually evaluated on a few benchmark datasets. Only recently, have random graph ensembles been recognized as a possible testbed [1,2,3].

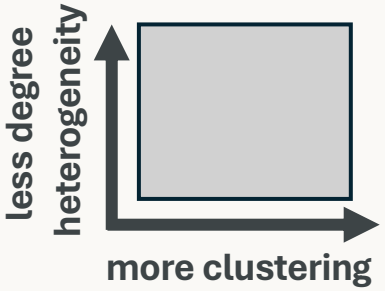


[1] *Palowitch et al.* KDD (2022) [2] *Aliakbarisani et al.* arXiv:2406.02772 (2024) [3] *Vasiliauskaite & Antulov-Fantulin* Comms Phys. 7 1 (2024)

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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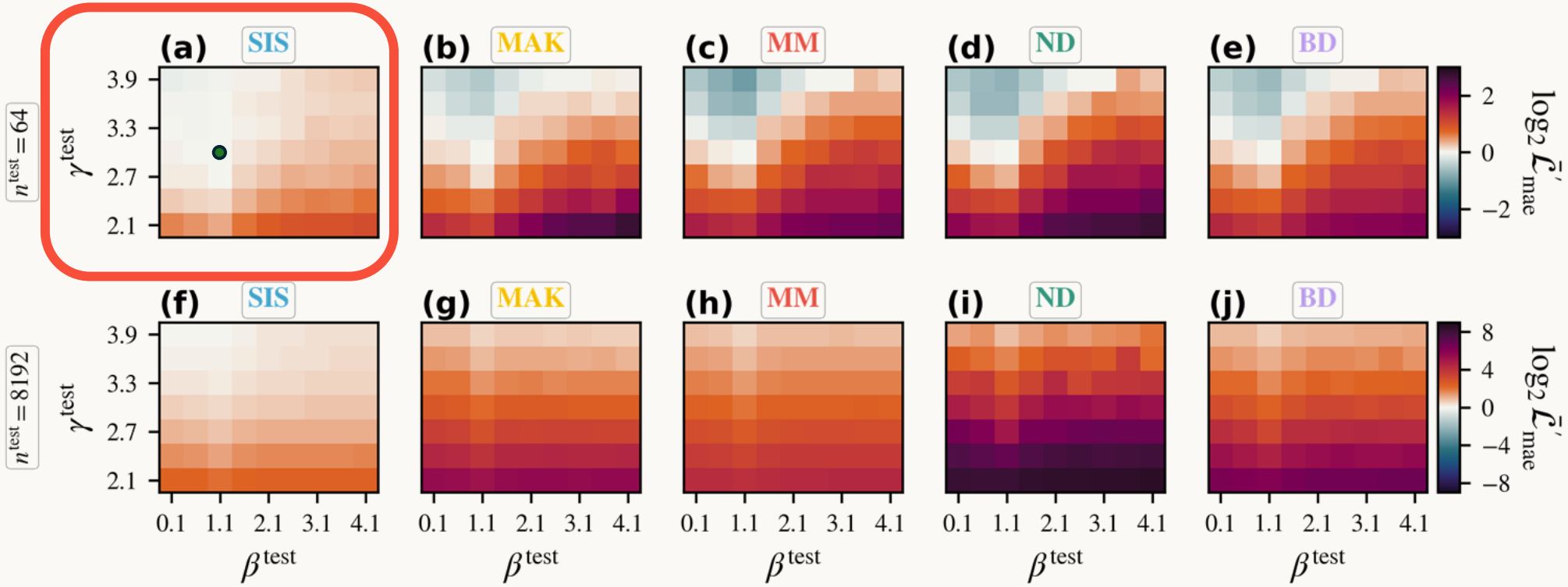

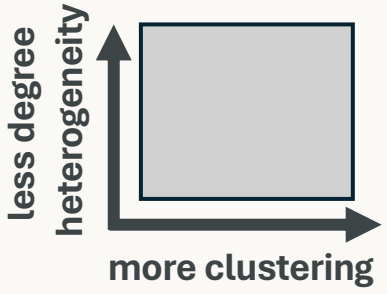

Training Parameters $(\gamma^{\text{train}}, \beta^{\text{train}}) = (3.0, 1.1)$

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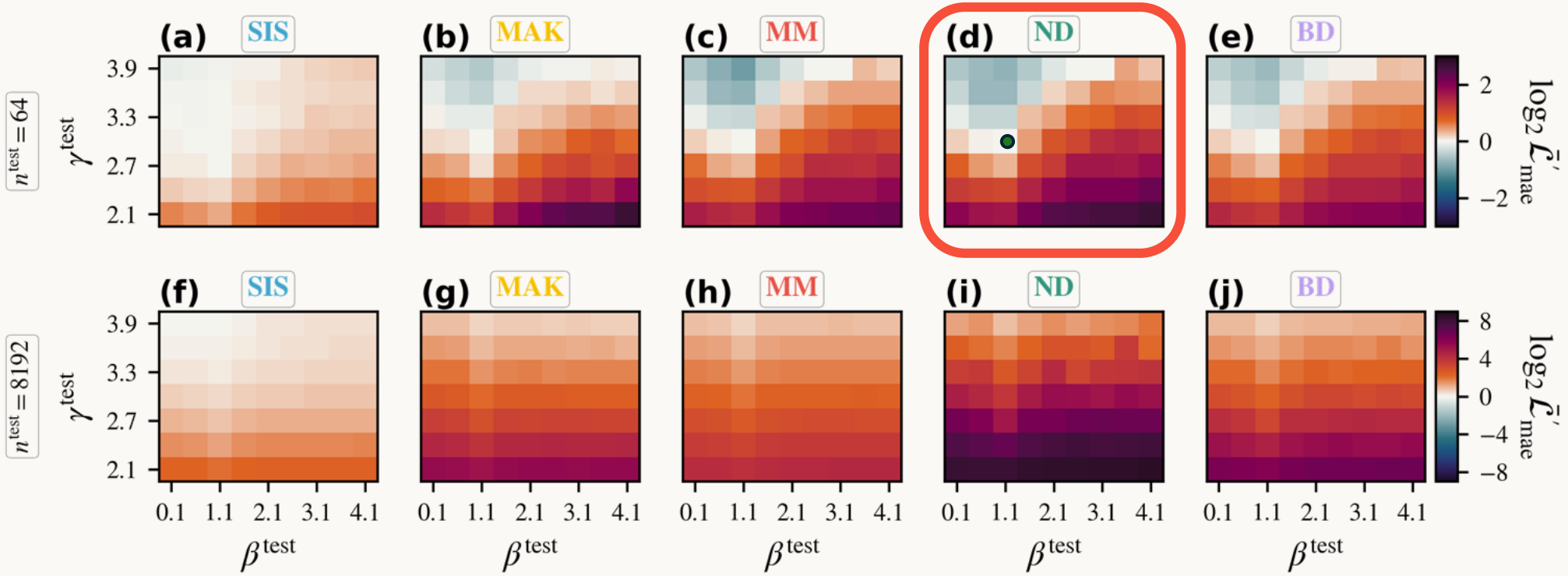

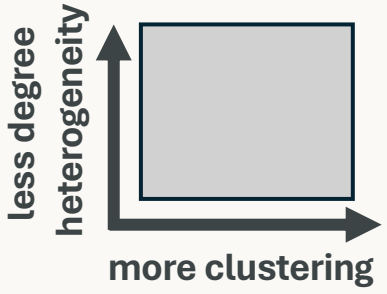

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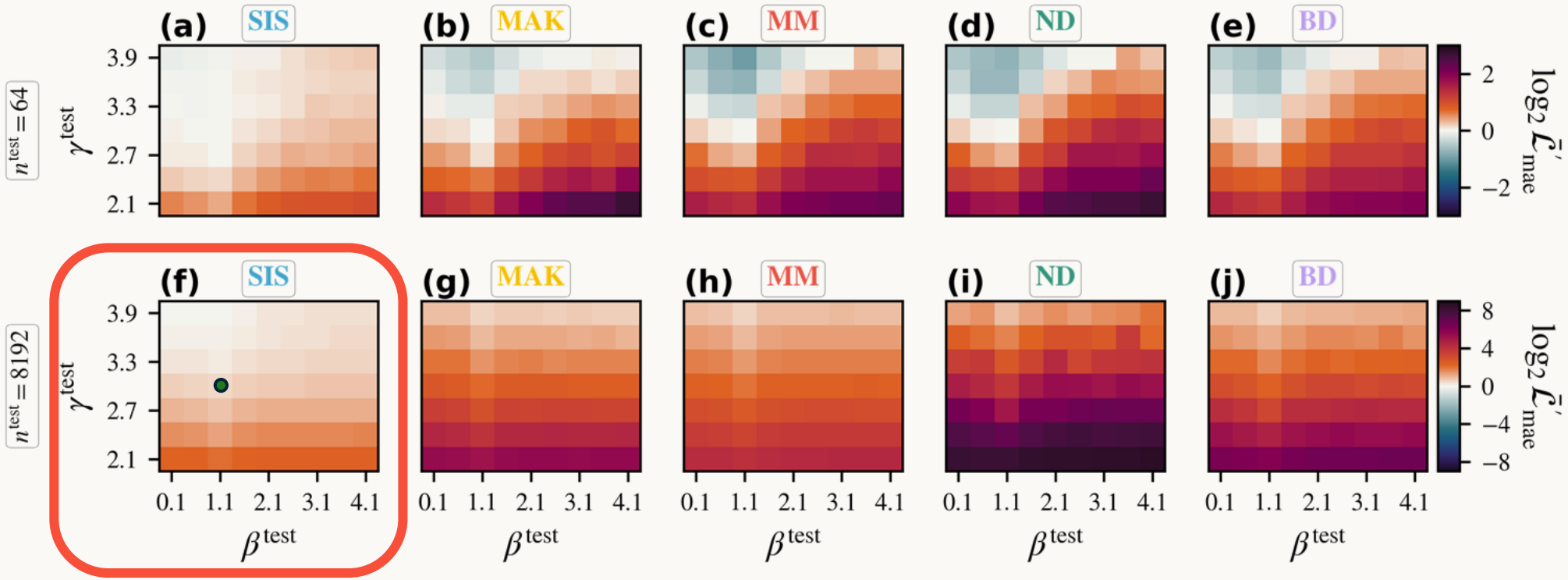

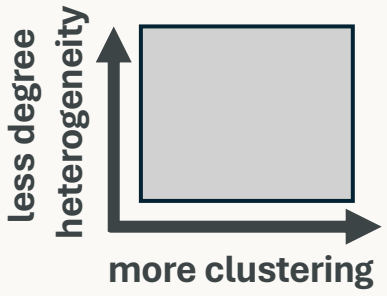

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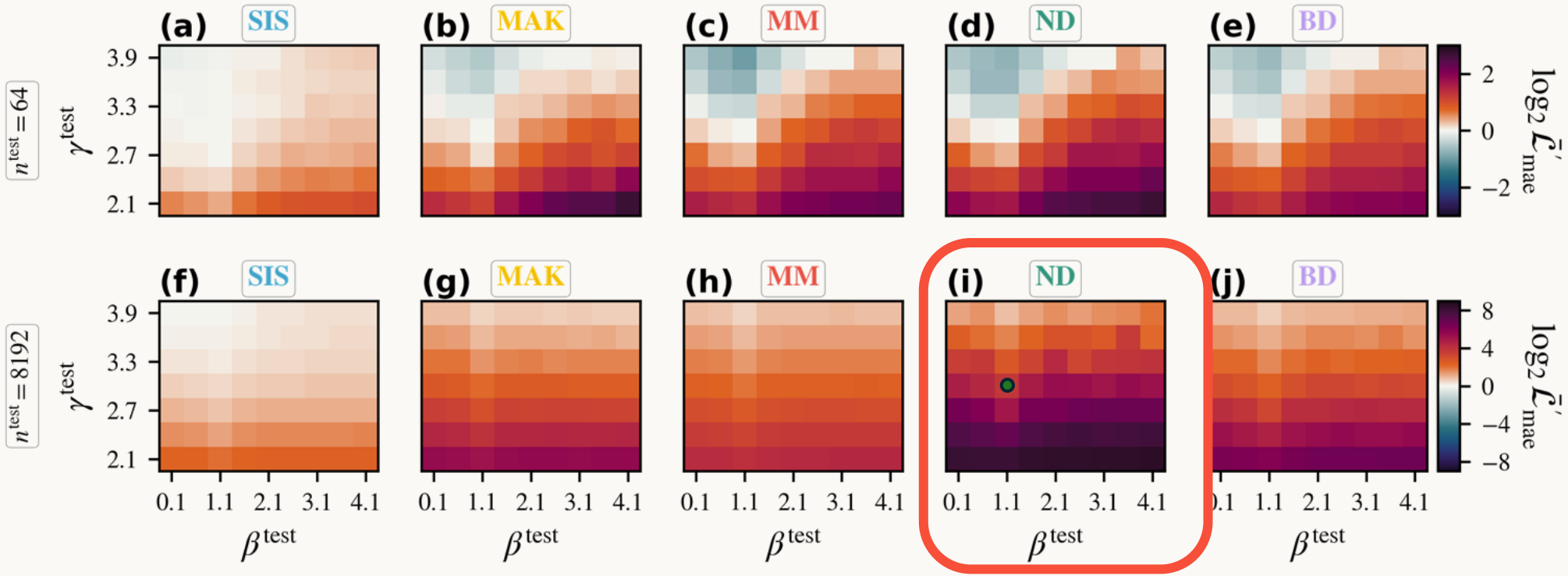

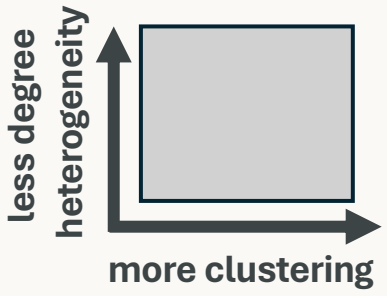

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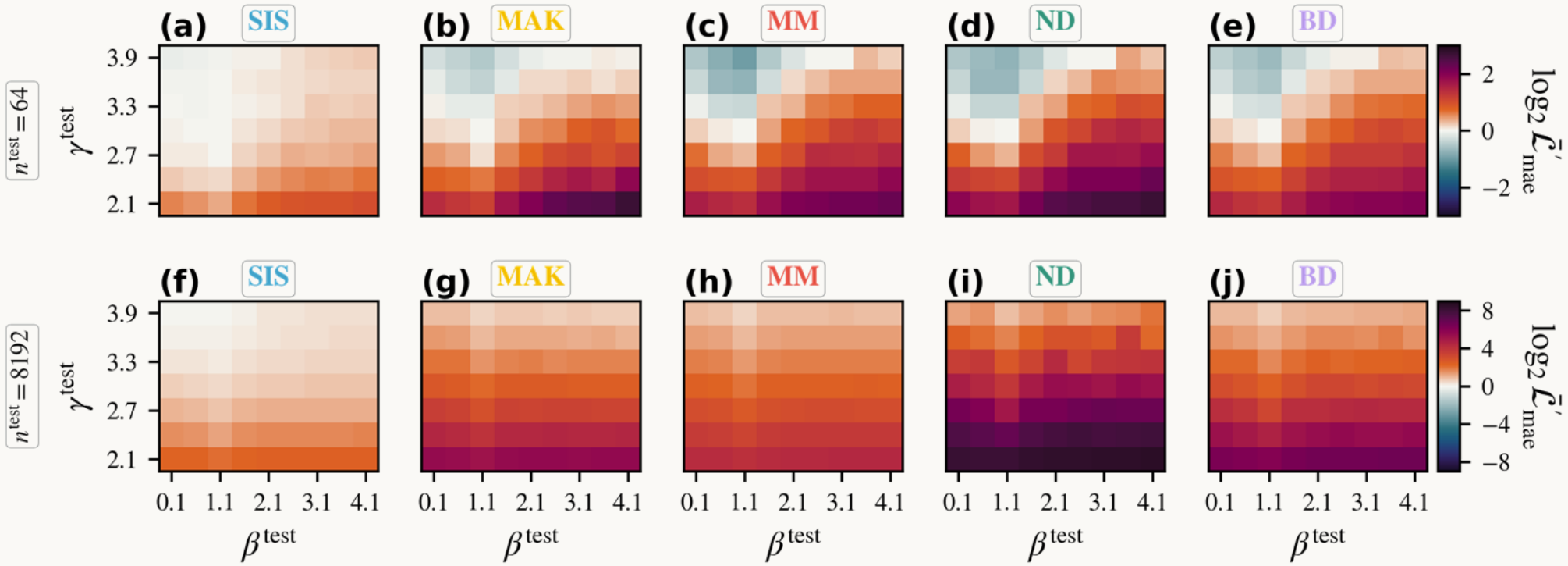

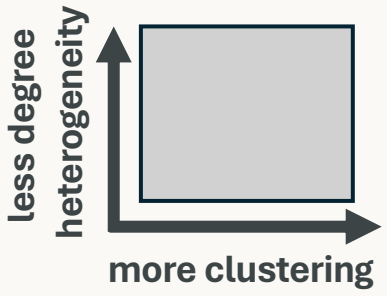

Conclusion

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.

Preprint!

https://arxiv.org/abs/2602.08980

✉ **laber.m@northeastern.edu**

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