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Degree Heterogeneity Impacts Generalization and Robustness of Neural ODEs on Graphs

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Background: Dynamical Systems on Graphs

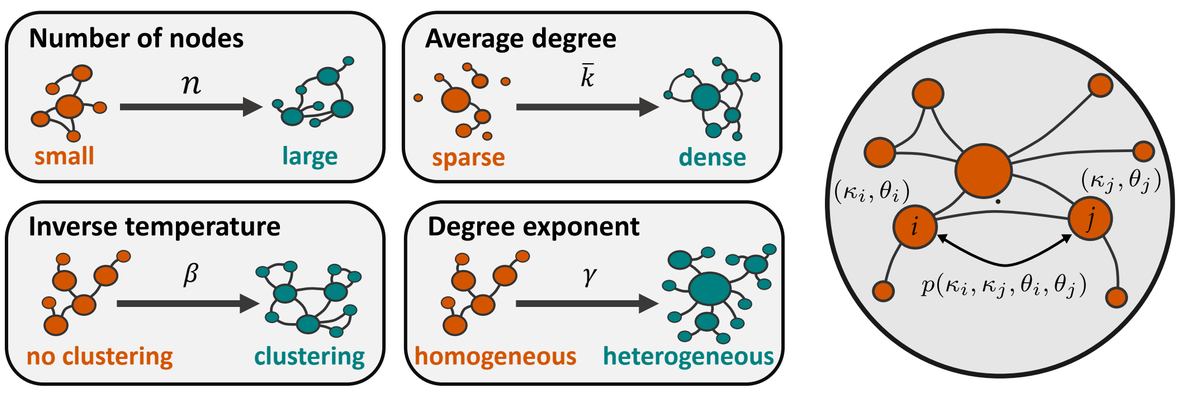
We consider **dynamical systems** in Barabási-Barzel (BB) form.

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

Five different **domains**

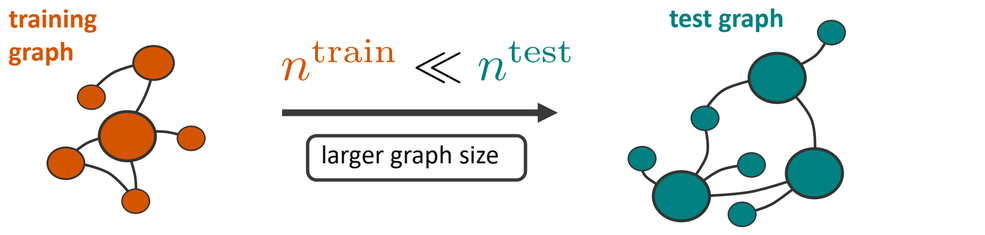
- Gene Regulation: MM model
- Epidemiology: SIS model
- Population Dynamics: BD model
- Chemistry: MAK model
- Neuroscience: ND model

Background: $\mathbb{S}^1$ Random Graph Model



Evaluation 1: Generalization across Graph Sizes

nODEs generalize across graph sizes on graphs with low degree heterogeneity but fail to do so on graphs with high degree heterogeneity.



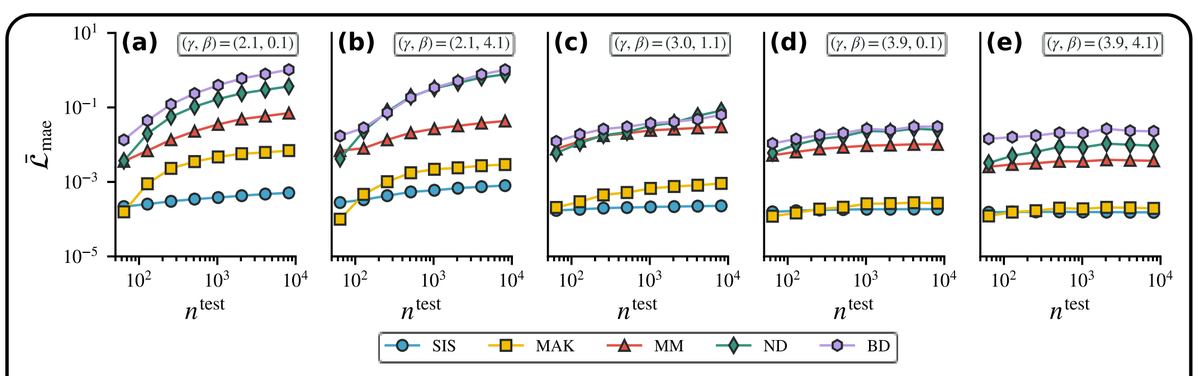
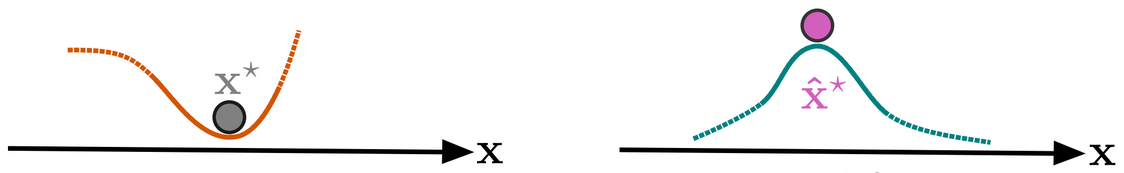


Figure 1: The ability of nODEs trained on small graphs ($n^{train} = 64$) to generalize to larger graphs ($64 \leq n^{\text{test}} \leq 8192$) with the same $\mathbb{S}^1$-model parameters depends on the exponent γ of the degree distribution but varies only weakly with inverse temperature β, which controls the clustering coefficient. The average node-wise MAE, $\overline{\mathcal{L}}_{\text{mae}}$, increases substantially with graph size on graphs with **(a)**, **(b)** strong degree heterogeneity, but less on graphs with **(c)** moderate or **(d)**, **(e)** low degree heterogeneity.

Evaluation 3: Approximating Fixed Points

We find stable fixed points of nODEs at all test graph sizes. nODEs approximate fixed points well across graph sizes on graphs with low degree heterogeneity, but on very degree-heterogeneous graphs the quality of the fixed-point approximation declines with graph size.



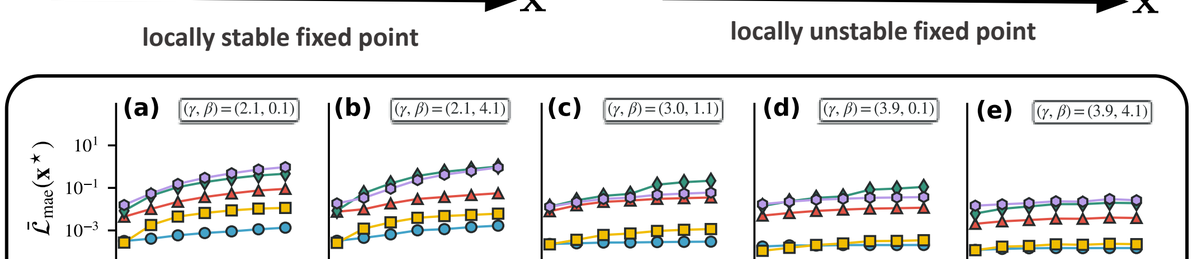


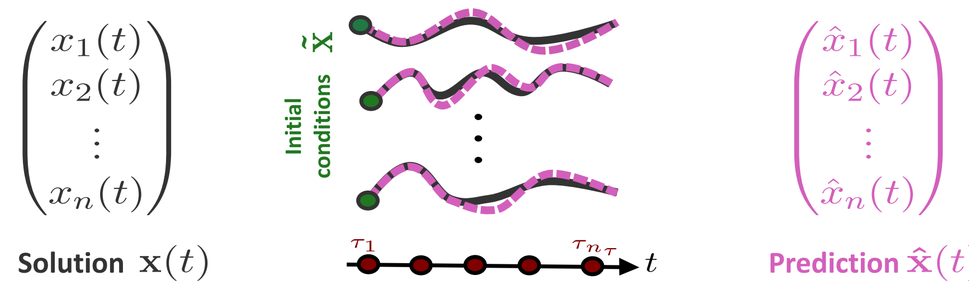
Figure 3: When nODEs trained on small graphs ($n^{\text{train}} = 64$) are evaluated on test graphs of increasing size ($64 \leq n^{\text{test}} \leq 8192$), the mean node-wise MAE, $\bar{\mathcal{L}}_{\text{mae}}(\mathbf{x}^\star)$, at the fixed point $\mathbf{x}^\star$ increases most with test graph size on graphs with **(a)**, **(b)** high degree heterogeneity, less on graphs with **(c)** moderate degree heterogeneity, and least on graphs with **(d)**, **(e)** low degree heterogeneity.

Setup: nODE Architecture

The **nODE architecture** mirrors the BB form, using 3 independent MLPs.

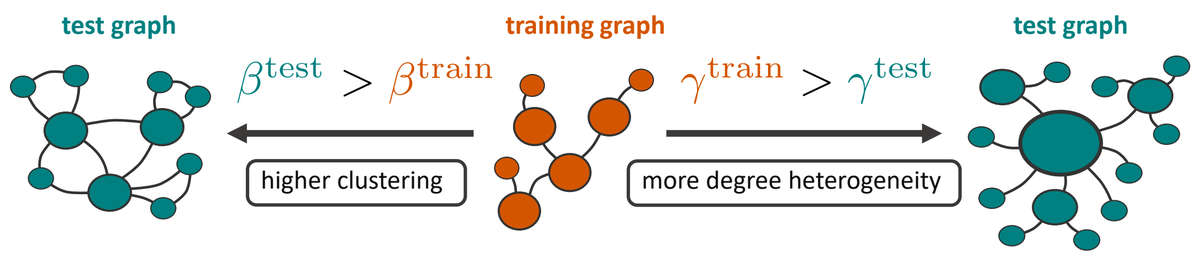
$$\frac{dx_i(t)}{dt} = f_\omega(x_i(t)) + \sum_{j\in\mathcal{V}} h^{\text{ego}}_\omega(x_i(t)) A_{ij} h^{\text{alt}}_\omega(x_j(t))$$

Input: initial conditions $\tilde{\mathbf{x}}$ and graph A. **Output:** prediction $\hat{\mathbf{x}}(t)$ at arbitrary times t.



Evaluation 2: Generalization across Properties

On small graphs, nODEs generalize to graphs with lower clustering and less degree heterogeneity but not to graphs with higher clustering and greater degree heterogeneity. Larger graph size exacerbates performance decline.



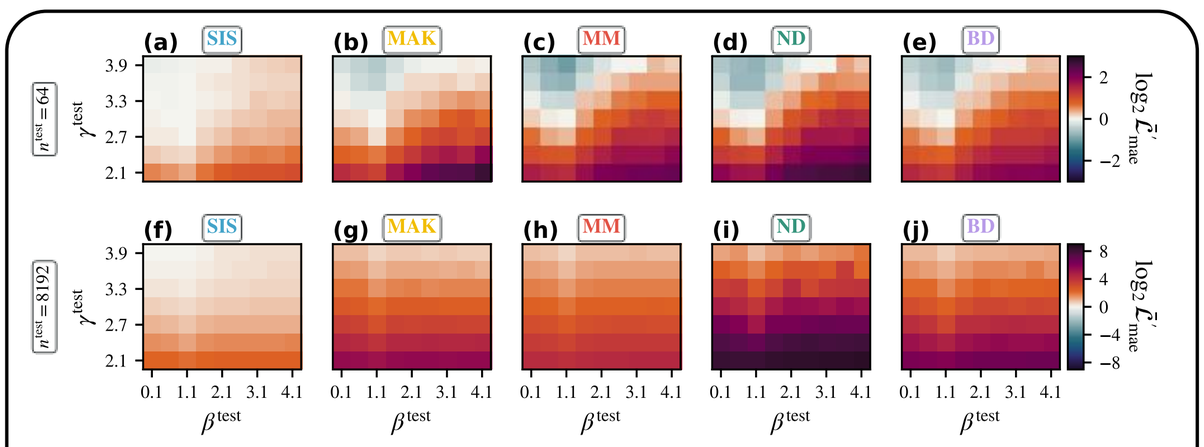


Figure 2: When nODEs trained on small graphs with moderate degree heterogeneity and clustering ($n^{train} = 64$, $\gamma = 3.0$, $\beta = 1.1$) are evaluated on graphs of the same size **(a)**-**(e)** or larger size ($n^{\text{test}} = 8192$) **(f)**-**(j)** that differ from the training graphs in γ and β, node-wise MAE relative to graphs with the same properties as the training graphs, $\overline{\mathcal{L}}'_{\text{mae}}$, increases towards more degree-heterogeneous graphs and graphs with higher clustering.

Evaluation 4: Robustness to Unobserved Nodes

When some nodes are unobserved at test time, nODEs are more robust on graphs with greater degree heterogeneity, i.e., they can tolerate a larger number of unobserved nodes before prediction error increases.

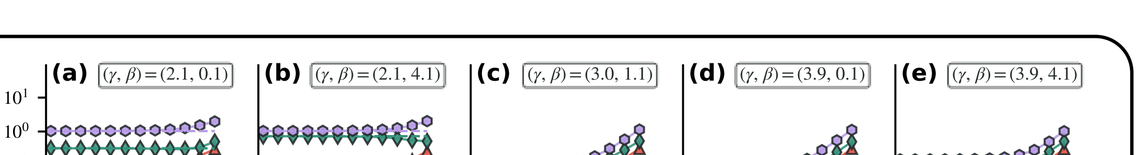


Figure 4: nODEs trained on small graphs ($n^{train} = 64$) show an increase in mean node-wise MAE, $\overline{\mathcal{L}}_{\text{mae}}$, as the number of unobserved nodes $n^{\text{test}} - n^{\text{obs}}$ increases on larger test graphs ($n^{\text{test}} = 8192$) with the same $\mathbb{S}^1$-model parameters ($\bar{k}$, γ, β) as the training graph. The increase sets in later on **(a)**, **(b)** degree-heterogeneous graphs than on graphs with **(c)** moderate or **(d)**, **(e)** low degree heterogeneity.

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