Injecting Hamiltonian Architectural Bias into Deep Graph Networks

AI4Science Talk by Simon Heilig[1] & Alessio Gravina[2]

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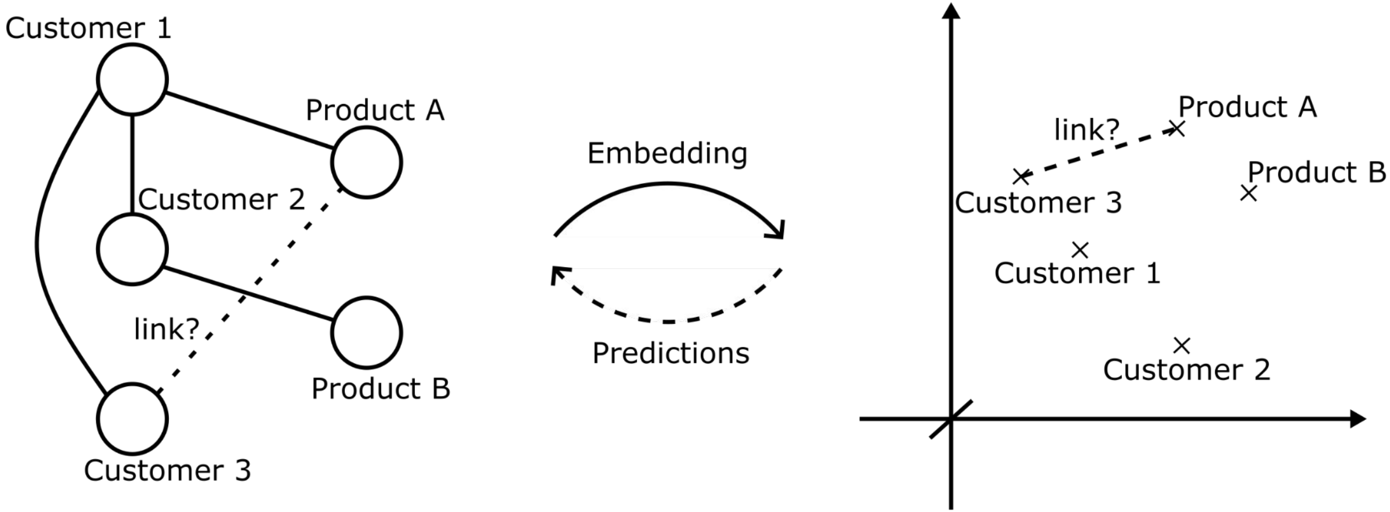
Outline

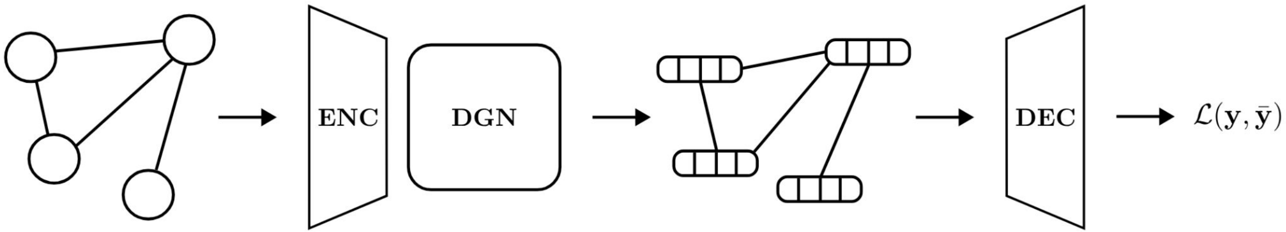
- Background
  - ML on Graphs
  - Message Passing Neural Networks
  - Neural ODEs and Hamiltonian Dynamics
- Contribution
  - (Port-)Hamiltonian Graph Neural ODE
  - Theoretical Properties
- Experimental Validation
  - Graph Transfer
  - Graph Property Prediction
  - Long Range Graph Benchmark

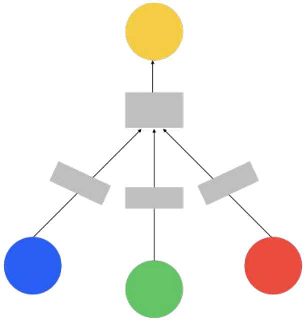
Background

Motivation: ML on Graphs



Message Passing Neural Networks





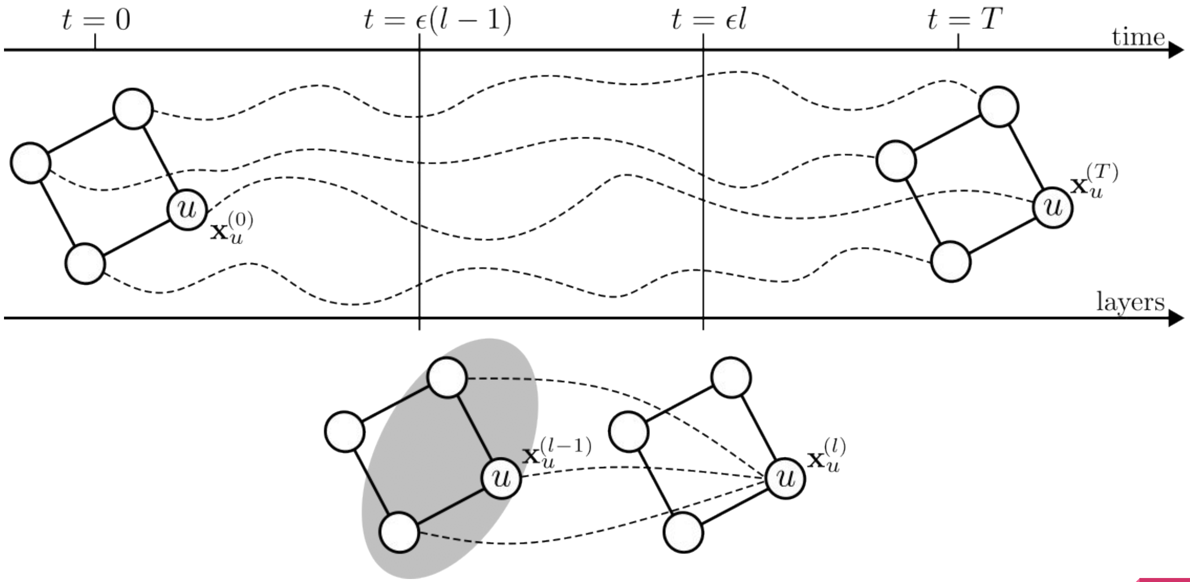
$$\mathbf{x}_u^{(l+1)} = \mathrm{UP}^{(l+1)}\left(\mathbf{x}_u^{(l)}, \mathrm{AGG}^{(l+1)}\left(\left\{\mathbf{x}_v^{(l)} \, : \, v \in \mathcal{N}_u\right\}\right)\right)$$

$$\mathbf{x}_u^{(l+1)} = \sigma\left(\mathbf{W}_{\text{self}}^{(l+1)}\mathbf{x}_u^{(l)} + \sum_{v\in\mathcal{N}_u} \mathbf{W}_{\text{msg}}^{(l+1)}\mathbf{x}_v^{(l)}\right)$$

$$\mathbf{X}^{(l+1)} = \mathbf{X}^{(l)} + \sigma\left(-\mathbf{X}^{(l)}\mathbf{W}_{\text{self}}^{(l+1)} + \mathbf{A}_{\text{agg}}\mathbf{X}^{(l)}\mathbf{W}_{\text{msg}}^{(l+1)} - \mathbf{X}^{(0)}\mathbf{W}_{\text{skip}}^{(l+1)}\right)$$

Ref: [1]

Graph Coupled Neural ODEs

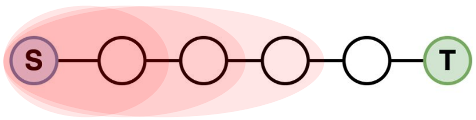


$$\frac{\mathrm{d}\mathbf{x}_u(t)}{\mathrm{d}t} = \sigma\left(\mathbf{W}_{\text{self}}(t)\mathbf{x}_u(t) + \Phi_{\mathcal{G}}(\{\mathbf{x}_v(t) : v \in \mathcal{N}_u\}, t) + \mathbf{b}(t)\right)$$

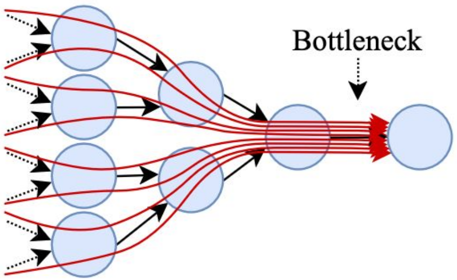
Ref: [4]

The Long-Range Regime

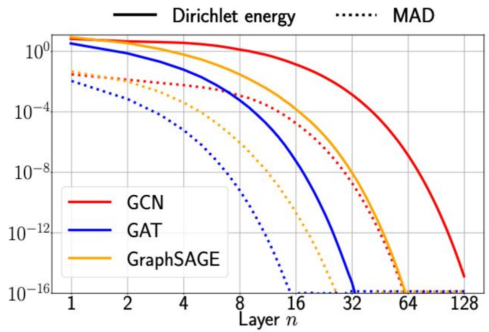
Under Reaching



Over Squashing



Over Smoothing



Hamiltonian Dynamics

Example (Equations of Motion)

$$H(\mathbf{p},\mathbf{q}) = T(\mathbf{p}) + U(\mathbf{q}), \quad \text{with } T = \frac{1}{2}\sum_{i=1,\dots,n}\frac{\|\mathbf{p}_i\|^2}{m_i}, U = -\sum_{1\leq i<j\leq n}\frac{Gm_im_j}{\|\mathbf{q}_j-\mathbf{q}_i\|}, \mathbf{p},\mathbf{q}\in\mathbb{R}^{3n}$$

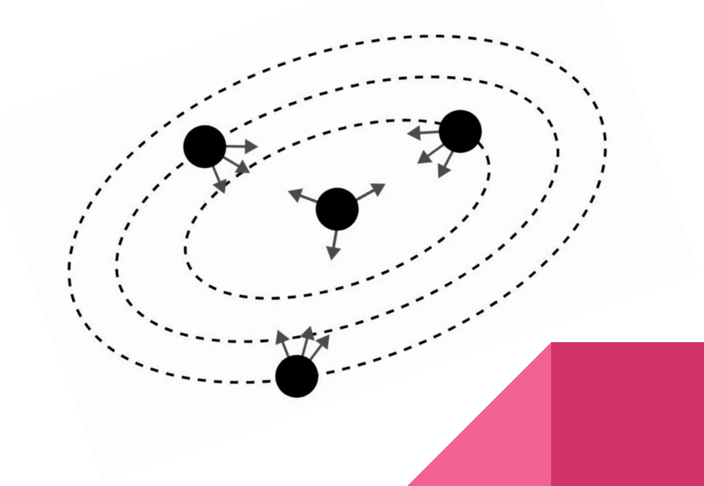
Definition (Hamiltonian Dynamics)

$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -\frac{\partial H}{\partial \mathbf{q}}(\mathbf{p},\mathbf{q}), \quad \frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \frac{\partial H}{\partial \mathbf{p}}(\mathbf{p},\mathbf{q})$$

$$\Leftrightarrow$$

$$\frac{\mathrm{d}\mathbf{y}(t)}{\mathrm{d}t} = \mathcal{J}\nabla_{\mathbf{y}}H(\mathbf{y}(t)),$$

where $\mathbf{y} = (\mathbf{p},\mathbf{q})^\top \in \mathbb{R}^{2d}$ and $\mathcal{J} = \begin{pmatrix} \mathbf{0} & -\mathbf{I}_d \\ \mathbf{I}_d & \mathbf{0} \end{pmatrix}$



Ref: [5]

(Port-)Hamiltonian DGN

Hamiltonian Inspired Message Passing

Step 1)

$$\mathbf{y} := \begin{pmatrix} \mathbf{p}_1 \\ \vdots \\ \mathbf{p}_n \\ \mathbf{q}_1 \\ \vdots \\ \mathbf{q}_n \end{pmatrix} = \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix} \in \mathbb{R}^{nd}, \text{with } \begin{pmatrix} \mathbf{p}_u \\ \mathbf{q}_u \end{pmatrix} := \mathbf{x}_u \in \mathbb{R}^d, \text{ and } H_{\mathcal{G}}(\mathbf{y}) := \sum_{u \in \mathcal{V}}^{n} \tilde{\sigma}(\mathbf{W}\mathbf{x}_u + \Phi_{\mathcal{G}}(\mathbf{y}, \mathcal{N}_u) + \mathbf{b})^\top \mathbf{1}_d$$

Step 2)

$$\frac{\mathrm{d}\mathbf{y}(t)}{\mathrm{d}t} = \mathcal{J}\nabla_{\mathbf{y}} H_{\mathcal{G}}(\mathbf{y}(t)) \Leftrightarrow \frac{\mathrm{d}\mathbf{p}(t)}{\mathrm{d}t} = -\nabla_{\mathbf{q}} H_{\mathcal{G}}(\mathbf{y}(t)), \frac{\mathrm{d}\mathbf{q}(t)}{\mathrm{d}t} = \nabla_{\mathbf{p}} H_{\mathcal{G}}(\mathbf{y}(t))$$

$$\Leftrightarrow$$

$$\frac{\mathrm{d}\mathbf{x}_u(t)}{\mathrm{d}t} = \begin{pmatrix} -\nabla_{\mathbf{q}_u} H_{\mathcal{G}}(\mathbf{y}(t)) \\ \nabla_{\mathbf{p}_u} H_{\mathcal{G}}(\mathbf{y}(t)) \end{pmatrix} = \mathcal{J}_u \nabla_{\mathbf{x}_u} H_{\mathcal{G}}(\mathbf{y}(t)) \quad , \forall\, u \in \mathcal{V}$$

$$\frac{\mathrm{d}H_{\mathcal{G}}}{\mathrm{d}t} = 0$$

Continuous and Discrete Perspective

The Continuous Dynamic

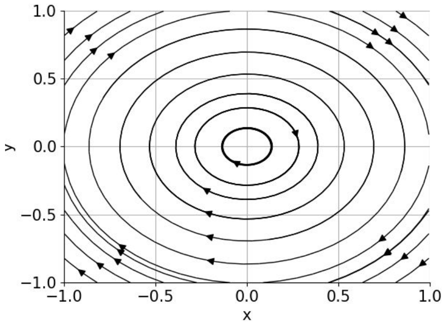
$$\frac{\mathrm{d}\mathbf{x}_u(t)}{\mathrm{d}t} = \mathcal{J}_u \nabla_{\mathbf{x}_u} H_{\mathcal{G}}(\mathbf{y}(t)) = \mathcal{J}_u \left[\mathbf{W}^\top \sigma(\mathbf{W}\mathbf{x}_u(t) + \Phi_{\mathcal{G}}(\mathbf{y}, \mathcal{N}_u) + \mathbf{b}) + \sum_{v \in \mathcal{N}_u \cup \{u\}} \frac{\partial \Phi_{\mathcal{G}}(\mathbf{y}, \mathcal{N}_v)}{\partial \mathbf{x}_u(t)}^\top \sigma(\mathbf{W}\mathbf{x}_v(t) + \Phi_{\mathcal{G}}(\mathbf{y}, \mathcal{N}_v) + \mathbf{b}) \right]$$

Symplectic Integration

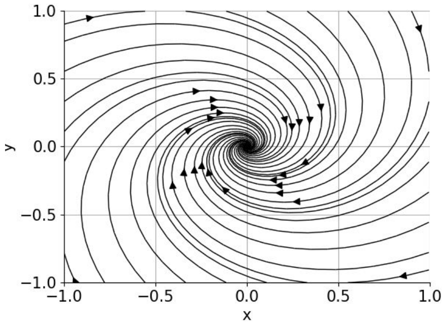
$$\begin{pmatrix} \mathbf{p}_u^{(n+1)} \\ \mathbf{q}_u^{(n+1)} \end{pmatrix} = \begin{pmatrix} \mathbf{p}_u^{(n)} \\ \mathbf{q}_u^{(n)} \end{pmatrix} + \epsilon \mathcal{J}_u \begin{pmatrix} \nabla_{\mathbf{p}_u} H_{\mathcal{G}}(\mathbf{p}^{(n+1)}, \mathbf{q}^{(n)}) \\ \nabla_{\mathbf{q}_u} H_{\mathcal{G}}(\mathbf{p}^{(n+1)}, \mathbf{q}^{(n)}) \end{pmatrix} \quad , \forall u \in \mathcal{V}$$

Assumptions on $\mathbf{W}$ and $\mathbf{V}$ for $\Phi_{\mathcal{G}}((\mathbf{p}^{(n+1)}, \mathbf{q}^{(n)}), \mathcal{N}) = \sum_{i \in \mathcal{N}} \mathbf{V} \begin{pmatrix} \mathbf{p}_i^{(n+1)} \\ \mathbf{q}_i^{(n)} \end{pmatrix}$: $\mathbf{W} = \begin{pmatrix} \mathbf{W}_p & \mathbf{0} \\ \mathbf{0} & \mathbf{W}_q \end{pmatrix}$ and $\mathbf{V} = \begin{pmatrix} \mathbf{V}_p & \mathbf{0} \\ \mathbf{0} & \mathbf{V}_q \end{pmatrix}$

Conservation and Dissipation



vs.

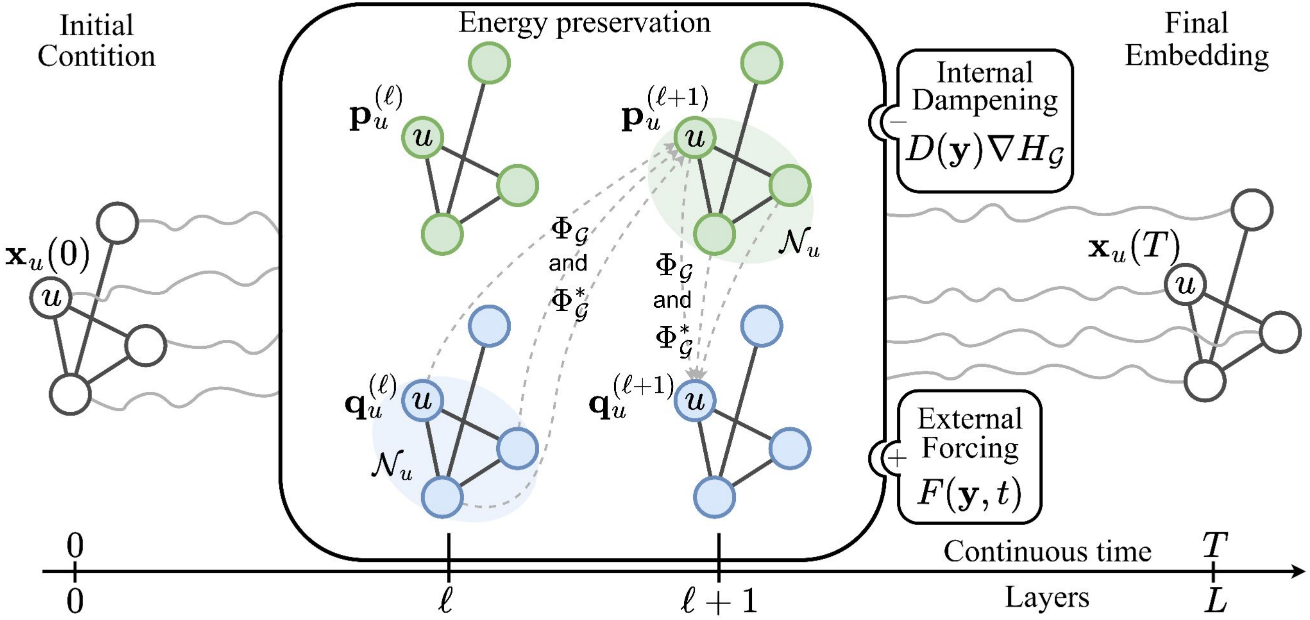


Port-Hamiltonian Dynamics

$$\frac{\mathrm{d}\mathbf{x}_u(t)}{\mathrm{d}t} = \left(\mathcal{J}_u - \begin{bmatrix} D(\mathbf{q}) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}\right) \nabla_{\mathbf{x}_u} H_{\mathcal{G}}(\mathbf{y}) + \begin{bmatrix} F(\mathbf{q}, t) \\ \mathbf{0} \end{bmatrix}, \quad \forall u \in \mathcal{V}.$$

Ref: [2]

Big Picture: Port-Hamiltonian DGN



Stability Analysis

Lemma (Eigenvalues of the Jacobian)

The local dynamics possess an Jacobian with eigenvalues purely on the imaginary axis, i.e.

$$\mathrm{Re}\left(\lambda_i\left(\frac{\partial}{\partial \mathbf{x}_u}\mathcal{J}_u \nabla_{\mathbf{x}_u} H_{\mathcal{G}}(\mathbf{y}(t))\right)\right) = 0 \quad , \forall i$$

Lemma (Divergence-Free Hamiltonian Vector Field)

The vector field defined by the local dynamics is divergence-free everywhere, which means:

$$\nabla \cdot \mathcal{J}_u \nabla_{\mathbf{x}_u} H_{\mathcal{G}}(\mathbf{y}(t)) = 0, \text{ everywhere}$$

Hence, no sources or sinks can exist in the nonlinear dynamic.

→ Allows for long-range propagation!

Sensitivity Analysis I

Theorem (Lower Bound)

Given a Hamiltonian graph ODE, the BSM for each node can not vanish. In particular, for any sub-multiplicative matrix norm $\|\cdot\|$, the lower bound is:

$$\left\| \frac{\partial \mathbf{x}_u(T)}{\partial \mathbf{x}_u(T-t)} \right\| \geq 1, \forall t \in [0, T].$$

Given a discrete Hamiltonian graph ODE obtained by a symplectic discretization scheme, the BSM can not vanish:

$$\left\| \frac{\partial \mathbf{x}_u^{(L)}}{\partial \mathbf{x}_u^{(L-j)}} \right\| \geq 1, \forall j = 0, \dots, L-1.$$

Ref: [3]

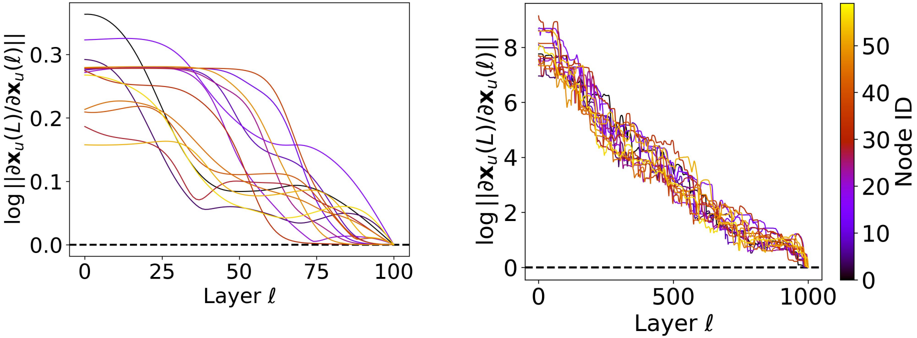
Sensitivity Analysis II

Theorem (Upper Bound)

Given a Hamiltonian graph ODE, with a nonlinearity whose derivative is bounded globally, i.e., $\exists M > 0, |\sigma'(x)| \leq M$*, and a neighborhood coupling of the form* $\Phi_{\mathcal{G}} = \sum_{v \in \mathcal{N}_u} \mathbf{V}\mathbf{x}_v$*, the BSM can be bounded above as:*

$$\left\| \frac{\partial \mathbf{x}_u(T)}{\partial \mathbf{x}_u(T-t)} \right\|_2 \leq \sqrt{d}\, \mathit{exp}(QT), \quad \forall t \in [0, T]$$

Where $Q = \sqrt{d}\, M \|\mathbf{W}\|_2^2 + \sqrt{d}\, M\, \mathit{max}_{i \in [n]} |\mathcal{N}_i| \|\mathbf{V}\|_2^2$.



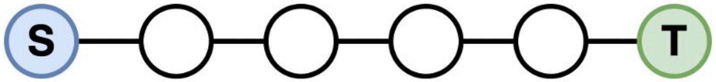
Experiments

Experimental outline

- Assess the efficacy in **preserving long-range information** between nodes
  - Graph transfer tasks
  - Graph property prediction tasks
  - Long Range Graph Benchmark

Graph Transfer task

- Propagate a label from a source to a target node



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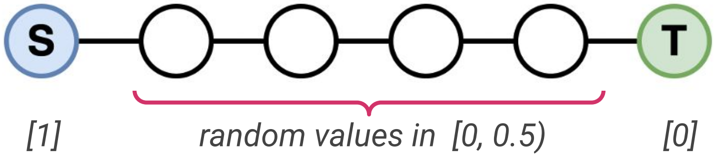
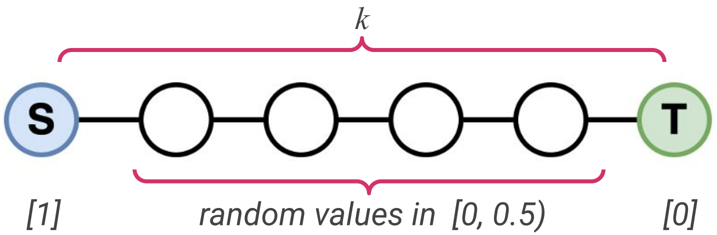


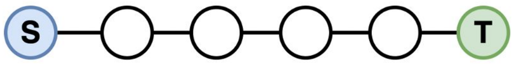
Graph Transfer task

- Propagate a label from a source to a target node
    - Increasing distance k

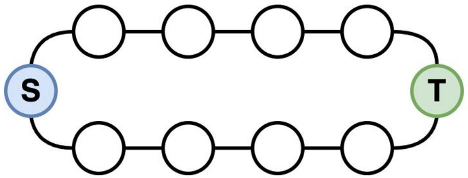


Graph Transfer task

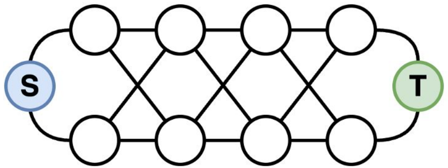
- Propagate a label from a source to a target node
  - Increasing distance k
  - Multiple graph topologies



Line graph



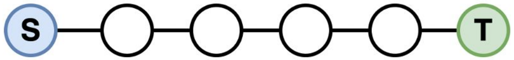
Ring graph



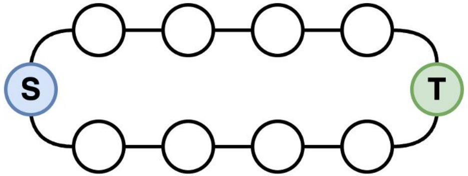
Crossed-Ring graph

Graph Transfer task

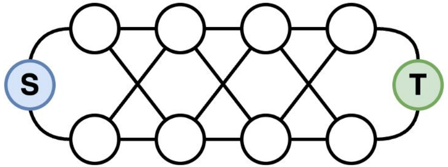
- Propagate a label from a source to a target node
  - Increasing distance k
  - Multiple graph topologies
  - MSE as metric



Line graph

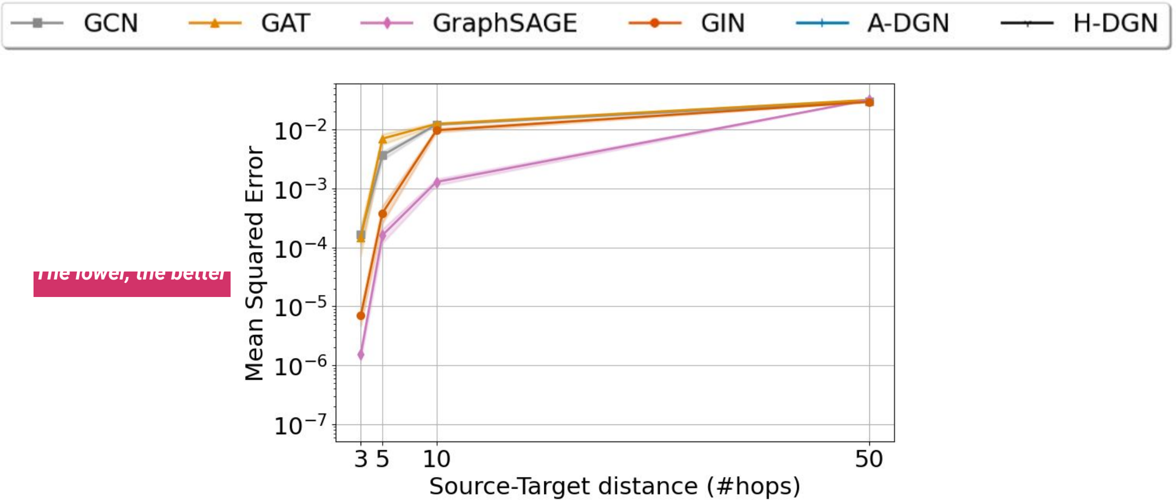


Ring graph



Crossed-Ring graph

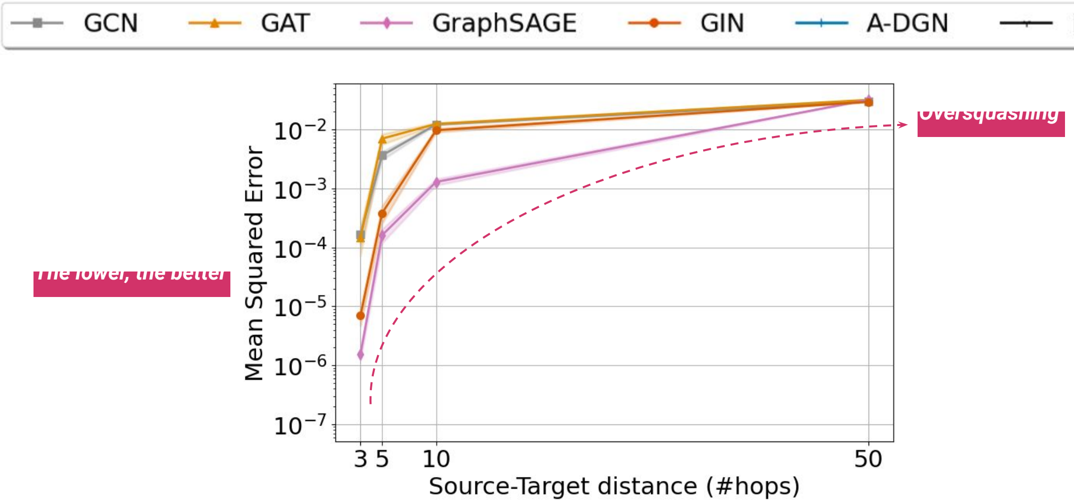
Graph Transfer task



The lower, the better

Line graph

Graph Transfer task



Line graph

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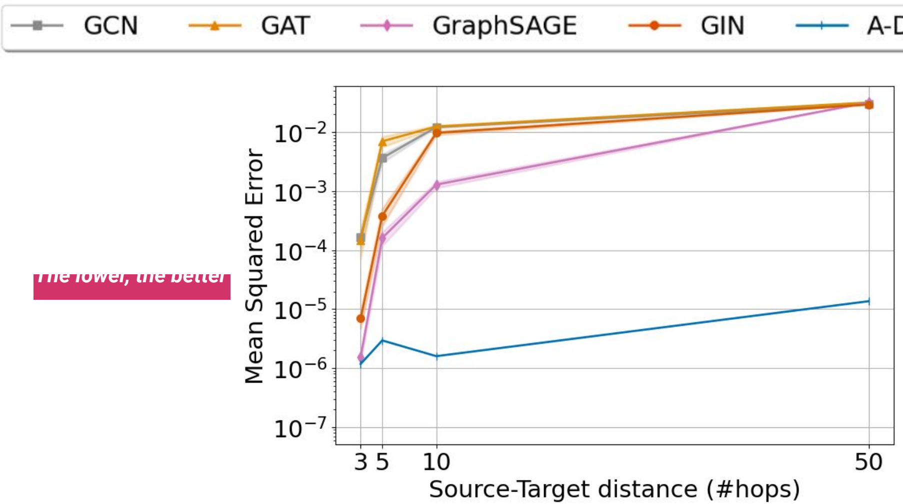


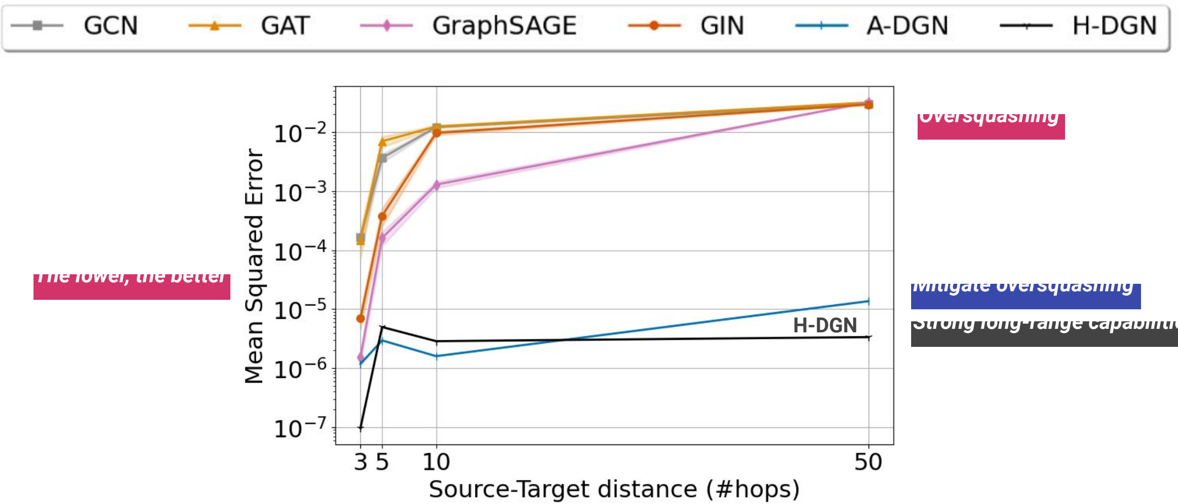
The lower, the better

Oversquashing

Mitigate oversquashing

Line graph

Graph Transfer task



Oversquashing

The lower, the better

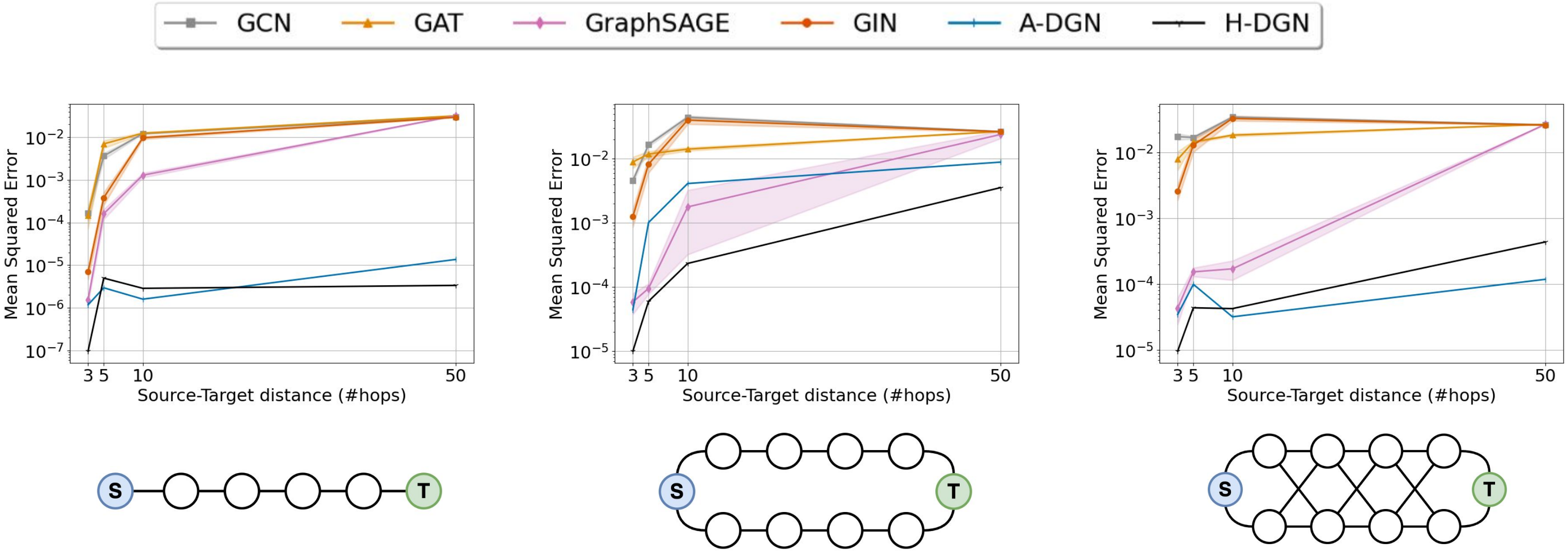
Mitigate oversquashing

Strong long-range capabilities

Line graph

Graph Transfer task

The lower, the better



Graph Property Prediction

- Introduced in [4]
- Predict 3 graph properties

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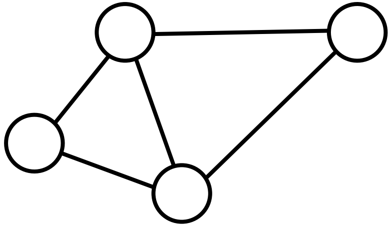

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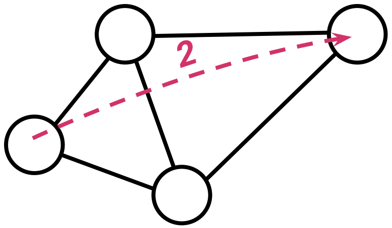

Graph Property Prediction

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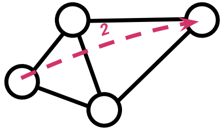
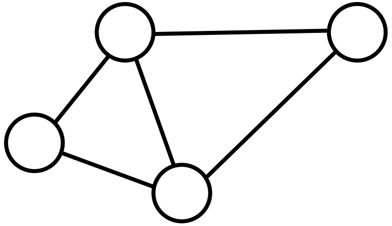
  - Single source shortest path (SSSP)





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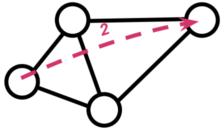

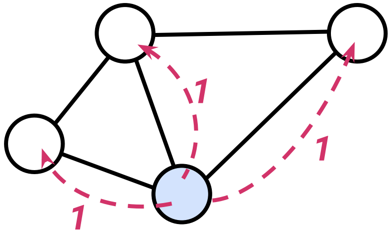

Graph Property Prediction

- Introduced in [4]
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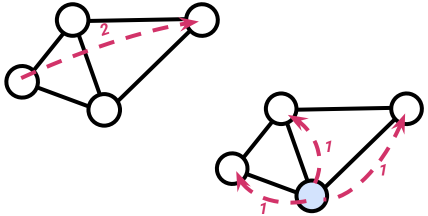
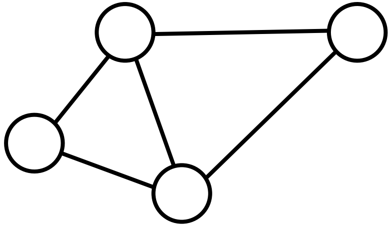
  - Graph diameter
  - Single source shortest path (SSSP)
  - Node eccentricity





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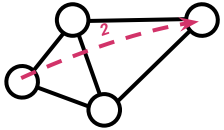

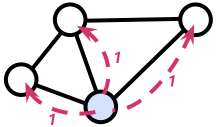

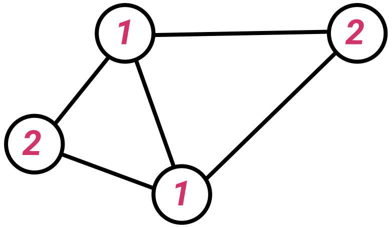

Graph Property Prediction

Table 1: Mean test log_{10}(MSE) and std average over 4 training seeds on the Graph Property Prediction. Our methods and DE-DGN baselines are implemented with weight sharing. The **first**, **second**, and **third** best scores are colored.

The lower, the better

Model	Eccentricity	Diameter	SSSP
MPNNs			
GCN	$0.8468_{\pm 0.0028}$	$0.7424_{\pm 0.0466}$	$0.9499_{\pm 9.2 \cdot 10^{-5}}$
GAT	$0.7909_{\pm 0.0222}$	$0.8221_{\pm 0.0752}$	$0.6951_{\pm 0.1499}$
GraphSAGE	$0.7863_{\pm 0.0207}$	$0.8645_{\pm 0.0401}$	$0.2863_{\pm 0.1843}$
GIN	$0.9504_{\pm 0.0007}$	$0.6131_{\pm 0.0990}$	$-0.5408_{\pm 0.4193}$
GCNII	$0.7640_{\pm 0.0355}$	$0.5287_{\pm 0.0570}$	$-1.1329_{\pm 0.0135}$
DE-DGNs			
DGC	$0.8261_{\pm 0.0032}$	$0.6028_{\pm 0.0050}$	$-0.1483_{\pm 0.0231}$
GraphCON	$0.6833_{\pm 0.0074}$	$0.0964_{\pm 0.0620}$	$-1.3836_{\pm 0.0092}$
GRAND	$0.6602_{\pm 0.1393}$	$0.6715_{\pm 0.0490}$	$-0.0942_{\pm 0.3897}$
A-DGN	$\mathbf{0.4296}_{\pm 0.1003}$	$\mathbf{-0.5188}_{\pm 0.1812}$	$\mathbf{-3.2417}_{\pm 0.0751}$
Ours			
H-DGN	$\mathbf{-0.7248}_{\pm 0.1068}$	$\mathbf{-0.5473}_{\pm 0.1074}$	$\mathbf{-3.0467}_{\pm 0.1615}$
PH-DGN	$\mathbf{-0.9348}_{\pm 0.2097}$	$\mathbf{-0.5385}_{\pm 0.0187}$	$\mathbf{-4.2993}_{\pm 0.0721}$

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GraphCON	$0.6833_{\pm 0.0074}$	$0.0964_{\pm 0.0620}$	$-1.3836_{\pm 0.0092}$
GRAND	$0.6602_{\pm 0.1393}$	$0.6715_{\pm 0.0490}$	$-0.0942_{\pm 0.3897}$
A-DGN	$\mathbf{0.4296}_{\pm 0.1003}$	$\mathbf{-0.5188}_{\pm 0.1812}$	$\mathbf{-3.2417}_{\pm 0.0751}$
Ours			
H-DGN	$\mathbf{-0.7248}_{\pm 0.1068}$	$\mathbf{-0.5473}_{\pm 0.1074}$	$\mathbf{-3.0467}_{\pm 0.1615}$
PH-DGN	$\mathbf{-0.9348}_{\pm 0.2097}$	$\mathbf{-0.5385}_{\pm 0.0187}$	$\mathbf{-4.2993}_{\pm 0.0721}$

0.33 log(MSE) better than the best baseline on average

Graph Property Prediction

Table 1: Mean test log_{10}(MSE) and std average over 4 training seeds on the Graph Property Prediction. Our methods and DE-DGN baselines are implemented with weight sharing. The **first**, **second**, and **third** best scores are colored.

The lower, the better

Model	Eccentricity	Diameter	SSSP
MPNNs			
GCN	$0.8468_{\pm 0.0028}$	$0.7424_{\pm 0.0466}$	$0.9499_{\pm 9.2 \cdot 10^{-5}}$
GAT	$0.7909_{\pm 0.0222}$	$0.8221_{\pm 0.0752}$	$0.6951_{\pm 0.1499}$
GraphSAGE	$0.7863_{\pm 0.0207}$	$0.8645_{\pm 0.0401}$	$0.2863_{\pm 0.1843}$
GIN	$0.9504_{\pm 0.0007}$	$0.6131_{\pm 0.0990}$	$-0.5408_{\pm 0.4193}$
GCNII	$0.7640_{\pm 0.0355}$	$0.5287_{\pm 0.0570}$	$-1.1329_{\pm 0.0135}$
DE-DGNs			
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PH-DGN	$\mathbf{-0.9348}_{\pm 0.2097}$	$\mathbf{-0.5385}_{\pm 0.0187}$	$\mathbf{-4.2993}_{\pm 0.0721}$

0.33 log(MSE) better

0.81 log(MSE) better than the best baseline on average

Graph Property Prediction

Table 1: Mean test log_{10}(MSE) and std average over 4 training seeds on the Graph Property Prediction. Our methods and DE-DGN baselines are implemented with weight sharing. The **first**, **second**, and **third** best scores are colored.

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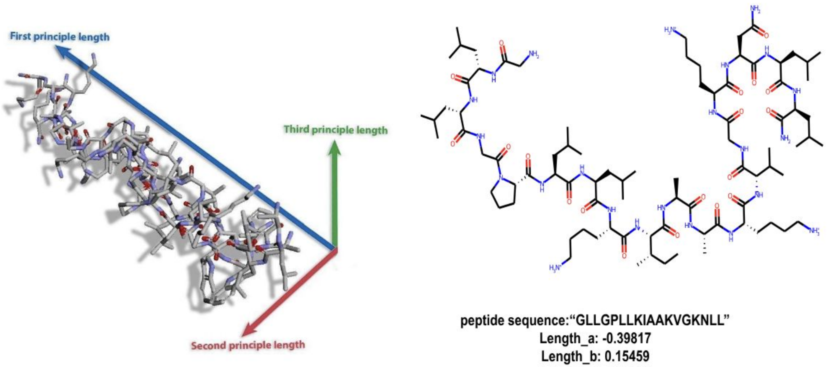
1.98 log(MSE) better *than the best MPNN on average*

0.33 log(MSE) better

0.81 log(MSE) better *than the best baseline on average*

Long Range Graph Benchmark

- Real-world benchmark
  - **Peptide-func** and **Peptide-struct**



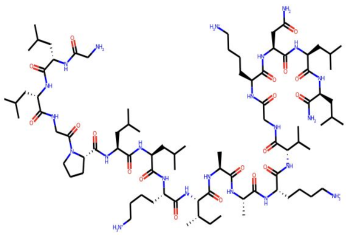
peptide sequence:"GLLGPLLKIAAKVGKNLL"
Length_a: -0.39817
Length_b: 0.15459
Length_c: -0.27048

Long Range Graph Benchmark

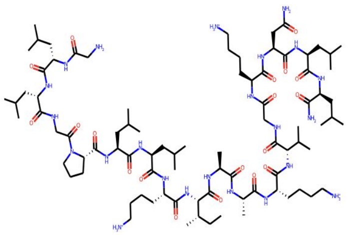
- Real-world benchmark
  - **Peptide-func** and **Peptide-struct**

- Multi-label graph **classif**.
- Predict the peptide **function**

- Multi-dim graph **regression**
- Predict **structural properties** of peptides



Is it an antiviral peptide?
Is it an antibacterial peptide?
...



Inertia mass?
Length?
Sphericity?
...

Long Range Graph Benchmark

Table 2: Results for Peptides-func and Peptides-struct averaged over 3 training seeds. The first, second, and **third** best scores are colored.

Model	Peptides-func AP ↑	Peptides-struct MAE ↓
MPNNs		
GCN	$0.6860_{\pm 0.0050}$	$\mathbf{0.2460}_{\pm 0.0007}$
GCNII	$0.5543_{\pm 0.0078}$	$0.3471_{\pm 0.0010}$
GINE	$0.6621_{\pm 0.0067}$	$0.2473_{\pm 0.0017}$
GatedGCN	$0.6765_{\pm 0.0047}$	$0.2477_{\pm 0.0009}$
Multi-hop DGNs		
DIGL+MPNN+LapPE	$0.6830_{\pm 0.0026}$	$0.2616_{\pm 0.0018}$
MixHop-GCN+LapPE	$0.6843_{\pm 0.0049}$	$0.2614_{\pm 0.0023}$
DRew-GCN+LapPE	$\mathbf{0.7150}_{\pm 0.0044}$	$0.2536_{\pm 0.0015}$
Transformers		
Transformer+LapPE	$0.6326_{\pm 0.0126}$	$0.2529_{\pm 0.0016}$
SAN+LapPE	$0.6384_{\pm 0.0121}$	$0.2683_{\pm 0.0043}$
GraphGPS+LapPE	$0.6535_{\pm 0.0041}$	$\mathbf{0.2500}_{\pm 0.0005}$
DE-DGNs		
GRAND	$0.5789_{\pm 0.0062}$	$0.3418_{\pm 0.0015}$
GraphCON	$0.6022_{\pm 0.0068}$	$0.2778_{\pm 0.0018}$
A-DGN	$0.5975_{\pm 0.0044}$	$0.2874_{\pm 0.0021}$
Ours		
H-DGN	$\mathbf{0.6961}_{\pm 0.0070}$	$0.2581_{\pm 0.0020}$
PH-DGN	$\mathbf{0.7012}_{\pm 0.0045}$	$\mathbf{0.2465}_{\pm 0.0020}$

Long Range Graph Benchmark

include PE and SE

Table 2: Results for Peptides-func and Peptides-struct averaged over 3 training seeds. The **first**, **second**, and **third** best scores are colored.

Model	Peptides-func AP ↑	Peptides-struct MAE ↓
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Long Range Graph Benchmark

include PE and SE

Better than MPNN, DE-DGN, graph transformers and rewiring

Table 2: Results for Peptides-func and Peptides-struct averaged over 3 training seeds. The first, second, and **third** best scores are colored.

Model	Peptides-func AP ↑	Peptides-struct MAE ↓
MPNNs		
GCN	$0.6860_{\pm 0.0050}$	$0.2460_{\pm 0.0007}$
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Conclusions

- PH-DGN is a new framework for DGNs
  - **Non-dissipative** and **non-conservative** behaviors equilibrium
  - Effectively explore long-range dependencies
- PH-DGN can be used to reinterpret and extend any classical DGN
- Our results show that:
  - PH-DGN outperforms state-of-the-art models
  - Data-driven forces maximize long-range propagation efficacy

References

[1] Di Giovanni, Francesco, et al. “Understanding convolution on graphs via energies”. Transactions on Machine Learning Research (2023).

[2] Desai, Shaan A., et al. “Port-Hamiltonian neural networks for learning explicit time-dependent dynamical systems”. Phys. Rev. E 104 (3 Sept. 2021): 034312.

[3] Galimberti, Clara Lucía, et al. “Hamiltonian Deep Neural Networks Guaranteeing Nonvanishing Gradients by Design”. IEEE Transactions on Automatic Control 68, no. 5 (2023): 3155–3162.

[4] Gravina, Alessio, Davide Bacciu, and Claudio Gallicchio. “Anti-Symmetric DGN: a stable architecture for Deep Graph Networks”. In The Eleventh International Conference on Learning Representations. 2023.

[5] Meyer, Kenneth R, and Daniel C Offin. Introduction to Hamiltonian Dynamical Systems and the N-Body Problem. 3rd ed. Springer, Cham, 2017.

The Team

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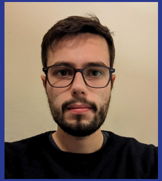

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Thank you for your attention

Arxiv

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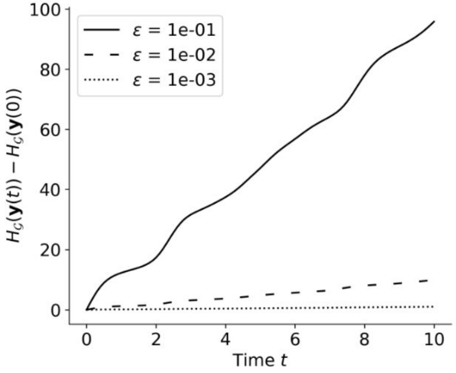
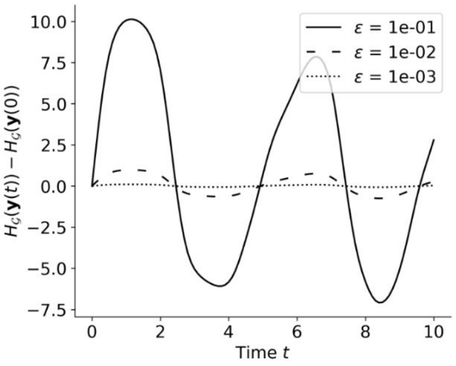
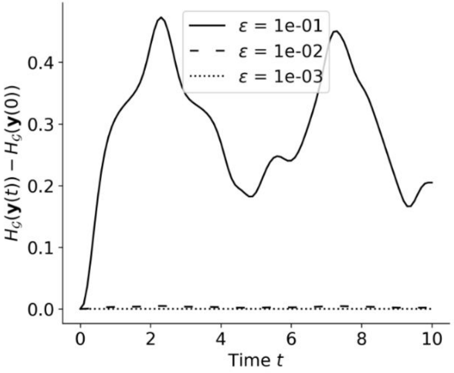
Backup I



Forward Euler



Symplectic Euler



Strömer-Verlet

method	H error	solution error
Forward Euler	$\mathcal{O}(t\epsilon)$	$\mathcal{O}(t^2\epsilon)$
Symplectic Euler	$\mathcal{O}(\epsilon)$	$\mathcal{O}(t\epsilon)$
Störmer-Verlet	$\mathcal{O}(\epsilon^2)$	$\mathcal{O}(t\epsilon^2)$

Backup II

Architecture

Coupling: $\Phi_{\mathbf{p}}, \Phi_{\mathbf{q}} \in \{$Vanilla , GCN$\}$

Decoding: $\{\mathbf{p}, \mathbf{q}, (\mathbf{p}, \mathbf{q})\}$

Dimension: $d \in \{10, 20, 30\}$

Port-Hamiltonian

Dampening: $$D_u(\mathbf{q}) = \begin{cases} \mathbf{w} \in \mathbb{R}^d \\ \mathrm{ReLU}(\mathbf{w}) \in \mathbb{R}^d \\ \mathrm{lin}(\tilde{d}, d) \circ \mathrm{ReLU} \circ \mathrm{lin}(\tilde{d}, \tilde{d}) \circ \mathrm{ReLU} \circ \mathrm{lin}(\tilde{d}, \tilde{d}) \circ \mathrm{ReLU} \circ \mathrm{lin}(d, \tilde{d}) \\ \mathrm{ReLU} \circ \sum_{i \in \mathcal{N}_v} \mathrm{lin}(d, d) \end{cases}$$

External Force: $$F_u(\mathbf{q}, t) = \begin{cases} \mathrm{lin}(\tilde{d}, d) \circ \sin \circ \mathrm{lin}(\tilde{d}, \tilde{d}) \circ \sin \circ \mathrm{lin}(\tilde{d}, \tilde{d}) \circ \sin \circ \mathrm{lin}(d+1, \tilde{d}) \\ \sigma \circ \sum_{i \in \mathcal{N}_v} \mathrm{lin}(d+1, d) \end{cases}$$

Integration

Layers: $L \in \{1, 5, 10, 20, 30\}$

Time: $T \in \{0.1, 1, 2, 3\}$

Backup III

H-DGN:

$$\mathbf{x}_u^{(\ell+1)} = \begin{pmatrix} \mathbf{p}_u^{(\ell+1)} \\ \mathbf{q}_u^{(\ell+1)} \end{pmatrix} = \begin{pmatrix} \mathbf{p}_u^{(\ell)} \\ \mathbf{q}_u^{(\ell)} \end{pmatrix} + \epsilon \mathcal{J}_u \begin{pmatrix} \nabla_{\mathbf{p}_u} H_{\mathcal{G}}(\mathbf{p}^{(\ell+1)}, \mathbf{q}^{(\ell)}) \\ \nabla_{\mathbf{q}_u} H_{\mathcal{G}}(\mathbf{p}^{(\ell+1)}, \mathbf{q}^{(\ell)}) \end{pmatrix}, \quad \forall u \in \mathcal{V}$$

$$\mathbf{p}_u^{(\ell+1)} = \mathbf{p}_u^{(\ell)} - \epsilon \Bigg[\mathbf{W}_q^\top \sigma(\mathbf{W}_q \mathbf{q}_u^{(\ell)} + \Phi_{\mathcal{G}}(\{\mathbf{q}_v^{(\ell)}\}_{v \in \mathcal{N}_u}) + \mathbf{b}_q) + \sum_{v \in \mathcal{N}_u \setminus \{u\}} \mathbf{V}_q^\top \sigma(\mathbf{W}_q \mathbf{q}_v^{(\ell)} + \Phi_{\mathcal{G}}(\{\mathbf{q}_j^{(\ell)}\}_{j \in \mathcal{N}_v}) + \mathbf{b}_q) \Bigg]$$

$$\mathbf{q}_u^{(\ell+1)} = \mathbf{q}_u^{(\ell)} + \epsilon \Bigg[\mathbf{W}_p^\top \sigma(\mathbf{W}_p \mathbf{p}_u^{(\ell+1)} + \Phi_{\mathcal{G}}(\{\mathbf{p}_v^{(\ell+1)}\}_{v \in \mathcal{N}_u}) + \mathbf{b}_p) + \sum_{v \in \mathcal{N}_u \setminus \{u\}} \mathbf{V}_p^\top \sigma(\mathbf{W}_p \mathbf{p}_v^{(\ell+1)} + \Phi_{\mathcal{G}}(\{\mathbf{p}_j^{(\ell+1)}\}_{j \in \mathcal{N}_v}) + \mathbf{b}_p) \Bigg].$$

PH-DGN:

$$\mathbf{p}_u^{(\ell+1)} = \mathbf{p}_u^{(\ell)} + \epsilon \Bigg[-\nabla_{\mathbf{q}_u} H_{\mathcal{G}}(\mathbf{p}^{(\ell)}, \mathbf{q}^{(\ell+1)}) - D_u(\mathbf{q}^{(\ell+1)}) \nabla_{\mathbf{p}_u} H_{\mathcal{G}}(\mathbf{p}^{(\ell)}, \mathbf{q}^{(\ell+1)}) + F_u(\mathbf{q}^{(\ell+1)}, t) \Bigg].$$