Graph-Coupled Oscillator Networks

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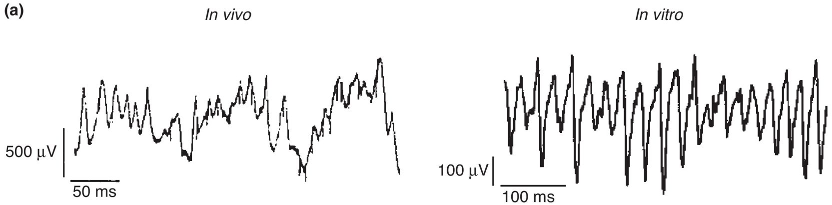
Oscillators (for GNNs?)

Oscillators are ubiquitous in nature and engineering systems



Why oscillators for GNNs:

- Neurobiological motivation for networks of oscillatory neurons
- Expressivity of oscillators (Fourier series approximation)
- Well-behaved gradients of oscillators $\rightarrow$ Exploding/vanishing gradients problem mitigated?
- Desirable stability properties: A solution for the oversmoothing problem?

Oscillatory inductive bias for GNNs

Set-up:

- Undirected Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E} \subseteq \mathcal{V} \times \mathcal{V})$
- Edges $\mathcal{E}$: pairs of nodes $\{i, j\}$ (denoted $i \sim j$)
- Node features $\mathbf{X}$

GraphCON based on graph dynamical system:

$$\mathbf{X}'' = \sigma(\mathbf{F}_\theta(\mathbf{X}, t)) - \gamma \mathbf{X} - \alpha \mathbf{X}' \iff \begin{cases} \mathbf{Y}' = \sigma(\mathbf{F}_\theta(\mathbf{X}, t)) - \gamma \mathbf{X} - \alpha \mathbf{Y}, \\ \mathbf{X}' = \mathbf{Y} \end{cases}$$

- General learnable 1-neighborhood coupling $\mathbf{F}_\theta$ (e.g. GCN, GAT,...):

$$\left(\mathbf{F}_\theta(\mathbf{X}, t)\right)_{ij} = \mathbf{F}_\theta\left(\mathbf{X}_i(t), \mathbf{X}_j(t), t\right) \quad \forall i \sim j,$$

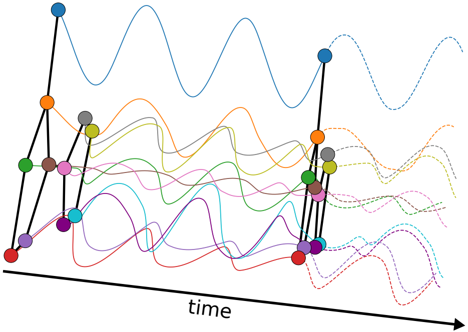
- Activation function σ
- Control parameters $\gamma, \alpha > 0$

IMEX discretizaton yields GraphCON:

$$\mathbf{Y}^n = \mathbf{Y}^{n-1} + \Delta t[\sigma(\mathbf{F}_\theta(\mathbf{X}^{n-1}, t^{n-1})) - \gamma \mathbf{X}^{n-1} - \alpha \mathbf{Y}^{n-1}],$$
$$\mathbf{X}^n = \mathbf{X}^{n-1} + \Delta t \mathbf{Y}^n,$$

for $n = 1, \ldots, N$, and

- $\Delta t > 0$ time-step
- $\mathbf{X}^n, \mathbf{Y}^n$ hidden node features at time $t^n = n\Delta t$

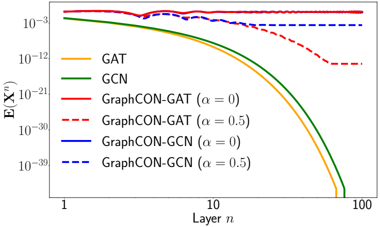


Properties of GraphCON

We provide mathematical definition of oversmoothing: exponential convergence to zero of layer-wise Dirichlet energy

Main result:

GraphCON mitigates the oversmoothing problem



We further show:

- GraphCON mitigates the exploding gradients problem
- GraphCON mitigates the vanishing gradients problem
- Naive multi-layer stacking of GNNs corresponds to fixed-point iteration of GraphCON $\rightarrow$ higher expressive power of GraphCON

Table: Transductive node classification test accuracy (MAP in %) on heterophilic datasets.

Homophily level	**Texas** **0.11**	**Wisconsin** **0.21**	**Cornell** **0.30**
GPRGNN	78.4 ± 4.4	82.9 ± 4.2	80.3 ± 8.1
H2GCN	$\mathbf{84.9 \pm 7.2}$	$\mathbf{87.7 \pm 5.0}$	$\mathbf{82.7 \pm 5.3}$
GCNII	77.6 ± 3.8	80.4 ± 3.4	77.9 ± 3.8
Geom-GCN	66.8 ± 2.7	64.5 ± 3.7	60.5 ± 3.7
PairNorm	60.3 ± 4.3	48.4 ± 6.1	58.9 ± 3.2
GraphSAGE	$\mathbf{82.4 \pm 6.1}$	81.2 ± 5.6	76.0 ± 5.0
MLP	80.8 ± 4.8	85.3 ± 3.3	81.9 ± 6.4
GAT	52.2 ± 6.6	49.4 ± 4.1	61.9 ± 5.1
GraphCON-GAT	82.2 ± 4.7	$\mathbf{85.7 \pm 3.6}$	$\mathbf{83.2 \pm 7.0}$
GCN	55.1 ± 5.2	51.8 ± 3.1	60.5 ± 5.3
GraphCON-GCN	$\mathbf{85.4 \pm 4.2}$	$\mathbf{87.8 \pm 3.3}$	$\mathbf{84.3 \pm 4.8}$

Table: Test accuracy in % on MNIST Superpixel 75.

Model	Test accuracy
ChebNet	75.62
MoNet	91.11
PNCNN	**98.76**
SplineCNN	95.22
GIN	97.23
GraphCON-GIN	98.53
GatedGCN	97.95
GraphCON-GatedGCN	98.27
GCN	88.89
GraphCON-GCN	**98.68**
GAT	96.19
GraphCON-GAT	**98.91**

Table: Test mean absolute error on ZINC (**without edge features, small 12k version**) restricted to small network sizes of $\sim 100k$ parameters.

Model	Test MAE
GIN	0.41 ± 0.008
GatedGCN	0.42 ± 0.006
GraphSAGE	0.41 ± 0.005
MoNet	0.41 ± 0.007
PNA	$\mathbf{0.32 \pm 0.032}$
DGN	$\mathbf{0.22 \pm 0.010}$
GCN	0.47 ± 0.002
GraphCON-GCN	$\mathbf{0.22 \pm 0.004}$
GAT	0.46 ± 0.002
GraphCON-GAT	$\mathbf{0.23 \pm 0.004}$

Conclusion / Outlook

- GraphCON: physics-inspired framework to construct very deep GNNs
- GraphCON provably overcomes the oversmoothing problem as well as exploding/vanishing gradient problem
- GraphCON reaches SOTA on a variety of different graph learning tasks

Main message: "Don't stack GNNs naively – use GraphCON!"

Future projects:

- Physics-inspired methods work – GraphCON is only the start

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