NEURAL INFORMATION PROCESSING SYSTEMS

KAIST

Parameter-Free Hypergraph Neural Network for Few-Shot Node Classification

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Most real-world data are connected

- **Social networks:** User−User
- **Recommendation:** User−Item
- **Academic:** Author−Paper
- **Entertainment:** Movie−Actor
- **Chemistry:** Atom−Atom

Figure: Sa Wang. “Social Network Graphs: Concepts, Metrics & Tools” PuppyGraph.

Hypergraph models diverse relations

- **Hyperedges** connect multiple nodes
  - e.g., Author (node) − Paper (hyperedge)
- Pair-wise interactions can also be hyperedges

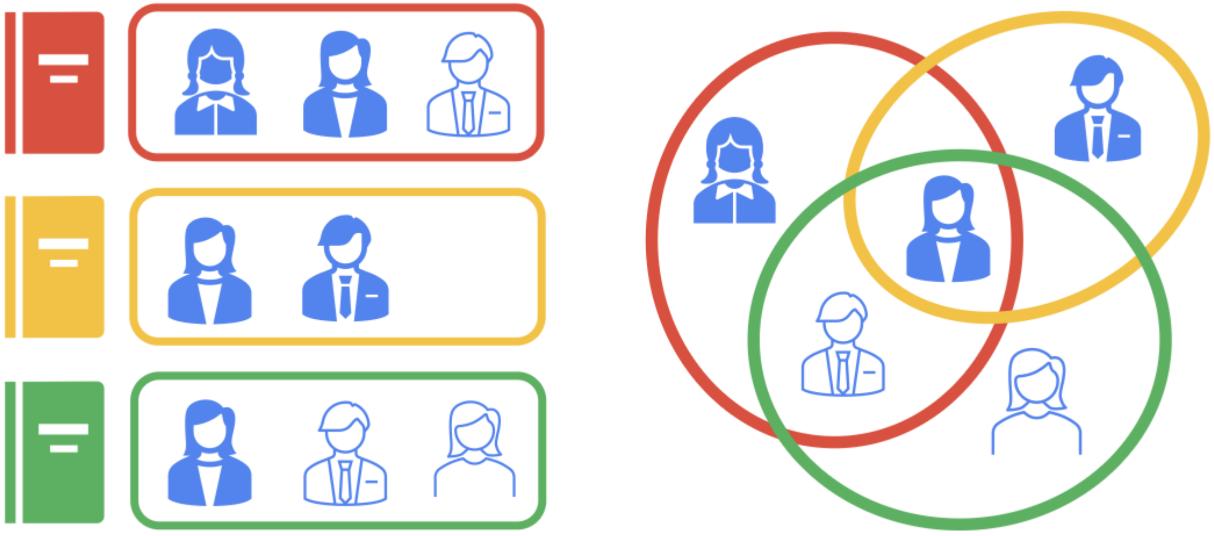

Figure: Kim et al. “Hypergraph Neural Networks: An In-Depth and Step-By-Step Guide.” KDD 2024.

Hypergraph models are complex

- Capturing higher-order interactions increases model complexity

- **Key limitations:**
  - Generalizability
  - Scalability
  - Interpretability

Label scarcity is a key challenge

- Complex models **fail** under scarce labels on real-world data

- **Our goal:** Simplify model without losing expressive power
- **Result: We reduce the number of parameters to ZERO!**

ZEN: Method overview

- Zero-Parameter Hypergraph Neural Network

- ZEN consists of three main ideas:
  1. Linearize existing models
  2. Remove remaining parameters
  3. Refine the propagation scheme

Start by linearizing existing models

- Simplify existing models via linearization − general form:

$$\mathbf{Y}_{\text{pred}} = \mathbf{PXW}^{\top}$$

  - $\mathbf{Y}_{\text{pred}} \in \mathbb{R}^{|\mathcal{V}| \times c}$: Prediction matrix
  - $\mathbf{P} \in \mathbb{R}^{|\mathcal{V}| \times |\mathcal{V}|}$: Propagation matrix
  - $\mathbf{W} \in \mathbb{R}^{c \times d}$: Weight matrix

Remove remaining parameter W

- Boost efficiency via approximated closed-form solution:

$$\mathbf{W} \approx \mathbf{Y}_{\mathrm{trn}}^{\top}\mathbf{P}\mathbf{X}$$

$$\therefore \mathbf{Y}_{\mathrm{pred}} = (\mathbf{P}\mathbf{X})(\mathbf{P}\mathbf{X})^{\top}\mathbf{Y}_{\mathrm{trn}}$$

  - $\mathbf{Y}_{\mathrm{trn}} \in \{0,1\}^{|\mathcal{V}| \times c}$: One-hot label matrix for training nodes; otherwise, 0

Refine propagation matrix $\mathbf{P}$

- Remove strong self-correlation from $\mathbf{P}$:

$$\mathbf{P}^* = \sum_l \alpha_l \left(\mathbf{A}_l - \mathrm{RSI}(\mathbf{A}_l)\right)$$

$$\therefore \mathbf{Y}_{\mathrm{pred}} = (\mathbf{P}^*\mathbf{X})(\mathbf{P}^*\mathbf{X})^\top \mathbf{Y}_{\mathrm{trn}}$$

- Residual self-information $\mathrm{RSI}(\mathbf{A}_l)$: Degree of correlation to $\mathbf{A}_0$

ZEN is accurate

- Outperforms all on 8 of 10 datasets (classification accuracy)

Methods	**Cora**	**Citeseer**	**Pubmed**	**Cora_CA**	**20News**	**MN40**	**Congress**	**Wallmart**	**Senate**	**House**	**Avg Rank**
HGNN	$44.4_{\pm 8.9}$	$40.1_{\pm 6.5}$	$52.5_{\pm 9.1}$	$54.3_{\pm 3.6}$	$\mathbf{73.1}_{\pm \mathbf{2.3}}$	$94.7_{\pm 0.3}$	$86.7_{\pm 1.1}$	$39.6_{\pm 2.4}$	$56.8_{\pm 5.0}$	$63.4_{\pm 4.3}$	5.9
HNHN	$36.7_{\pm 5.8}$	$36.0_{\pm 3.7}$	$51.8_{\pm 3.7}$	$39.2_{\pm 5.2}$	$41.2_{\pm 5.7}$	$90.8_{\pm 1.4}$	$51.1_{\pm 2.7}$	$15.9_{\pm 3.0}$	$69.7_{\pm 11.6}$	$67.4_{\pm 8.3}$	7.9
HCHA	$44.4_{\pm 8.7}$	$41.2_{\pm 6.5}$	$52.9_{\pm 10.4}$	$54.5_{\pm 4.2}$	$\underline{72.9_{\pm 2.5}}$	$94.7_{\pm 0.2}$	$86.6_{\pm 1.3}$	$39.3_{\pm 2.5}$	$53.0_{\pm 5.0}$	$63.5_{\pm 4.6}$	5.9
UniGCN	$48.5_{\pm 8.3}$	$41.6_{\pm 3.7}$	$54.2_{\pm 10.3}$	$55.3_{\pm 4.3}$	$70.4_{\pm 2.8}$	$95.9_{\pm 0.3}$	$\mathbf{91.6}_{\pm \mathbf{0.4}}$	$40.1_{\pm 2.8}$	$61.4_{\pm 4.4}$	$67.9_{\pm 5.1}$	3.9
UniGCNII	$43.3_{\pm 9.9}$	$38.9_{\pm 6.7}$	$54.5_{\pm 8.4}$	$52.0_{\pm 4.5}$	$66.5_{\pm 4.6}$	$\underline{96.4_{\pm 0.4}}$	$83.5_{\pm 6.4}$	$23.5_{\pm 2.4}$	$\mathbf{70.4}_{\pm \mathbf{8.5}}$	$\underline{70.7_{\pm 7.4}}$	5.5
AllDeepSets	$48.6_{\pm 4.7}$	$42.6_{\pm 4.4}$	$53.2_{\pm 5.8}$	$55.3_{\pm 5.1}$	$51.4_{\pm 4.4}$	$94.7_{\pm 0.3}$	$69.5_{\pm 4.7}$	$24.5_{\pm 3.7}$	$65.3_{\pm 10.3}$	$63.4_{\pm 8.3}$	5.7
AllSetTransformer	$\underline{50.5_{\pm 4.4}}$	$\underline{44.8_{\pm 2.7}}$	$\underline{60.4_{\pm 4.5}}$	$\underline{59.6_{\pm 3.4}}$	$70.3_{\pm 1.5}$	$95.5_{\pm 0.2}$	$88.2_{\pm 1.1}$	$38.3_{\pm 6.4}$	$63.1_{\pm 10.7}$	$66.3_{\pm 8.3}$	$\underline{3.6}$
ED-HNN	$48.4_{\pm 6.4}$	$44.5_{\pm 3.5}$	$56.5_{\pm 6.6}$	$58.8_{\pm 3.8}$	$67.7_{\pm 3.7}$	$96.0_{\pm 0.2}$	$\underline{89.1_{\pm 4.0}}$	$\underline{42.9_{\pm 5.7}}$	$63.1_{\pm 9.1}$	$62.8_{\pm 10.4}$	4.1
ZEN (proposed)	$\mathbf{51.9}_{\pm \mathbf{10.1}}$	$\mathbf{49.1}_{\pm \mathbf{4.8}}$	$\mathbf{62.6}_{\pm \mathbf{3.9}}$	$\mathbf{60.0}_{\pm \mathbf{6.2}}$	$68.6_{\pm 4.8}$	$\mathbf{97.6}_{\pm \mathbf{0.3}}$	$87.0_{\pm 4.8}$	$\mathbf{43.9}_{\pm \mathbf{3.1}}$	$\mathbf{70.4}_{\pm \mathbf{10.0}}$	$\mathbf{73.2}_{\pm \mathbf{6.3}}$	**1.7**

ZEN is extremely fast

- Overwhelming speed advantage (relative running time)

Methods	Cora	Citeseer	Pubmed	Cora_CA	20News	MN40	Congress	Wallmart	Senate	House
HGNN	8.65	3.81	3.00	8.95	<u>10.54</u>	20.05	53.10	30.16	777.14	388.05
HNHN	<u>7.61</u>	<u>2.71</u>	3.56	<u>7.23</u>	15.51	<u>13.78</u>	<u>42.11</u>	21.47	696.85	345.93
HCHA	12.37	4.74	5.51	10.19	12.21	20.63	71.62	<u>12.73</u>	1008.85	699.41
UniGCN	17.12	2.63	8.29	8.97	28.79	21.86	91.16	32.90	716.43	<u>292.95</u>
UniGCNII	15.77	5.18	<u>2.56</u>	17.25	16.98	19.41	80.17	36.37	<u>696.63</u>	369.10
AllDeepSets	58.11	24.92	11.01	57.56	35.52	47.51	273.58	90.16	4048.55	1748.67
AllSetTransformer	9.76	4.30	10.98	12.37	60.21	24.94	65.59	76.89	997.43	524.15
ED-HNN	16.04	6.06	5.46	23.55	46.71	28.70	426.91	46.31	714.73	379.41
ZEN (ours)	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**

ZEN is interpretable

- Domain-aligned representations by ZEN (color-coded $\mathbf{W}^\top$)

	Mammal	Bird	Reptile	Fish	Amphibian	Bug	Invertebrate
Hair	0.1735	0.0719	0.0778	0.0819	0.0661	0.0800	0.0465
Feathers	0.0251	0.1726	0.0383	0.0414	0.0311	0.0305	0.0276
Eggs	0.1072	0.2440	0.2255	0.2931	0.1979	0.1792	0.1850
Milk	0.1720	0.0664	0.0740	0.0826	0.0626	0.0432	0.0409
Airborne	0.0310	0.1417	0.0450	0.0456	0.0376	0.0979	0.0361
Aquatic	0.0807	0.0688	0.0727	0.2522	0.1606	0.0492	0.1437
Predetor	0.1796	0.1054	0.1878	0.2841	0.1601	0.1006	0.1688
Toothed	0.1707	0.1001	0.1946	0.2921	0.1959	0.0682	0.0745
Backbone	0.2280	0.2768	0.2687	0.3380	0.2304	0.1012	0.1049
Breathes	0.2239	0.2769	0.2597	0.1652	0.2235	0.1939	0.1064
Venomous	0.0109	0.0141	0.0628	0.0217	0.0465	0.0415	0.171
Fins	0.0246	0.0272	0.0337	0.2027	0.0301	0.0183	0.0273
Legs	0.8380	0.7794	0.7956	0.5875	0.8520	0.9333	0.9310
Tail	0.1836	0.2642	0.2542	0.3204	0.1522	0.0913	0.0963
Domestic	0.0225	0.0266	0.0234	0.0253	0.0197	0.0179	0.0146
Capsize	0.1416	0.1515	0.1134	0.1887	0.0687	0.0487	0.0744

ZEN: Summary

- Parameter-free (training-free)
- Highly expressive, low complexity
- Accurate, fast, and interpretable

Paper