

One for Two: A **Unified** Framework for Imbalanced Graph Classification via **Dynamic Balanced Prototype**

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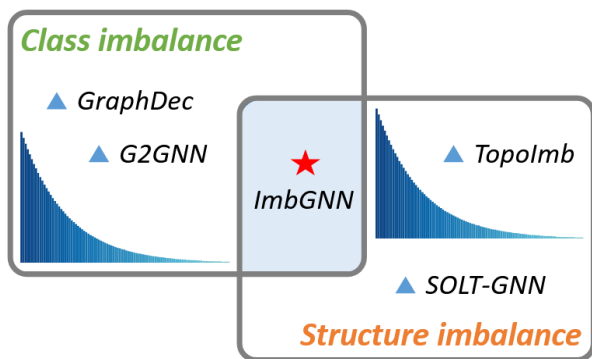
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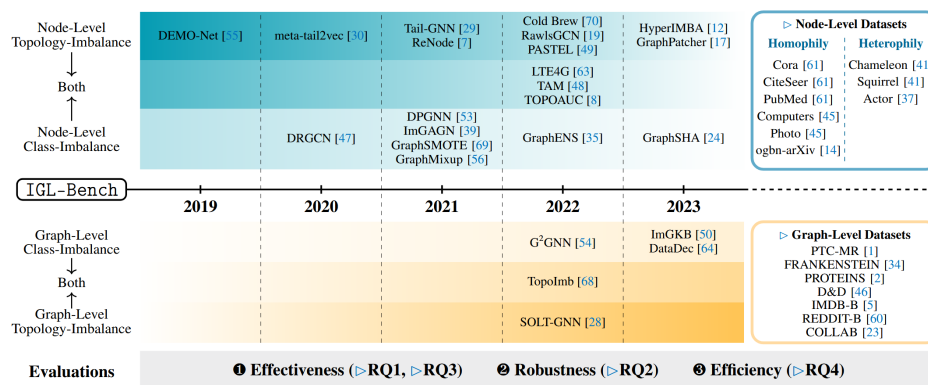
Insight and Motivation

One for Two: A **Unified** Framework for Imbalanced Graph Classification via **Dynamic Balanced Prototype**

- (1) **Unified Insight.** Class Imbalance and Topological Imbalance.
- (2) Practical Solution and Theoretical Explanation. **Dynamic Balanced Prototype.**
- (3) Empirical Study. **Richest benchmarks** for the community.

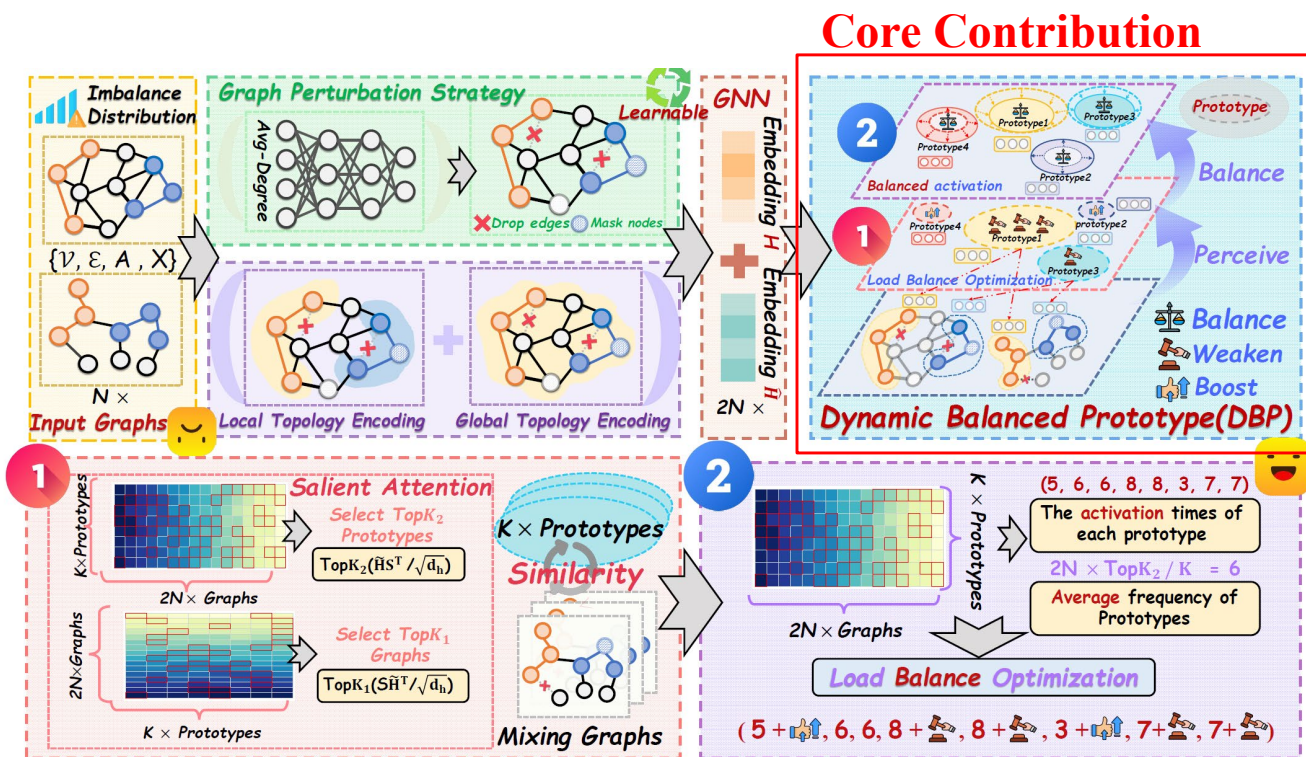


From WWW 2024 ImbGNN



From ICLR 2025 Spotlight

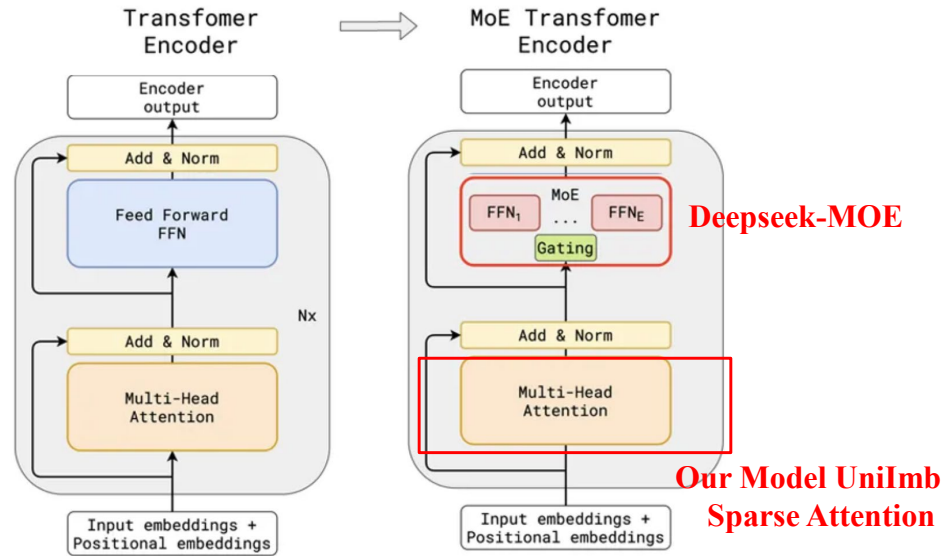
Model Architecture



- (1) Graph topology encoding
- (2) Personalized graph perturbation strategy
- (3) **Dynamic balanced prototype** based on information bottleneck

Dynamic Balanced Prototype

Dynamic balanced prototype



$$\min I(\mathbf{S}; \mathbf{G}) - \beta I(\mathbf{S}; \mathbf{Y})$$

$$\min I(\mathbf{S}; \mathbf{G}) = \sum_{\mathcal{G}, s} p(\mathcal{G}) p(s|\mathcal{G}) \log \frac{p(s|\mathcal{G})}{p(s)} \Rightarrow \min \text{KL}(\mathbf{P}||\mathbf{U}) \approx \min \frac{1}{2} \sum_{k=1}^K (p_k - u_k)^2$$

$$\hat{\mathbf{H}} = \text{Sigmoid} \left(\text{TopK}_2 \left(\tilde{\mathbf{H}} \mathbf{S}^T / \sqrt{d_h} + \eta \right) + \gamma \right) \tilde{\mathbf{H}}_S,$$

$$\tilde{\mathbf{H}}_S = \text{Softmax} \left(\text{TopK}_1 \left(\tilde{\mathbf{S}} \mathbf{H}^T / \sqrt{d_h} \right) \right) \tilde{\mathbf{H}} \mathbf{W}_v \in \mathbb{R}^{K \times d_h}$$

Prototype-balance Optimization

Load Balancing Optimization

$$\mathcal{L}_{\text{Balance}} = \alpha \sum_{i=1}^N f_i P_i,$$

$$f_i = \frac{N}{KT} \sum_{t=1}^T \mathbb{1}(\text{Token } t \text{ selects Expert } i),$$

$$P_i = \frac{1}{T} \sum_{t=1}^T s_{i,t},$$

$$s_{i,t} = \text{Softmax}_i(\mathbf{u}_t^T \mathbf{e}_i^t),$$

$$\mathcal{L}_{\mathcal{M}} = \frac{1}{2} \sum_{k=1}^K \left| n_k - \frac{2 * N * \text{TopK}_2}{\frac{1}{u_k}} \right|^2 = \frac{1}{2} \sum_{k=1}^K \left| \eta + \text{StopGrad}(n_k - \eta) - \frac{2 * N * \text{TopK}_2}{\frac{1}{u_k}} \right|^2$$

$$\eta \leftarrow \eta - \varphi \nabla \mathcal{L}_{\mathcal{M}} = \eta - \varphi \text{sgn}(n_k - 2 * N * \text{TopK}_2 * u_k)$$

(a) Common Auxiliary Loss of Mixture of Experts

(c) Unilmb Optimized Bias Term

$$g_{i,t} = \begin{cases} s_{i,t}, & s_{i,t} + b_i \in \text{Topk}(\{s_{j,t} + b_j \mid 1 \leq j \leq N\}, K) \\ 0, & \text{otherwise.} \end{cases}$$

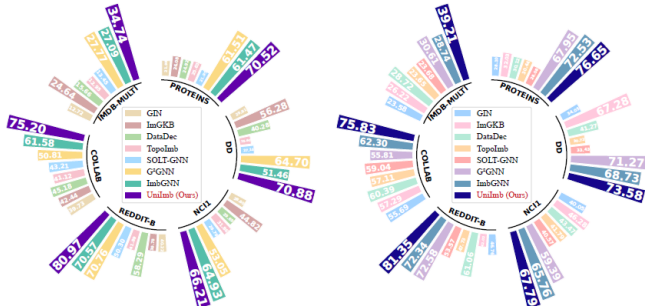
(b) DeepSeek-MOE Optimized Bias Term

Table 1: Macro-F1 and Micro-F1 scores on *class imbalance* datasets with *extreme imbalance degree* under *different U distributions*. The best results are **marked** and the runner-ups are underlined.

Distribution	PROTEINS		D&D		NCII		COLLAB	
	Macro-F1	Micro-F1	Macro-F1	Micro-F1	Macro-F1	Micro-F1	Macro-F1	Micro-F1
Zipf (Axtell, 2001)	67.80 ± 3.71	73.29 ± 4.00	44.05 ± 2.29	79.02 ± 7.38	65.69 ± 3.11	79.78 ± 1.58	69.25 ± 10.26	69.79 ± 10.08
Exponential (Marshall & Olkin, 1967)	66.45 ± 3.34	71.99 ± 4.94	<u>44.99 ± 2.95</u>	<u>82.31 ± 9.36</u>	65.03 ± 2.41	79.85 ± 2.09	73.51 ± 6.73	74.47 ± 6.09
Poisson (Consul & Jain, 1973)	<u>68.49 ± 1.70</u>	<u>73.94 ± 3.40</u>	41.62 ± 3.72	71.98 ± 10.64	<u>67.67 ± 5.50</u>	<u>80.60 ± 5.09</u>	<u>75.56 ± 2.03</u>	<u>75.85 ± 2.18</u>
Uniform (Kuipers & Niederreiter, 2012)	70.44 ± 4.72	74.50 ± 4.99	46.63 ± 3.42	83.60 ± 6.50	68.30 ± 5.19	80.68 ± 4.22	75.73 ± 2.52	76.34 ± 2.60

Experimental Results

A comprehensive and thorough benchmark



New Scenario Setting

Figure 3: Macro-F1 (left) and Micro-F1 (right) on intertwined imbalance datasets.

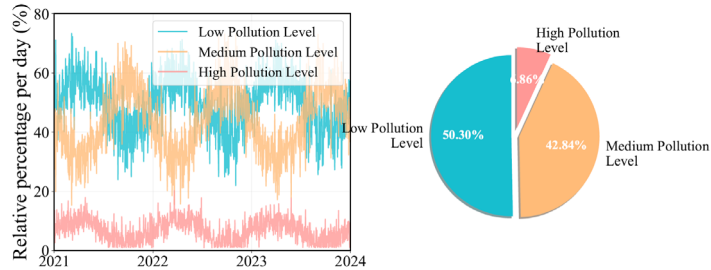


Figure 7: Distribution of Pollution Levels in the AirGraph Dataset: High (6.86%), Medium (42.84%), and Low (50.30%).

Open Source AirGraph

Table 2: Performance on *class imbalance* datasets with *extreme imbalance degree*. The best results are **marked** and the runner-ups are **underlined**. We report the average and standard deviation over 20 runs. Numbers marked with * indicated that the improvement is statistically significant compared with the best baseline (Wilcoxon Signed-Rank Test with *p-value* < 0.05).

Method	Backbone	PROTEINS		D&D		NCI		REDDIT-B		COLLAB		IMDB-MULTI	
		Macro-F1	Micro-F1	Macro-F1	Micro-F1	Macro-F1	Micro-F1	Macro-F1	Micro-F1	Macro-F1	Micro-F1	Macro-F1	Micro-F1
Classic	GIN	25.33 ± 7.53	28.50 ± 5.82	9.99 ± 7.44	11.88 ± 9.49	18.24 ± 7.58	18.94 ± 7.12	33.19 ± 14.26	36.02 ± 17.38	32.58 ± 3.66	57.31 ± 4.12	13.25 ± 6.19	14.92 ± 5.43
	InfoGraph	35.91 ± 7.58	36.81 ± 6.51	21.41 ± 4.51	27.68 ± 7.52	33.09 ± 4.88	34.03 ± 3.68	57.67 ± 3.80	67.10 ± 4.91	43.48 ± 4.29	59.10 ± 3.80	17.28 ± 7.28	29.18 ± 4.47
	GraphCL	40.86 ± 6.94	41.24 ± 6.38	21.02 ± 3.05	26.89 ± 4.95	31.02 ± 2.69	31.62 ± 3.05	53.40 ± 4.06	62.19 ± 5.68	45.02 ± 5.61	60.22 ± 3.47	16.20 ± 9.22	32.18 ± 8.90
GTs	GraphGPS	25.79 ± 7.05	28.71 ± 5.46	10.12 ± 4.41	11.97 ± 3.91	14.94 ± 2.41	15.62 ± 2.07	11.68 ± 7.76	12.71 ± 8.13	25.58 ± 12.93	39.92 ± 13.66	14.20 ± 5.61	28.54 ± 13.78
	Expformer	25.52 ± 4.79	28.38 ± 3.57	9.79 ± 4.18	10.85 ± 4.28	14.56 ± 3.92	15.36 ± 3.60	22.68 ± 10.79	27.33 ± 21.65	32.61 ± 17.44	42.02 ± 15.44	20.81 ± 5.43	28.14 ± 8.30
up-sampling	GraphMamba	31.12 ± 5.10	32.79 ± 4.02	4.99 ± 7.93	6.12 ± 10.36	14.11 ± 3.26	14.94 ± 3.82	15.27 ± 12.46	17.02 ± 14.71	42.53 ± 11.15	50.63 ± 5.58	16.89 ± 4.57	28.69 ± 12.47
	GIN	65.64 ± 2.67	71.55 ± 3.19	41.15 ± 3.74	70.56 ± 10.28	59.19 ± 3.39	71.80 ± 7.02	66.71 ± 3.92	83.00 ± 5.18	64.30 ± 2.67	66.10 ± 3.28	22.27 ± 10.01	38.32 ± 10.04
re-weight	InfoGraph	62.68 ± 2.70	66.02 ± 3.18	41.55 ± 2.32	71.34 ± 6.76	53.38 ± 1.88	62.20 ± 2.63	67.01 ± 3.34	78.68 ± 1.71	63.28 ± 2.90	65.14 ± 3.29	21.79 ± 6.68	37.29 ± 10.02
	GraphCL	64.21 ± 2.53	65.76 ± 2.61	38.96 ± 3.01	64.23 ± 8.10	49.92 ± 2.15	58.29 ± 3.30	62.01 ± 3.97	75.84 ± 3.98	64.57 ± 4.20	66.79 ± 4.11	23.02 ± 6.91	40.29 ± 6.90
G ² GNN	GIN	54.54 ± 6.29	55.77 ± 7.11	28.49 ± 5.92	40.79 ± 11.84	36.84 ± 4.46	39.19 ± 10.05	43.17 ± 8.46	51.92 ± 12.29	57.83 ± 3.03	60.09 ± 4.59	22.07 ± 11.13	36.69 ± 11.14
	InfoGraph	45.73 ± 3.10	49.60 ± 3.68	41.92 ± 2.28	72.43 ± 6.63	53.05 ± 1.12	62.45 ± 1.89	65.79 ± 3.38	77.35 ± 3.96	62.22 ± 3.80	64.48 ± 3.14	21.16 ± 8.79	38.02 ± 5.70
dynamic sparsity	GraphCL	63.46 ± 2.42	64.97 ± 2.41	40.29 ± 3.31	67.96 ± 8.98	50.05 ± 2.09	58.18 ± 3.08	62.79 ± 6.93	76.15 ± 4.15	63.18 ± 4.55	65.29 ± 3.87	22.48 ± 6.82	39.57 ± 5.89
	remove edge	67.70 ± 2.96	73.10 ± 4.05	43.25 ± 3.91	77.03 ± 9.38	63.60 ± 1.57	72.97 ± 1.81	68.39 ± 2.67	86.35 ± 1.80	37.63 ± 3.12	54.98 ± 4.28	20.54 ± 9.49	35.78 ± 11.08
mask node	GIN	67.39 ± 2.99	73.30 ± 4.19	43.93 ± 3.46	79.03 ± 10.78	64.78 ± 2.86	74.91 ± 2.14	67.52 ± 2.60	85.43 ± 1.87	53.92 ± 6.37	61.29 ± 4.87	21.54 ± 9.49	35.78 ± 11.08
	TopoLab	53.95 ± 6.68	56.00 ± 7.88	7.72 ± 5.68	9.47 ± 4.26	16.41 ± 9.19	17.14 ± 5.68	10.38 ± 2.94	11.20 ± 2.69	19.24 ± 0.02	40.71 ± 0.05	9.37 ± 1.51	15.24 ± 0.90
ImbGKB	DataDc	29.48 ± 9.98	31.25 ± 2.98	15.79 ± 2.38	18.86 ± 3.47	18.14 ± 3.86	18.52 ± 3.64	56.11 ± 4.65	65.35 ± 6.16	41.73 ± 1.20	57.27 ± 0.65	11.68 ± 1.15	16.29 ± 0.72
	GIN	53.99 ± 7.22	55.31 ± 8.17	31.15 ± 6.29	46.31 ± 11.72	32.93 ± 5.46	34.85 ± 7.14	11.00 ± 8.34	14.00 ± 1.34	18.84 ± 1.46	39.58 ± 4.90	16.52 ± 5.23	34.12 ± 12.71
ImbGNN	/	67.69 ± 2.95	73.24 ± 3.85	46.06 ± 7.21	83.24 ± 10.03	65.48 ± 3.39	74.58 ± 5.49	68.36 ± 8.10	80.56 ± 4.27	56.62 ± 4.28	62.79 ± 3.83	17.52 ± 9.88	34.54 ± 8.24
	Unilab	/	70.44* ± 4.72	74.50* ± 4.99	46.63* ± 5.42	83.60* ± 6.59	68.30* ± 5.19	80.68* ± 4.22	76.24* ± 4.09	88.82* ± 2.93	75.73* ± 2.52	76.34* ± 2.69	33.55* ± 7.13
Promotion		4.05%↑	1.64%↑	1.24%↑	0.43%↑	4.31%↑	7.70%↑	11.48%↑	2.61%↑	17.28%↑	14.30%↑	41.62%↑	13.48%↑

+41.62%

Table 3: Performance comparison on *topological imbalance* datasets with *extreme imbalance degree*.

Method	PROTEINS		D&D		NCI		REDDIT-B		COLLAB		IMDB-MULTI	
	Macro-F1	Micro-F1	Macro-F1	Micro-F1	Macro-F1	Micro-F1	Macro-F1	Micro-F1	Macro-F1	Micro-F1	Macro-F1	Micro-F1
GIN	53.48 ± 2.03	58.00 ± 4.19	57.98 ± 4.51	60.68 ± 6.89	61.60 ± 2.20	61.84 ± 2.29	66.60 ± 2.27	67.41 ± 2.23	64.92 ± 2.18	67.05 ± 4.26	20.80 ± 4.91	34.73 ± 2.16
InfoGraph	55.31 ± 3.30	60.68 ± 3.52	59.46 ± 4.03	64.22 ± 4.11	62.25 ± 1.53	57.99 ± 2.01	69.56 ± 3.46	69.63 ± 4.28	63.28 ± 1.68	66.20 ± 1.33	33.36 ± 1.60	36.42 ± 1.10
GraphCL	57.62 ± 5.50	61.91 ± 3.84	62.01 ± 1.18	65.29 ± 2.33	63.62 ± 5.43	56.93 ± 4.75	67.25 ± 7.92	68.31 ± 6.36	68.16 ± 4.68	59.88 ± 4.01	30.39 ± 2.53	33.90 ± 1.57
GraphGPS	65.54 ± 4.22	69.26 ± 2.48	63.33 ± 12.97	63.85 ± 2.08	62.96 ± 3.51	64.02 ± 2.40	66.16 ± 4.19	68.42 ± 5.32	24.11 ± 8.74	56.65 ± 2.81	16.87 ± 0.53	34.49 ± 0.62
Expformer	64.01 ± 2.18	67.33 ± 2.78	59.43 ± 8.06	60.26 ± 5.92	62.16 ± 3.19	63.23 ± 7.21	66.48 ± 14.59	67.81 ± 7.45	21.03 ± 7.89	36.71 ± 15.27	25.52 ± 5.03	33.60 ± 2.70
GraphMamba	68.46 ± 3.91	72.09 ± 3.16	43.36 ± 9.73	54.45 ± 9.53	63.09 ± 2.82	63.63 ± 2.14	64.81 ± 12.47	67.06 ± 8.99	13.64 ± 5.97	27.37 ± 14.82	17.63 ± 1.07	33.21 ± 0.52
TopoLab	44.79 ± 14.19	54.89 ± 13.58	63.97 ± 2.78	64.16 ± 2.96	63.57 ± 1.69	64.17 ± 1.33	68.41 ± 5.34	69.14 ± 4.83	65.65 ± 6.03	67.52 ± 0.27	32.59 ± 5.45	40.63 ± 3.12
ImbGNN	66.87 ± 2.59	67.07 ± 2.75	68.67 ± 6.33	70.71 ± 6.99	61.24 ± 1.72	61.66 ± 1.17	65.19 ± 6.11	66.96 ± 5.03	51.35 ± 0.12	52.31 ± 0.14	23.85 ± 5.05	33.91 ± 1.78
SOLT-GNN	70.70 ± 2.20	72.14 ± 2.18	58.50 ± 10.48	64.97 ± 3.24	61.99 ± 1.44	62.13 ± 1.44	54.80 ± 3.23	60.24 ± 2.21	64.68 ± 2.21	67.12 ± 3.28	33.55 ± 4.77	39.69 ± 2.00
Unilab	71.32 ± 1.88	74.89* ± 1.12	74.49* ± 1.13	76.73* ± 1.04	64.99* ± 9.58	65.76* ± 7.24	77.14* ± 10.05	78.22* ± 7.41	75.54* ± 1.63	70.51* ± 1.48	64.67* ± 3.91	46.67* ± 2.31
Promotion	0.88%↑	3.80%↑	8.48%↑	8.51%↑	2.15%↑	2.48%↑	10.90%↑	12.34%↑	11.97%↑	11.88%↑	20.57%↑	14.87%↑

+20.57%

Thank you for your attention!

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