Relieving the Over-Aggregating Effect in Graph Transformers

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Abstract

Graph attention has demonstrated superior performance in graph learning tasks. However, learning from global interactions can be challenging due to the large number of nodes. In this paper, we discover a new phenomenon termed over-aggregating. Over-aggregating arises when a large volume of messages is aggregated into a single node with less discrimination, leading to the dilution of the key messages and potential information loss. To address this, we propose Wideformer, a plug-and-play method for graph attention. Wideformer divides the aggregation of all nodes into parallel processes and guides the model to focus on specific subsets of these processes. The division can limit the input volume per aggregation, avoiding message dilution and reducing information loss. The guiding step sorts and weights the aggregation outputs, prioritizing the informative messages. Evaluations show that Wideformer can effectively mitigate over-aggregating. As a result, the backbone methods can focus on the informative messages, achieving superior performance compared to baseline methods.

1 Introduction

Transformers have achieved remarkable success in modeling Euclidean-structured data, including natural language processing [47, 26, 25], image understanding [27, 40, 38, 39], and video processing [2, 5, 52]. Built on this success, significant efforts have been devoted to adapting transformers to graph-structured data, giving rise to various graph transformer models [23, 58, 55]. Leveraging the attention mechanism, graph transformers can learn from long-range dependencies and capture global features. These strengths provide effective solutions to address the challenges of over-smoothing [30] and over-squashing [1, 46], commonly encountered in traditional graph neural networks (GNNs) [17, 14, 48, 43, 13, 44, 45]. Evaluations across diverse downstream tasks highlight the promising performance of graph transformers [55, 42, 9].

Nevertheless, the dense global attention in graph transformers incurs a space complexity of $O(n^2)$, where the memory consumption increases quadratically with the number of input nodes. This high complexity hinders graph transformers from scaling to large datasets. To enhance the scalability of graph transformers, two primary approaches have been proposed, including sparse attention [19, 42] and linear global attention [50, 49, 51, 9]. Sparse methods reduce the density of dense global attention, which, in its original form, corresponds to a fully connected graph. The sparsified attention graph contains fewer edges, resulting in reduced memory overhead but also smaller receptive fields for each node. In contrast, linear methods preserve pairwise interactions between nodes and reduce complexity by eliminating the need for explicitly computing the dense attention.

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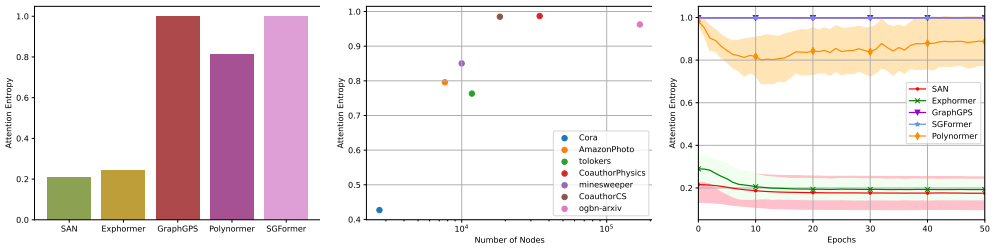


(a) Average Attention Entropy (b) Entropy across Node Scales (c) Entropy during Training

Figure 1: **Over-Aggregating in Graph Transformers.** The entropy values are normalized to $[0, 1]$, with higher entropy indicating a more uniform distribution of attention scores. In (b), we show the attention entropy with different numbers of nodes for Polynormer [9], a typical linear attention method.

However, learning from pairwise interactions is challenging due to the large number of graph nodes. Fig. 1 illustrates the average attention entropy on different models. Attention entropy denotes the confidence of the nodes in discriminating informative messages during aggregation. Higher entropy indicates a more uniform distribution of attention scores and less confidence. From Fig. 1(a), we can see that linear methods tend to aggregate messages from nodes with higher attention entropy and similar attention scores. When the number of nodes increases in Fig. 1(b), the attention scores become more and more similar. As a result, a large volume of messages is aggregated into a single node with less discrimination, leading to potential information loss. We name this uniform aggregation phenomenon as over-aggregating.

To tackle over-aggregating in graph transformers, we propose Wideformer, a plug-and-play method for graph attention. Wideformer divides the aggregation of all nodes into parallel processes and guides the model to focus on specific subsets of these processes. Specifically, the aggregation inputs are divided into distinct clusters, with each cluster aggregated separately. Instead of compressing messages from all nodes into a single target node, Wideformer limits the input volumes for each aggregation, thereby avoiding message dilution and reducing information loss. To ensure target nodes focus on the informative messages, the aggregation results are sorted and weighed based on the attention scores between the clusters and the target nodes. In contrast to the sparse attention methods that reduce the number of inputs for each target node, Wideformer maintains the global receptive field and distributes the inputs into multiple aggregation processes. By integrating with three popular linear methods GraphGPS [34], SGFormer [51], and Polynormer [9], Wideformer demonstrates effectiveness in tackling over-aggregating. It can consistently benefit the backbones to achieve superior performance over baselines. Codes are available at `https://github.com/sunjss/over-aggregating`.

The contribution of this paper can be summarized as follows:

- We discover a new phenomenon in graph attention, termed over-aggregating, which aggregates a large volume of messages with less discrimination.
- We propose a novel method to relieve over-aggregating, named Wideformer, which divides the aggregation process and guides the model to focus on the informative messages.
- We demonstrate the effectiveness of Wideformer on thirteen real-world datasets, which consistently relieves over-aggregating and benefits backbones to achieve superior performance.

2 Related Work

GNNs perform message passing on input graphs, enabling nodes to learn from their connected neighbors and capture topological features [61]. Among the different message passing methods, GAT [48] first adopts the attention mechanism to aggregate messages. It utilizes attention scores between connected nodes to help central nodes filter out noisy neighbors and focus on the most informative ones. Following GAT, subsequent methods further adopt dense global attention to graphs [23]. A primary challenge for these methods lies in how to effectively encode the graph structure, as global attention performs message passing between all pairs of nodes while neglecting

the underlying graph structure. Several solutions have been proposed, including combining global attention with GNNs to simultaneously encode global features and graph structures [62, 53, 29], learning positional or structural encodings as node features [62, 11, 10, 19], and incorporating graph structures as an attention bias [55].

Another challenge arising from the dense global attention is a space complexity of $O(n^2)$. Efforts to address this challenge can be broadly categorized into two approaches: sparse attention and linear global attention. Sparse attention stems from the Big Bird model [59], which utilizes random masks, sliding windows, and partial global masks to achieve sparsification in traditional transformer architectures. Built upon Big Bird, GraphGPS incorporates these sparse mechanisms into a comprehensive framework for constructing graph transformers [34]. In addition to Big Bird, GAT, which employs input graphs as attention graphs, can also be considered a form of sparse attention. Exphormer [42] and Spexphormer [41] further transform the input graphs into expander graphs, thus better approximating the fully connected graph. However, all of these sparsification methods shrink the receptive fields of each node, leading to a trade-off between model complexity and the ability to capture global information. Different from sparse attentions, Wideformer maintains the global receptive field while requiring linear computing complexity.

In contrast to sparse attention, linear global attention focuses on directly simplifying the computation of dense attention. For example, GraphGPS [34] and Nodeformer [50] extend the linear attention method, Performer [8], from traditional transformer architectures to graph transformers. Performer enables nearly unbiased estimations of dense attention without explicitly computing the attention matrix. In addition to approximation methods, several models have been proposed to model pairwise relations in linear time [51, 9]. However, as shown in Fig. 1(a), the linear methods that maintain the global receptive field during aggregation encounter over-aggregating, leading to dilution of important messages and potential loss of information.

3 Over-Aggregating in Graph Transformers

Graph transformers facilitate global or approximated global message passing between nodes. However, extracting informative features from these global interactions becomes challenging as the number of graph nodes increases. To investigate the behavior of global interactions in graph transformers, we utilize entropy as a measure of attention scores and examine how graph nodes distribute their attention in the receptive field.

3.1 Attention Entropy

In graph attention, input features are projected into query, key, and value features. The value features are aggregated based on the similarity between the query and key features. Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ denote the input node features, where n denotes the number of nodes and d denotes the number of features. Node features are mapped to the query, key, and value features through $\mathbf{Q} = \mathbf{X}\mathbf{W}_Q$, $\mathbf{K} = \mathbf{X}\mathbf{W}_K$, and $\mathbf{V} = \mathbf{X}\mathbf{W}_V$, respectively. Let $\mathbf{R} = \mathbf{Q}\mathbf{K}^\top$, we now have graph attention as

$$\mathbf{H} = \boldsymbol{\alpha}\mathbf{V}, \quad \boldsymbol{\alpha}_{i,j} = \texttt{softmax}(\mathbf{R})_{i,j} = \frac{\texttt{exp}(\mathbf{R}_{i,j})}{\sum_k \texttt{exp}(\mathbf{R}_{i,k})}. \tag{1}$$

Given the attention scores $\{\boldsymbol{\alpha}_{i,1}, \cdots, \boldsymbol{\alpha}_{i,n}\}$ between the target node v_i and all graph nodes, the attention entropy can be formulated as

$$\mathcal{H}(v_i) = -\sum_{j=1}^{n} \boldsymbol{\alpha}_{i,j} \log \boldsymbol{\alpha}_{i,j}. \tag{2}$$

To ensure comparable results across different datasets, the entropy values are normalized by $\log\ n$ to range $[0, 1]$ for visualizations. Attention entropy measures the distribution of attention scores, indicating the confidence of the target nodes in discriminating informative messages. Lower entropy indicates that each target node focuses on a subset of graph nodes with higher attention scores (confidence), while higher entropy reflects more uniformly distributed attention and lower confidence.

Fig. 1(a) compares the attention entropy in sparse attention and linear global attention methods, including linear methods GraphGPS with Performer [34], Polynormer [9], and SGFormer [51], as

well as sparse methods SAN [19] and Exphormer [42]. The entropy values are averaged over all graph nodes throughout the training process. As shown in Fig. 1(a), linear and sparse methods exhibit distinct attention distribution patterns. Specifically, sparse methods demonstrate low attention entropy, which can be attributed to their sparsification strategies that enable nodes to filter out noisy messages and focus on the most informative ones. Conversely, linear methods involve all the graph nodes for aggregation and tend to assign similar attention scores in the receptive field, resulting in higher entropy. The distinct distribution patterns of the sparse and linear methods indicate the relation between the number of nodes in aggregation and the attention entropy.

Theorem 3.1 (Monotonic Lower Bond of Attention Entropy)**.** *Let $\boldsymbol{\alpha}_{i,\cdot} \in \mathbb{R}^n$ be the attention distribution of node v_i over n nodes. The attention entropy $\mathcal{H}(v_i)$ admits a lower bound that increases monotonically with n.*

The proof is provided in Appendix A. Theorem 3.1 indicates that graph attention will be more likely to have higher attention entropy when aggregating more graph nodes, which is further demonstrated in Fig. 1(b).

3.2 Over-Aggregating

We refer to the aggregation process with high attention entropy as over-aggregating, typically demonstrated as uniform and small attention scores, offering limited discrimination among nodes. As a result, over-aggregating prevents graph nodes from prioritizing the informative messages, leading to message dilution and potential information loss.

To empirically evaluate the effect of over-aggregating with high attention entropy, we add an entropy regularization term to the optimization loss for linear methods GraphGPS with Performer, SGFormer, and Polynormer. The best results among the three backbones are reported. Tab. 1 shows that directly reducing the attention entropy during training gives rise to better model performance. This indicates that over-aggregating with high attention entropy does harm the model performance. However, although directly regularizing attention entropy during training can benefit model performance, this process requires the explicit computation of the whole attention matrix, making it inapplicable to large graphs. As a result, it remains an open problem to alleviate over-aggregating for learning on graphs.

Table 1: **Effect of Over-Aggregating by Attention Entropy Regularization (Measured by accuracy except for ROC-AUC for minesweeper: %).**

	ORI	+REG
CORA	86.03$_{\pm 0.54}$	**86.23**$_{\pm 0.32}$
CITESEER	77.96$_{\pm 0.37}$	**78.19**$_{\pm 0.39}$
AMZPHOTO	95.47$_{\pm 0.53}$	**95.52**$_{\pm 0.44}$
MSWEEPER	97.13$_{\pm 0.17}$	**97.20**$_{\pm 0.32}$

Over-aggregating stems from the optimization of attention scores. As shown in Fig. 1(c), models are typically initialized with high attention entropy, which gradually decreases during training. Throughout this process, models update the parameters $\mathbf{W}_Q$ and $\mathbf{W}_K$ with back-propagation, and thus optimize the attention scores. Take $\mathbf{W}_Q$ as an example, the gradient of $\boldsymbol{\alpha}_{i,j}$ with respect to $\mathbf{W}_Q$ can be derived as

$$\frac{\partial \boldsymbol{\alpha}_{i,j}}{\partial \mathbf{W}_Q}\downarrow = \boldsymbol{\alpha}_{i,j}\downarrow \left(\mathbf{X}_{i,\cdot}^\top \mathbf{X}_{j,\cdot} \mathbf{W}_K^\top - \sum_{k=1}^{n} \boldsymbol{\alpha}_{i,k} \mathbf{X}_{i,\cdot}^\top \mathbf{X}_{k,\cdot} \mathbf{W}_K^\top \right). \tag{3}$$

For more details, please refer to Appendix B. A higher initial attention entropy implies smaller attention scores, which in turn attenuate the signals to update these scores. As a result, models converge with persistently high attention entropy, reflecting suboptimal attention distributions. Eq. 3 can also provide insights for the aggravated over-aggregating problem on large-scale graphs (indicated by Theorem 3.1 and Fig. 1(b))

$$\frac{\partial \boldsymbol{\alpha}_{i,j}}{\partial \mathbf{W}_Q} = \boldsymbol{\alpha}_{i,j}(g_{v_j} - g_{\texttt{others}}\uparrow) = \boldsymbol{\alpha}_{i,j} \left[(1-\boldsymbol{\alpha}_{i,j}) \mathbf{X}_{i,\cdot}^\top \mathbf{X}_{j,\cdot} \mathbf{W}_K^\top - \sum_{\substack{k=1 \\ k\neq j}}^{n\uparrow} \boldsymbol{\alpha}_{i,k} \mathbf{X}_{i,\cdot}^\top \mathbf{X}_{k,\cdot} \mathbf{W}_K^\top \right], \tag{4}$$

where g_{v_j} corresponds to the update signals based on the interaction between node v_i and v_j, and $g_{\texttt{others}}$ corresponds to the cumulative impact of all other nodes. As the number of graph nodes grows, $g_{\texttt{others}}$ increasingly incorporates more irrelevant signals, diluting the relative strength of the meaningful update signals in g_{v_j}. This dilution hinders the optimization of $\boldsymbol{\alpha}_{i,j}$, preventing the model from learning discriminative attention distributions and amplifying the over-aggregating issue on large-scale graphs.

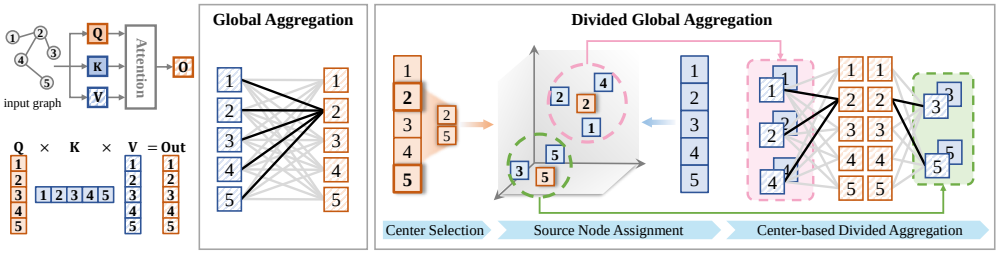


Figure 2: **Attention Comparison between Global Aggregation and Our Divided Global Aggregation.** Global attention employs global aggregation to aggregate source messages into a one-dimensional representation. To relieve the over-aggregating, we assign source nodes into distinct clusters and aggregate each cluster separately, giving rise to multiple aggregation results.

3.3 Discussion

Similar to the occurrence of over-aggregating on the attention graphs, a recent study highlights a phenomenon known as over-globalizing in graph transformers, where models struggle to learn from neighboring nodes in homophilic datasets [54]. While over-globalizing specifically concerns nodes at varying distances, over-aggregating focuses on the discrimination of all nodes during aggregation.

In the context of message passing on input graphs, over-dilution studies aggregation for both feature dimensions and neighboring nodes [21]. Specifically, intra-node dilution focuses on the volumes of the node features, while inter-node dilution focuses on whether a node's own information is preserved during aggregation. Different from over-dilution, over-aggregating focuses on the volumes of the input nodes and emphasizes the preservation of messages from the informative nodes, regardless of whether that includes the node itself.

Besides over-dilution, over-smoothing occurs when node features become increasingly similar as the number of layers grows [30]. This results from the low-pass aggregation among connected nodes in the input graph. In contrast, over-aggregating occurs in the attention graph due to the large number of nodes in the global receptive field. Designing high-pass aggregating functions can tackle over-smoothing. Conversely, for over-aggregating on graph transformers, even when a high-pass behavior is desired, the optimization of attention weights may still be hindered by the overwhelming number of nodes involved in aggregation.

Another notable issue on input graphs is over-squashing, which occurs when message pathways include edges with negative curvatures. It leads to an exponential expansion of the receptive field as the message-passing distance increases [1]. In consequence, a large volume of messages is compressed into fixed-dimensional representations, impeding the effective message exchange between long-range nodes. Unlike over-squashing that occurs during multi-step message passing, over-aggregating arises in one step. It aggregates a large volume of messages into a single node with limited discrimination, leading to the loss of informative messages from one-hop neighbors.

4 Wideformer: Relieving the Over-Aggregating

Based on the analysis in Sec. 3, global attention, including both dense and linear methods, faces a critical trade-off between mitigating over-aggregating and maintaining a global receptive field. To address this challenge, we propose Wideformer, a plug-and-play method designed to enhance graph transformer backbones. Unlike sparse attention methods that reduce the input volume, Wideformer maintains the total inputs and increases the output volume. Specifically, it partitions the inputs into distinct clusters, giving rise to multiple aggregation results for each node and guiding the nodes to focus on the informative clusters. The following subsections detail the two key components of Wideformer: dividing the aggregation and guiding the attention.

4.1 Dividing the Aggregation

Message passing involves aggregating messages from source nodes to target nodes. For each target node v_i in global attention, it treats all the input nodes $\{v_j\}, j \in \{1, \cdots, n\}$ as the source nodes, and aggregate messages $\mathbf{V}_{j,\cdot}$ based on the attention scores between its query features $\mathbf{Q}_{i,\cdot}$ and the

source key features $\mathbf{K}_{j,\cdot}$. As a result, messages from all source nodes at each feature dimension are compressed into a single-dimensional representation, leading to the potential dilution of the key messages.

To relieve the dilution, we propose to divide the source nodes into different clusters based on their attention scores and aggregate each cluster separately. Therefore, source nodes with the highest level of attention can be aggregated together, excluding the other nodes and relieving the message dilution. However, explicitly computing the attention matrix requires a space complexity of $O(n^2)$. To address this issue, Wideformer approximates the division with attention scores by first selecting cluster centers among the query features, and then assigning the source nodes to the clusters based on the similarity between their key features and the centers.

Algorithm 1 Center-selection Function `Cluster`

Input: query $\mathbf{Q} \in \mathbb{R}^{n\times d}$, number of clusters m
Initialize center $\mathbf{C} = \{0\}_{m\times d}$
$\mathbf{C}_{1,\cdot} = \mathbf{Q}_{t,\cdot},\ t = \arg\max_i \sum_j \mathbf{Q}_{i,j}$
for $t = 1$ **to** m **do**
  Compute distances: $\mathbf{q} = \max_j \left[(\mathbf{Q}\mathbf{C}^\top)_{\cdot,j}\right]$
  Select next center indices: $q = \arg\min_i(\mathbf{q}_i)$
  Update centers: $\mathbf{C}_{t,\cdot} = \mathbf{Q}_{q,\cdot}$
end for
Output: centers $\mathbf{C} \in \mathbb{R}^{m\times d}$

Let m be the number of clusters, $\mathbf{C} = \texttt{Cluster}(\mathbf{Q}, m) \in \mathbb{R}^{m\times d}$ be the cluster centers. The center-selection function `Cluter` in Algorithm 1 is implemented based on K-Means++ [3]. The query of the source node with the largest summation across feature dimensions is selected as the initial cluster center. Notably, this initial center is solely used to initiate the selection process and does not participate in the aggregation. `Cluter` then select m centers sequentially, where the node that minimizes the maximum similarity to all previously selected centers is designated as a new cluster center.

The source nodes are assigned to the identified query clusters based on the similarity between $\mathbf{K}$ and $\mathbf{C}$. The assignment result $\mathbf{k} \in \mathbb{R}^n$ can be formulated as

$$\mathbf{k}_i = \arg\max_j \left[\left(\mathbf{K}\mathbf{C}^\top\right)_{i,j}\right]. \tag{5}$$

By performing aggregation within distinct clusters, Wideformer produces multiple outputs for each target node. The aggregation result of the t-th cluster $\mathbf{H}^{(t)} \in \mathbb{R}^{n\times d}$ can be formulated as

$$\mathbf{H}^{(t)} = \sum_{i\in\{j|\mathbf{k}_j=t\}} \texttt{softmax}(\mathbf{Q}\mathbf{K}_{i,\cdot}^\top)\mathbf{V}_{i,\cdot}\,. \tag{6}$$

To illustrate the effect of aggregation, for each target node v_i and the j-th feature dimension of the source message $\mathbf{V}$, the original aggregation method in Eq. 1 compresses messages from all nodes into a one-dimensional representation $\mathbf{H}_{i,j}$, which leads to the dilution of key messages and over-aggregating. In contrast, Wideformer with Eq. 6 increases the output volume, yielding a m-dimensional representation $\{\mathbf{H}_{i,j}^{(1)}, \cdots, \mathbf{H}_{i,j}^{(m)}\}$. Only a limited volume of messages is aggregated for each cluster, preventing the dilution of the key messages. Even when the target nodes apply uniform attention scores to the source nodes, the messages in different clusters remain separate from being over-aggregated.

4.2 Guiding the Attention

The aggregation results $\{\mathbf{H}^{(1)}, \cdots, \mathbf{H}^{(m)}\}$ are concatenated for the subsequent modules in backbones. During the concatenation, the current ordering of the aggregated results depends on the cluster-selection order. However, since each target node assigns different attention scores to the clusters, this order does not reflect the importance of each cluster for the target node. To ensure consistent ordering and enable the target nodes to focus on the informative clusters, Wideformer sorts and weights the clusters for each target node based on the cluster attention score $\bar{\boldsymbol{\alpha}}_{i,j} \in \mathbb{R}^{n\times m}$. These scores can be formulated as

$$\bar{\boldsymbol{\alpha}}_{i,j} = \texttt{softmax}(\mathbf{Q}\bar{\mathbf{K}}^\top)_{i,j}, \qquad \bar{\mathbf{K}}_{t,\cdot} = \frac{1}{|\{v_i|\mathbf{k}_i = t\}|} \sum_{i\in\{j|\mathbf{k}_j=t\}} \mathbf{K}_{i,\cdot}, \tag{7}$$

where $\bar{\mathbf{K}} \in \mathbb{R}^{m\times d}$ denotes the average key features of the clusters. The sorted and weighted aggregation result $\hat{\mathbf{H}}^{(t)} \in \mathbb{R}^{n\times d}$ is then obtained as

$$\hat{\mathbf{H}}_{i,\cdot}^{(t)} = \bar{\boldsymbol{\alpha}}_{i,\mathbf{S}_{i,t}} \mathbf{H}_{i,\cdot}^{(\mathbf{S}_{i,t})}, \qquad \mathbf{S}_{i,\cdot} = \arg\texttt{sort}_j\left[\bar{\boldsymbol{\alpha}}_{i,j}\right], \tag{8}$$

Table 2: **Comparison Results on Homophilic Datasets (Measured by accuracy: %).** OOM indicates out-of-memory under the experimental setups.

	AMAZONCOMPUTERS	COAUTHORCS	AMAZONPHOTO	COAUTHORPHYSICS
#NODES	13,381	18,333	7,487	34,493
#FEATURES	767	6,805	745	8,415
#CLASSES	10	15	8	5
GCN	89.65±0.52	92.92±0.12	92.70±0.20	96.18±0.07
GRAPHSAGE	91.20±0.29	93.91±0.13	94.59±0.14	96.49±0.06
GAT	90.78±0.13	93.61±0.14	93.87±0.11	96.17±0.08
GPRGNN	89.32±0.29	95.13±0.09	94.49±0.14	96.85±0.08
NAGPHORMER	91.19±0.14	95.75±0.09	95.49±0.11	97.34±0.03
NODEFORMER	86.98±0.62	95.64±0.22	93.46±0.35	96.45±0.28
DIFFORMER	91.99±0.76	94.78±0.20	95.10±0.47	96.60±0.18
GOAT	90.96±0.90	94.21±0.38	92.96±1.48	96.24±0.24
EXPHORMER	91.47±0.17	94.93±0.01	95.35±0.22	96.89±0.09
GRAPHGPS	90.62±0.36	95.44±0.03	94.98±0.16	96.75±0.07
+ENTROPY REG	90.68±0.37	95.50±0.19	95.28±0.28	OOM
+WIDEFORMER	90.84±0.57	**95.85**±0.07	95.55±0.74	96.95±0.03
SGFORMER	91.66±0.23	93.50±0.32	95.47±0.66	96.87±0.08
+ENTROPY REG	91.78±0.37	93.59±0.41	95.51±0.49	96.88±0.09
+WIDEFORMER	92.19±0.17	93.86±0.41	95.64±0.57	**97.39**±0.19
POLYNORMER	91.98±0.09	94.53±0.61	95.47±0.53	96.67±0.29
+ENTROPY REG	92.08±0.07	94.57±0.43	95.52±0.44	96.69±0.31
+WIDEFORMER	**92.39**±0.07	94.60±0.27	**95.64**±0.36	96.79±0.20

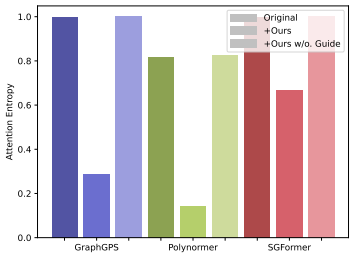
where arg `sort` returns the indices of the sorted elements in ascending order. Eq. 7 and 8 inject the importance of each cluster into the aggregation, guiding the focus of the target nodes. The weighted results are concatenated for the following computation.

5 Experiment

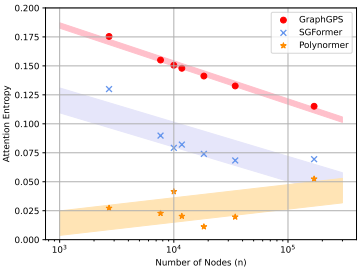
To evaluate the effectiveness of Wideformer, we conduct empirical evaluations on real-world datasets. The detailed setups are presented in Appendix D.

5.1 Effectiveness in tackling Over-Aggregating

Wideformer is evaluated on three linear methods, including GraphGPS with Performer [34], SGFormer [51], and Polynormer [9]. To ensure consistent comparison, these methods are implemented under the framework of GraphGPS. As presented in Fig. 3(a), Wideformer can effectively reduce the attention entropy of all backbone methods. This reduction allows target nodes to focus on informative source nodes within the global receptive field, effectively preventing the dilution of key messages and mitigating over-aggregating.



(a) Attention Entropy Comparison



(b) Cluster Attention Entropy

Figure 3: **Effectiveness Evaluation for Over-Aggregating.** "+ Ours" denotes using our proposed Wideformer. "+ Ours w/o. Guide" employs Wideformer without attention guidance.

However, Wideformer without the attention-guiding process still exhibits high attention entropy in Fig. 3(a). This partial method only avoids message dilution but fails to effectively guide the attention of the target nodes. To further investigate the attention-guiding process in Wideformer, we conduct an empirical analysis of cluster attention $\bar{\alpha}$. As shown in Fig. 3(b), Wideformer provides low cluster attention entropy for all three backbones, indicating that only a subset of input messages is crucial for the target nodes. The attention-guiding process in Wideformer allows backbone methods to concentrate on these informative subsets, enhancing their ability to mitigate over-aggregating. As the number of nodes increases, GraphGPS and SGFormer exhibit increasingly divergent attention scores across clusters, while Polynormer maintains much lower cluster attention entropy, albeit with a slight upward trend. This indicates that Wideformer consistently supports different backbone methods in prioritizing informative messages, even when the graph size grows.

Table 3: **Comparison Results on Heterophilic Datasets (Measured by ROC-AUC except for accuracy for amazon-ratings and roman-empire: %).** OOM indicates out-of-memory under the experimental setups.

	AMAZON-RATINGS	MINESWEEPER	QUESTIONS	ROMAN-EMPIRE	TOLOKERS
#NODES	24,492	10,000	48,921	22,662	11,758
#FEATURES	300	7	301	300	10
#CLASSES	5	2	2	18	2
GCN	48.70±0.63	89.75±0.52	76.09±1.27	73.69±0.74	83.64±0.67
GRAPHSAGE	53.63±0.39	93.51±0.57	76.44±0.62	85.74±0.67	82.43±0.44
GAT	52.70±0.62	93.91±0.35	76.79±0.71	88.75±0.41	83.78±0.43
GPRGNN	44.88±0.34	86.24±0.61	55.48±0.91	64.85±0.27	72.94±0.97
NAGPHORMER	51.26±0.72	84.19±0.66	68.17±1.53	74.34±0.77	78.32±0.95
NODEFORMER	43.86±0.35	86.71±0.88	74.27±1.46	64.49±0.73	78.10±1.03
DIFFORMER	47.84±0.65	90.89±0.58	72.15±1.31	79.10±0.32	83.57±0.68
GOAT	44.61±0.50	81.09±1.02	75.76±1.66	71.59±1.25	83.11±1.04
EXPHORMER	53.51±0.46	84.19±0.53	73.94±1.06	89.03±0.37	83.77±0.78
GRAPHGPS	49.73±0.11	93.26±0.10	75.48±0.66	81.46±0.40	83.95±0.81
+ENTROPY REG	OOM	93.35±0.23	OOM	OOM	84.23±0.51
+WIDEFORMER	49.96±0.41	93.52±0.07	75.69±1.17	82.12±0.39	84.67±0.66
SGFORMER	52.38±0.22	88.60±0.49	76.81±0.09	75.20±0.89	82.24±0.13
+ENTROPY REG	52.86±0.29	88.87±0.33	76.83±0.18	75.84±0.43	82.39±0.19
+WIDEFORMER	53.47±0.14	89.02±0.22	76.94±0.05	77.03±0.38	82.55±0.03
POLYNORMER	54.71±0.17	97.13±0.17	78.66±0.50	91.83±0.16	85.09±0.21
+ENTROPY REG	54.79±0.23	97.20±0.32	78.69±0.24	91.94±0.34	85.21±0.33
+WIDEFORMER	**55.05**±0.08	**97.26**±0.01	**79.00**±0.20	**92.16**±0.24	**85.33**±0.23

Table 4: **Comparison Results on Datasets with Broader Scales (Measured by accuracy: %).** OOM indicates out-of-memory under the experimental setups.

	OGB-ARXIV	CITESEER	CORA	TWITCH-GAMER
#NODES	169,343	3,327	2,708	168,114
#FEATURES	128	3,703	1,433	7
#CLASSES	40	6	7	2
GCN	71.74±0.29	71.60±0.40	81.60±0.40	62.18±0.26
GRAPHSAGE	71.49±0.27	71.93±0.85	82.68±0.47	64.37±0.39
GAT	71.95±0.36	72.10±1.10	83.00±0.70	59.89±4.12
EXPHORMER	72.44±0.28	71.63±1.19	82.77±1.38	64.30±0.16
GRAPHGPS	70.47±1.56	77.96±0.37	86.03±0.54	64.98±0.26
+ENTROPY REG	OOM	78.19±0.39	86.23±0.32	OOM
+WIDEFORMER	70.66±1.29	**78.61**±0.35	**86.70**±0.83	65.46±0.20
SGFORMER	72.23±0.73	69.93±0.31	80.83±0.52	65.85±0.02
+ENTROPY REG	OOM	70.12±0.41	81.04±0.38	OOM
+WIDEFORMER	**72.58**±0.39	70.63±0.78	81.20±0.37	66.34±0.37
POLYNORMER	70.77±1.16	66.43±1.50	78.70±0.94	67.15±0.03
+ENTROPY REG	OOM	67.21±0.35	79.28±0.51	OOM
+WIDEFORMER	70.88±0.10	68.10±0.42	79.90±0.86	**67.33**±0.15

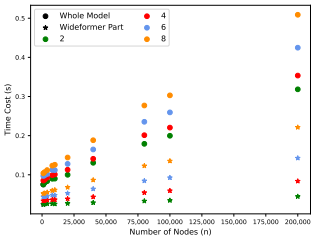


Figure 4: **Time Cost on GraphGPS.** The point shape "." denotes the whole model and "*" denotes the Wideformer part. The color of the points indicates the number of the clusters m.

5.2 Model Comparison

Experimental Setup. We adopt thirteen real-world datasets, including both heterophilic and homophilic graphs. For baseline methods, both GNNs and graph transformers are adopted. Please refer to Appendix D.2 for detailed experimental setups. To address the out-of-memory issue associated with the entropy regularization baseline, we divide the target nodes into mini-batches. Each batch is sequentially processed to compute attention scores with all source nodes. The results of the backbone methods GraphGPS with Performer, SGFormer, and Polynormer are reproduced under the framework of GraphGPS.

Performance. We present the comparison results on datasets where the number of nodes is around 10k in Tab. 2 and Tab. 3. Wideformer consistently enhances the performance of all backbone models across various datasets. Specifically, backbones integrated with Wideformer achieve superior performance compared to baseline methods. For instance, in Tab. 2, Wideformer enables backbone methods to outperform the previous best-performing baselines, including DIFFormer on AmazonComputers and NAGphormer on CoauthorsCS, CoauthorPhysics, and AmazonPhoto. Compared to the entropy regularization method, we can see that regularizing entropy results in inferior performance to Wideformer and even marginal gains on larger graphs. This is consistent with our analysis in Sec. 3.2. Entropy regularization does not divide the aggregation process, and thus suffers from optimization challenges when aggregating over a large number of source nodes. In contrast, Wideformer separates

the aggregation into parallel processes. Each process only involves a small ratio of the source nodes to be aggregated, preventing the dilution of the key messages. We also compare the gains with zero to evaluate the statistical significance of the performance gains. Paired t-tests on all backbones consistently give rise to p-values smaller than 0.05, and the confidence interval results do not contain 0, validating the statistical significance of the performance gains with Wideformer. These results demonstrate that relieving over-aggregating improves the effectiveness of graph attention.

To further verify Wideformer's ability to mitigate over-aggregating, we extend our experiments to datasets with broader node scales, including 1k and 0.1M nodes. Results in Tab. 4 show that Wideformer can benefit backbones with different scales of nodes. Among the three backbones, SGFormer achieves better results on large-scale graphs ogb-arxiv and twitch-gamer, but inferior results on small-scale graphs CiteSeer and Cora. This is due to the trade-off between noise filtering and information loss in SGFormer, which is further investigated in Sec. 5.3.1.

5.3 Model Analysis

5.3.1 Informative Source Nodes

Wideformer empowers backbone methods to focus on informative source nodes within the global receptive field. To investigate the attention mechanism in Wideformer, we conduct additional experiments on source nodes assigned to the cluster with the highest attention score, analyzing both their volumes and their relations with the target nodes.

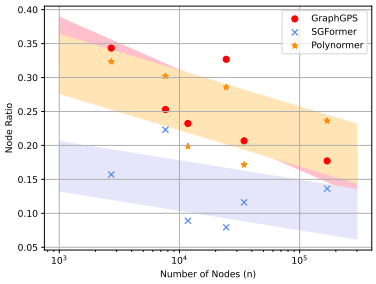


Figure 5: **Informative Source Node Ratio.** The ratio is the number of nodes assigned to the cluster with the highest attention score relative to the total number of graph nodes.

Node Ratio. To analyze the node volume, we calculate the ratio of nodes assigned to the cluster with the highest attention score relative to the total number of graph nodes. As shown in Fig. 5, the node ratio decreases as the total number of nodes increases. This suggests that the proportion of informative nodes diminishes in larger graphs, leading to noisier source messages. Wideformer addresses this by assigning a smaller ratio of nodes to the cluster with the highest attention score, guiding the backbones to focus on the most informative nodes. Among the three backbones, SGFormer focuses on fewer source nodes than GraphGPS and Polynormer. This results in a trade-off between noise filtering and information loss, where SGFormer performs better on large-scale graphs (ogb-arxiv and twitch-gamer) but lags behind on smaller graphs (CiteSeer and Cora).

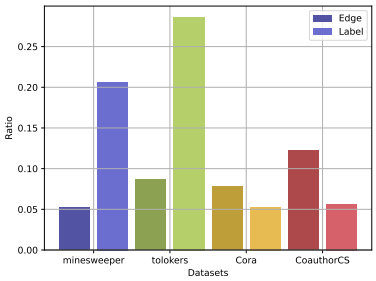


Figure 6: **Node Relations.** Label/Edge denotes the ratio of source nodes sharing the same label/connected with the target nodes.

Node Relations. To analyze the relations between target and source nodes in the cluster with the highest attention score, we compute the ratio of the source nodes (1) that have the same label as the target nodes, and (2) that are connected with the target nodes, both relative to the total number of source nodes in the cluster. The results with GraphGPS are presented in Fig. 6. For the other two backbones, please refer to Appendix E. As shown in Fig. 6, we can see that approximately 10% of source nodes are connected with their target nodes. The label distribution diverges between heterophilic graphs and homophilic graphs, where target nodes assign larger attention scores to the same-class source nodes on heterophilic graphs.

5.3.2 Complexity Analysis

The time and space complexity of Wideformer is $O(nm)$, where n and m denote the number of nodes and clusters, respectively. In practice, m is chosen from $\{2, ..., 8\}$, which ensures the model's scalability to large graphs. We provide a time cost study regarding the number of nodes (n) and clusters (m), comparing the whole model with the part of Wideformer. The results on GraphGPS are presented in Fig. 4, where the time cost of Wideformer scales linearly to n and remains a small ratio of the total cost. For detailed experimental setup and full results, please refer to Appendix F.

5.3.3 Model Ablation

To evaluate the contribution of the aggregation-dividing and attention-guiding process in Wideformer, we conduct an ablation study on the three backbone methods.

Cluster Ablation. Wideformer partitions the source nodes into distinct clusters. To examine the impact of this division, we perform an ablation study on the number of clusters m regarding performance gains. The gain is defined as $\frac{p_m - p_1}{p_1}$, where p_1 and p_m denote the performance with a single cluster and m clusters, respectively. The average performance gains across various datasets for all three backbones are shown in Fig. 7. We can see that increasing the number of clusters initially increases the performance gain. However, when m exceeds 6, the performance gain starts to decline. This is because a relatively larger number of clusters can effectively reduce the input message volume, mitigating the dilution of key information. Nevertheless, excessively partitioning the source nodes disperses critical information into multiple clusters. This leads to the distracted attention of the target nodes, reducing the values of attention scores and increasing attention entropy. In practice, the optimal number of clusters is around $3 \sim 5$.

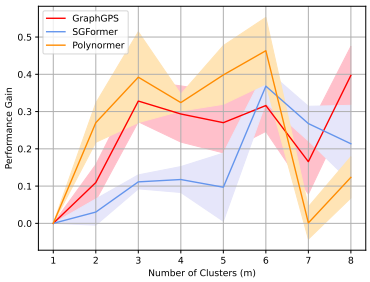


Figure 7: **Comparison with Different Numbers of Clusters.**

Center Selection. To ensure computing efficiency, Wideformer employs a non-iterative strategy for center selection. We now compare this simple choice with (1) multi-step iterative clustering and (2) parameterized centers, to shed light on the future directions. Tab. 5 shows that applying iterative clustering can achieve better results, indicating the efficiency-performance trade-offs. Further modeling centers as parameters can address this trade-off, which does not require iterations and achieves the best results.

Table 5: **Comparison on the Center Selection Methods.** Results are averaged on amazon-ratings, questions, CoauthorCS, and AmazonPhoto.

	GRAPHGPS	SGFORMER	POLYNORMER
ORIGINAL	78.91±0.24	79.54±0.32	80.84±0.45
+WIDEFORMER	79.26±0.59	79.98±0.29	81.07±0.23
+ITER=2	79.93±0.45	80.58±0.39	81.44±0.29
+ITER=4	79.95±0.57	80.42±0.37	81.43±0.21
+ITER=6	79.85±0.44	80.55±0.34	81.52±0.23
+LEARNABLE	**80.05**±0.46	**80.60**±0.39	**81.54**±0.20

Module Ablation. Tab. 6 shows that combining divided aggregation and attention guidance generally achieves better performance. However, using only divided aggregation can also benefit the backbones, such as on CoauthorCS and AmazonPhoto with Polynormer. This is likely due to the simple attention-guiding strategy, which directly determines the importance of each cluster as a whole. Under circumstances where fewer source nodes contain informative messages, this simple strategy leads to limited benefit capability. Exploring alternative guiding strategies will be the focus of our future work.

Table 6: **Module Ablation Results (Measured by accuracy: %).** "Div."/"All" denotes the divided aggregation without/with attention-guidance.

	AMAZON -RATINGS	COAUTHOR CS	AMAZON PHOTO	ROMAN -EMPIRE
GRAPHGPS	49.73±0.11	95.44±0.03	94.98±0.16	81.46±0.40
+DIV.	49.58±0.54	95.56±0.30	94.98±0.61	81.40±0.54
+ALL	**49.96**±0.41	**95.65**±0.07	**95.55**±0.74	**82.12**±0.39
SGFORMER	52.38±0.22	93.50±0.32	95.47±0.66	75.20±0.89
+DIV.	52.42±0.54	93.53±0.21	95.58±0.53	**77.38**±0.54
+ALL	**53.47**±0.14	**93.86**±0.41	**95.64**±0.57	77.03±0.38
POLYNORMER	54.71±0.17	94.53±0.61	95.47±0.53	91.83±0.16
+DIV.	54.82±0.11	**94.90**±0.30	**96.74**±0.30	92.04±0.15
+ALL	**55.05**±0.08	94.60±0.27	95.64±0.36	**92.16**±0.24

6 Conclusion

In this paper, we discovered a phenomenon in graph attention, termed over-aggregating. Attention with over-aggregating assigns uniformly distributed attention scores to the messages. As a result, the key messages are diluted during aggregation, leading to potential information loss. To relieve this problem, we proposed a novel plug-and-play method, Wideformer. Wideformer divides the source nodes for aggregation into distinct clusters and aggregates each cluster separately. To ensure focus on the informative source nodes, Wideformer applies attention guidance to sort and weight the clusters. Experiments on thirteen datasets show that Wideformer can consistently enhance the performance of backbones and effectively relieve over-aggregating. Please refer to Appendix. I for the limitation discussion.

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A Proof for Monotonic Lower Bound of Attention Entropy

Lemma A.1 (Lower Bound of Attention Entropy)**.** *Let $\boldsymbol{\alpha}_{i,\cdot} \in \mathbb{R}^n$ be the attention distribution of node v_i over n nodes. Suppose each entry satisfies $\boldsymbol{\alpha}_{i,j} \geq \epsilon > 0$. Then the attention entropy $\mathcal{H}(v_i)$ admits the following strict lower bound:*

$$\mathcal{H}(v_i) \geq -\left[1-(n-1)\epsilon\right]\log\left[1-(n-1)\epsilon\right] - (n-1)\epsilon\log\epsilon.$$

Proof. Assume $\epsilon > 0$ is a lower bound for all elements of $\boldsymbol{\alpha}_{i,\cdot}$. The minimum entropy under this constraint is attained when one entry takes the maximum possible weight and the remaining $(n-1)$ entries equal ϵ, *i.e.*,

$$\hat{\boldsymbol{\alpha}}_{i,\cdot} = \left(1-(n-1)\epsilon, \epsilon, \ldots, \epsilon\right).$$

The attention entropy of this distribution is

$$\mathcal{H}_{\min}(v_i) = -\left[1-(n-1)\epsilon\right]\log\left[1-(n-1)\epsilon\right] - (n-1)\epsilon\log\epsilon.$$

Since the Shannon entropy is strictly concave, any deviation from this distribution increases the entropy. Therefore, for any valid distribution $\boldsymbol{\alpha}_{i,\cdot}$ with elements bounded below by ϵ, it holds that

$$\mathcal{H}(v_i) \geq \mathcal{H}_{\min}(v_i).$$

□

We now provide the proof for Theorem 3.1 based on Lemma A.1.

Theorem 3.1 (Monotonic Lower Bound of Attention Entropy). *Let $\boldsymbol{\alpha}_{i,\cdot} \in \mathbb{R}^n$ be the attention distribution of node v_i over n nodes. The attention entropy $\mathcal{H}(v_i)$ admits a lower bound that increases monotonically with n.*

Proof. To show that $\mathcal{H}_{\min}(v_i)$ increases monotonically with n, we compute its derivative with respect to n

$$\begin{aligned}
\frac{d\mathcal{H}_{\min}(v_i)}{dn} &= \epsilon\log\left[1-(n-1)\epsilon\right] + \left[1-(n-1)\epsilon\right]\frac{\epsilon}{\left[1-(n-1)\epsilon\right]} - \epsilon\log\epsilon \\
&= \epsilon\log\left[1-(n-1)\epsilon\right] + \epsilon - \epsilon\log\epsilon \\
&= \epsilon\log\frac{1-(n-1)\epsilon}{\epsilon} + \epsilon.
\end{aligned}$$

Since $\hat{\boldsymbol{\alpha}}_{i,\cdot} = (1-(n-1)\epsilon, \epsilon, \cdots, \epsilon)$ denoting the most non-uniform distribution $\boldsymbol{\alpha}_{i,\cdot}$ requires $0 < \epsilon \leq 1/n$, it follows that $1-(n-1)\epsilon \geq \epsilon$, and thus

$$\frac{d\mathcal{H}_{\min}(v_i)}{dn} > 0.$$

This confirms that $\mathcal{H}_{\min}(v_i)$ increases monotonically with n. □

B Detailed Derivation

In this section, we provide a detailed derivation for Eq. 3. Let $\mathbf{R} = \mathbf{Q}\mathbf{K}^\top$. Given the attention scores formulated in Eq. 1, the gradient of $\boldsymbol{\alpha}_{i,j}$ with respect to $\mathbf{W}_Q$ can be derived as

$$\begin{aligned}
\frac{\partial\boldsymbol{\alpha}_{i,j}}{\partial\mathbf{W}_Q} &= \sum_{k=1}^{n}\frac{\partial\boldsymbol{\alpha}_{i,j}}{\partial\mathbf{R}_{i,k}}\frac{\partial\mathbf{R}_{i,k}}{\mathbf{W}_Q} \\
&= \sum_{k=1}^{n}\boldsymbol{\alpha}_{i,j}\left(\delta_{j,k}-\boldsymbol{\alpha}_{i,k}\right)\frac{\partial}{\partial\mathbf{W}_Q}\mathbf{X}_{i,\cdot}\mathbf{W}_Q\mathbf{W}_K^\top\mathbf{X}_{k,\cdot}^\top \\
&= \sum_{k=1}^{n}\boldsymbol{\alpha}_{i,j}\left(\delta_{j,k}-\boldsymbol{\alpha}_{i,k}\right)\mathbf{X}_{i,\cdot}^\top\mathbf{X}_{k,\cdot}\mathbf{W}_K^\top \\
&= \boldsymbol{\alpha}_{i,j}\left(\mathbf{X}_{i,\cdot}^\top\mathbf{X}_{j,\cdot}\mathbf{W}_K^\top - \sum_{k=1}^{n}\boldsymbol{\alpha}_{i,k}\mathbf{X}_{i,\cdot}^\top\mathbf{X}_{k,\cdot}\mathbf{W}_K^\top\right),
\end{aligned}$$

where $\delta_{j,k}$ is a sign function. When $k=j$, $\delta_{j,k}=1$, otherwise $\delta_{j,k}=0$.

Table S7: **Comparison Results with Entropy Regulation on the Cluster Attention (Measure by accuracy: %).** "Reg." denotes employing the attention entropy of the cluster attention scores as part of the optimization target.

	ROMAN-EMPIRE	COAUTHORCS
GRAPHGPS	81.46	95.44
+WIDEFORMER	82.12	95.85
+WIDEFORMER W/ REG.	**82.23**	**96.14**
SGFORMER	75.20	93.50
+WIDEFORMER	77.03	93.86
+WIDEFORMER W/ REG.	**77.83**	**94.16**
POLYNORMER	91.83	94.53
+WIDEFORMER	92.16	94.60
+WIDEFORMER W/ REG.	**92.36**	**95.42**

C Over-Aggregating Measurement

In this paper, we propose to employ entropy to quantify over-aggregating. This stems from the observation that the attention scores distribute uniformly among different source nodes. To quantify the uniformity of the distribution, we adopt entropy as the measure following the common practice in the community [56, 6, 32]. Except for entropy, other potential metrics include standard deviation (STD), Kullback-Leibler divergence (KLD), and Jensen-Shannon divergence (JSD). STD focuses on the dispersion of values. When the total number of values is large, but the number of dispersed values is small, the STD may remain small despite the distribution being uneven. Therefore, using STD to assess uniformity is not an accurate approach. KLD and JSD are used to assess the similarity between two distributions. It can measure the uniformity of a distribution by setting the reference distribution to be uniform. However, when the reference distribution is uniform, KLD equals the difference between the maximum entropy and the entropy of the given distribution, while JSD can be viewed as a combination of entropy and KLD. Therefore, we opted for the simpler and more commonly used entropy to directly measure the uniformity.

Entropy also demonstrates effectiveness in benefiting model performance. In addition to the entropy regularization method on the whole attention matrix (Tab. 1), we compute the entropy of the cluster attention scores in Wideformer and employ the results as part of the optimization target. Results on roman-empire and CoauthorCS in Tab. S7 show that optimizing the cluster attention entropy for backbones with Wideformer can also benefit the model performance. This also indicates that the value of the attention entropy properly quantifies over-aggregating.

In Fig. 3(a), a more significant entropy reduction occurs on Polynormer, but its associated performance gains are not superior to those of the other two backbone architectures. This is due to the distinct architectural design of the backbones. Different architectures inherently prioritize different attention patterns for optimal representation learning. While high attention entropy consistently indicates over-aggregating, the optimal entropy level varies across models. Thus, although Polynormer exhibits the most significant entropy reduction, this may still fall short of what is needed for its optimal performance.

D Details on Experiments

D.1 Datasets

We adopt thirteen real-world datasets, including heterophilic graphs (amazon-ratings, minesweeper, questions, roman-empire, tolokers [32], and twitch-gamer [24]) and homophilic graphs (Cora, CiteSeer [36], CoauthorCS, CoauthorPhysics, AmazonComputers, AmazonPhoto [37], and ogb-arxiv [15]).

Questions is derived from Yandex Q, spanning user activity from September 2021 to August 2022. Nodes represent users interested in "medicine" and edges indicate answers to others' questions. The binary classification task predicts whether users remained active without account deletion or blocking. Node features are averaged FastText embeddings of profile descriptions.

Amazon-ratings is based on the Amazon product co-purchase network from the SNAP Datasets [22]. Nodes represent products, and edges capture frequent co-purchase relationships. The task is to predict the average reviewer rating for each product, grouped into five ordinal classes. Node features are the average FastText embeddings of product descriptions.

Tolokers represents crowdsourcing participation data from the Toloka platform. Nodes correspond to contributors ("tolokers") active in at least one of 13 projects, with edges connecting those who completed the same tasks. The binary classification task predicts whether tolokers were banned from projects. Node features include profile attributes and task performance statistics.

Minesweeper is a synthetic 100x100 grid graph where nodes represent grid cells, with 20% randomly assigned as mines. The task is to classify nodes as mines or non-mines. Node features are one-hot vectors encoding the count of neighboring mines, but 50% of nodes have their features reset to unknown values, marked by a binary indicator.

Twitch-gamer is collected from the Twitch website with nodes representing users. Only users with mutual relations are incorporated in the dataset. The task is to predict whether the user accounts contain explicit content.

Cora and CiteSeer are citation graphs. In the Cora dataset, machine learning papers are grouped into seven distinct classes, while the CiteSeer dataset categorizes papers into six classes. Node features are derived from high-frequency words appearing in the content of the papers.

CoauthorCS and CoauthorPhysics are derived from the Microsoft Academic Graph. These datasets represent co-authorship networks, where nodes correspond to researchers, and edges signify their collaborative relationships. The features of each node reflect the frequency of keywords extracted from the publications of the respective authors. Graph labels identify the primary research domain of each author, distinguishing between computer science and physics.

AmazonComputers and AmazonPhoto are co-purchase networks constructed from Amazon. In these graphs, nodes represent products, while edges indicate co-purchase relationships between item pairs. Node features are derived from encoded customer review texts associated with each product, and graph labels classify the products into specific categories.

OGB-arXiv is a citation graph composed of Computer Science papers from arXiv. In this dataset, nodes correspond to individual articles, and directed edges represent citation relationships. Node features are computed as the average of 128-dimensional word embeddings extracted from the title and abstract of each paper. The task involves predicting the primary category of arXiv articles among 40 possible classes.

D.2 Experimental Setup

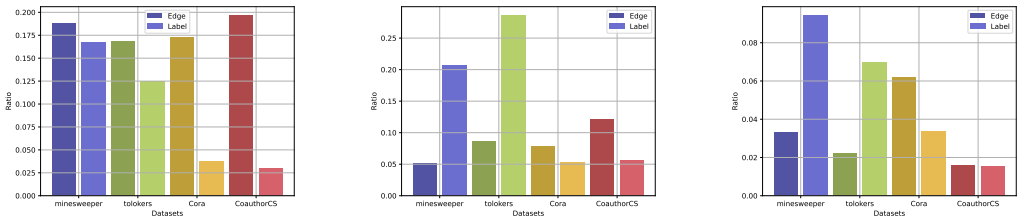
The attention entropy experiments in Fig. 1, Fig. 3, and Fig. 5 are conducted on Cora, Amazon-Photo, AmazonComputers, CoauthorCS, CoauthorPhysics, tolokers, amazon-ratings, minesweeper, and ogb-arxiv. The cluster ablation study in Fig. 7 is conducted and averaged on all the datasets included in this paper. The number of clusters is 4 in Fig. 3, Fig. 5-6, Fig. S8, and Tab. 5-6. Other experiments choose m from $\{2, \cdots, 8\}$. For baseline methods, both GNNs (GCN [17], GraphSAGE [14], GAT [48], GPRGNN [7]) and graph transformers (NAGphormer [4], NodeFormer [50], DIFFormer [49], GOAT [18]) are included. The results of the backbone methods, including GraphGPS with Performer, SGFormer, and Polynormer, are reproduced under the framework of GraphGPS. The framework is implemented with PyTorch [31] and PyTorch Geometric [12], and trained on a single NVIDIA A100. We perform grid search based on the validation performance of the models as follows:

GraphGPS. We search the number of graph transformer layers in $\{1, \cdots, 6\}$, the number of hidden dimensions in $\{64, 80, 128, 256\}$, the number of heads in $\{1, 2, 4\}$, dropout in $\{0.1, 0.2, 0.3, 0.5\}$, and learning rate in $\{5e-4, 1e-3, 1e-2\}$. The rest hyperparameters are fixed as in the original implementation.

SGFormer. The GNN backbone is implemented as GCN [17]. The number of GCN layers is searched in $\{1, \cdots, 10\}$, the number of hidden dimensions in $\{64, 80, 128, 256\}$, the number of

heads in $\{1, 2, 4\}$, dropout in $\{0.1, 0.2, 0.3, 0.5\}$, and learning rate in $\{1e-3, 5e-3, 1e-2\}$. The rest hyperparameters are fixed as in the original implementation.

Polynormer. The GNN backbone is implemented as GAT [48]. We search the number of graph transformer layers in $\{1, \cdots, 6\}$, the number of GAT layers in $\{1, \cdots, 10\}$, the number of hidden dimensions in $\{64, 80, 128, 256\}$, the number of heads in $\{1, 2, 4, 8\}$, dropout in $\{0.1, 0.2, 0.3, 0.5\}$, and learning rate in $\{5e-4, 1e-3\}$. The rest hyperparameters are fixed following the original implementation.

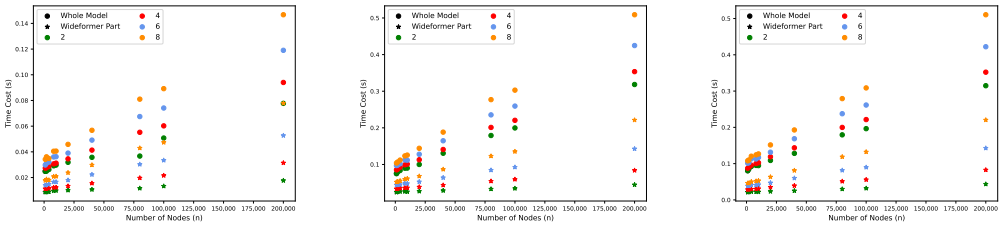


(a) SGFormer (b) GraphGPS (c) Polynormer

Figure S8: **Full Results for Relations between Source and Target Nodes.**

E Full Results for Informative Source Nodes

To analyze the relations between target and source nodes in the cluster with the highest attention score, we compute the ratio of the source nodes (1) that have the same label as the target nodes, and (2) that are connected with the target nodes, both relative to the total number of source nodes in the cluster. The results for all three backbones are presented in Fig. S8. The ratio of source nodes that are connected to their target nodes varies across the different backbones. Among the backbones, SGFormer assigns more attention to source nodes connected with the target nodes than Polynormer and GraphGPS. The label distribution differs between heterophilic and homophilic graphs, yet remains consistent across the backbones. On heterophilic graphs, target nodes assign higher attention scores to source nodes that have the same label as them. This stems from the heterophily of these graphs, where connected nodes often have different labels. Therefore, models only aggregate messages from nodes with different labels via local message passing and turn to global attention to collect messages from nodes with the same label as the target nodes.



(a) SGFormer (b) GraphGPS (c) Polynormer

Figure S9: **Time Cost.** Different colors of the points denote the number of clusters m. The point shape "." denotes the whole model with Wideformer. "*" denotes the Wideformer part.

F Complexity Analysis

We construct synthetic graphs to test the time cost across different graph scales. The average degree is set to 8, with a maximum number of edges equals $100,000$. The number of classes is set to 10. Both the number of input features and hidden dimensions are set to 64. Following the common configuration of the backbones, we set the number of local layers and global layers as (3, 1), (3, 3),

Table S8: **Average Cost Increase Ratio.** Comparing the time and memory cost of 4 clusters against 1 cluster. m denotes the number of clusters. The results are averaged across datasets with different numbers of graph nodes.

	M	TIME (S)	MEMORY (MB)
GRAPHGPS	1	0.0973	13,870
	4	$0.1408_{30.93\%\uparrow}$	$15{,}546_{10.78\%\uparrow}$
SGFORMER	1	0.0258	50,206
	4	$0.0413_{37.56\%\uparrow}$	$51{,}332_{2.19\%\uparrow}$
POLYNORMER	1	0.1042	29,338
	4	$0.1435_{27.37\%\uparrow}$	$30{,}180_{2.78\%\uparrow}$

Table S9: **Comparison Results with ENACT (Measure by accuracy except for ROC-AUC for questions: %).** The bold values denote the best results among comparisons with the same backbone.

	AMAZON-RATINGS	COAUTHORCS	AMAZONPHOTO	QUESTIONS
GRAPHGPS	49.73	95.44	94.98	75.48
+ENACT	48.52	95.16	94.76	**75.74**
+WIDEFORMER	**49.96**	**95.85**	**95.55**	75.69
SGFORMER	52.38	93.50	95.47	76.81
+ENACT	53.32	93.21	95.53	76.53
+WIDEFORMER	**53.47**	**93.86**	**95.64**	**76.94**
POLYNORMER	54.71	94.53	95.47	78.66
+ENACT	54.94	94.60	95.55	78.78
+WIDEFORMER	**55.05**	**94.94**	**95.64**	**79.00**

and (6, 3) for SGFormer, GraphGPS, and Polynormer, respectively. All models have 4 attention heads. From the results in Fig. S9, we can see that the time cost of Wideformer scales linearly with the number of nodes and remains a small ratio of the total time cost as the number of clusters increases.

In Sec 5.3.3, we show that increasing the number of clusters m can benefit the model performance, while the optimal value of m is around $3 \sim 5$. In practice, m is chosen from $\{2, \cdots, 8\}$ to remain a small value. Therefore, although a larger m increases the memory and runtime cost linearly, the additional cost is minor. We further present the average cost increase ratio (calculated as $\frac{\texttt{cost}(m=4)-\texttt{cost}(m=1)}{\texttt{cost}(m=1)}$) across different numbers of graph nodes in Tab. S8. We can see that the additional costs are relatively minor, amounting to only $\sim$ 30% of the original time cost and less than 11% of the memory cost.

G Broader Related Work

Our study is also related to other works beyond graph transformers. Wideformer employs the center selection method to assign source nodes to different clusters. Traditional cluster pooling methods focus on learning hierarchical features of input graphs [56, 20, 57, 28]. They can collect global information by stacking multiple layers. In contrast, Wideformer and other graph transformer models can collect global information in a single layer, giving rise to shallow architectures for large graphs.

To better optimize the learning process of the attention matrix with dense interactions, a previous study proposes to inject uniform attention to vision transformers [16]. However, this solution cannot be directly adopted for graph transformers. It requires explicitly computing the whole attention matrix, which demands a space complexity of $O(n^2)$ and is not scalable to large graphs. Moreover, different from the occasional observation of the uniform attention [16], we discover that uniform attention with high attention entropy consistently exists across different global graph attention methods on different datasets. To further reduce the computing complexity, ENACT proposes to cluster source nodes during attention-based aggregation for vision transformers [35]. However, ENACT cannot effectively alleviate over-aggregating. Specifically, their clustering process is based on the features of each individual node, while Wideformer clusters nodes based on the source-target relation, which better enables the selection of the informative sources for the targets. ENACT also applies attention

aggregation at the cluster level, while Wideformer applies attention aggregation at the node level within each cluster. Node-level aggregation allows the model to adjust the attention scores at a finer level and capture the node feature distribution within each cluster. To further compare Wideformer against ENACT for tackling over-aggregating, we implement ENACT in graph transformers by directly clustering source nodes based on their own features, and only applying cluster-level attention aggregation. Results in Tab. S9 show that ENACT cannot effectively tackle over-aggregating and gains worse performance than Wideformer. This demonstrates the effectiveness of our method in tackling over-aggregating and benefiting backbone performance.

H Societal Impact

This paper presents work whose goal is to advance the field of graph representation learning by proposing a plug-and-play method to tackle over-aggregating problem in graph transformers. The proposed method remains independent of specific downstream applications and can potentially benefit a wide range of domains, such as computational biology [60, 55] and intelligent transportation [33]. At present, we do not anticipate any evident ethical concerns or foreseeable adverse societal impacts.

I Limitation

This paper discovers the over-aggregating phenomenon in graph attention and proposes a plug-and-play method to tackle over-aggregating. To keep the simplicity of our proposed method, we only explore a simple division method based on KMeans++ [3] and an attention-guiding method with cluster weighting. In Sec. 5.3.3, the center selection study primarily shows that a learnable center selection strategy can solve the trade-off between efficiency and model performance. The module ablation study demonstrates that the simple weighting method may fail to benefit backbones under certain circumstances. All these ablation results and the informative source node study in Sec. 5.3.1 indicates that it lacks further exploration of a learnable division strategy and adaptive weighting method.

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