BENCHMARKING GRAPHORMER ON LARGE-SCALE MOLECULAR MODELING DATASETS

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Abstract
This technical note describes the recent updates of Graphormer, including architecture design modifications, and the adaption to 3D molecules. With these simple modifications, Graphormer attained better results on large-scale molecular modeling datasets, and the performance gain could be consistently obtained on 2D and 3D molecular graph modeling tasks. In addition, we show that with a global receptive field and an adaptive aggregation strategy, Graphormer is more powerful than classic message-passing-based GNNs. Empirically, Graphormer could achieve much less MAE than the originally reported results on the PCQM4M quantum chemistry dataset used in KDD Cup 2021. In the meanwhile, it greatly outperforms the competitors in the recent Open Catalyst Challenge, which is a competition track on NeurIPS 2021 workshop, and aims to model the catalyst-adsorbate reaction system with advanced AI models. All code can be found at this link.

1. Introduction
Graphormer (Ying et al., 2021) is a recently proposed deep learning model built upon the standard Transformer, which aims to break through the limitations of conventional graph neural networks (Xu et al., 2019; Hamilton et al., 2017) on expressiveness and over-smoothing. The architecture design of Graphormer is quite simple, where a standard Transformer (Vaswani et al., 2017) is equipped by three structural encodings (i.e., centrality, spatial, and edge encodings), which is attractively effective on a wide range of graph representation tasks. Graphormer enjoys the great power of expressiveness from Transformer architecture, while also incorporates the structural information of the graph with high efficiency.

In this note, we report several design improvements built in the Graphormer framework. We first investigate the change of placement of layer normalization, and find that the Post-LN variant could lead to significantly better results on molecular property prediction tasks. Furthermore, we extend Graphormer to 3D molecule graph modeling by designing specific centrality encoding, spatial encoding, and 3D attention sub-layer. After a series of architecture design modifications, the upgraded Graphormer establishes stronger and more feasible baselines on large-scale molecular modeling datasets, i.e., PCQM4M (Hu et al., 2021) and OC20 (Chanussot et al., 2020).

Finally, we endeavor to obtain a better theoretical understanding of Graphormer via the lens of distributed computing theory. Specifically, we show that with a global receptive field, Graphormer enjoys a greater expressiveness compared to classic message-passing-based GNNs.

2. Empirical Analysis
2.1. The Placement of Layer Normalization Matters
The originally designed Graphormer follows the architecture of a prevailing variant of Transformer, i.e., the Pre-LN Transformer, where layer normalization is placed inside the residual blocks. Recent literature (Xiong et al., 2020) shows that with this modification, the gradients are well-behaved at initialization, leading to a much faster convergence compared to the vanilla Post-LN Transformer (Vaswani et al., 2017). Yet, we observe that the latter leads to a better generalization performance on the large-scale quantum chemical property prediction dataset PCQM4M (Hu et al., 2021). Therefore, we adopt this simple modification to Graphormer and establish a stronger baseline built in the Graphormer framework.

2.1.1. Molecular Property Prediction
Datasets. The experiment is conducted on the large-scale molecular graph dataset PCQM4M (Hu et al., 2021), which contains 3.8M graphs and 55.4M edges in total. It is a
Table 1. Graphormer’s PreLN variant vs. PostLN variant: Mean absolute error on PCQMv2 dataset.

| Case       | #params. | MAE on PCQMv2 | MAE on PCQMv2 |
|------------|----------|---------------|---------------|
|            |          | train. | valid. | train. | valid. |
| PreLN\textsubscript{Base} | 48.3M    | 0.0266 | 0.1229 | 0.0266 | 0.0889 |
| PreLN\textsubscript{Large} | 159.3M   | 0.0172 | 0.1213 | 0.0173 | 0.0879 |
| PostLN\textsubscript{Base} | 48.3M    | 0.0416 | \textbf{0.1193} | 0.0348 | \textbf{0.0864} |
| PostLN\textsubscript{Large} | 159.3M   | 0.0212 | 0.1228 | 0.0186 | 0.0883 |

\footnote{https://ogb.stanford.edu/docs/lsc/pcqm4mv2/}
Title Suppressed Due to Excessive Size

| case                      | ID   | OOD Ads. | OOD Cat. | OOD Both | avg.  |
|--------------------------|------|----------|----------|----------|-------|
| Graphormer$_{Base}$*     | 0.4329 | 0.5850  | 0.4441  | 0.5299 | 0.4980 |
| Graphormer$_{Base}$ (ensemble) | 0.3976 | 0.5719  | 0.4166  | 0.5029 | 0.4722 |

Table 2. Results on IS2RE task by direct approach. * denotes evaluation on the OC20 validation split.

In addition to predicting the relaxed energy of the entire system, inspired by Godwin et al. (2022), we further adopt an auxiliary node-level objective to predict the displacement of each atom between the initial and relaxed structures. In Table 2 we report the performance on the IS2RE Direct track, which directly estimates the relaxed energy from the initial structure. As shown in the table, the energy prediction of unseen element compositions for catalysts (Out of Domain (OOD) Catalyst) is much accurate than OOD Adsorbates, and OOD Both, which implies that Graphormer may have the potential to help the catalyst discovery process for well-known but important chemical species involved in the chemical reactions of interest, such as OH, O$_2$, or H$_2$O.

3. Understanding Graphormer from a Theoretical Perspective

In this section, we develop a better theoretical understanding of Graphormer based on distributed computing theory. Compared with the classic message-passing-based GNNs (MPGNNs), Graphormer enjoys two unique characteristics: a global receptive field and an adaptive aggregation strategy. We first analyze the impact of the global receptive field on expressiveness. In literature, the $k$-Weisfeiler-Lehman ($k$-WL) graph isomorphism test is often adopted as a metric to characterize the expressiveness of MPGNNs. For example, it was shown in (Xu et al., 2019) that the anonymous MPGNN is equivalent to 1-WL test, which implies that anonymous MPGNN has a very limited ability in graph isomorphism test. Higher-order GNNs have been developed to go beyond 1-WL test (Morris et al., 2019; Balcilar et al., 2021) and achieve the same power as 3-WL test. In these papers, one essential assumption is that the nodes share the same feature. For wide and deep MPGNNs with discriminative features, their expressive power goes beyond $k$-WL (for any $k$) and becomes universal (Abboud et al., 2021). The discriminative features can be easily achieved by adding random features (Sato et al., 2021) or unique identifiers (Loukas, 2020), which is often adopted in practice. Thus, to characterize the expressiveness of more practical MPGNNs, a new metric is needed.

In (Loukas, 2020), the expressiveness of GNNs with discriminative features was studied via the metrics in distributed computing theory. Specifically, it was proved that a $d$ layer MPGNN with width $w$ has equivalent expressiveness to a CONGEST model with $d$ communication round and $w \log n$ communication bits in each round, where $n$ is the number of nodes in the graph. Thus, the expressiveness bound of CONGEST models in distributed computing literature can be used for characterizing the expressiveness of MPGNNs. Due to the locality of the message-passing scheme in CONGEST models, they lose a significant power when $d$ and $w$ is limited. Specifically, several graph problems cannot be solved unless the product of $d$ and $w$, i.e., communication complexity, is large enough. By repurposing these results in CONGEST models, it was shown in (Loukas, 2020) that several graph problems cannot be solved unless the product of MPGNN’s depth $d$ and width $w$, i.e., model capacity, exceeds a polynomial of the graph size. The impossibility results in (Loukas, 2020) are summarized in the column “Local MP” in Table 3.

In contrast to the local message-passing in MPGNNs, each node is allowed to send different messages to any other node in Graphormer. This paradigm is called CONGESTED CLIQUE in distributed computing literature (Drucker et al., 2014) and breaks the expressiveness barrier of the CONGEST model. We summarize the corresponding possibility results of CONGESTED CLIQUE in the column “Non-local MP” of Table 3. Detailed theorems are listed in Appendix A. These bounds demonstrate that a global receptive field qualitatively improves the expressiveness of the model.

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Table 3. A comparison of local message passing and non-local message passing in the model capacity for solving different graph problems. Results for local MP are from (Loukas, 2020) and results for non-local MP are shown in Appendix A.

| Problem              | Local MP                      | Non-local MP                   |
|----------------------|-------------------------------|--------------------------------|
| 4-cycle detection    | $dw = \Omega(\sqrt{n}/\log n)$ | $dw = O(1)$                    |
| subgraph verification| $dw = \Omega(\sqrt{n}/\log n)$ | $dw = O(1)$                    |
| diam. $3/2$-approx.  | $dw = \Omega(\sqrt{n}/\log n)$ | $dw = O(n^{0.158})$            |
| 5-cycle detection    | $dw = \Omega(n/\log n)$      | $dw = O(n^{0.158})$            |
| diam. computation    | $dw = \Omega(n/\log n)$      | $dw = O(n^{1/3} \log n)$      |
| min. vertex cover    | $dw = \Omega(n^2/\log^2 n)$  | $dw = O(1)$ for $w = O(1)$     |
| max. indep. set      | $dw = \Omega(n^2/\log^2 n)$  | $dw = O(n^{1-2/n})$ for $w = O(1)$ |

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A. Theorems for Table 3

Theorem A.1. (4-cycle detection) (Theorem 4 in (Censor-Hillel et al., 2019)) Given \( w = O(1) \), the existence of 4-cycle can be detected in \( O(1) \) rounds.

Theorem A.2. (5-cycle detection) (Theorem 3 in (Censor-Hillel et al., 2019)) Given \( w = O(1) \), for directed and undirected graphs, the existence of \( k \) cycles can be detected in \( d = 2^{O(k)} n^{1-2/\omega} \log n \) rounds, where \( \omega \) is the matrix multiplication time.

For 5-cycle detection problem, taking \( k = 5 \) results in the desired bound.

Theorem A.3. (Diameter computation) (Corollary 6 in (Censor-Hillel et al., 2019)) Given \( w = O(1) \), for weighed and directed graphs with integer weights \( \{0, \pm 1, \cdots, \pm M\} \), all-pair shortest path can be computed in \( d = O(n^{1/3} \log n [\log M / \log n]) \).

Theorem A.4. (Diameter approximation) (Theorem 9 in (Censor-Hillel et al., 2019)) Given \( w = O(1) \), for directed graphs with integer weights in \( \{0, 1, \cdots, 2^{n^{o(1)}}\} \), we can compute \( (1 + o(1)) \)-approximate all-pairs shortest path in \( d = O(n^{1-2/\omega+o(1)}) \) rounds.

Theorem A.5. (Subgraph verification) (Corollary 1 in (Jurdziński & Nowicki, 2018)) Given \( w = O(1) \), there are randomized distributed algorithms that solve the following verification problems in congested clique model in \( O(1) \) rounds with high probability: bipartiteness verification, cut verification, s-t connectivity, and cycle containment.

Theorem A.6. (Subgraph Detection) (Dolev et al., 2012) Given \( w = O(1) \), there are distributed algorithms that count the number of \( d \)-vertex subgraph in \( d = O(n^{(d-2)/d} / \log n) \) rounds.

The bound of the maximum independent set can be obtained by using the relationship between \( k \)-independent set and maximum independent set, and the minimum vertex cover is equivalent to the maximum independent set.