Attending to Graph Transformers

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Abstract

Recently, transformer architectures for graphs emerged as an alternative to established techniques for machine learning with graphs, such as graph neural networks. So far, they have shown promising empirical results, e.g., on molecular prediction datasets, often attributed to their ability to circumvent graph neural networks' shortcomings, such as over-smoothing and over-squashing. Here, we derive a taxonomy of graph transformer architectures, bringing some order to this emerging field. We overview their theoretical properties, survey structural and positional encodings, and discuss extensions for important graph classes, e.g., 3D molecular graphs. Empirically, we probe how well graph transformers can recover various graph properties, how well they can deal with heterophilic graphs, and to what extent they prevent over-squashing. Further, we outline open challenges and research direction to stimulate future work. Our code is available at https://github. com/luis-mueller/probing-graph-transformers.

1 Introduction

Graph-structured data are prevalent across application domains ranging from chemo- and bioinformatics [Barabasi and Oltvai, 2004; Reiser *et al.*, 2022] to image [Simonovsky and Komodakis, 2017] and social-network analysis [Easley and Kleinberg, 2010], clearly indicating the importance of machine learning methods for such data. In recent years, *graph neural networks* (GNNs) [Chami *et al.*, 2022; Gilmer *et al.*, 2017; Morris *et al.*, 2021] were the dominant paradigm in machine learning for graphs. However, with the rise of transformer architectures [Vaswani *et al.*, 2017] in natural language processing [Lin *et al.*, 2021b] and computer vision [Han *et al.*, 2022], recently, a large number of works in the field focused on designing transformer architectures capable of dealing with graphs, so-called *graph transformers* (GTs).

Graph transformers have already shown promising performance [Ying et al., 2021], e.g., by topping the leaderboard of the OGB Large-Scale Challenge [Hu et al., 2021; Masters et al., 2022] in the molecular property prediction track. The superiority of GTs over standard GNN architecture is often explained by GNNs' bias towards encoding local structure

and being unable to capture global or long-range information, often attributed to phenomena such as *over-smoothing* [Li *et al.*, 2018], *under-reaching* or *over-squashing* [Alon and Yahav, 2021]. Many papers speculate that GTs [Rampášek *et al.*, 2022] do not suffer from such effects as they aggregate information over all nodes in a given graph and hence are not limited to local structure bias. However, to make GTs aware of graph structure, one has to equip them with so-called *structural* and *postional encodings*. Here, structural encodings are, e.g., additional node features to make the GT aware of (sub-)graph structure. In contrast, positional encodings make a node aware of its position in the graph concerning the other nodes.

Present Work. Here, we derive a taxonomy of state-of-theart GT architectures, giving a structured overview of recent developments. Moreover, we survey common positional and structural encodings and clarify how they are related to GTs' theoretical properties, e.g., their expressive power to capture graph structure. Additionally, we investigate these properties empirically by probing how well GTs can recover various graph properties, deal with heterophilic graphs, and to what extent GTs alleviate the over-squashing phenomenon. Further, we outline open challenges and research direction to stimulate future work. Our categorization, theoretical clarification, and experimental study present a useful handbook for the GT and the broader graph machine-learning community. Its insights and principles will help spur novel research results and avenues.

Related Work. Since GTs emerged recently, only a few surveys exist. Notably, Min *et al.* [2022a] provide a high-level overview of some of the recent GT architectures. Different from the present work, they do not discuss GT's theoretical and practical shortcomings and miss out on recent architectural advancements. Chen *et al.* [2022a] gives an overview of GTs for computer vision. Finally, Rampášek *et al.* [2022] provide a general recipe for classifying GT architectures, focusing on devising empirically well-performing architectures rather than giving a detailed, principled overview of the literature.

1.1 Background

A graph G is a pair (V, E) with a finite set of nodes V(G) and a set of edges $E(G) \subseteq \{\{u,v\} \subseteq V \mid u \neq v\}$. For ease of notation, we denote an edge $\{u,v\}$ as (u,v) or (v,u). In the case of directed graphs, $E(G) \subseteq \{(u,v) \in V^2 \mid u \neq v\}$. Throughout the paper, we set n := |V(G)| and m := |E(G)|.

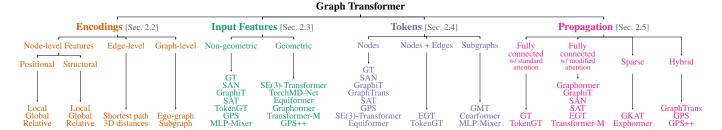


Figure 1: Categorization of graph transformers along four main categories with representative architectures.

A node-attributed graph G is a triple (V, E, \mathbf{X}) , where $\mathbf{X} \in \mathbb{R}^{n \times d}$, for d > 0, is a node feature matrix and \mathbf{X}_v is the node feature of node $v \in V(G)$. Similarly, we can represent edge features by an edge feature matrix $\mathbf{E} \in \mathbb{R}^{m \times e}$, for e > 0, where \mathbf{E}_{vw} is the edge feature of edge $(v, w) \in E(G)$. The neighborhood of $v \in V(G)$ is $N(v) \coloneqq \{u \in V(G) \mid (v, u) \in E(G)\}$. We say that two graphs G and H are isomorphic if there exists an edge-preserving bijection $\varphi \colon V(G) \to V(H)$, i.e., (u, v) is in E(G) if and only if $(\varphi(u), \varphi(v))$ is in E(H) for all $u, v \in V(G)$. We denote a multiset by $\{\!\{\ldots\}\!\}$.

Equivariance and Invariance. Operations on graphs need to respect their symmetries, such as being agnostic to the node permutations or other (group) transformations, such as rotation, leading to the definitions of equivariance and invariance. In general [Fuchs et al., 2021], given a transformation \mathbf{T} , a function f is equivariant if transforming the vector input \mathbf{x} is equal to transforming the output of the function f, i.e., $f(\mathbf{T}\mathbf{x}) = \mathbf{T}f(\mathbf{x})$. A function g is invariant if transforming the vector input \mathbf{x} does not change the output, i.e., $g(\mathbf{T}\mathbf{x}) = g(\mathbf{x})$. In the 3D Euclidean space, 3D translations, rotations, and reflections form the E(3) group. Translation and rotation form the SE(3) group. Rotations form the SO(3) group, rotations and reflections form the O(3) group.

Graph Transformers. A transformer is a stack of alternating blocks of *multi-head attention* and fully-connected *feed-forward networks*. Let G be a graph with node feature matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$. In each layer, t > 0, given node feature matrix $\mathbf{X}^{(t)} \in \mathbb{R}^{n \times d}$, a single attention head computes

$$\mathsf{Attn}(\mathbf{X}^{(t)}) \coloneqq \mathsf{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^T}{\sqrt{d_k}}\right)\mathbf{V},\tag{1}$$

where the softmax is applied row-wise, d_k denotes the feature dimension of the matrices \mathbf{Q} and \mathbf{K} , with $\mathbf{X}^{(0)} := \mathbf{X}$. Here, the matrices \mathbf{Q} , \mathbf{K} , and \mathbf{V} are the result of projecting $\mathbf{X}^{(t)}$ linearly,

$$\mathbf{Q}\coloneqq \mathbf{X}^{(t)}\mathbf{W}_Q, \mathbf{K}\coloneqq \mathbf{X}^{(t)}\mathbf{W}_K, \text{ and } \mathbf{V}\coloneqq \mathbf{X}^{(t)}\mathbf{W}_V,$$

using three matrices $\mathbf{W}_Q, \mathbf{W}_K \in \mathbb{R}^{d \times d_K}$, and $\mathbf{W}_V \in \mathbb{R}^{d \times d}$, with optional bias terms omitted for clarity. Now, multi-head attention MultiHead($\mathbf{X}^{(t)}$) concatenates multiple (single) attention heads, followed by an output projection to the feature space of $\mathbf{X}^{(t)}$. By combining the above with additional residual

connections and normalization, the transformer layer updates features $\mathbf{X}^{(t)}$ via

$$\mathbf{X}^{(t+1)} \coloneqq \mathsf{FFN} \big(\mathsf{MultiHead} \big(\mathbf{X}^{(t)} \big) + \mathbf{X}^{(t)} \big).$$
 (2)

As noticed by Mialon et al. [2021], we can rewrite Eq. (1) as

$$\mathsf{Attn}(\mathbf{X}^{(t)})_v = \sum_{u \in V(G)} \frac{k_{\mathrm{exp}}(\mathbf{X}_v^{(t)}, \mathbf{X}_u^{(t)})}{\sum_{w \in V(G)} k_{\mathrm{exp}}(\mathbf{X}_v^{(t)}, \mathbf{X}_w^{(t)})} \mathbf{X}_w^{(t)} \mathbf{W}_V,$$

for $v \in V(G)$, where

$$k_{\exp}(\mathbf{X}_v^{(t)}, \mathbf{X}_w^{(t)}) \coloneqq \exp(\mathbf{X}_v^{(t)} \mathbf{W}_Q \mathbf{X}_w^{(t)} \mathbf{W}_K / \sqrt{d_K}).$$

Hence, we can view GTs as a special GNN, which we define below, operating on a complete graph, where the attention score weights the importance of each node during the sum aggregation.

Graph Neural Networks. Intuitively, GNNs learn a vector representing each node in a graph by aggregating information from neighboring nodes. Formally, let G be a graph with node feature matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$. A GNN architecture consists of a stack of neural network layers, i.e., a composition of permutation-equivariant parameterized functions. Each layer aggregates local neighborhood information, i.e., the neighbors' features, around each node and then passes this aggregated information on to the next layer. Following Gilmer *et al.* [2017] and Scarselli *et al.* [2009], in each layer, $t \geq 0$, we compute vertex features

$$\mathbf{h}_v^{(t+1)} \coloneqq \mathsf{UPD}^{(t)}\Big(\mathbf{h}_v^{(t)},\,\mathsf{AGG}^{(t)}\big(\{\!\!\{\mathbf{h}_u^{(t)}\mid u\in N(v)\}\!\!\}\big)\Big) \in \mathbb{R}^d,$$

where $\mathsf{UPD}^{(t)}$ and $\mathsf{AGG}^{(t)}$ may be differentiable parameterized functions, e.g., neural networks. For example, GNNs often compute a vector for node v by using sum aggregation [Morris et al., 2019], i.e.,

$$\mathbf{h}_v^{(t+1)} \coloneqq \sigma \Big(\mathbf{h}_v^{(t)} \mathbf{W}_1^{(t)} + \sum_{w \in N(v)} \mathbf{h}_w^{(t)} \mathbf{W}_2^{(t)} \Big),$$

where σ is a non-linearity applied pointwise, $\mathbf{W}_1^{(t)}$ and $\mathbf{W}_2^{(t)} \in \mathbb{R}^{d \times d}$ are parameter matrices, and $\mathbf{h}_v^{(0)} \coloneqq \mathbf{X}_v$.

2 The Landscape of Graph Transformers

In the following, we outline our taxonomy of GTs, see also Figure 1, bringing some order to the growing set of GT architectures. We start by discussing the theoretical properties of

¹For simplicity, we learn attention between a graph's nodes. However, in Section 2.4, we extend this to, e.g., edges or subgraphs.

GTs that heavily rely on structural and positional encodings, which we study subsequently. Further, we discuss different approaches to dealing with essential classes of input node features, e.g., 3D coordinates in the case of molecules. We then study how to *tokenize* a graph, i.e., partition a graph into atomic entities between which the attention is computed, e.g., nodes. Then, we review how GTs organize message propagation in the graph through global, sparse, or hybrid attention. Finally, we overview representative applications of GTs.

2.1 Theoretical Properties

It is crucial to understand that the general GT architecture of Eq. (2) is less expressive in distinguishing non-isomorphic graphs than standard GNNs. Hence, it is also weaker in approximating permutation-invariant and -equivariant functions over graphs [Chen et al., 2019]. GTs are weaker since, without sufficiently expressive structural and positional encodings, they cannot capture any graph structure besides the number of nodes and hence equal DeepSets-like architectures [Zaheer et al., 2020] in expressive power. Thus, for GTs to capture non-trivial graph structure information, they are crucially dependent on such encodings; see below. In fact, by leveraging the results in Chen et al. [2019], it is easy to show that GTs can only become maximal expressive, i.e., universal function approximators, if they have access to maximally expressive structural bias, e.g., structural encodings. However, this is equivalent to solving the graph isomorphism problem [Chen et al., 2019]. Moreover, we stress that GNN architectures equipped with the same encodings will also possess the same expressive power. Hence, in terms of expressive power, GTs do not have an advantage over GNNs.

2.2 Structural and Positional Encodings

As outlined in the previous subsection, GTs are crucially dependent on structural and positional encodings to capture graph structure. Although there is no formal definition or distinction between the two, structural encodings make the GT aware of graph structure on a local, relative, or global level. Such encodings can be attached to node-, edge-, or graph-level features. Examples of local structural encodings include annotating node features with node degree [Chen et al., 2022b], the diagonal of the m-step random-walk matrix [Dwivedi et al., 2022], the timederivative of the heat-kernel diagonal [Kreuzer et al., 2021], enumerate or count predefined substructures and the node's role within [Bouritsas et al., 2022], or Ricci curvature [Topping et al., 2022]. Examples of edge-level relative structural encodings include relative shortest-path distances [Chen et al., 2022a] or Boolean features indicating if two nodes are in the same substructure [Bodnar et al., 2021]. Examples of graph-level global structural encodings include eigenvalues of the adjacency or Laplacian matrix [Kreuzer et al., 2021] or graph properties such as diameter, number of connected components, or treewidth.

On the other hand, positional encodings make, e.g., a node, aware of its relative position to the other nodes in a graph. Hence, two such encodings should be close to each other if the corresponding nodes are close in the graph. Again, we can distinguish between local, global, or relative encodings. Examples of node-level local positional encodings include the shortest-path distance of a node to a hub or central node or

the sum of each column of the non-diagonal elements of the m-step random walk matrix. An example of edge-level relative positional encodings is pair-wise node distances [Chen et~al., 2022a; Beaini et~al., 2021; Kreuzer et~al., 2021; Mialon et~al., 2021; Li et~al., 2020]. Examples of node-level global positional encodings include eigenvalues of the adjacency or Laplacian matrix [Kreuzer et~al., 2021; Dwivedi and Bresson, 2020] or unique identifiers for each connected component of the graph.

When designing such encodings, one must ensure equivariance or invariance to the nodes' ordering. Such equivariance is trivially satisfied for simple encodings such as node degree but not for more powerful encodings based on eigenvalues of the adjacency or Laplacian matrix [Lim *et al.*, 2022]. It is an ongoing effort to design equivariant Laplacian-based encodings [Lim *et al.*, 2022; Wang *et al.*, 2022].

2.3 Input Features

Besides characterizing GTs based on their use of structural and positional encodings, we can also characterize them based on their ability to deal with different node and edge features. To this end, we devise two families of input features. First, we consider so-called *non-geometric features* where nodes and edges have feature vectors in \mathbb{R}^d , i.e., graphs are described with a tuple $(V, E, \mathbf{X}, \mathbf{E})$. Secondly, we consider so-called *geometric features* where nodes and edges features contain geometric information, e.g., 3D coordinates for nodes $\mathbf{X}^{3D} \in \mathbb{R}^3$. Therefore, graphs are described with $(V, E, \mathbf{X}, \mathbf{E}, \mathbf{X}^{3D}, \mathbf{E}^{3D})$. We categorize GT architectures as non-geometric and those supporting both features in the following.

Non-geometric GTs [Chen et al., 2022b; Choromanski et al., 2021; Dwivedi and Bresson, 2020; He et al., 2022; Kim et al., 2022; Kreuzer et al., 2021; Jain et al., 2021; Mialon et al., 2021; Rampášek et al., 2022] are most common and follow equations in Section 1.1. Graphs with non-geometric features do not have explicit geometric inductive bias. Examples of such features include encoded node attributes in citation networks or learnable atom-type embeddings in molecular graphs. Non-geometric features are supposed to be equivariant to node permutations, and transformers provide such equivariance by default. Structural and positional features, see Section 2.2, are often added to non-geometric features to increase the expressive power of GTs.

3D molecular graphs provide geometric features describing nodes and edges, e.g., 3D coordinates of atoms, angles of bonds, or torsion angles of planes. Building GTs supporting geometric features is more challenging as geometric features have to be *invariant* or *equivariant* to certain group transformations, such as rotation, depending on the task. Further, the architectures must be invariant for graph-level molecular property prediction tasks. In contrast, models must be equivariant in node-level tasks such as predicting structural conformers or force fields.

SE(3)-Transformer [Fuchs et al., 2020] was one of the first attempts to incorporate SE(3) equivariance. By using irreducible representations, Clebsch-Gordan coefficients, and spherical harmonics, the authors encode SE(3) equivariance into the attention operation. Equiformer [Liao and Smidt, 2023] further extends this mechanism to complete E(3) equivariance. In contrast, TorchMD-NET [Thölke and Fabritiis, 2022] achieves SO(3) equivariance by incorporating inter-

atomic distances into the attention operation via exponential normal radial basis functions (RBF). Graphormer [Shi *et al.*, 2022], Transformer-M [Luo *et al.*, 2022a] and GPS++ [Masters *et al.*, 2022] take a similar approach, using Gaussian kernels to encode 3D distances between all pairs of atoms. Tailored for graph-level prediction tasks, GPS++ remains SE(3)-invariant, while Graphormer and Transformer-M introduce an additional SE(3)-equivariant prediction head for node-level molecular dynamics tasks.

2.4 Graph to Sequence Tokenization

The nature of *graph tokenization*, i.e., mapping a graph into a sequence of *tokens*, directly affects the supported features and computational complexity. Here, we identify three approaches to graph tokenization: (1) nodes as tokens, (2) nodes and edges as tokens, and (3) patches or subgraphs as tokens.

Using nodes as input tokens is the most common approach followed by many GTs, e.g., [Dwivedi and Bresson, 2020; Fuchs et al., 2020; Kreuzer et al., 2021; Luo et al., 2022b; Rampášek et al., 2022; Thölke and Fabritiis, 2022; Ying et al., 2021]. Here, we often treat structural and positional features as additional node features. Given a graph with n nodes and the attention procedure of Eq. (1), the complexity of such GTs is in $\mathcal{O}(n^2)$. We note that more scalable, sparse attention mechanisms are also possible; see Section 2.5. Edge features, e.g., shortest-path distances [Ying et al., 2021] or relative 3D distances [Luo et al., 2022b; Thölke and Fabritiis, 2022], may be added as an attention bias given the fully computed attention score matrix with n^2 entries. Alternatively, Mialon et al. [2021]; Jain et al. [2021]; Chen et al. [2022b] leverage a GNN to incorporate node and edge features before applying a transformer on the resulting node features. However, the transformer's quadratic complexity remains the bottleneck.

The second approach uses nodes and edges in the input sequence as employed by EGT [Hussain et~al., 2022] and TokenGT [Kim et~al., 2022]. Turning an input graph into a graph of its edges is often used in molecular GNNs [Gasteiger et~al., 2021] and NLP [Yao et~al., 2020]. In addition to soft modeling the edges, i.e., the node-to-node interactions, the attention operation also possibly models higher-order node-edge and edge-edge interactions that theoretically result in an expressiveness boost Kim et~al. [2022]. The input sequence can naturally incorporate node features, their positional encodings, and edge features. A pitfall of this approach is its $\mathcal{O}(n+m)^2$ computational complexity. However, since the approach includes edge features in the input sequence, such GTs might benefit from sparse attention mechanisms that do not materialize the full attention matrix.

The third approach relies on *patches* or *subgraphs* as tokens. In visual transformers [Dosovitskiy *et al.*, 2021], such patches correspond to $k \times k$ image slices. A generalization of patches to the graph domain often corresponds to graph coarsening or partitioning [Baek *et al.*, 2021; Kuang *et al.*, 2022; He *et al.*, 2022]. There, tokens are small subgraphs extracted with various strategies. Initial representations of tokens are obtained by passing subgraphs through a GNN using a form of pooling to a single vector. He *et al.* [2022] adds token position features to the resulting vectors to distinguish coarsened subgraphs better. Finally, these tokens are passed through a transformer

with $O(k^2)$ complexity for a graph with k extracted subgraphs.

2.5 Message Propagation

Most GTs follow the global all-to-all attention of Vaswani et al. [2017] between all pairs of tokens. In the initial GT [Dwivedi and Bresson, 2020] and TokenGT [Kim et al., 2022] this mechanism is unchanged, relying on token representations augmented with graph structural or positional information. Other models alter the global attention mechanism to bias it explicitly, typically based on the input graph's structural properties. Graphormer [Ying et al., 2021] incorporates shortestpath distances, representation of edges along a shortest path, and node degrees. Transformer-M [Luo et al., 2022a] follows Graphormer and adds kernelized 3D inter-atomic distances. GRPE [Park et al., 2022] considers multiplicative interactions of keys and queries with node and edge features instead of Graphormer's additive bias and additionally augments output token values. SAN [Kreuzer et al., 2021] relies on positional encodings and only adds preferential bias to interactions along input-graph edges over long-distance virtual edges. GraphiT [Mialon et al., 2021] employs diffusion kernel bias, while SAT [Chen et al., 2022b] develops a GNN-based structure-aware attention kernel. EGT [Hussain et al., 2022] includes a mechanism akin to cross-attention to edge tokens to bias inter-node attention and update edge representations.

As standard global attention incurs quadratic computational complexity, it limits the application of graph transformers to graphs of up to several thousands of nodes. To alleviate this scaling issue, Choromanski *et al.* [2022] proposed GKAT based on a kernelized attention mechanism of the Performer [Choromanski *et al.*, 2021], scaling linearly with the number of tokens. Another approach to improve GTs' scaling is to consider a reduced attention scope, e.g., based on locality or sparsified instead of dense all-to-all, following expander graph-based propagation [Deac *et al.*, 2022].

Finally, hybrid approaches combine several propagation schemes. For example, GPS and GPS++ [Rampášek *et al.*, 2022; Masters *et al.*, 2022] fuse local GNN-like models with global all-to-all attention in one layer. While GPS employs standard attention and can utilize linear attention mechanisms such as Performer [Choromanski *et al.*, 2022], GPS++ follows Transformer-M's attention conditioning. GraphTrans [Jain *et al.*, 2021] is also a hybrid but applies a stack of GNNs layers first, followed by a stack of global transformer layers.

3 Applications of Graph Transformers

Although GTs only emerged recently, they have already been applied in various application areas, most notably in molecular property prediction. In the following, we give a representative overview of the applications of GTs.

Kan et al. [2022] propose the Brain Network Transformers to predict properties of brain networks, e.g., the presence of diseases, stemming from magnetic resonance imaging. To that, they leverage rows of the adjacency matrix of each node as structural encodings, which showed superior performance over Laplacian-based encodings in previous studies. Moreover, they devise a custom pooling layer leveraging the fact that nodes in the same functional module tend to have similar properties.

Table 1: Hyper-parameter sets for GTs and GNNs with or without PE/SE (SET 1), and for Graphormer models (SET 2).

Hyper-parameter	SET 1	SET 2
Embed. dim.	64	72
Self-attn. heads	4	4
Weight decay	10^{-5}	10^{-2}
Learning rate	10^{-3}	10^{-3}
Gradient clip norm	1.0	5.0
LR scheduler	cosine, warm-up	constant
Batch size	96	256

Table 2: Average test accuracy of GTs with structural bias (± SD) over five random seeds on the structural awareness tasks. Difficulty level on top derived from GIN performance. We additionally report the performance of a transformer without any structural bias serving as a baseline.

Model	Easy Edges	Medium TRIANGLES-SMALL TRIANGLES-LARGE		Hard CSL
	2-way Accuracy \(\ \)	10-way Accuracy ↑	10-way Accuracy ↑	10-way Accuracy ↑
GIN	98.11 ±1.78 55.84 ±0.32	71.53 ±0.94	33.54 ±0.30	10.00 ±0.00
Transformer		12.08 ±0.31	10.01 ±0.04	10.00 ±0.00
Transformer (LapPE)		78.29 ±0.25	10.64 ±2.94	100.00 ±0.00
Transformer (RWSE)		99.40 ±0.10	54.76 ±7.24	100.00 ±0.00
Graphormer		99.09 ±0.31	42.34 ±6.48	90.00 ±0.00

Liao and Smidt [2023]; Thölke and Fabritiis [2022] devise an equivariant transformer architecture to predict quantum mechanical properties of molecules. To capture the molecular structure, they encode atom types and the atomic neighborhood into a vectorial representation, followed by a multi-head attention mechanism. To predict scalar atom-wise prediction, they rely on gated equivariant blocks [Schütt *et al.*, 2021], which are then aggregated into single molecular predictions.

Yao et al. [2020] use transformers to tackle the graph-to-sequence problem, i.e., the problem of translating a graph to word sequences. They first translate a graph to its Levi graph, replacing labeled edges with additional nodes to incorporate edge labels. They then split such a graph into multiple sub-graphs according to the different edge nodes. Each subgraph uses a standard transformer architecture to learn the vectorial representation for each node. To incorporate graph structure, they mask out non-neighbors of a node, concentrating on the local structure. Finally, they concatenate multiple node representations. Further applications use transformers for rumor detection in microblogs [Khoo et al., 2020], predicting properties of crystals [Yan et al., 2022] or click-through rates [Min et al., 2022b], or leverage them for 3D human pose and mesh reconstruction from a single image [Lin et al., 2021a].

4 Experimental Study

We empirically evaluate two highly discussed aspects of graph transformers: (1) the effectiveness of incorporating *graph structural bias* into GTs, and (2) their ability to reduce *over-smoothing* and *over-squashing* affecting GNNs. Concretely, we aim to answer the following questions.

- **Q1** How well do different strategies for incorporating structural awareness into GTs contribute to recovering fundamental structural properties of graphs?
- **Q2** Does the ability of transformers to reduce over-smoothing lead to improved performance on heterophilic datasets?
- **Q3** Do graph transformers alleviate over-squashing better than GNN models?

4.1 Structural Awareness of GTs

For question **Q1**, we evaluate the two most prevalent strategies for incorporating graph structure bias into transformers.

Positional and Structural Encodings (Sec. 2.2). Random-walk structural encodings (RWSE) and Laplacian positional encodings (LapPE), two popular positional or structural encodings for transformers [Rampášek *et al.*, 2022].

Attention Bias (Sec. 2.5). Attention bias based on spatial information such as shortest-path distance between nodes, following the Graphormer architecture [Ying *et al.*, 2021].

We propose a benchmark of three tasks that require increasingly higher structural awareness of non-geometric graphs. We determine the level of structural awareness necessary to solve a task according to the baseline performance of GIN [Xu *et al.*, 2019], a 1-WL-equivalent GNN reference model. In addition, we report the performance of a vanilla transformer without any structural bias to understand the relative impact of the positional or structural encodings (PE/SE) and attention biasing.

We first describe the tasks in our benchmark and their estimated difficulty, then outline task-specific hyper-parameters of evaluated models, and interpret the observed results; see Table 2 for quantitative results.

Detect Edges (Easy). Detecting whether an edge connects two nodes can be considered the fundamental test for structural awareness. We investigate this task using a custom dataset, EDGES, derived from the ZINC [Dwivedi *et al.*, 2023] dataset. For each graph, we treat the pairs of nodes connected by an edge as positive examples and select an equal number of unconnected nodes as negative examples, resulting in a binary edge detection task with balanced classes. Let P denote the set of pairs selected as either positive or negative examples, and let $\mathbf{h}_v^{(T)}$ denote the feature vector of node v after the last layer T of a model. We make predictions as follows. We first compute the cosine similarity between $\mathbf{h}_v^{(T)}$ and $\mathbf{h}_w^{(T)}$ for each pair (v, w) of nodes in P, resulting in a scalar similarity score. Finally, we apply a linear layer to each similarity score, followed by a sigmoid activation, resulting in binary class probabilities.

Count Triangles (Medium). Counting triangles only requires information within a node's immediate neighborhood. However, more than 1-WL expressivity is required to solve it [Morris et al., 2019]. For this task, we evaluate models on the TRIANGLES dataset proposed by Knyazev et al. [2019], which poses triangle counting as a 10-way classification problem. Here, graphs have between 1 and 10 triangles, each corresponding to one class. The dataset specifies a fixed train/validation/test split which we adopt in our experiments. Graphs in the train and validation split are roughly the same size. The test set is a mixture of two graph distributions, where 50% are graphs with a similar size to those in the training and validation set (TRIANGLES-SMALL) and 50% are graphs of larger size (TRIANGLES-LARGE). We separately report model performance for TRIANGLES-SMALL

and TRIANGLES-LARGE to study the ability of transformers with different structural biases to generalize to larger graphs. We analyzed the datasets' class balance and report that each test set contains 5000 graphs with 500 graphs per class. For more details about the dataset, see Knyazev *et al.* [2019].

Distinguish Circular Skip Links (CSL) (Hard). A 1-WL limited model cannot distinguish non-isomorphic CSL graphs [Murphy *et al.*, 2019] as the task requires an understanding of distance [Morris *et al.*, 2019]. Here, we evaluate models on the CSL dataset [Dwivedi *et al.*, 2023], which contains 150 graphs with skip-link lengths ranging from 2 to 16 and poses a 10-way classification problem. We follow Dwivedi *et al.* [2023] in training with 5-fold cross-validation.

Hyper-parameters. To simplify hyper-parameter selection, we hand-designed two general sets of hyper-parameters; see Table 1. For EDGES and TRIANGLES, we fix a parameter budget of around 200k for the transformer models, resulting in six layers for each model with the respective embedding sizes specified in Table 1. Further, we train Graphormer on 1k epochs. Due to the small number of graphs in the CSL dataset, we fix a parameter budget of around 100k for the transformer models, resulting in three layers for each model with the exact embedding sizes as above. Further, we train Graphormer on 2k epochs. We repeat each experiment on five random seeds and report the model accuracy's mean and standard deviation.

For our 1-WL-equivalent reference model, we chose the GIN-layer [Xu et al., 2019]. To improve comparability with the transformer models, we use a feed-forward network composed of the same components and using the same hyper-parameters as for transformers. For Graphormer, we use the feed-forward network specified by Ying et al. [2021]. Further, we train GIN with the SET 1 hyper-parameters. For EDGEs and TRIANGLES, this results in around 150k parameters, while for CSL, the GIN model contains approximately 75k parameters.

Answering Q1. Table 2 shows that GTs supplemented with structural bias generally perform well on all three tasks with a few exceptions. First, the GT with Laplacian positional encodings performs sub-par on the TRIANGLES task. However, it is still an improvement over the 1-WL-equivalent GIN. We hypothesize this is due to an expressivity limit of Laplacian encodings regarding triangle counting. Secondly, we observe that all models generalize poorly to larger graphs on the TRIANGLES dataset. Lastly, we observe that on CSL, Graphormer cannot surpass 90% accuracy. A deeper analysis revealed that the shortest-path distributions can only distinguish 9 out of the 10 classes correctly, meaning that Graphormer is theoretically limited to at most 90% accuracy on CSL.

The above failure cases highlight that current graph transformers still suffer from limited expressivity, and no clear expressivity hierarchy exists for the used positional or structural encodings. Moreover, GTs may generalize poorly to larger graphs. At the same time, we demonstrate a general superiority of structurally biased GTs over standard 1-WL-equivalent models such as GIN. Both the transformer with RWSE as well as Graphormer solve EDGES, TRIANGLES-SMALL, and CSL almost perfectly, two of which pose a challenge for GIN, especially on CSL where GIN performs no better than random.

4.2 Reduced Over-smoothing in GTs?

Graph transformers are often ascribed with an ability to circumvent GNNs' over-smoothing problem due to their global attention mechanism. Thus, we set out to benchmark several variants of GCN [Kipf and Welling, 2017], hybrid GPS models, and Graphormer on six heterophilic transductive datasets: ACTOR [Tang *et al.*, 2009]; CORNELL, TEXAS, WISCONSIN [CMU, 2001]; CHAMELEON and SQUIRREL [Rozember-czki *et al.*, 2021]. In these datasets, we expect over-smoothing and under-reaching to be limiting factors.

We broadly follow the SET 1 hyper-parameters (Table 1). However, we perform a grid search for each model variant to select the embedding size (32, 64, or 96) and dropout rates while we fix the number of layers to two. We implement the GCN and GT models following GPS with hybrid GCN+Transformer aggregation layers but with the latter or former component disabled, respectively. We train all models in full-batch mode using the entire graph as input.

Answering Q2. All transformer-based models outperform a 2-layer GCN, and often the specialized Geom-GCN [Pei et al., 2020], which experimental setup we follow. With the exemption of node degree encodings (DEG), other PE/SE had minimal effect on GCN's performance. Adding global attention to the GCN, i.e., following the GPS model, universally improves the performance. Most interestingly, disabling the local GCN in GPS, i.e., becoming the Transformer model, increases the performance even further. Such results indicate that GNN-like models are unfit for these heterophilic datasets, while the global attention of a transformer empirically facilitates considerably more successful information propagation. Graphormer, which utilizes node degree encodings, performs comparably to the Transformer counterparts. Surprisingly, the attention bias of Graphormer had no impact on its performance. The shortestpath distance bias appears uninformative in these datasets, unlike, e.g., in ZINC, where we observed degradation from 0.12 test mean absolute error to 0.54 when disabling the attention bias.

We conclude that we empirically confirm the expected benefits of global attention, albeit GTs do not achieve overall SOTA performance (e.g., see Luan *et al.* [2022]), which is a reminder that specialized architectures can achieve similar or higher performance without global attention still.

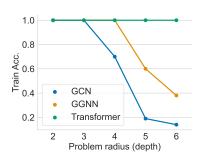
4.3 Reduced Over-squashing in GTs?

To answer question **Q3**, we evaluate a GT on the NEIGHBORS-MATCH problem proposed by Alon and Yahav [2021]. This synthetic dataset requires long-range interaction between leaf nodes and the root node of a tree graph of depth d. The problem demonstrates GNNs' difficulty in transmitting information through a receptive field growing exponentially with d. We run our experiments with minimal changes to the code of Alon and Yahav [2021] and train our transformer on depths 2 to 6. Note that GNN models fail to perfectly fit the training set of trees with depth 4. Convergence on NEIGHBORSMATCH can sometimes take up to $100\,000$ epochs for large depths d. Since the structure of the graphs in NEIGHBORSMATCH is irrelevant to solving the problem, we did not need to augment node features with positional/structural encodings or attention

Table 3: Benchmarking of multiple model variants on six heterophilic transductive datasets. Here we report average test accuracy (± SD) over ten random seeds. We follow the dataset protocol of Pei *et al.* [2020]; for additional model comparison; see Luan *et al.* [2022].

Model (PE/SE type)	ACTOR	CORNELL	TEXAS	Wisconsin	CHAMELEON	SQUIRREL
Geom-GCN [Pei et al., 2020]	31.59 ±1.15	60.54 ±3.67	64.51 ±3.66	66.76 ±2.72	60.00 ±2.81	38.15 ±0.92
GCN (no PE/SE)	33.92 ±0.63	53.78 ±3.07	65.95 ±3.67	66.67 ±2.63	43.14 ±1.33	30.70 ±1.17
GCN (LapPE)	34.30 ±1.12	56.22 ±2.65	65.95 ±3.67	66.47 ±1.37	43.53 ±1.45	30.80 ±1.38
GCN (RWSE)	33.69 ±1.07	53.78 ±4.09	62.97 ±3.21	69.41 ±2.66	43.84 ±1.68	31.77 ±0.65
GCN (DEG)	33.99 ±0.91	53.51 ±2.65	66.76 ±2.72	67.26 ±1.53	46.36 ±2.07	34.50 ±0.87
GPSGCN+Transformer (LapPE)	37.68 ±0.52	66.22 ±3.87	75.41 ±1.46	74.71 ±2.97	48.57 ±1.02	35.58 ±0.58
GPSGCN+Transformer (RWSE)	36.95 ±0.65	65.14 ±5.73	73.51 ±2.65	78.04 ±2.88	47.57 ±0.90	34.78 ±1.21
GPSGCN+Transformer (DEG)	36.91 ±0.56	64.05 ±2.43	73.51 ±3.59	75.49 ±4.23	52.59 ±1.81	42.24 ±1.09
Transformer (LapPE)	38.43 ±0.87	69.46 ±1.73	77.84 ±1.08	76.08 ±1.92	49.69 ±1.11	35.77 ±0.50
Transformer (RWSE)	38.13 ±0.63	70.81 ±2.02	77.57 ±1.24	80.20 ±2.23	49.45 ±1.34	35.35 ±0.75
Transformer (DEG)	37.39 ±0.50	71.89 ±2.48	77.30 ±1.32	79.80 ±0.90	56.18 ±0.83	43.64 ± 0.65
Graphormer (DEG only)	36.91 ±0.85	68.38 ±1.73	76.76 ±1.79	77.06 ±1.97	54.08 ±2.35	43.20 ±0.82
Graphormer (DEG, attn. bias)	36.69 ±0.70	68.38 ±1.73	76.22 ±2.36	77.65 ±2.00	53.84 ±2.32	43.75 ±0.59

Figure 2: Average train accuracy over ten random seeds of a GT on the NEIGHBORSMATCH dataset, compared to models from Alon and Yahav [2021].



bias. Otherwise, we used the same transformer architecture as in Section 4.1.

Answering Q3. Figure 2 shows that the GT performs exceedingly better than the GNN baselines and can perfectly fit the training set even for depth d=6. However, we note that the NEIGHBORSMATCH problem is idealized and has only limited practical implications. The core issue of over-squashing, which is squashing an exponentially growing amount of information into a fixed-size vector representation, is not resolved by transformers. Nonetheless, our results demonstrate that the ability of transformers to model long-range interactions between nodes can circumvent the problem posed by Alon and Yahav [2021].

5 Open Challenges and Future Work

Since the area of GTs is a new, emerging field, there are still many open challenges, both from practical and theoretical points of view. On the theoretical side, although it is often claimed that GTs offer better predictive performance over GNNs, are more capable of capturing long-range dependencies and preventing over-smoothing and over-squashing, a principled explanation still needs to be formed. Moreover, there needs to be a clearer understanding of the properties of structural and positional encodings. For example, it has yet to be understood when certain encodings are helpful and how they compare. A first step could be precisely characterizing different encodings in terms of distinguishing non-isomorphic graphs, similar to the WL hierarchy. Further, understanding GTs' generalization performance on larger graphs has yet to be understood, at least on a similar level to GNNs [Yehudai et al., 2021; Zhou et al., 2022].

On the practical side, one major downside of GTs is their quadratic running time in the number of nodes, preventing them from scaling to truly large graphs typical in real-world node-level prediction tasks. Moreover, due to the attention mechanism's nature, it still needs to be determined how best to incorporate edge-feature information into GT architectures. Further, our experimental analysis reveals a disadvantage of local GNN-like model when used in conjunction with transformers as in Rampášek *et al.* [2022] on heterophilic datasets. Dealing with heterophilic data is thus an open challenge also

for GTs. Moreover, it is crucial to incorporate expert or domain knowledge, e.g., physical or chemical knowledge for molecular prediction, into the attention matrix, in a principled manner.

Explaining and interpreting the performance of GTs remains an open research area where we draw parallels with NLP. We posit that studying graph transformers in the graph machine learning community follows a similar path of studying transformer language models in NLP unified under the name of Bertology [Rogers et al., 2021; Vulić et al., 2020]. Numerous Bertology studies reported that more than dissecting attention matrices and attention scores in transformer layers is needed for understanding how language models work. Instead, the community converged on designing datasets and tasks tailored to language model features such as co-reference resolution or mathematical reasoning. Therefore, we hypothesize that understanding GTs' performance through attention scores is limited, and the community should focus on designing diverse benchmarks probing particular GTs' properties. Further, studying scaling laws and emergent behavior of GTs and GNNs is still in its infancy, with few examples in chemistry [Frey et al., 2022] and protein representation learning [Lin et al., 2022].

6 Conclusion

We have provided a taxonomy of graph transformers (GTs). To this end, we overviewed GTs' theoretical properties and their connection to structural and positional encodings. We then thoroughly surveyed how GTs can deal with different input features, e.g., 3D information, and discussed the different ways of mapping a graph to a sequence of tokens serving as GTs' input. Moreover, we thoroughly discussed different ways GTs propagate information and recent real-world applications. Most importantly, we showed empirically that different encodings and architectural choices drastically impact GTs' predictive performance. We verified that GTs can deal with heterophilic graphs and prevent over-squashing to some extent. Finally, we proposed open challenges and outlined future work. We hope our survey presents a helpful handbook of graph transformers' methods, perspectives, and limitations, and that its insights and principles will help spur and shape novel research results in this emerging field.

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